Supplementary table 1: Metabolomics results (in asceding order according to p-value from progressive ALD vs non-progressive ALD comparison, with molecular features with ID_level of 1-2 first)

								all_ALD_vs_control			Prog_ALD_vs_non-prog_ALD			Prog_ALD_vs_control_ALD			Non-prog_ALD_vs_control			Healthy_control		all_ALD		Non-prog_ALD		Progressive_ALD	
								t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA								
Feature_ID	RP_HILIC	POS_NEG	Average.Rt	Average.Mz	Metabolite.name	curated_MSMS	ID_level	p	d	VIP	p	d	VIP	p	d	VIP	p	d	VIP	Mean	SD	Mean	SD	Mean	SD	Mean	SD
HILIC_NEG_146_04582a6_342	HILIC	NEG	6.34	146.0458	Glutamic acid	116.9214(100), 102.0555(65), 128.0349(30), 146.0464(18)	1	9.01E-11	0.82	1.38	1.45E-06	1.01	2.57	2.59E-09	1.32	1.82	2.24E-05	0.31	1.39	490105	322685	1589809	1441092	905598	512451	2274019	1725651
HILIC_POS_148_06041a6_375	HILIC	POS	6.38	148.0604	Glutamic acid	84.0452(100), 102.0553(40), 130.056(35), 143.068(25)	1	1.43E-10	0.80	1.36	2.09E-06	1.00	2.54	4.66E-09	1.30	1.79	2.12E-05	0.30	1.38	1454208	993547	5034590	4789916	2792354	1685027	7276825	5766720
RP_NEG_464_30231a8_82	RP	NEG	8.82	464.3023	Glycocholic acid (BA 24:1;O4;G)	464.3029(100), 74.0236(30)	2	6.18E-05	0.50	0.95	1.55E-05	0.97	2.60	1.43E-05	0.98	1.36	7.95E-01	0.01	0.35	2923786	4426418	12023014	20479776	3163347	3358869	20882681	25998632
RP_POS_786_60083a13_874	RP	POS	13.87	786.6008	PC 36:2	184.0731(100), 786.5901(3)	2	3.66E-07	0.74	1.30	3.77E-05	0.85	2.41	1.09E-07	1.17	1.70	1.05E-02	0.31	1.12	46148766	15528004	69551474	33501449	55991356	18012964	83111592	39596383
RP_POS_754_53552a12_975	RP	POS	12.98	754.5355	PC 32:1 [M+Na]+	146.9823(100), 86.0965(40), 571.468(35), 754.5403(35), 695.4633(30), 549.4855(15)	2	4.01E-24	1.34	2.16	4.81E-05	0.73	2.38	4.48E-16	1.70	2.43	2.69E-14	0.97	2.21	11679509	5507836	36320929	17075318	29557975	11566328	43083884	19025283
RP_POS_732_55353a12_969	RP	POS	12.97	732.5535	PC 32:1 | PC 16:0_16:1	184.0735(100), 732.5476(3)	2	7.50E-23	1.32	2.15	4.84E-05	0.73	2.36	5.26E-16	1.69	2.41	1.73E-13	0.96	2.16	43071534	21118949	126931501	58675467	103711675	40266409	150151327	65070511
RP_POS_466_31628a8_815	RP	POS	8.82	466.3163	Glycocholic acid	412.2819(100), 337.2529(50), 319.2395(25), 430.2958(21), 76.0396(20),	1	1.03E-04	0.47	0.93	4.88E-05	0.91	2.47	4.05E-05	0.93	1.30	7.07E-01	0.02	0.39	2653271	4036434	12134584	22473567	2979056	3433285	21290112	28940863
RP_NEG_448_30701a9_311	RP	NEG	9.31	448.3070	Glycochenodeoxycholic acid	448.3033(100), 74.0236(35)	1	1.28E-04	-0.18	0.92	5.65E-05	0.90	2.46	4.73E-05	0.92	1.29	7.28E-01	0.02	0.55	11300301	13292022			12301616	11584875	68349588	89400521
RP_POS_852_55029a12_638	RP	POS	12.64	852.5503	PC 40:8 [M+Na]+	146.9819(100), 669.4792(75), 86.0969(65), 793.4791(30), 852.5507(25)	2	1.24E-05	-0.95	1.70	6.64E-05	-0.69	2.30	4.41E-08	-1.29	2.12	6.68E-03	-0.60	1.12	3405928	995319	2442054	910131	2793812	911172	2090295	768654
RP_POS_488_29803a8_816	RP	POS	8.82	488.2980	Glycocholic acid [M+Na]+	488.2962(100)	2	1.18E-04	0.47	0.93	7.09E-05	0.90	2.44	5.66E-05	0.91	1.29	6.56E-01	0.02	0.39	566880	900054	2916311	5670496	654497	805158	5178124	7340066
RP_POS_704_52209a12_381	RP	POS	12.38	704.5221	PC 30:1 | PC 14:0 16:1	184.0732(100), 704.5137(3)	2	1.73E-11	0.90	1.66	1.01E-04	0.80	2.30	3.23E-09	1.30	1.92	2.77E-06	0.51	1.48	2886253	2302752	8558751	6519937	6057546	3384371	11059957	7852726
HILIC_POS_166_07256a1_475	HILIC	POS	1.48	166.0726	7-Methylguanine	166.0732(100)	2	5.36E-07	0.76	1.31	1.50E-04	0.77	1.97	4.48E-08	1.15	1.96	1.13E-02	0.38	0.88	1289673	216127	1589919	410468	1437934	300377	1741903	450597
RP_POS_450_32062a9_303	RP	POS	9.30	450.3206	Glycochenodeoxycholic acid	414.2982(100), 339.2652(20), 76.0396(15), 321.2572(15)	1	2.66E-04	0.44	0.90	1.54E-04	0.86	2.35	1.34E-04	0.87	1.23	7.53E-01	0.01	0.54	5923344	7431856	24069969	46374378	6431272	6548859	41708665	60557589
RP_POS_432_31018a9_303	RP	POS	9.30	432.3102	Glycochenodeoxycholic acid [M-H2O+H]+	414.2975(100), 76.0396(30), 339.2647(30), 321.2564(20)	2	2.77E-04	0.44	0.90	1.60E-04	0.85	2.35	1.40E-04	0.87	1.23	7.60E-01	0.01	0.53	5674106	7076859	23005822	44447792	6145088	6283264	39866555	58067886
RP_POS_756_55298a12_652	RP	POS	12.65	756.5530	PC 34:3 | PC 14:0_20:3	184.0732(100), 756.5563(3)	2	1.23E-03	0.55	1.08	1.91E-04	0.76	2.19	2.53E-05	0.93	1.47	2.95E-01	0.17	0.80	39842308	13732763	50357103	19777472	43131694	13838629	57582511	22186208
RP_POS_806_56873a12_736	RP	POS	12.74	806.5687	PC 38:6 | PC 16:1_22:5 AND 18:2_20:4	184.0732(100), 806.5739(3)	2	2.29E-05	-0.98	1.63	2.46E-04	-0.61	2.13	2.18E-07	-1.29	2.15	4.37E-03	-0.67	1.13	52627067	17662994	36403143	14184013	41476307	14784089	31329979	11635487
RP_POS_726_50385a12_379	RP	POS	12.38	726.5039	PC 30:1 [M+Na]+	146.9813(100), 86.0966(40), 726.5051(30), 543.436(30), 667.4315(22), 521.457(17)	2	2.35E-10	0.87	1.62	3.56E-04	0.74	2.10	1.78E-08	1.24	1.85	1.03E-05	0.51	1.42	765449	779490	2430167	1981264	1730065	1069012	3130268	2405795
RP_NEG_748_51483a12_381	RP	NEG	12.38	748.5148	PC 30:1 | PC 14:0 16:1 [M+HCOO]-	253.2183(100), 227.2001(60), 688.4893(30)	2	3.09E-11	0.92	1.68	3.68E-04	0.73	2.10	4.79E-09	1.28	1.90	2.44E-06	0.56	1.51	902980	795130	2677702	1984571	1978917	1119472	3376488	2389074
RP_POS_432_31091a8_33	RP	POS	8.33	432.3109	Glycohyodeoxcholic acid [M-H2O+H]+	414.2974(100), 76.0394(35), 321.2565(20), 158.0813(20), 339.2697(20)	2	2.34E-06	0.57	0.96	5.69E-04	0.76	2.02	1.74E-05	0.95	1.32	1.26E-02	0.19	0.96	389130	330816	1829421	2825934	859405	1225059	2799437	3565633
RP_NEG_850_56183a12_745	RP	NEG	12.75	850.5618	PC 38:6 | PC 16:1_22:5 AND 18:2_20:4 [M+HCOO]-	279.2334(100), 329.2498(85), 253.2187(70), 303.2316(55), 790.5417(50)	2	9.83E-06	-0.97	1.59	6.44E-04	-0.59	1.97	6.83E-08	-1.27	2.16	3.44E-03	-0.68	1.17	12955409	3729219	9306256	3315589	10416856	3633457	8195656	2547820
RP_POS_770_50861a12_974	RP	POS	12.97	770.5086	PC O-37:10	184.0728(100), 770.5153(3)	2	5.14E-20	1.26	2.03	7.71E-04	0.62	1.98	2.32E-14	1.57	2.32	2.13E-11	0.94	2.00	697778	638379	2883117	1643966	2339832	1248765	3426401	1816213
RP_POS_830_56824a12_639	RP	POS	12.64	830.5682	PC 40:8	184.0732(100), 830.5507(1)	2	4.90E-05	-0.87	1.59	8.46E-04	-0.60	1.96	4.34E-07	-1.17	2.01	1.21E-02	-0.57	1.04	10336707	2889994	7761593	2731898	8655792	2852282	6867393	2304672
RP_POS_450_32138a8_33	RP	POS	8.33	450.3214	Glycoursodeoxycholic acid	414.2946(100), 339.2654(25), 76.403(25)	2	3.52E-06	0.56	0.94	8.63E-04	0.74	1.96	2.78E-05	0.93	1.28	1.22E-02	0.19	0.96	335596	303140	1620487	2570585	766502	1116795	2474472	3258081
HILIC_POS_450_32153a1_027	HILIC	POS	1.03	450.3215	Glycochenodeoxycholic acid	414.3001(100), 339.268(30), 321.2579(20), 76.0398(20)	2	6.17E-04	0.41	0.73	8.67E-04	0.76	1.87	5.92E-04	0.79	1.07	3.69E-01	0.03	0.64	605931	635131	2778871	6052439	749370	794600	4808371	8060669
RP_NEG_540_32928a10_375	RP	NEG	10.38	540.3293	LPC 16:0 [M+HCOO]-	255.2333(100), 480.3058(18), 224.069(1)	2	3.52E-01	0.19	0.99	9.79E-04	-0.65	2.02	5.39E-01	-0.14	0.69	1.87E-02	0.51	1.12	120531302	24796683	125297572	25699440	133607547	22438460	116987597	26267601
RP_POS_810_59705a14_755	RP	POS	14.76	810.5971	PC 36:1 [M+Na]+	146.9821(100), 86.097(45), 810.6053(35), 627.5277(30), 751.5237(20), 605.5495(15)	2	3.23E-04	0.60	1.03	1.18E-03	0.67	1.92	3.26E-05	0.94	1.34	8.60E-02	0.27	0.66	12664017	6545605	18384831	9877240	15216469	6343043	21553193	11678603
RP_POS_854_56775a12_547	RP	POS	12.55	854.5678	PC 42:10	184.0732(100), 854.5798(1)	2	9.24E-03	-0.51	1.17	1.27E-03	-0.63	1.88	8.78E-05	-0.83	1.65	3.87E-01	-0.19	0.59	2631334	973529	2085035	1071379	2424548	1160733	1745522	858247
RP_NEG_540_32928a10_504	RP	NEG	10.50	540.3293	LPC 16:0 [M+HCOO]-	255.2331(100), 480.3054(37), 224.0681(9)	2	9.32E-01	0.02	0.91	1.49E-03	-0.63	1.98	1.96E-01	-0.30	0.79	1.12E-01	0.33	0.94	391151674	45168578	391947965	47529940	406804377	38834283	377091554	51046628
RP_POS_734_56848a13_573	RP	POS	13.57	734.5685	PC 32:0 | PC 16:0_16:0	184.0732(100), 734.5657(3)	2	4.26E-02	0.38	0.84	1.54E-03	0.64	1.84	2.39E-03	0.70	1.14	7.64E-01	0.06	0.25	8567632	4045209	10361672	4894580	8832446	3626112	11890897	5521008
RP_POS_450_32156a9_451	RP	POS	9.45	450.3216	Glycodeoxycholic acid	434.2901(100)	2	4.29E-04	0.42	0.81	1.90E-03	0.70	1.86	6.98E-04	0.77	1.13	1.26E-01	0.07	0.85	3383123	3241080	12727886	25074945	4896809	5608941	20558963	33372483
RP_POS_480_30869a10_519	RP	POS	10.52	480.3087	LPE 18:1	339.2899(100), 480.3412(4), 60.0817(22)	2	1.74E-03	0.53	1.24	1.95E-03	0.64	2.08	1.57E-04	0.85	1.41	1.97E-01	0.21	0.95	2301424	1002107	3050940	1482721	2596318	995581	3505562	1740348
RP_POS_195_08778a3_862	RP	POS	3.86	195.0878	Caffeine	195.0876(100), 138.0663(25)	1	6.60E-02	0.28	0.56	2.22E-03	0.67	1.80	6.63E-03	0.61	1.00	7.02E-01	-0.05	0.58	80499529	93647137	124844619	171725980	72507967	88808760	177181272	214719375
HILIC_NEG_131_07137a0_617	HILIC	NEG	0.62	131.0714	2-Hydroxy-4-methylpentanoic acid	85.0656(100), 131.0721(60)	2	2.43E-08	0.68	1.42	2.28E-03	0.67	1.80	3.62E-06	1.01	1.42	1.73E-04	0.35	1.25	1507805	663631	4238507	4393411	2903847	2323016	5573166	5474148
HILIC_POS_144_10197a4_656	HILIC	POS	4.66	144.1020	(2R)-6-methylpiperidine-2-carboxylic acid	85.0289(100), 144.01012(70)	2	2.52E-06	0.72	1.28	2.34E-03	0.63	1.67	1.41E-06	1.04	1.59	6.39E-03	0.41	0.96	1012369	371015	1487910	690091	1280169	491193	1695650	795503
RP_NEG_590_34692a10_397	RP	NEG	10.40	590.3469	LPC 20:3 [M+HCOO]-	305.2499(100), 530.3265(20)	2	1.93E-02	0.47	1.09	2.64E-03	-0.59	1.76	4.29E-01	0.18	0.61	5.07E-04	0.77	1.33	3884128	1496574	4625213	1562089	5088011	1371413	4162415	1616218
RP_POS_496_33841a10_503	RP	POS	10.50	496.3384	LPC 16:0 (16:0/0:0)	184.0733(100), 496.3362(25), 478.3312(5), 104.1067(65)	2	3.52E-01	0.18	0.99	3.21E-03	-0.59	1.90	6.04E-01	-0.12	0.69	2.36E-02	0.48	1.09	1415784776	211859329	########	233774656	1525135336	202769164	1389224088	244697246
HILIC_POS_126_06646a1_936	HILIC	POS	1.94	126.0665	5-Methylcytosine	126.0661(100), 109.389(3)	1	2.16E-03	0.51	1.02	3.32E-03	0.61	1.64	1.36E-04	0.82	1.41	2.29E-01	0.21	0.46	820442	241676	998545	364606	892786	293922	1104303	399215
RP_POS_804_55328a12_408	RP	POS	12.41	804.5533	PC 38:7	184.0736(100), 804.5588(2), 338.0778(1)	2	3.68E-01	-0.19	0.76	3.49E-03	-0.58	1.73	2.88E-02	-0.47	0.97	6.66E-01	0.10	0.40	7072383	3998100	6336960	3954987	7478556	4355696	5195364	3157736
HILIC_POS_131_11803a3_335	HILIC	POS	3.34	131.1180	N-Acetylputrescine	114.0914(100), 86.0606(70), 72.018(45), 131.1177(20)	1	1.19E-06	0.67	1.14	4.43E-03	0.61	1.63	7.16E-06	0.98	1.47	2.82E-03	0.37	1.09	4558200	951317	6035213	2349966	5369822	1433148	6700604	2863547
HILIC_POS_176_10301a6_376	HILIC	POS	6.38	176.1030	Citrulline	159.0767(100), 113.0718(50), 70.0658(45)	1	1.47E-07	0.74	1.19	4.54E-03	0.60	1.67	6.44E-07	1.04	1.55	1.78E-03	0.44	1.03	5169686	1796996	8122856	4225487	6934780	3136671	9310933	4832648
RP_NEG_832_60986a14_761	RP	NEG	14.76	832.6099	PC 36:1 | PC 18:0_18:1 [M+HCOO]-	281.2503(100), 283.2653(35), 772.5747(20)	2	2.13E-04	0.70	1.13	4.82E-03	0.56	1.70	2.69E-05	0.97	1.42	2.27E-02	0.42	0.89	11420568	5936068	16412238	7132947	14418850	5204401	18405643	8221981
RP_NEG_526_35291a10_776	RP	NEG	10.78	526.3529	LPC O-16:0 [M+HCOO]-	466.3308(100), 78.5974(20), 168.0423(12), 377.2458(7)	2	4.63E-03	-0.64	1.23	4.90E-03	-0.51	1.82	2.34E-04	-0.90	1.55	1.06E-01	-0.39	0.85	7114304	2172510	5850938	1799569	6351186	1855810	5350691	1608003
HILIC_NEG_145_06169a6_093	HILIC	NEG	6.09	145.0617	Glutamine	115.9206(100), 100.9334(30), 127.0514(13), 145.062(12),	1	2.50E-01	-0.18	0.95	5.05E-03	-0.61	1.54	1.42E-02	-0.48	1.01	4.92E-01	0.12	1.15	11895182	2377826	11209627	4169022	12364548	3780880	10054706	4254295
RP_POS_496_33997a10_375	RP	POS	10.38	496.3400	LPC 16:0 (0:0/16:0)	184.0733(100), 496.3366(3), 478.3301(1)	2	1.66E-01	0.27	1.03	5.65E-03	-0.56	1.79	9.52E-01	-0.01	0.65	1.01E-02	0.55	1.18	309977343	73888194	331680098	83257195	354456126	74704884	308904070	85822476
RP_POS_828_55005a12_957	RP	POS	12.96	828.5501	PC 38:6 [M+Na]+	146.9816(100), 645.4805(80), 86.097(70), 769.4818(40), 828.5576(30), 623.5005(10)	2	2.08E-09	-1.06	1.92	7.59E-03	-0.50	1.62	2.68E-10	-1.31	2.22	1.40E-05	-0.82	1.60	102717189	15155406	79505475	20611932	84951417	19324676	74059533	20601060
RP_POS_788_6153a14_755	RP	POS	14.76	788.6153	PC 36:1 | PC 18:0 18:1	184.0735(100), 788.6064(3)	2	5.36E-06	0.66	1.12	7.62E-03	0.57	1.58	1.44E-05	0.94	1.36	5.46E-03	0.38	1.00	25267766	11915154	41120426	25636726	34311227	16707250	47929626	30889180
RP_POS_184_07434a10_375	RP	POS	10.38	184.0743	Phosphocholine	184.0735(100), 86.097(37), 125.0002(20), 60.0815(7)	2	1.43E-01	0.28	1.05	8.34E-03	-0.54	1.77	9.51E-01	0.01	0.64	9.12E-03	0.55	1.20	3474080	857506	3741706	975202	3996524	861825	3486888	1022835
HILIC_POS_518_32288a1_172	HILIC	POS	1.17	518.3229	LPC 18:3 [M+Na]+	146.9822(100), 184.0743(80), 459.2502(55), 313.2715(55)	2	4.71E-03	0.52	0.81	8.56E-03	-0.53	1.43	2.27E-01	0.25	0.50	1.35E-04	0.79	1.37	2695604	974578	3312292	1211632	3627806	1087631	2996779	1256966
HILIC_POS_100_07619a0_569	HILIC	POS	0.57	100.0762	2-Piperidone	100.076(100), 56.0504(10), 86.0651(3)	2	1.50E-05	0.51	0.95	8.87E-03	0.59	1.45	1.87E-04	0.81	1.26	1.52E-02	0.22	0.74	4747185	6244349	42623624	82570636	21037446	45232113	64209803	103817493
RP_POS_806_56537a13_293	RP	POS	13.29	806.5654	PC 36:3 [M+Na]+	146.9818(75), 86.0964(50), 623.4926(20), 806.5719(18), 747.4955(13), 601.5135(6), 184.0732	2	1.34E-02	-0.43	0.85	8.90E-03	0.54	1.58	4.39E-01	-0.16	0.64	2.60E-04	-0.71	1.25	116832105	18004191	106636825	24522895	100276745	20552468	11299604	26646979
RP_POS_595_34937a6_222	RP	POS	6.22	595.3494	Stercobilin	595.348(100), 345.1794(90), 470.2667(85), 166.0874(13), 126.0916(7),	2	5.78E-03	0.33	0.85	8.97E-03	0.60	1.67	6.57E-03	0.63	1.06	3.56E-01	0.03	0.60	717235	1508155	4571468	13418985	1033677	1495221	8109259	18331250
RP_POS_780_5528a12_577	RP	POS	12.58	780.5528	PC 36:5 | PC 16:0 20:5	184.0732(100), 780.5327(2)	2	1.09E-06	0.86	1.48	9.82E-03	0.51	1.61	1.04E-06	1.11	1.68	3.04E-04	0.61	1.41	14743398	6077631	21991760	8338970	19847748	5587874	24135772	9994522
HILIC_POS_482_323a1_209	HILIC	POS	1.21	482.3230	LPC 15:0	184.0743(100), 482.3315(5)	2	1.23E-04	-0.87	1.67	9.94E-03	-0.45	1.49	4.79E-06	-1.10	1.99	7.37E-03	-0.65	1.29	688418	280717	458182	233062	517801	257760	398564	189869
RP_POS_510_39182a11_174	RP	POS	11.17	510.3918	LPC O-18:0	104.1074(100), 510.3875(25), 184.0727(15), 86.0969(10), 125(6),	2	1.96E-05	-1.10	1.88	1.03E-02	-0.38	1.73	1.68E-06	-1.30	1.98	4.55E-04	-0.91	1.59	5748881	2225912	3722889	1378184	4073476	1474393	3372302	1188643
HILIC_POS_147_07639a6_13	HILIC	POS	6.13	147.0764	Glutamine	130.0506(100), 84.0453(80), 102.0559(50)	1	2.67E-01	-0.18	0.98	1.05E-02	-0.55	1.44	2.38E-02	-0.46	0.93	6.39E-01	0.09	1.00	105370043	27844529	98113861	42386366	108865188	39368668	87362533	42942768
RP_NEG_798_53076a12_467	RP	NEG	12.47	798.5308	PC 34:4 | PC 14:0 20:4 [M+HCOO]-	303.2313(100), 227.1998(60), 738.5117(30)	2	5.35E-01	0.14	0.71	1.14E-02	-0.47	1.50	6.98E-01	-0.09	0.96	1.34E-01	0.38	0.74	3405520	1994949	3647527	1598823	4048698	1654765	3246356	1448428
HILIC_POS_510_35559a1_135	HILIC	POS	1.14	510.3556	LPC 17:0	184.0741(100), 72.0816(10)	2	5.10E-05	-0.90	1.72	1.19E-02	-0.45	1.44	2.16E-06	-1.12	2.08	3.99E-03	-0.67	1.25	1080264	392170	735382	343952	821258	367755	649506	297869
RP_POS_482_36081a10_775	RP	POS	10.78	482.3608	LPC O-16:0	104.1075(100), 482.3635(25), 184.073(15), 86.097(10), 125.0002(6)	2	1.94E-03	-0.73	1.31	1.19E-02	-0.44	1.71	1.58E-04	-0.95	1.57	3.85E-02	-0.51	0.97	15170131	4818100	12103598	3721374	13032136	3820510	11175060	3409401
RP_NEG_564_33008a10_325	RP	NEG	10.33	564.3301	LPC 18:2 [M+HCOO]-	279.2348(100), 504.3116(17)	2	3.15E-02	-0.51	1.18	1.19E-02	-0.45	1.73	4.68E-03	-0.74	1.26	2.39E-01	-0.29	0.88	256643826	71808914	225968093	53942674	239417501	48735550	212518685	55988374
RP_NEG_850_5625a12_96	RP	NEG	12.96	850.5625	PC 38:6 | PC 16:0_22:6 [M+HCOO]-	250.2334(100), 327.2307(80), 790.5433(40)	2	1.11E-06	-0.89	1.69	1.25E-02	-0.48	1.51	9.97E-08	-1.13	1.97	9.27E-04	-0.64	1.33	62758050	10247435	50730982	13241825	54012081	12551459	47449882	13219703
RP_POS_766_57336a13_116	RP	POS	13.12	766.5734	PC O-36:5	184.0732(100), 766.5707(2)	2	4.21E-01	-0.18	0.53	1.27E-02	-0.48	1.48	7.38E-02	-0.42	0.73	8.07E-01	0.06	0.34	3238011	2330194	2866150	2011983	3364208	2188689	2368092	1697692
RP_POS_615_49512a14_633	RP	POS	14.63	615.4951	DG 34:2 [M+Na]+	615.4916(100)	2	3.44E-05	0.55	1.00	1.35E-02	0.54	1.46	2.72E-04	0.82	1.16	5.48E-03	0.28	1.00	2721780	2231429	6030132	6622314	4389734	3044304	7670530	8593350
RP_NEG_331_26471a11_275	RP	NEG	11.28	331.2647	FA 22:4	331.2646(100)	2	6.88E-11	0.88	1.75	1.63E-02	0.50	1.53	5.45E-08	1.13	1.83	6.91E-06	0.63	1.68	1760523	1112056	4396658	3138992	3645830	2379393	5147487	3618788
RP_POS_542_32184a10_198	RP	POS	10.20	542.3218	LPC 18:2 [M+Adduct]	483.2499(50), 542.3265(40) , 337.2713(30), 86.0964(35), 104.107(3), 146.9807(100)	2	5.47E-02	-0.46	1.15	1.68E-02	-0.43	1.69	9.42E-03	-0.67	1.18	3.26E-01	-0.24	0.88	30307056	13532690	25173245	10162955	27587117	9500759	22759373	10321016
RP_POS_566_32135a10_199	RP	POS	10.20	566.3214	LPC 20:4	507.2521(60), 86.097(46), 566.3217(35), 361.2737(8), 104.1077(4)	2	2.34E-01	0.24	0.84	1.71E-02	-0.48	1.76	9.86E-01	0.00	0.45	2.83E-02	0.48	1.03	4916834	1793328	5357161	1827379	5790091	1588982	4924232	1959441
RP_POS_452_27689a10_003	RP	POS	10.00	452.2769	LPE 16:1	311.2559(100)	2	2.76E-15	0.98	1.85	1.84E-02	0.49	1.47	8.59E-09	1.23	1.90	1.84E-09	0.74	1.80	183839	120090	1008375	871218	803497	590969	1213253	1048154
RP_NEG_586_31628a9_909	RP	NEG	9.91	586.3163	LPC 20:5 [M+HCOO]-	301.2173(100), 526.2935(32), 224.0689(3)	2	1.55E-01	0.31	0.94	1.86E-02	-0.45	1.43	6.99E-01	0.09	0.52	2.75E-02	0.54	1.01	1805702	1441279	2216007	1249343	2508120	1258855	1923894	1180980
RP_POS_520_34045a10_324	RP	POS	10.32	520.3405	LPC 18:2 (18:2/0:0)	184.0736(100), 520.331(25), 502.3302(6), 104.1077(75)	2	8.77E-02	-0.40	1.11	1.92E-02	-0.42	1.69	1.78E-02	-0.62	1.12	4.31E-01	-0.19	0.85	905685662	316593824	799262164	239989786	855148604	213420877	743375723	253856386
RP_NEG_722_5144a13_381	RP	NEG	13.38	722.5144	PE O-36:5 | PE O-16:1_20:4	303.2314(100), 436.2796(15), 722.518(13)	2	4.86E-01	-0.15	0.75	1.92E-02	-0.46	1.37	9.01E-02	-0.38	0.79	7.48E-01	0.08	0.59	1964491	1073176	1814494	984331	2043959	1111626	1585029	783849
HILIC_POS_282_11938a4_449	HILIC	POS	4.45	282.1194	1-Methyladenosine	150.078(100), 282.1189(5)	1	2.29E-05	0.64	0.96	1.96E-02	0.49	1.40	5.66E-06	0.89	1.48	2.37E-02	0.39	0.88	2634220	319233	3004249	613961	2861835	572467	3146664	626481

Supplementary table 1: Metabolomics results (in asceding order according to p-value from progressive ALD vs non-progressive ALD comparison, with molecular features with ID_level of 1-2 first)

								all_ALD_vs_control			Prog_ALD_vs_non-prog_ALD			Prog_ALD_vs_control_ALD			Non-prog_ALD_vs_control			Healthy_control		all_ALD		Non-prog_ALD		Progressive_ALD	
								t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA								
Feature_ID	RP_HILIC	POS_NEG	Average.Rt	Average.Mz	Metabolite.name	curated_MSMS	ID_level	p	d	VIP	p	d	VIP	p	d	VIP	p	d	VIP	Mean	SD	Mean	SD	Mean	SD	Mean	SD
HILIC_NEG_124_99135a0_735	HILIC	NEG	0.74	124.9914	Isetheonic acid	96.9596(100), 124.9917(45)	2	8.43E-08	0.64	1.21	2.06E-02	0.51	1.27	1.00E-05	0.90	1.38	1.81E-03	0.39	0.94	95435	189266	2301078	3801349	1423664	2838097	3178492	4423741
RP_POS_482_32394a10_107	RP	POS	10.11	482.3239	LPC 15:0	184.0733(100), 482.3246(3)	2	3.44E-07	-1.12	1.90	2.18E-02	-0.39	1.61	1.38E-08	-1.32	2.15	6.25E-05	-0.93	1.52	2774748	866525	1760499	770473	1936498	865034	1584501	622794
RP_POS_184_06049a1_807	RP	POS	1.81	184.0605	4-Pyridoxate	166.0506(100), 184.0614(30), 148.0391(18)	2	6.03E-03	0.32	1.08	2.24E-02	0.53	1.63	1.15E-02	0.58	1.34	1.16E-02	0.06	1.07	40703	26516	1510674	5237528	303387	707589	2717960	7207494
RP_POS_810_59979a13_542	RP	POS	13.54	810.5998	PC 38:4|PC 18:2_20:2	184.0732(100), 810.5881(2)	2	3.65E-01	0.19	0.48	2.26E-02	0.45	1.34	8.16E-02	0.42	0.66	8.95E-01	-0.03	0.70	31027692	10610512	32967835	9883772	30726981	9150471	35208689	10168216
HILIC_POS_170_09241a6_372	HILIC	POS	6.37	170.0924	N-Methylhistidine	124.0868(100), 170.0929(40), 109.0757(10)	2	6.45E-07	0.76	1.16	2.30E-02	0.47	1.35	9.45E-06	1.00	1.39	1.63E-04	0.52	1.34	5370796	4455880	11504195	8441803	9583610	4997719	13424781	10558285
RP_NEG_564_33142a10_198	RP	NEG	10.20	564.3314	LPC 18:2 [M+HCOO]-	279.2348(100), 504.3116(17)	2	5.30E-02	-0.48	1.17	2.31E-02	-0.39	1.61	1.14E-02	-0.68	1.17	2.67E-01	-0.28	0.90	64774366	28531293	53992029	19593327	58418752	18191566	49565307	20117329
RP_NEG_478_29431a10_515	RP	NEG	10.52	478.2943	LPE 18:1	281.2492(100), 478.2928(6), 214.0502(2), 196.0375(1), 78.9581(1)	2	2.80E-03	0.53	1.30	2.34E-02	0.47	1.68	9.85E-04	0.77	1.30	8.13E-02	0.30	1.07	2085171	1078202	2824416	1433442	2499772	957877	3149060	1737477
RP_POS_504_30548a10_247	RP	POS	10.25	504.3055	LPC 15:0 [M+Na]+	104.1075(100), 445.2271(60), 504.3061(25), 299.2548(10), 86.097(15)	2	1.28E-06	-1.10	1.90	2.40E-02	-0.38	1.61	7.27E-08	-1.29	2.08	1.17E-04	-0.91	1.53	4357765	1468554	2757217	1227729	3033028	1347350	2481406	1036725
RP_POS_568_33978a10_192	RP	POS	10.19	568.3398	LPC 22:6 (0:0/22:6)	184.0736(100), 568.3354(3), 550.330(0.6)	2	6.75E-01	-0.08	0.99	2.44E-02	-0.47	1.39	1.37E-01	-0.31	0.77	4.77E-01	0.15	0.90	7255418	3056201	6981217	3627388	7793263	3703003	6169170	3395060
RP_NEG_450_26285a10_138	RP	NEG	10.14	450.2629	LPE 16:1	253.2184(100), 450.2629(18), 196.0373(11), 78.9574(3), 214.0472(2.3)	2	7.52E-18	1.08	1.92	2.47E-02	0.45	1.41	3.20E-10	1.31	2.02	3.47E-10	0.85	1.86	1080988	619883	5125148	3791214	4276218	2867799	5974078	4398282
RP_POS_784_586a13_296	RP	POS	13.30	784.5860	PC 36:3	184.0732(100), 784.5887(3)	2	3.03E-02	-0.47	0.88	2.49E-02	0.43	1.36	2.54E-01	-0.26	0.59	4.92E-03	-0.69	1.23	217912908	57811395	192380842	51364781	180917591	53133676	203844094	47319784
RP_NEG_812_58368a13_592	RP	NEG	13.59	812.5837	PC O-36:4|PC O-16:0_20:4 [M+HCOO]-	303.235(100), 752.5616(50), 466.33(14), 448.3212(5), 279.2336(90)	2	2.01E-02	-0.45	0.82	2.50E-02	-0.45	1.32	1.06E-03	-0.67	1.21	3.28E-01	-0.22	0.47	10478619	2552581	9196806	2904004	9845160	3250182	8548453	2370026
RP_POS_520_34009a10_198	RP	POS	10.20	520.3401	LPE 18:2 (0:0/18:2)	184.0733(100), 520.3419(3), 502.3257(1)	2	6.57E-02	-0.45	1.14	2.67E-02	-0.39	1.63	1.44E-02	-0.64	1.13	3.17E-01	-0.25	0.88	161435926	78088733	133294869	55755768	145587092	52383302	121002647	56823297
HILIC_POS_184_06052a0_827	HILIC	POS	0.83	184.0605	4-Pyridoxic acid	166.0505(100), 184.0604(25), 148.0393(25)	1	1.77E-03	0.37	1.08	2.72E-02	0.51	1.34	6.69E-03	0.62	1.13	1.40E-02	0.11	1.23	214175	122474	5624468	16834392	1878162	4613807	9370774	22861483
RP_POS_568_33813a10_52	RP	POS	10.52	568.3381	LPC 20:3 [M+Na]+	104.1076(100), 509.2663(50), 568.3379(20), 86.0964(17), 363.2902(3)	2	1.15E-02	0.50	1.06	2.81E-02	-0.44	1.30	1.98E-01	0.28	0.71	1.06E-03	0.72	1.24	5574627	1682654	6483998	1804641	6878362	1680026	6089634	1854735
RP_POS_706_53735a12_843	RP	POS	12.84	706.5374	PC 30:0|PC 14:0_16:0	184.0735(100), 706.5386(4),	2	5.45E-03	0.54	1.00	2.86E-02	0.44	1.31	1.16E-03	0.76	1.21	1.03E-01	0.32	0.59	6773192	4093088	9245456	4574934	8247036	3684313	10243876	5165138
RP_POS_542_3241a9_91	RP	POS	9.91	542.3241	LPC 20:5 (0:0/20:5)	184.0736(100), 542.3288(5)	2	1.27E-01	0.32	0.96	2.89E-02	-0.43	1.35	6.36E-01	0.11	0.55	2.37E-02	0.53	1.02	3305299	2601355	4117951	2498097	4661356	2563504	3574547	2331128
RP_POS_247_1441a2_845	RP	POS	2.85	247.1441	Lenticin	188.0712(100), 60.0814(50), 146.0599(20)	2	7.41E-02	-0.50	0.92	2.92E-02	-0.33	1.45	1.91E-02	-0.67	1.16	2.56E-01	-0.34	0.45	10136039	13105818	5702513	6678016	7158351	8149974	4246674	4399364
RP_POS_398_32635a8_935	RP	POS	8.94	398.3264	CAR 16:1	85.0288(100), 398.3235(60)	2	6.46E-11	1.01	1.76	2.92E-02	0.43	1.56	3.30E-10	1.23	2.01	6.32E-06	0.80	1.57	2802052	1777237	6117985	3248397	5412966	3101562	6823003	3268859
HILIC_POS_496_33926a1_309	HILIC	POS	1.31	496.3393	LPC 16:0	184.0741(100), 104.1071(70), 496.3452(20), 86.0971(18)	2	2.91E-02	0.40	1.00	2.96E-02	-0.45	1.30	4.05E-01	0.17	0.30	3.12E-03	0.62	1.10	690900610	188706862	782707945	240981525	834910418	235722738	730505471	237071090
RP_POS_538_38635a11_132	RP	POS	11.13	538.3864	LPC 19:0	184.0722(100), 538.3342(60), 520.3745(5), 104.107(80), 538.8439(40)	2	3.92E-06	-1.26	2.08	3.04E-02	-0.28	1.47	6.97E-07	-1.40	2.04	3.68E-05	-1.12	1.72	2323884	1141243	1182873	596840	1311577	617025	1054169	552431
HILIC_POS_137_071a2_193	HILIC	POS	2.19	137.0710	1-Methylnicotinamide	137.0708(100), 94.0657(5)	1	3.85E-01	-0.15	0.46	3.06E-02	-0.46	1.21	8.71E-02	-0.38	0.59	6.76E-01	0.08	0.25	24372493	13299135	21783032	18036759	25672336	14259557	17893727	20568978
RP_NEG_612_33154a10_191	RP	NEG	10.19	612.3315	LPC 22:6 [M+HCOO]-	327.2362(100), 552.3096(40),	2	6.49E-01	-0.08	0.98	3.09E-02	-0.45	1.30	1.36E-01	-0.31	0.75	5.05E-01	0.14	0.90	3124791	1176762	3008417	1461373	3322467	1482672	2694368	1383912
RP_POS_724_52667a13_381	RP	POS	13.38	724.5267	PE P-36:4|PE P-16:0_20:4	361.2745(100), 266.2842(20), 583.5109(10), 60.0815(30), 81.0704(30), 95.0855(30)	2	5.16E-01	-0.14	0.87	3.17E-02	-0.43	1.26	9.93E-02	-0.35	0.80	7.59E-01	0.08	0.67	5471775	2674330	5119989	2559848	5669397	3069128	4570581	1789918
RP_POS_590_32159a10_295	RP	POS	10.30	590.3216	LPC 22:6 (22:6/0:0)	104.1076(100), 531.2495(50), 86.0964(18)	2	6.92E-01	-0.07	0.95	3.21E-02	-0.45	1.30	1.50E-01	-0.30	0.74	4.76E-01	0.15	0.90	8724385	3197915	8448679	4004895	9303466	4089330	7593891	3767217
RP_POS_132_07686a0_577	RP	POS	0.58	132.0769	Creatine	90.0559(100), 132.0767(90), 114.067(4)	2	8.25E-02	0.32	0.51	3.26E-02	-0.44	1.45	6.36E-01	0.10	0.57	1.05E-02	0.54	0.88	6109140	3726232	7526688	4601188	8505782	4466996	6547594	4567658
HILIC_POS_520_34039a1_279	HILIC	POS	1.28	520.3404	LPC 18:2	184.0745(100), 104.1073(70), 520.3422(40), 86.0972(20)	2	1.66E-01	-0.33	0.88	3.34E-02	-0.39	1.24	4.05E-02	-0.52	0.92	5.96E-01	-0.13	0.34	28587134	140419696	247808939	106870268	270452220	105279845	225165658	104620197
RP_POS_544_33948a10_199	RP	POS	10.20	544.3399	LPC 20:4	184.0734(100), 544.333(3), 526.3271(0.8)	2	2.73E-01	0.23	0.81	3.36E-02	-0.42	1.67	9.19E-01	0.02	0.44	5.16E-02	0.44	0.96	26610415	10934134	29038706	10271102	31213360	9012565	26864052	11057416
RP_POS_744_58899a14_128	RP	POS	14.13	744.5890	PC O-34:2	184.0732(100), 744.5767(3)	2	4.27E-01	-0.15	0.37	3.40E-02	0.44	1.28	7.59E-01	0.07	0.28	6.12E-02	-0.37	0.69	4631243	1474922	4380447	1743056	4011603	1372412	4749291	1994326
RP_POS_776_51837a12_466	RP	POS	12.47	776.5184	PC 34:4 [M+Na]+	146.9817(100), 593.4515(75), 86.0968(65), 776.52(40), 717.4384(38)	2	6.71E-01	0.10	0.67	3.42E-02	-0.40	1.26	6.74E-01	-0.10	0.92	2.40E-01	0.30	0.57	3652681	2316282	3844969	1864747	4238527	1940924	3451411	1715296
RP_NEG_253_21748a10_827	RP	NEG	10.83	253.2175	FA 16:1 (Palmitoleic acid)	253.2186(100)	2	2.78E-11	1.00	1.88	3.53E-02	0.42	1.48	1.55E-09	1.21	2.02	2.11E-06	0.79	1.73	1274513	1078853	3403496	2130919	2956491	1892457	3850502	2277088
RP_POS_426_35754a9_373	RP	POS	9.37	426.3575	CAR 18:1 (Oleoylcarnitine)	85.0288(100), 426.3528(60)	1	2.87E-11	1.11	1.78	3.79E-02	0.47	1.26	1.71E-10	1.31	1.98	2.73E-07	0.84	1.75	12749926	5215526	22162205	8020179	19880440	7244677	23821726	8476643
HILIC_POS_595_34918a1_11	HILIC	POS	1.11	595.3492	Stercobilin	345.182(100), 470.2632(95), 595.3523(75)	2	5.87E-02	0.27	0.76	3.81E-02	0.46	1.19	2.56E-02	0.50	0.85	7.16E-01	0.05	0.22	1811623	5587625	4755204	11826975	2294365	6220026	7216044	15217161
RP_POS_288_25229a9_361	RP	POS	9.36	288.2523	Lauryl diethanolamide	106.0876(100), 88.0762(55), 288.2547(20), 227.1991(20)	2	1.23E-01	-0.30	0.93	3.84E-02	0.42	1.23	7.04E-01	-0.09	0.59	9.98E-03	-0.51	0.95	5894523	336613	5784749	370759	5707977	258685	5861521	445851
HILIC_POS_482_32376a1_354	HILIC	POS	1.35	482.3238	LPC 15:0	104.1073(100), 184.0728(80), 482.3219(10)	2	2.00E-04	-0.77	1.59	3.88E-02	-0.39	1.26	9.94E-06	-0.97	1.88	1.33E-02	-0.58	1.24	7418106	2569083	5333328	2552824	5860067	2918578	4806590	2020517
RP_POS_247_1440a3_062	RP	POS	3.06	247.1441	Lenticin	188.0716(100), 60.0815(65), 146.0603(25)	2	7.97E-02	-0.48	0.89	3.91E-02	-0.33	1.37	2.01E-02	-0.64	1.14	2.80E-01	-0.31	0.42	15471256	18466578	9308453	10197530	11413623	12475016	7203284	6740258
RP_POS_564_30579a10_032	RP	POS	10.03	564.3058	LPC 20:5 (20:5/0:0)	104.1076(100), 505.2331(55), 564.306(15), 86.0964	2	9.73E-02	0.33	0.97	3.94E-02	-0.41	1.26	5.45E-01	0.13	0.57	2.14E-02	0.54	1.06	4287268	4057287	5690204	4202907	6553623	4546296	4826784	3674116
RP_POS_494_32391a9_984	RP	POS	9.98	494.3239	LPC 16:1 (0:0/16:1)	184.0735(100), 494.3196(3)	1	4.78E-16	1.03	1.87	3.99E-02	0.42	1.30	7.97E-09	1.24	1.90	3.32E-11	0.82	1.95	7841732	3270524	22226873	14253052	19295243	9331322	25158502	17488042
RP_POS_140_06783a0_552	RP	POS	0.55	140.0678	Glycine betaine [M+Na]+	140.0682(100), 74.0968(50), 114.0889(4), 96.0793(1)	2	1.40E-04	0.53	0.90	4.05E-02	0.45	1.41	1.74E-04	0.76	1.23	4.22E-02	0.31	0.97	4371724	747724	5240577	1769607	4878721	1461769	5602433	1980639
RP_POS_466_29263a9_501	RP	POS	9.50	466.2926	LPC 14:1	184.0729(100), 466.2884(25), 448.2802(7), 104.1073(85)	2	4.38E-08	0.69	1.41	4.06E-02	0.45	1.33	3.42E-05	0.92	1.44	4.98E-06	0.47	1.38	231674	192158	717867	761817	561373	408196	874361	977738
RP_POS_494_32336a10_125	RP	POS	10.13	494.3234	LPC 16:1 (16:1/0:0)	184.073(100), 494.3183(25), 476.3127(8) , 104.1075(90)	1	2.34E-17	1.09	1.92	4.08E-02	0.41	1.30	1.55E-09	1.29	1.97	5.13E-12	0.88	2.01	68531727	27857219	186186962	108750645	163926128	72991453	208447795	132497921
RP_POS_832_5813a13_541	RP	POS	13.54	832.5813	PC 38:4|PC 18:2_20:2 [M+Na]+	146.9818(100), 86.0968(50), 649.5152(40), 832.5806(30), 773.5119(25), 627.5269(8)	2	5.66E-01	0.12	0.41	4.20E-02	0.40	1.19	1.78E-01	0.32	0.51	7.40E-01	-0.08	0.58	11126733	3779757	11561935	3479644	10856349	3264812	12267522	3576020
RP_POS_728_5191a12_844	RP	POS	12.84	728.5191	PC 30:0 [M+Na]+	146.982(100), 86.0964(40), 728.5206(35), 545.4542(28), 669.4459(25), 523.475(20)	2	5.85E-03	0.54	1.00	4.24E-02	0.40	1.25	1.47E-03	0.74	1.19	9.17E-02	0.34	0.61	2059118	1339049	2856377	1464392	2559677	1210547	3153077	1639382
HILIC_POS_520_34064a1_15	HILIC	POS	1.15	520.3406	LPC 18:2	184.0742(100), 520.3424(3)	2	1.52E-01	-0.35	0.91	4.29E-02	-0.36	1.19	4.32E-02	-0.53	0.92	5.01E-01	-0.17	0.40	33603138	21239096	27713055	14783984	30697598	14622840	24728511	14477115
HILIC_POS_118_08664a3_699	HILIC	POS	3.70	118.0866	Glycine betaine	118.0868(100), 59.0739(3)	1	3.95E-03	0.40	0.92	4.30E-02	0.45	1.28	3.61E-03	0.63	1.09	1.78E-01	0.18	0.46	1273942568	475380563	#########	#########	1459132488	758423818	1921096284	#########
RP_POS_285_07895a8_02	RP	POS	8.02	285.0790	Diazepam	285.0785(100), 257.084(6), 154.0414(5)	2	1.11E-03	0.43	1.09	4.35E-02	0.45	1.60	2.27E-03	0.66	1.41	8.86E-02	0.21	0.66	11402119	32370412	48986848	97019506	29371300	61578263	68602397	120168798
HILIC_POS_132_0768a5_591	HILIC	POS	5.59	132.0768	Creatine	90.0554(100), 132.0771(80)	1	1.24E-01	0.29	0.55	4.36E-02	-0.41	1.41	6.89E-01	0.09	0.46	1.90E-02	0.50	0.91	70737110	43324146	85010278	49894417	95051813	46875568	74968743	51250478
RP_POS_790_57318a13_242	RP	POS	13.24	790.5732	PC O-38:7	184.0732(100), 790.5635(2)	2	1.12E-05	-0.89	1.58	4.37E-02	-0.38	1.27	9.99E-07	-1.08	1.82	1.36E-03	-0.70	1.21	6139808	1553615	4596776	1618897	4922485	1700229	4271068	1479142
RP_NEG_746_56818a13_32	RP	NEG	13.32	746.5682	PC 33:1	184.0732(100), 746.5707(2)	2	3.13E-01	0.19	0.62	4.38E-02	0.41	1.19	7.09E-02	0.40	0.78	9.50E-01	-0.01	0.14	7128338	2260132	7611328	2567856	7094923	2426857	8127734	2624589
RP_NEG_588_33154a10_199	RP	NEG	10.20	588.3315	LPC 20:4 [M+HCOO]-	303.2313(100), 528.3049(20)	2	2.10E-01	0.27	0.76	4.52E-02	-0.39	1.57	7.69E-01	0.07	0.40	4.06E-02	0.46	0.94	10870500	3867576	11852951	3614053	12575463	3118238	11130440	3949753
RP_NEG_538_31592a9_984	RP	NEG	9.98	538.3159	LPC 16:1 [M+HCOO]-	253.2186(100), 478.2944(19)	2	1.96E-17	1.08	1.92	4.60E-02	0.40	1.26	1.69E-09	1.28	1.97	1.07E-11	0.88	1.98	3969272	1490259	10898932	6465544	9607670	4454467	12190194	7823976
RP_NEG_750_53046a12_847	RP	NEG	12.85	750.5305	PC 30:0|PC 14:0_16:0 [M+HCOO]-	227.2(100), 255.2332(90), 690.5033(30)	2	1.56E-03	0.63	1.11	4.76E-02	0.39	1.24	4.62E-04	0.83	1.30	3.10E-02	0.44	0.79	1799787	1106129	2559304	1176475	2326573	965534	2792034	1324251
RP_NEG_824_54694a12_579	RP	NEG	12.58	824.5469	PC 36:5|PC 16:0_20:5 [M+HCOO]-	279.235(100), 303.2319(45), 764.5127(35), 253.2187(30)	2	8.72E-07	0.90	1.59	4.78E-02	0.39	1.20	2.19E-06	1.09	1.67	6.69E-05	0.70	1.51	4284188	1700215	6301584	2193104	5867254	1522576	6735914	2648461
RP_POS_448_34177a9_121	RP	POS	9.12	448.3418	CAR 20:4	448.3451(100), 85.0292(75)	2	5.96E-11	0.97	1.63	4.81E-02	0.40	1.62	3.57E-09	1.17	1.86	3.59E-06	0.78	1.59	362310	219099	789495	441156	702478	397058	876512	469149
RP_POS_146_11719a0_566	RP	POS	0.57	146.1172	Deoxycarnitine	146.1178(100), 87.0447(48), 60.0814(25), 130.0506(5)	1	8.53E-01	0.03	0.68	4.81E-02	-0.42	1.34	4.01E-01	-0.18	0.83	1.97E-01	0.24	0.90	4981390	1143859	5029489	1623826	5349850	1402946	4709128	1774746
HILIC_POS_229_11833a6_131	HILIC	POS	6.13	229.1183	Proline-hydroxyproline	70.0659(100), 229.1171(35), 132.0657(20)	2	6.49E-01	-0.09	0.79	4.86E-02	-0.41	1.14	1.63E-01	-0.29	1.02	6.04E-01	0.12	0.67	1254657	714354	1185899	816997	1346739	876914	1025058	725822
RP_NEG_824_54712a12_695	RP	NEG	12.70	824.5471	PC 36:5|PC 16:0_20:5 [M+HCOO]-	301.2184(100), 255.2334(90), 764.5135(35)	2	2.08E-03	0.61	1.21	4.94E-02	-0.39	1.22	5.43E-02	0.41	0.85	3.24E-04	0.80	1.31	32791967	13192168	41645017	14464217	44481186	14340857	38808848	14164059
RP_NEG_826_56226a13_071	RP	NEG	13.07	826.5623	PC 36:4|PC 16:0_20:4 [M+HCOO]-	303.2315(100), 255.233(60), 766.5427(25)	2	3.04E-01	0.22	0.51	5.64E-02	-0.38	1.15	9.03E-01	0.03	0.62	6.65E-02	0.41	0.83	97630208	17676945	101308268	16658455	104485244	13470099	98131293	18937522
RP_POS_480_34473a10_699	RP	POS	10.70	480.3447	LPC O-16:1	104.1076(100), 480.3414(100), 86.0964(45), 184.0733(35), 124.9998(22)	2	7.83E-02	-0.40	1.01	5.84E-02	-0.36	1.71	2.00E-02	-0.58	1.07	3.58E-01	-0.22	0.80	24664467	8272414	21752908	6887758	23054488	6652345	20451328	6938266
RP_POS_802_53503a12_693	RP	POS	12.69	802.5350	PC 36:5 [M+Na]+	146.9814(100), 619.4614(65), 86.0966(61), 743.4567(35), 802.5381(30), 597.4855(7)	2	3.75E-03	0.58	1.22	5.86E-02	-0.37	1.18	6.92E-02	0.40	0.85	6.45E-04	0.77	1.29	50431049	22187141	64247045	23305019	68648086	22959866	59846004	23035790
RP_NEG_538_31543a10_125	RP	NEG	10.13	538.3154	LPC 16:1 [M+HCOO]-	253.2184(100), 478.2941(35), 224.0698(9)	2	3.43E-19	1.18	2.00	5.89E-02	0.37	1.22	9.36E-11	1.37	2.07	4.20E-13	1.00	2.09	33339917	11811190	78152681	36966331	71162082	26517576	85143280	44249223
RP_POS_782_56714a13_72	RP	POS	13.72	782.5671	PC 34:1 [M+Na]+	146.9823(100), 86.0965(45), 782.5644(35), 599.5015(30), 723.4892(22), 577.5145(15)	2	4.35E-08	0.94	1.54	5.91E-02	0.37	1.13	5.43E-09	1.12	1.90	1.75E-04	0.75	1.38	137918081	23555194	170752270	34350960	164274492	37061767	17723047	30411312
RP_POS_363_21646a7_048	RP	POS	7.05	363.2165	Cortisol	363.217(100), 121.0645(50), 327.1921(20), 309.1825(15), 267.1724(13), 345.2052(10)	1	8.94E-02	-0.43	2.00	6.02E-02	0.32	1.13	3.02E-01	-0.27	1.18	2.87E-02	-0.59	1.53	11348473	5945582	9399844	3840044	8679111	3848208	10120577	3731487
SCFA_Acetic acid	SCFA	SCFA			FA 02:0 (Acetic acid)	targeted SCFA analysis	1	8.11E-05	0.47	0.93	6.27E-02	0.42	1.37	6.83E-04	0.68	1.08	4.29E-02	0.26	0.69	683499	304851	3458037	6692952	2213096	5191490	4728386	7789915
RP_POS_160_13326a2_925	RP	POS	2.93	160.1333	Pregabalin	160.1332(30), 142.1218(100), 97.103(40)	2	1.30E-01	0.18	0.65	6.32E-02	0.43	1.25	8.77E-02	0.39	0.69	3.53E-01	-0.03	0.57	2839223	3829715	6912062	25812476	2070246	3289444	11753879	35881776
RP_POS_752_55762a14_271	RP	POS	14.27	752.5576	PE P-38:4|PE P-18:0_20:4	361.2746(100), 392.2911(45), 294.313(22), 611.5332(7), 752.5183(2), 81.0704(30), 95.0856(28), 67.055(25), 119.0853(20)	2	9.28E-01	-0.02	0.35	6.37E-02	-0.39	1.11	2.73E-01	-0.21	0.59	4.51E-01	0.18	0.43	7183164	3729739	7111071	4433800	7933899	5229530	6288244	3314913
RP_POS_384_08264a6_157	RP	POS	6.16	384.0826	Pantoprazole	138.0552(100), 200.038(90), 153.0791(38), 122.0599(8), 107.073(2)	2	2.97E-03	0.46	0.74	6.51E-02	0.40	1.15	3.49E-03	0.66	1.00	6.58E-02	0.26	0.85	20031232	10627979	28144547	18827616	24661018	11410497	31628075	23690247
RP_POS_806_56885a12_958	RP	POS	12.96	806.5689	PC 38:6|PC 16:0_22:6	184.0735(100), 806.5713(3)	2	2.18E-06	-0.86	1.68	6.51E-02	-0.36	1.16	1.01E-06	-1.04	1.87	5.14E-04	-0.68	1.35	318435243	57973748	252580794	75168567	266430165	70770947	238731424	77562707
RP_POS_152_07077a2_588	RP	POS	2.59	152.0708	Paracetamol	152.0712(100), 110.0598(60), 134.0595(2)	2	4.01E-02	0.24	0.44	6.73E-02	-0.42	1.23	2.92E-01	0.03	0.36	5.07E-02	0.45	0.55	364824	1076657	3175612	13386174	5648548	18609003	702676	1805763
RP_POS_225_19606a7_999	RP	POS	8.00	225.1961	Dicyclohexylurea	225.1955(100), 100.1126(25), 143.1169(2)	2	5.79E-01	0.12	0.79	6.90E-02	-0.35	1.21	8.10E-01	-0.06	0.59	2.27E-01	0.30	0.68	3974241	1891928	4182909	1673631	4487083	1800031	3878736	1493423

Supplementary table 1: Metabolomics results (in asceding order according to p-value from progressive ALD vs non-progressive ALD comparison, with molecular features with ID_level of 1-2 first)

								all_ALD_vs_control			Prog_ALD_vs_non-prog_ALD			Prog_ALD_vs_control_ALD			Non-prog_ALD_vs_control			Healthy_control		all_ALD		Non-prog_ALD		Progressive_ALD	
								t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA								
Feature_ID	RP_HILIC	POS_NEG	Average.Rt	Average.Mz	Metabolite.name	curated_MSMS	ID_level	p	d	VIP	p	d	VIP	p	d	VIP	p	d	VIP	Mean	SD	Mean	SD	Mean	SD	Mean	SD
RP_POS_808_58398a13_996	RP	POS	14.00	808.5840	PC 36:2 [M+Na]+	146.9816(100), 86.0968(50), 625.5158(35), 808.5881(30), 749.5114(20), 603.5292(12)	2	2.75E-02	-0.49	0.93	7.30E-02	0.34	1.16	1.66E-01	-0.32	0.78	8.24E-03	-0.66	1.05	144384054	35035668	128654819	30721124	123147605	33371798	134162034	27041860
RP_POS_786_5993a13_998	RP	POS	14.00	786.5993	PC 36:2|PC 18:0_18:2	184.0732(100), 786.5901(2)	2	6.72E-02	-0.44	0.88	7.43E-02	0.32	1.17	2.68E-01	-0.28	0.72	1.95E-02	-0.60	0.94	351706188	103721029	314465290	75224639	301046862	72260900	327883718	76445287
RP_POS_768_58923a13_584	RP	POS	13.58	768.5892	PC O-36:4|PC O-16:0_20:4	184.0735(100), 768.5784(3)	2	3.81E-02	-0.40	0.72	7.61E-02	-0.36	1.05	3.86E-03	-0.58	1.10	3.49E-01	-0.22	0.44	48776751	12803373	43061071	14623388	45653811	17089862	40463831	11234814
RP_NEG_854_59454a13_547	RP	NEG	13.55	854.5945	PC 38:4|PC 18:2_20:2 [M+HCOO]-	305.2496(100), 279.2349(56), 794.5665(27), 112.9847(50)	2	3.81E-01	0.19	0.50	7.73E-02	0.35	1.05	1.34E-01	0.36	0.57	9.57E-01	0.01	0.62	8015170	2517849	8460242	2352571	8044654	2155254	8875830	2486872
RP_POS_396_31055a8_634	RP	POS	8.63	396.3106	CAR 16:2	85.0287(100), 396.3098(75)	1	8.44E-01	-0.04	0.88	7.91E-02	-0.37	1.81	2.16E-01	-0.22	0.87	5.37E-01	0.15	0.81	623133	365171	607586	448948	686685	562543	528486	279282
RP_POS_836_61517a14_022	RP	POS	14.02	836.6152	PC 40:5|PC 20:1_20:4	184.0732(100), 836.6042(2)	2	4.88E-06	0.80	1.35	7.98E-02	0.35	1.30	1.03E-05	0.97	1.53	4.89E-04	0.62	1.25	12909805	3994816	17361747	5616739	16376770	4482236	18346723	6455150
RP_POS_752_52142a12_164	RP	POS	12.16	752.5214	PC 34:5	184.0732(100), 752.5291(3)	2	6.78E-02	0.29	0.96	8.03E-02	-0.38	1.05	5.79E-01	0.10	0.70	2.00E-02	0.48	0.79	1912517	995420	2367099	1718067	2667636	1872980	2066563	1507103
RP_POS_589_48016a14_415	RP	POS	14.42	589.4802	DG 32:1 [M+Na]+	589.4122(100)	2	2.30E-03	0.36	0.81	8.26E-02	0.40	1.03	1.38E-02	0.56	0.82	4.69E-03	0.17	0.86	1053388	805056	2870563	5646389	1882594	1741226	3858532	7706503
RP_POS_437_323a11_2	RP	POS	11.20	437.3230	DG 21:0 [M+Na]+	437.3226(100), 96.9217(6), 232.8979(3)	2	2.16E-06	0.56	1.22	8.73E-02	-0.38	1.41	9.45E-04	0.37	1.37	3.14E-04	0.75	1.34	186157	84912	1967283	3535936	2573735	4352974	1360832	2358366
RP_POS_218_13847a0_71	RP	POS	0.71	218.1385	CAR 03:0 (Propionylcarnitine)	85.0288(100), 218.1379(60), 159.0644(15), 60.0816(13),	1	9.97E-01	0.00	0.76	8.81E-02	-0.36	1.10	3.78E-01	-0.18	0.48	3.72E-01	0.18	0.74	4835877	1610774	4834366	2190131	5207936	2126468	4460796	2210105
RP_POS_147_0766a0_525	RP	POS	0.53	147.0766	Glutamine	130.0501(100), 84.0446(80), 147.0766(8), 101.0714(8), 102.055(5)	1	7.19E-01	0.05	0.69	8.91E-02	-0.38	1.09	4.89E-01	-0.13	0.48	1.66E-01	0.24	0.82	8636320	1416022	8771704	2803172	9248586	2544964	8294823	2989139
RP_POS_279_17035a4_44	RP	POS	4.44	279.1704	Phenylalanylisoleucine	120.0814(100), 279.1688(5)	2	1.34E-04	0.45	1.19	9.06E-02	0.38	1.38	2.58E-03	0.64	1.30	1.06E-02	0.26	1.21	309627	56920	3092948	7001992	1903257	4239362	4282640	8842831
RP_NEG_498_26358a10_049	RP	NEG	10.05	498.2636	LPE 20:5	301.2183(100), 196.0374(33), 498.2665(25), 78.9574(18), 214.0472(9)	2	1.51E-05	0.69	1.30	9.27E-02	-0.35	0.99	2.74E-03	0.52	1.19	3.23E-05	0.87	1.43	2757964	1983553	4970776	3327237	5530700	3686656	4410852	2852311
RP_NEG_748_53003a13_52	RP	NEG	13.52	748.5300	PE O-38:6|PE O-16:1_22:5	303.2315(100), 748.5336(17), 462.298(13)	2	9.29E-01	-0.02	0.67	9.33E-02	-0.35	0.99	3.60E-01	-0.19	0.41	4.70E-01	0.16	0.74	3724098	1252949	3700310	1488718	3950268	1547911	3450352	1397947
RP_POS_290_15967a2_242	RP	POS	2.24	290.1597	Adipoyl-L-carnitine	290.1582(100), 85.0287(75), 129.0542(35),	2	7.56E-04	0.39	0.91	9.40E-02	0.38	1.13	6.14E-03	0.59	0.90	3.36E-02	0.20	0.69	144185	263519	2252546	6049336	1234762	3514193	3270330	7711819
RP_POS_800_51837a12_377	RP	POS	12.38	800.5184	PC 36:6	146.9818(100), 86.0968(85), 617.4538(80), 741.4485(50), 800.5135(40), 595.4698(13)	2	6.99E-02	-0.37	1.15	9.52E-02	-0.33	1.02	1.41E-02	-0.54	1.31	3.81E-01	-0.21	0.51	1734074	918196	1388579	923368	1542813	1019718	1234345	796394
RP_POS_307_11127a4_916	RP	POS	4.92	307.1113	Fluconazole	220.0664(100), 238.0788(95), 73.0652(50), 307.1103(50), 169.046(40)	2	5.03E-01	0.10	1.12	9.69E-02	-0.37	1.25	4.85E-01	-0.09	0.58	2.13E-01	0.28	1.10	8241731	6150336	9366239	12746109	11494257	16618577	7238222	6543953
RP_NEG_309_28049a11_691	RP	NEG	11.69	309.2805	FA 20:1	309.2805(100)	2	1.08E-08	0.88	1.72	9.78E-02	0.34	1.20	3.73E-07	1.05	1.76	1.62E-05	0.71	1.66	610296	367575	1194941	673196	1083337	565645	1306544	755157
RP_POS_806_56622a13_401	RP	POS	13.40	806.5662	PC 36:3 [M+Na]+	146.9818(100), 86.0969(55), 623.5042(40), 806.5659(30), 747.4948(20), 601.5248(12)	2	8.74E-01	0.04	0.45	9.79E-02	-0.30	1.11	6.57E-01	-0.11	0.47	4.54E-01	0.19	0.61	88907602	22752977	89606398	16904216	92406024	16315726	86806772	17179583
RP_POS_500_27722a10_049	RP	POS	10.05	500.2772	LPE 20:5	359.2576(100), 62.0608(80), 500.2825(7)	2	3.24E-05	0.67	1.28	9.80E-02	-0.35	0.98	4.50E-03	0.49	1.16	5.62E-05	0.84	1.40	4463281	3374428	8053286	5620557	8984339	6204516	7122233	4853958
SCFA_Propionic acid	SCFA	SCFA			FA 03:0 (Propionic acid)	targeted_SCFA_analysis	1	5.25E-04	0.82	1.34	1.03E-01	-0.61	2.12	6.95E-02	0.52	1.16	8.22E-04	1.14	1.81	64210	19974	102246	49802	116877	49285	88476	47620
RP_NEG_773_58307a12_915	RP	NEG	12.92	773.5831	SM 36:2;2O [M+HCOO]-	713.558(100), 168.042(80), 78.9573(65)	2	5.29E-05	-0.98	1.66	1.05E-01	-0.27	1.04	2.31E-05	-1.11	1.62	4.38E-04	-0.84	1.61	3993036	1320025	2857256	961379	3013473	779715	2701039	1099819
RP_NEG_498_29181a9_012	RP	NEG	9.01	498.2918	BA 24:1;O3;T	498.2869(100)	2	2.29E-01	0.15	1.00	1.06E-01	0.37	1.11	1.37E-01	0.34	0.82	7.25E-02	0.03	0.52	1005164	725715	1338747	2440956	941266	904064	1736229	3301267
RP_POS_760_58386a14_257	RP	POS	14.26	760.5839	PC 34:1	184.0729(100), 760.5709(3)	2	2.46E-04	0.56	0.94	1.08E-01	0.35	0.97	7.22E-04	0.73	1.11	1.14E-02	0.39	0.95	4780197	3049904	7759241	5681084	6842537	4140477	8675946	6808052
HILIC_NEG_151_02615a1_655	HILIC	NEG	1.66	151.0262	Xanthine	151.0262(100), 108.0202(35)	1	4.61E-11	0.81	1.25	1.09E-01	0.35	1.18	9.90E-07	0.98	1.50	4.81E-06	0.64	1.51	162912	52861	443926	373197	383947	300214	503905	428863
HILIC_POS_177_10217a1_624	HILIC	POS	1.624	177.1022	Serotonin	159.95.10(100)	1	9.65E-03	0.31	0.80	1.11E-01	-0.36	1.04	1.53E-01	0.13	1.02	2.40E-02	0.49	0.95	88995	91959	246301	574894	338491	749945	154111	296627
RP_NEG_733_55182a12_477	RP	NEG	12.48	733.5518	SM 33:1;2O [M+HCOO]-	673.5261(100), 168.042(80), 78.9574(60)	2	4.02E-07	-1.21	2.08	1.13E-01	-0.25	0.93	6.56E-08	-1.34	2.18	1.03E-05	-1.09	1.77	2724529	900097	1692107	664593	1797552	758457	1586663	542619
RP_POS_271_06332a7_721	RP	POS	7.72	271.0633	Nordiazepam	271.0631(100)	2	2.83E-01	0.14	0.71	1.13E-01	0.36	1.17	1.62E-01	0.32	0.95	5.95E-01	-0.04	0.74	56642121	51101091	78224786	178879406	49685995	66279471	106763577	242061076
RP_POS_583_25439a8_27	RP	POS	8.27	583.2544	Biliverdin	297.1203(100), 583.2581(85)	2	2.00E-02	0.35	0.92	1.16E-01	0.34	1.48	1.71E-02	0.52	0.90	2.30E-01	0.18	0.79	1087878	781914	1574386	1526217	1333894	1056215	1814879	1863489
HILIC_NEG_103_03985a0_701	HILIC	NEG	0.70	103.0399	3-Hydroxyisobutyric acid	73.0286(100), 59.0131(30), 101.9237(25), 103.0403(10)	2	5.86E-04	0.41	0.84	1.18E-01	0.36	1.28	1.05E-02	0.59	0.83	3.15E-05	0.23	1.33	3215470	3581770	15549168	34209436	10153756	10025035	20944581	4695252
RP_NEG_717_51996a11_856	RP	NEG	11.86	717.5200	SM 32:2;2O [M+HCOO]-	657.504(100), 168.0422(85), 78.9574(70)	2	2.19E-05	-1.01	1.85	1.18E-01	-0.26	0.93	5.47E-06	-1.14	1.84	3.28E-04	-0.88	1.56	2759531	911828	1924897	683868	2031919	707632	1817876	648674
RP_POS_804_54791a13_069	RP	POS	13.07	804.5479	PC 36:4 [M+Na]+	146.9817(100), 86.0968(65), 621.4869(60), 745.4814(30), 804.5549(30),	2	9.19E-01	-0.02	0.49	1.19E-01	-0.32	0.94	4.38E-01	-0.18	0.81	5.29E-01	0.14	0.45	146049367	21525980	145597052	22313269	149085560	20688795	142108544	23517281
RP_POS_182_08159a0_709	RP	POS	0.71	182.0816	Tyrosine	136.0752(100), 165.0546(50), 123.0443(30), 147.0445(17), 119.0495(15), 182.081(8)	2	3.33E-01	0.17	0.92	1.20E-01	0.33	1.07	1.30E-01	0.33	1.18	9.99E-01	0.00	0.55	75858953	16786033	79563368	23718637	75862569	19460052	83264166	27018219
RP_NEG_303_23337a10_942	RP	NEG	10.94	303.2334	FA 20:4 (Arachidonic acid, AA)	303.2318(100)	2	9.14E-08	0.88	1.70	1.21E-01	0.31	1.01	6.13E-07	1.04	1.74	4.43E-05	0.73	1.61	16296802	7773446	27066049	12218835	25167919	10767073	28964179	13355301
HILIC_NEG_89_02393a1_301	HILIC	NEG	1.30	89.0239	D-Lactic acid	89.024(100)	2	5.25E-11	0.91	1.54	1.22E-01	0.32	0.97	5.97E-08	1.07	1.67	3.24E-06	0.75	1.49	152280210	52610387	268871847	132788175	248289869	117509763	28945825	144748676
RP_POS_325_17111a5_597	RP	POS	5.60	325.1711	Escitalopram	325.1696(100), 109.045(50), 262.1021(20)	2	7.02E-02	0.31	0.79	1.23E-01	0.33	1.08	3.00E-02	0.47	1.22	4.23E-01	0.15	0.44	3727720	2896165	4935992	4130825	4296639	3432489	5575345	4675411
RP_POS_290_15964a2_595	RP	POS	2.60	290.1596	Adipoyl-L-carnitine	290.1571(100), 85.0291(85), 129.0557(40), 101.0242(30), 60.0808(18)	1	1.34E-03	0.38	0.82	1.24E-01	0.35	1.04	7.23E-03	0.55	0.87	7.57E-02	0.20	0.63	195902	326727	1915502	5182397	1114908	3560055	2716097	6346695
RP_POS_812_61475a14_294	RP	POS	14.29	812.6148	PC 38:3|PC 18:0_20:3	184.0732(100), 812.6267(2)	2	2.31E-01	0.23	0.60	1.25E-01	0.31	0.93	1.01E-01	0.39	0.70	7.01E-01	0.08	0.59	71201816	26309920	77847060	29097579	73375800	22584513	82318321	34055199
RP_POS_368_27936a8_076	RP	POS	8.08	368.2794	CAR 14:2	85.0288(100), 368.2795(65)	2	2.69E-01	-0.20	0.93	1.26E-01	-0.32	1.63	3.55E-02	-0.36	1.09	8.78E-01	-0.04	0.75	4088666	2344123	3515617	3038680	3982876	3896342	3048357	1740271
RP_POS_136_07573a0_71	RP	POS	0.71	136.0757	fragment of tyrosine	136.0752(100), 119.0495(55), 91.0544(70)	2	4.49E-01	0.13	0.92	1.27E-01	0.33	1.02	1.80E-01	0.29	1.14	8.50E-01	-0.03	0.57	8547988	1843248	8867594	2651282	8462445	2190009	9272743	3011797
RP_POS_832_58313a13_081	RP	POS	13.08	832.5831	PC 40:7	184.0732(100), 832.5811(3)	2	5.66E-04	-0.63	1.22	1.28E-01	0.31	0.97	3.37E-02	-0.47	0.83	4.48E-05	-0.78	1.54	17554628	4846216	13730096	6164731	12789313	4755761	14670279	7236171
RP_POS_751_5708a12_913	RP	POS	12.91	751.5708	SM 36:2;2O [M+Na]+	568.4996(100), 692.4962(60), 751.5734(40), 86.0967(50), 146.9814(42)	2	2.63E-05	-0.98	1.62	1.30E-01	-0.26	0.98	1.28E-05	-1.11	1.65	2.69E-04	-0.85	1.53	3784177	1274375	2626183	1006566	2779094	859235	2473271	1122953
RP_NEG_568_3634a10_934	RP	NEG	10.93	568.3634	LPC 18:0	283.2653(100), 508.3423(30), 224.0689(5)	2	7.69E-02	-0.42	1.11	1.32E-01	-0.27	1.62	3.29E-02	-0.56	1.06	2.44E-01	-0.29	0.91	171698079	45305571	155959303	33449538	161008780	30036375	150909825	36143579
RP_POS_754_53674a12_465	RP	POS	12.47	754.5367	PC 34:4|PC 14:0_20:4	184.0732(100), 754.5454(2),	2	4.88E-01	0.15	0.64	1.32E-01	-0.30	0.91	9.98E-01	0.00	0.86	2.04E-01	0.30	0.58	12099324	6464103	13001357	5999655	13906761	5810408	12095953	6106760
RP_POS_144_1019a0_615	RP	POS	0.62	144.1019	Proline betaine	144.1012(100)	1	3.96E-01	0.15	1.18	1.34E-01	0.32	1.22	1.53E-01	0.31	1.27	9.41E-01	-0.01	0.69	30747980	24502014	35473216	34475586	30292836	30526211	40653595	37613441
RP_POS_746_604a14_36	RP	POS	14.36	746.6040	PC O-34:1	184.0732(100), 746.6037(3)	2	3.99E-02	-0.38	0.78	1.37E-01	0.31	0.97	3.14E-01	-0.22	0.52	7.32E-03	-0.53	1.08	5499385	2075304	4560352	2566848	4177269	2169531	4943436	2881929
RP_NEG_307_2652a11_385	RP	NEG	11.39	307.2652	FA 20:2	307.263(100)	2	3.79E-10	0.91	1.76	1.40E-01	0.30	1.15	1.09E-07	1.06	1.81	4.23E-06	0.76	1.66	721152	378162	1446416	818870	1325126	721777	1567705	896546
HILIC_POS_160_13289a2_098	HILIC	POS	2.10	160.1329	5-AVAB	160.1328(100), 101.0603(30), 60.0815(20)	1	2.29E-04	0.56	0.99	1.44E-01	0.31	0.92	3.83E-04	0.72	1.20	1.88E-02	0.40	0.80	66495525	21776096	88074191	41316200	82022309	36803323	94126074	44940672
RP_POS_730_53711a12_533	RP	POS	12.53	730.5371	PC 32:2|PC 16:1_16:1	184.0732(100), 730.5381(3)	2	3.41E-01	0.19	0.74	1.45E-01	0.29	0.86	1.53E-01	0.34	0.80	8.34E-01	0.04	0.18	30342401	13380986	32974845	13840360	30951529	11810148	34998161	15465644
RP_POS_810_59827a13_871	RP	POS	13.87	810.5983	PC 38:4 + PC 36:1 [M+Na]+	146.9819(100), 86.0969(65), 649.5148(55), 773.5109(32), 832.5852(30), 627.5255(5)	2	6.61E-01	-0.09	0.51	1.48E-01	0.28	1.12	8.48E-01	0.05	0.49	2.90E-01	-0.24	0.44	192144519	59791051	186902926	54375499	179019144	44288490	194786708	62333099
RP_POS_786_59991a14_252	RP	POS	14.25	786.5999	PC 36:2	184.0732(100), 786.5897(2)	2	7.19E-01	-0.08	0.35	1.51E-01	0.28	0.99	7.80E-01	0.07	0.18	3.49E-01	-0.22	0.67	22208884	13236654	21250963	12360617	19471742	12137919	23030184	12445812
RP_POS_299_13901a5_809	RP	POS	5.81	299.1390	3-Hydroxy-3',4'-Dimethoxyflavone	299.1375(100)	2	5.42E-01	-0.08	0.61	1.51E-01	0.32	1.28	7.36E-01	0.08	0.39	1.27E-02	-0.25	1.15	634447	356246	567875	887307	439404	298073	696347	1211678
HILIC_POS_170_08121a0_885	HILIC	POS	0.89	170.0812	Pyridoxine (Vitamin B6)	152.0701(100), 170.0821(35), 134.0606(20)	1	1.52E-01	0.17	0.77	1.53E-01	0.33	0.94	1.53E-01	0.33	0.76	5.98E-01	0.00	0.67	12697	27027	7231305	49965431	15694	21414	14446916	70269360
RP_POS_256_01541a4_299	RP	POS	4.30	256.0154	Lamotrigine	256.0161(100)	2	1.31E-02	-0.43	0.70	1.54E-01	0.30	0.86	2.45E-01	-0.28	0.43	2.60E-04	-0.58	1.47	78735090	35582967	58391180	49334636	51301543	20112611	65480816	66410764
RP_NEG_810_56763a13_375	RP	NEG	13.38	810.5676	PC O-36:5|PC O-16:1_20:4 [M+HCOO]-	303.2352(100), 750.5476(28), 464.3197(16), 446.3023(5)	2	9.07E-01	-0.02	0.60	1.56E-01	-0.30	0.89	4.14E-01	-0.17	0.38	5.58E-01	0.13	0.48	6749295	1730732	6705597	2097411	7004093	2166605	6407102	2003004
SCFA_Isovaleric acid	SCFA	SCFA			FA 05:0 (Isovaleric acid)	targeted_SCFA_analysis	1	2.54E-02	0.31	0.57	1.58E-01	-0.34	1.00	1.84E-01	0.13	0.64	4.69E-02	0.47	0.74	85573	88255	179884	342948	230153	449977	125846	153145
RP_POS_804_55029a12_821	RP	POS	12.82	804.5503	PC 36:4 [M+Na]+	146.9823(100), 621.487(45), 804.5485(30), 745.4802(25), 599.5013(12)	2	2.00E-06	-1.15	1.84	1.58E-01	-0.23	0.94	6.68E-07	-1.26	1.93	2.36E-05	-1.03	1.60	57199483	20287995	35818086	14838236	37918326	14777569	33717846	14746565
HILIC_POS_130_1089a1_485	HILIC	POS	1.49	130.1089	Metformin	60.0567(100), 130.1095(100), 71.0604(40), 85.0518(25), 88.0869(25)	2	8.20E-01	-0.08	0.77	1.59E-01	0.14	0.98	9.81E-01	-0.01	0.11	6.67E-01	-0.14	0.53	34934212	114634732	30227260	29737331	26021555	23467144	34432966	34638996
RP_POS_369_35065a13_296	RP	POS	13.30	369.3507	Cholesterol	369.3474(100), 161.1315(45), 147.1173(40), 135.1167(30), 95.0857(30), 109.1011(28), 81.0705(26), 175.1472(18), 121.1013(13), 215.1801(10), 203.1797(8), 243.2101(8),	2	1.56E-01	-0.26	0.73	1.60E-01	0.30	0.88	6.24E-01	-0.11	0.47	3.95E-02	-0.40	0.79	45463844	7507204	43107547	9661312	41746480	8303662	44468614	10763615
HILIC_POS_143_08162a0_723	HILIC	POS	0.72	143.0816	Piracetam	98.0603(100), 126.055(45), 143.0815(5)	2	1.61E-01	0.16	0.46	1.63E-01	-0.32	0.83	7.27E-01	0.00	0.27	1.63E-01	0.32	0.42	298831	106519	5591106	37510234	10874710	52780343	307503	113783
HILIC_POS_250_18013a0_867	HILIC	POS	0.87	250.1801	N,O-Didesmethylvenlafaxine	232.17(100), 250.18(70), 202.127(50), 133.0645(40), 107.0498(40)	2	4.23E-02	0.24	0.76	1.64E-01	-0.32	1.18	8.30E-03	0.08	0.86	8.59E-02	0.40	0.78	212291	829562	4820054	22349360	7958255	31236633	1681854	3654550
RP_POS_524_37085a10_932	RP	POS	10.93	524.3709	LPC 18:0	184.0724(100), 524.3712(33), 506.3652(8), 104.107(85)	2	1.61E-01	-0.34	1.01	1.66E-01	-0.25	1.52	7.70E-02	-0.46	0.89	3.96E-01	-0.21	0.84	501365860	156623930	458681396	113229873	474399783	106128920	442963008	118895307
RP_NEG_826_56268a12_823	RP	NEG	12.82	826.5627	PC 36:4|PC 18:2_18:2 [M+HCOO]-	303.2315(100), 255.2332(60), 766.5427(25)	2	5.95E-06	-1.10	1.78	1.67E-01	-0.22	0.92	2.26E-06	-1.21	1.86	5.87E-05	-0.99	1.55	37010478	12647643	24497051	9124625	25760597	8884156	23233505	9275249
RP_POS_808_58411a13_2	RP	POS	13.20	808.5841	PC 38:5|PC 16:0_22:5 AND PC 18:1_20:4	184.0731(100), 808.5745(2)	2	2.82E-03	0.58	1.03	1.70E-01	0.27	1.08	2.63E-03	0.72	1.11	2.19E-02	0.44	0.93	103754159	21961484	118086635	24579272	114697631	18012137	121475639	29542072
RP_NEG_614_34747a10_447	RP	NEG	10.45	614.3475	LPC 22:5 [M+HCOO]-	329.2495(100), 554.3241(60), 224.0686(20)	2	8.20E-04	0.64	1.29	1.70E-01	-0.27	1.03	2.25E-02	0.50	1.00	2.00E-04	0.78	1.46	5655722	2979846	7878775	3473388	8356658	3119221	7400891	3765561
RP_POS_143_08138a0_71	RP	POS	0.71	143.0814	Piracetam	98.0602(100), 126.0553(48), 70.0657(4), 143.0808(2)	2	1.64E-01	0.16	0.58	1.73E-01	-0.32	0.84	1.54E-01	0.00	0.65	1.69E-01	0.32	0.58	15124	8615	2131963	15092452	4210996	21245182	52930	184106
RP_POS_818_60437a13_565	RP	POS	13.57	818.6044	PC O-40:7	184.0732(100), 818.6068(2)	2	4.01E-07	-1.21	2.15	1.73E-01	0.21	1.12	5.57E-06	-1.11	1.77	1.20E-07	-1.32	2.07	10007238	2902091	6677769	2147171	6384658	2035009	6970881	2235660
HILIC_POS_344_27966a0_66	HILIC	POS	0.66	344.2797	AC 12:0 (Lauroylcarnitine)	85.0287(100), 344.2782(50)	1	8.50E-01	0.03	0.49	1.79E-01	-0.28	1.13	5.56E-01	-0.11	0.23	4.47E-01	0.18	0.35	7382375	4208704	7556936	5364383	8281883	6447651	6831990	3936463
RP_POS_370_29504a8_374	RP	POS	8.37	370.2950	CAR 14:1	85.0288(100), 370.2921(50)	2	1.10E-08	0.81	1.50	1.80E-01	0.28	1.38	1.13E-07	0.95	1.77	2.46E-04	0.67	1.32	908317	739419	2226936	1701308	1997877	1768193	2455995	1616905

Supplementary table 1: Metabolomics results (in asceding order according to p-value from progressive ALD vs non-progressive ALD comparison, with molecular features with ID_level of 1-2 first)

								all_ALD_vs_control			Prog_ALD_vs_non-prog_ALD			Prog_ALD_vs_control_ALD			Non-prog_ALD_vs_control			Healthy_control		all_ALD		Non-prog_ALD		Progressive_ALD	
								t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA								
Feature_ID	RP_HILIC	POS_NEG	Average.Rt	Average.Mz	Metabolite.name	curated_MSMS	ID_level	p	d	VIP	p	d	VIP	p	d	VIP	p	d	VIP	Mean	SD	Mean	SD	Mean	SD	Mean	SD
RP_POS_810_59894a14_255	RP	POS	14.26	810.5989	PC 38:4|PC 18:0_20:4	184.0732(100), 810.5998(2)	2	6.54E-01	0.08	0.49	1.80E-01	0.28	0.97	3.07E-01	0.22	0.43	7.60E-01	-0.06	0.73	4183248	2772279	4456079	3551367	3978017	3218610	4934141	3828309
RP_POS_130_08647a0_708	RP	POS	0.71	130.0865	Pipecolinic acid	84.0811(100), 130.0865(45)	2	5.56E-01	-0.15	0.43	1.85E-01	0.23	0.88	8.85E-01	-0.04	0.17	3.08E-01	-0.27	0.58	10620882	6984902	9844225	4260787	9276387	2879758	10412062	5265744
RP_POS_150_0582a0_709	RP	POS	0.71	150.0582	Methione	104.053(100), 56.0503(55), 133.0317(55), 61.0114(22), 102.0557(22), 150.084(18)	2	4.36E-01	-0.10	0.47	1.85E-01	0.30	0.91	8.27E-01	0.05	0.27	4.80E-03	-0.25	1.35	24047617	3339034	23108607	10480655	21708594	3860482	24508621	14248739
RP_POS_760_58508a13_717	RP	POS	13.72	760.5851	PC 34:1|PC 16:0_18:1	184.0735(100), 760.5764(3)	2	2.71E-10	1.12	1.77	1.89E-01	0.25	0.95	3.28E-09	1.24	1.88	1.20E-07	0.99	1.76	373955781	79835411	505158758	109955123	490665858	99949055	519651658	118357596
RP_POS_346_1221a5_854	RP	POS	5.85	346.1221	Omeprazole	198.0595(100), 151.0994(55), 136.0752(20), 168.1014(20), 180.047(18), 149.0714(17), 179.0275(7(	1	8.40E-04	0.42	0.80	1.90E-01	0.30	1.00	1.27E-02	0.56	0.84	1.36E-03	0.27	1.12	8531556	4524457	15718151	19413277	13156028	8059284	18280274	26136049
RP_POS_633_45544a10_872	RP	POS	10.87	633.4554	DG 36:7	633.457(100)	2	3.08E-01	-0.17	0.61	1.93E-01	0.28	0.89	8.78E-01	-0.03	0.37	1.09E-01	-0.31	0.61	11935654	587890	11796531	870424	11682903	822046	11910160	910292
RP_POS_858_59827a14_026	RP	POS	14.03	858.5983	PC 40:5 [M+Na]+	146.9818(100), 86.0969(60), 675.5334(40), 858.6024(30), 790.5298(23),	2	5.73E-07	0.94	1.61	1.99E-01	0.25	1.00	2.12E-06	1.07	1.67	1.98E-05	0.82	1.58	4212446	1594384	6112688	1918470	5865129	1575601	6360247	2197402
RP_POS_675_54248a12_21	RP	POS	12.21	675.5425	SM 32:1;2O|SM 16:1;2O/16:0	184.0731(100), 675.5374(1)	2	2.72E-02	-0.45	0.89	2.01E-01	0.25	0.89	1.49E-01	-0.32	0.70	1.11E-02	-0.58	1.02	25226498	7692844	21663631	7815220	20660596	7761927	22666665	7816718
RP_POS_678_50568a12_274	RP	POS	12.27	678.5057	PC 28:0	184.0732(100), 678.4957(4)	2	1.32E-01	0.28	0.69	2.03E-01	0.26	0.88	8.14E-02	0.41	0.75	4.23E-01	0.15	0.36	1591769	1892679	2208760	2268407	1918358	1614868	2499163	2759791
RP_POS_231_08333a0_709	RP	POS	0.71	231.0833	Beta-Asarone	231.0833(100)	2	6.43E-16	1.00	1.69	2.03E-01	0.27	0.92	1.04E-08	1.14	1.82	6.89E-09	0.87	1.69	224878	245550	3142391	3015038	2756909	2557434	3527872	3394510
RP_NEG_297_24417a9_953	RP	NEG	9.95	297.2442	FA 18:1;O	297.2419(100)	2	5.36E-13	0.96	1.66	2.07E-01	0.26	1.37	1.22E-08	1.09	1.78	5.14E-07	0.82	1.71	979616	535994	2499039	1640250	2291411	1525638	2706667	1737872
RP_POS_246_16994a3_08	RP	POS	3.08	246.1699	Isovaleryl-L-carnitine	85.0292(100), 246.1712(70), 187.0963(30), 60.0806(15)	1	3.14E-01	0.17	0.34	2.09E-01	-0.27	0.92	8.55E-01	0.03	0.23	1.49E-01	0.30	0.50	2634111	1169158	2907202	1727959	3125028	1877701	2689375	1552425
RP_POS_570_35535a10_446	RP	POS	10.45	570.3554	LPC 22:5	184.0735(100), 570.3572(25), 552.3459(6), 104.1067(75)	2	1.93E-03	0.59	1.24	2.15E-01	-0.25	0.96	3.47E-02	0.47	0.96	5.86E-04	0.72	1.38	11812767	6682991	16404156	7803260	17374876	7013006	15433437	8480512
RP_NEG_566_34454a10_502	RP	NEG	10.50	566.3445	LPC 18:1 [M+HCOO]-	281.2505(100), 506.3257(18)	2	1.47E-03	0.63	1.34	2.16E-01	0.24	0.99	1.49E-03	0.76	1.34	1.12E-02	0.51	1.20	15587672	4647147	18803051	4978707	18184530	3925515	19421573	5821555
RP_POS_518_3241a9_905	RP	POS	9.91	518.3241	LPC 18:3 (0:0/18:3)	184.0733(100), 518.3215(5)	2	4.57E-01	0.16	0.65	2.17E-01	-0.24	0.82	8.76E-01	0.04	0.53	2.26E-01	0.28	0.79	1924825	1645354	2170945	1523536	2359599	1448777	1982291	1586854
RP_NEG_786_56799a13_501	RP	NEG	13.50	786.5680	PC O-34:3|PC O-16:1_18:2 [M+HCOO]-	279.2345(100), 762.5512(18), 464.3112(7), 446.3023(2)	2	3.73E-03	-0.67	1.07	2.22E-01	-0.22	0.78	1.89E-03	-0.78	1.21	1.97E-02	-0.56	0.87	6044899	2175038	4754311	1723762	4965562	1639086	4543060	1796015
RP_POS_134_06029a3_283	RP	POS	3.28	134.0603	Indoxyl sulfate	134.0598(100), 106.0653(13)	2	7.64E-02	-0.43	0.82	2.22E-01	-0.22	0.72	4.06E-02	-0.54	0.94	2.05E-01	-0.32	0.58	1275863	915445	957888	667633	1039688	616401	876088	712010
HILIC_NEG_151_02606a1_2	HILIC	NEG	1.20	151.0261	Oxypurinol	151.0262(100), 108.0202(3)	2	3.95E-04	0.46	0.72	2.23E-01	0.27	0.79	1.13E-03	0.59	1.01	5.20E-02	0.32	0.80	3445908	1931733	6169168	6660539	5355075	6370805	6983260	6905883
RP_POS_729_59027a12_915	RP	POS	12.92	729.5903	SM 36:2;2O|SM 18:2;2O/18:0	184.0735(100), 729.5819(1)	2	2.67E-05	-0.94	1.55	2.24E-01	-0.22	0.85	2.47E-05	-1.04	1.57	2.22E-04	-0.83	1.51	13766857	4428619	9705370	3845272	10174993	3198862	9235746	4380774
RP_POS_357_27863a9_858	RP	POS	9.86	357.2786	Chenodeoxycholic acid	357.2766(100), 135.1163(15), 161.1328(16), 147.1169(13)	1	4.78E-01	0.13	0.33	2.29E-01	0.25	0.73	2.47E-01	0.26	0.46	9.85E-01	0.00	0.64	3507680	5500233	4354029	6792344	3532830	6084803	5175229	7403536
RP_POS_344_2793a8_114	RP	POS	8.11	344.2793	CAR 12:0 (Lauroycarnitine)	85.0288(100), 344.2816(50)	1	5.04E-01	0.11	0.94	2.30E-01	-0.26	1.59	9.31E-01	-0.01	0.69	2.88E-01	0.24	0.87	8978813	4734950	9702562	6774667	10519459	8280170	8885665	4775540
RP_POS_391_28372a11_391	RP	POS	11.39	391.2837	Dioctyl phthalate	149.0228(100), 71.0858(15), 167.0348(13), 57.0706(11)	2	1.49E-01	-0.30	0.58	2.34E-01	0.24	1.01	4.62E-01	-0.18	0.38	5.32E-02	-0.41	0.82	7606524	745971	7384608	746943	7295379	610186	7473837	859452
RP_POS_834_59705a14_323	RP	POS	14.32	834.5971	PC 38:3 [M+Na]+	146.9816(100), 86.0967(60), 651.5278(45), 834.5889(35), 775.5125(27), 629.5432(8), 184.0726(60)	2	5.45E-01	0.14	0.61	2.35E-01	0.22	0.77	3.38E-01	0.25	0.60	9.01E-01	0.03	0.39	16605442	7519662	17492702	5880126	16790860	4668751	18194543	6859656
RP_POS_302_23242a6_351	RP	POS	6.35	302.2324	CAR 09:0	85.0288(100), 302.2323(60)	2	2.06E-04	-0.69	1.20	2.40E-01	-0.24	0.72	5.47E-05	-0.81	1.53	9.23E-03	-0.57	0.96	1506985	770353	853707	946260	965426	1063567	741988	807740
RP_POS_782_56873a12_82	RP	POS	12.82	782.5687	PC 36:4|PC 18:2_18:2	146.9817(100), 86.0968(55), 595.4709(40), 778.5302(30), 719.4662(25), 573.4848(13), 184.0727(70)	2	5.79E-06	-1.12	1.81	2.40E-01	-0.19	0.86	2.51E-06	-1.21	1.88	4.50E-05	-1.03	1.56	154503389	57779276	97390529	40074976	102116720	40851958	92664338	39119242
RP_NEG_329_24921a11_049	RP	NEG	11.05	329.2492	FA 22:5 (Docosapentaenoic acid)	329.2497(100)	2	3.30E-09	0.81	1.76	2.48E-01	0.25	0.90	2.01E-06	0.93	1.68	2.12E-05	0.68	1.70	4401558	2414017	9306262	6419022	8561027	5710115	10051497	7036316
RP_POS_308_12555a8_419	RP	POS	8.42	308.1256	Piperine [M+Na]+	308.124(100)	2	6.71E-01	0.09	0.28	2.52E-01	0.23	0.83	4.05E-01	0.20	0.45	8.97E-01	-0.03	0.43	5936843	7951066	6625229	7870886	5719508	6421431	7530950	9069568
RP_POS_502_29254a10_216	RP	POS	10.22	502.2925	LPE 20:4	361.2755(100), 502.4443(4), 81.0705(18)	2	4.31E-06	0.80	1.52	2.54E-01	-0.23	0.87	1.31E-03	0.69	1.22	9.97E-07	0.92	1.76	7062091	2213564	9539887	3090810	9893882	2523294	9185891	3560677
RP_POS_766_57379a13_372	RP	POS	13.37	766.5738	PC O-36:5|PC O-16:1_20:4	184.0732(100), 766.5822(2)	2	7.50E-01	-0.06	0.58	2.57E-01	-0.24	0.74	3.91E-01	-0.18	0.34	7.97E-01	0.06	0.52	34965066	9385991	34330258	10910026	35572430	11789755	33088086	9916613
RP_POS_583_25464a11_804	RP	POS	11.80	583.2546	Biliverdin	297.1208(100), 583.2571(70)	2	2.56E-02	-0.44	1.10	2.61E-01	0.23	1.31	1.88E-01	-0.32	0.68	4.15E-03	-0.55	1.32	25029179	13655694	18520394	14957052	16829226	8919142	20211562	19146917
RP_POS_342_26376a7_71	RP	POS	7.71	342.2638	CAR 12:1	85.0286(100), 342.2594(50)	2	1.44E-06	0.67	1.26	2.67E-01	0.24	1.19	7.80E-06	0.79	1.52	2.83E-03	0.55	1.15	4801668	3230454	9831589	8124748	8925156	8500035	10738022	7709919
RP_POS_287_05817a7_376	RP	POS	7.38	287.0582	Oxazepam	269.0463(100), 241.0513(90), 287.0583(85), 231.0684(10)	2	6.57E-01	-0.06	0.61	2.67E-01	0.25	0.84	7.60E-01	0.07	0.60	5.89E-03	-0.18	1.41	3346044	2483439	2898735	9034551	1885755	1814095	3911715	12630397
RP_NEG_498_29214a8_173	RP	NEG	8.17	498.2921	BA 24:1;O3;T	498.2869(100)	2	9.99E-01	0.00	0.46	2.74E-01	0.25	1.25	5.93E-01	0.12	0.75	8.23E-02	-0.13	0.74	14893306	15324236	14885460	49768241	9392660	10696649	20378260	69486061
RP_NEG_856_60919a14_325	RP	NEG	14.33	856.6092	PC 38:3|PC 18:0_20:3 [M+HCOO]-	305.2499(100), 283.2655(40), 796.5891(20)	2	4.30E-01	0.19	0.66	2.77E-01	0.20	0.70	2.76E-01	0.29	0.66	7.22E-01	0.09	0.43	14780571	6258658	15739205	4701016	15225118	3968675	16253292	5325445
RP_POS_130_06532a6_095	RP	POS	6.10	130.0653	Fragment of 3-indolepropionic acid	130.0655(100)	2	1.97E-03	-0.83	1.45	2.78E-01	-0.17	0.64	8.06E-04	-0.92	1.48	8.01E-03	-0.75	1.12	2248453	1963140	1036074	1110250	1157263	1330082	914886	831489
RP_NEG_774_53088a12_535	RP	NEG	12.54	774.5309	PC 32:2|PC 16:1_16:1 [M+HCOO]-	253.2185(100), 714.511(10)	2	1.86E-01	0.28	0.92	2.82E-01	0.21	0.66	1.10E-01	0.39	0.92	4.35E-01	0.18	0.36	8769586	3809302	9790903	3557157	9406090	3184891	10175716	3888346
RP_POS_190_08635a6_096	RP	POS	6.10	190.0864	3-Indolepropionic acid	130.0656(100), 172.0753(20), 190.0865(15), 55.0188(10)	1	2.95E-03	-0.81	1.41	2.86E-01	-0.16	0.63	1.24E-03	-0.89	1.43	1.10E-02	-0.73	1.08	10103276	9163283	4702484	5069929	5246524	6148672	4158444	3677327
RP_POS_780_55267a13_158	RP	POS	13.16	780.5527	PC 34:2 [M+Na]+	146.9818(100), 86.0968(50), 597.4879(35), 780.5561(33), 721.4839(25), 575.5069(10)	2	5.42E-01	0.15	0.42	2.88E-01	0.19	0.88	3.34E-01	0.24	0.60	8.48E-01	0.05	0.24	212402209	43212062	217478013	31237381	214140699	33936293	220815327	28232246
RP_POS_286_14368a8_418	RP	POS	8.42	286.1437	Piperine	201.0543(100), 286.1456(100), 135.0441(10)	2	6.28E-01	0.10	0.31	2.90E-01	0.21	0.77	4.03E-01	0.21	0.45	9.81E-01	-0.01	0.42	38318645	56925768	43907018	55221302	38036736	43533241	49777300	64773041
RP_POS_147_11279a0_465	RP	POS	0.47	147.1128	Lysine	84.0811(100), 130.0865(50), 147.1123(8), 129.1016(3), 101.0598(2)	1	8.43E-03	0.35	1.03	2.92E-01	-0.24	1.12	1.97E-01	0.23	0.95	6.83E-03	0.47	1.13	1149023	254914	1385970	762513	1466742	738331	1305198	785029
RP_POS_366_26373a7_689	RP	POS	7.69	366.2637	CAR 14:3	85.0287(100), 366.2627(70)	2	3.79E-01	-0.19	0.93	2.95E-01	-0.21	1.12	1.96E-01	-0.29	0.67	7.26E-01	-0.09	0.96	571309	431563	495026	393812	536501	443611	453550	336215
RP_POS_373_27377a9_323	RP	POS	9.32	373.2738	Cholic acid [M+H-H2O]+	355.2615(100), 373.2716(13), 245.1533(10), 337.2521(8), 319.2402(6),	1	2.71E-01	-0.32	0.63	2.98E-01	0.16	0.64	4.24E-01	-0.24	0.40	1.81E-01	-0.39	0.60	2689676	5464725	1570772	2620436	1296899	2358803	1844645	2855954
RP_POS_358_29498a8_357	RP	POS	8.36	358.2950	CAR 13:0	85.0289(100), 358.2919(55)	2	1.15E-01	-0.34	0.88	3.01E-01	-0.20	0.66	7.43E-02	-0.44	0.71	2.91E-01	-0.23	0.75	2300896	1413134	1847213	1319802	1984423	1133961	1710002	1481557
RP_NEG_498_29016a8_562	RP	NEG	8.56	498.2902	BA 24:1;O3;T	498.2869(100)	2	5.21E-01	0.09	0.41	3.01E-01	0.23	1.03	3.83E-01	0.21	0.66	8.06E-01	-0.02	0.40	9414707	24186815	13799276	52907046	8276804	12014207	19321748	73816363
RP_NEG_500_27905a10_216	RP	NEG	10.22	500.2791	LPE 20:4	303.2313(100), 500.2761(6), 214.0469(6), 78.9574(3), 196.0375(2)	2	1.51E-06	0.84	1.57	3.02E-01	-0.21	0.79	5.62E-04	0.74	1.28	4.43E-07	0.95	1.79	4205188	1288791	5723519	1788406	5909055	1452290	5537983	2069461
RP_POS_689_51117a14_537	RP	POS	14.54	689.5112	DG 40:7 [M+Na]+	689.5001(100)	2	5.33E-01	0.07	0.76	3.09E-01	0.24	0.62	4.08E-01	0.19	0.52	2.58E-01	-0.04	0.73	944636	848892	1293001	5358099	742363	663947	1843640	7546174
RP_NEG_305_2496a11_128	RP	NEG	11.13	305.2496	FA 20:3 (Eicosatrienoic acid)	305.2499(100)	2	6.54E-08	0.84	1.76	3.09E-01	0.21	1.01	3.99E-06	0.94	1.69	2.02E-05	0.73	1.69	1631321	792325	2808177	1443286	2660584	1264053	2955770	1601991
RP_POS_540_30707a10_04	RP	POS	10.04	540.3071	LPC 18:3 (18:3/0:0)	104.1076(100), 481.2313(55), 540.306(20), 84.0964(17), 335.2595(3)	2	2.70E-02	0.42	0.97	3.10E-01	-0.21	0.89	1.44E-01	0.31	0.90	1.53E-02	0.52	1.17	2692383	2242350	3774612	2664821	4046420	2647464	3502805	2680976
RP_POS_504_30762a10_523	RP	POS	10.52	504.3076	LPE 20:3	363.2895(100), 504.3085(10), 62.0608(50)	2	3.14E-05	0.76	1.30	3.12E-01	-0.20	0.66	1.38E-03	0.66	1.21	3.34E-05	0.86	1.44	2862796	1063758	3898839	1353557	4036340	1330341	3761338	1375949
HILIC_POS_204_123a2_968	HILIC	POS	2.97	204.1230	Acetylcarnitine	85.0289(100), 204.1229(50), 145.0495(20), 60.0802(10)	1	6.62E-12	0.90	1.47	3.14E-01	0.21	1.03	7.57E-09	1.00	1.77	1.11E-05	0.79	1.46	279367494	133412491	653939970	436106531	609788076	458550962	698091863	412324978
RP_POS_752_51874a12_533	RP	POS	12.53	752.5187	PC 32:2 [M+Na]+	146.9818(100), 86.0969(40), 752.5212(36), 569.4515(35), 693.454(24), 547.484(13)	2	5.34E-01	0.13	0.82	3.16E-01	0.20	0.60	3.41E-01	0.23	0.82	8.76E-01	0.04	0.14	10363194	4957354	10980674	4502024	10527000	4078847	11434348	4888051
RP_POS_264_19583a5_311	RP	POS	5.31	264.1958	Fragment of N-Desmethylvenlafaxine	246.1861(100), 264.1958(75), 215.1436(60), 121.0643(40), 147.0801(30)	2	5.35E-01	0.09	0.71	3.18E-01	0.22	0.62	2.13E-01	0.20	0.80	9.26E-01	-0.02	0.59	8225379	5839685	9195840	11679837	8022627	13433240	10369053	9610425
RP_POS_253_09724a5_873	RP	POS	5.87	253.0972	Carbamazepine-10,11-epoxide	180.0813(100), 210.092(95), 182.0969(18), 208.0767(9) 236.0683(4)	2	3.21E-01	0.11	0.75	3.22E-01	-0.23	0.78	1.93E-01	0.00	0.66	3.23E-01	0.23	0.83	33211	13675	2261995	22338745	4494705	31591922	29284	12365
RP_POS_271_1076a5_576	RP	POS	5.58	271.1076	10,11-Dihydro-10,11-dihydroxycarbamazepine	180.0809(100), 210.0915(95), 254.0795(80), 253.0953(25), 182.0963(18), 208.0767(10)	2	3.20E-01	0.11	0.75	3.23E-01	-0.23	0.78	8.98E-01	0.00	0.53	3.22E-01	0.23	0.83	19866	9507	1415342	13960788	2810528	19743661	20155	10576
RP_POS_320_25583a9_477	RP	POS	9.48	320.2558	NAE 18:4	320.2545(100)	2	3.74E-01	-0.24	0.83	3.24E-01	-0.16	0.67	2.47E-01	-0.32	0.72	5.82E-01	-0.16	0.49	26608500	36810984	20439017	21512887	22570750	23289768	18307285	19579742
RP_POS_394_29514a8_446	RP	POS	8.45	394.2951	CAR 16:3	394.2965(100), 85.0285(80)	2	2.92E-03	0.46	0.88	3.26E-01	-0.21	1.30	4.82E-02	0.36	0.81	4.25E-03	0.57	1.04	455024	211038	616365	373821	653287	396118	579443	350207
RP_POS_770_60498a13_833	RP	POS	13.83	770.6050	PC O-36:3	184.0732(100), 770.611(2)	2	3.28E-06	-1.06	1.64	3.26E-01	-0.17	0.67	3.92E-06	-1.14	1.67	2.10E-05	-0.97	1.58	6952886	2331850	4538736	1939134	4730172	1657171	4347299	2185456
RP_POS_237_10228a6_888	RP	POS	6.89	237.1023	Carbamazepine	194.0963(100), 237.1004(90), 192.081(15), 220.0761(3)	2	3.13E-01	0.12	0.75	3.27E-01	-0.23	0.78	7.01E-02	0.00	0.77	3.22E-01	0.23	0.83	476208	102899	9625906	90314430	18566062	12773450	685749	790714
HILIC_NEG_117_01951a1_1	HILIC	NEG	1.10	117.0195	Succinic acid	73.0287(100), 116.9285(60), 99.925(15), 99.0092(10)	2	8.82E-01	-0.03	0.74	3.29E-01	0.20	0.95	7.33E-01	0.07	0.17	5.52E-01	-0.13	0.69	1475727	366126	1464168	422123	1422728	429229	1505609	415054
RP_POS_782_56836a13_069	RP	POS	13.07	782.5684	PC 36:4|PC 16:0_20:4	184.0731(100), 782.5666(3)	2	3.60E-01	0.19	0.54	3.35E-01	-0.19	0.63	6.92E-01	0.09	0.75	1.96E-01	0.29	0.68	511754194	119073348	533931989	115178224	545091779	101352611	522772199	127578465
RP_POS_550_38635a11_005	RP	POS	11.01	550.3864	LPC 20:1	184.0733(100), 550.3918(30), 532.3806(6), 104.1077(85)	2	5.43E-01	-0.14	0.68	3.36E-01	0.18	1.22	8.57E-01	-0.05	0.43	3.32E-01	-0.23	0.79	6653730	2890816	6308041	2380998	6077450	2056184	6538633	2667882
RP_NEG_281_24884a11_254	RP	NEG	11.25	281.2488	FA 18:1 (Oleic/Elaidic acid)	281.2505(100)	2	6.60E-07	0.75	1.64	3.38E-01	0.20	1.00	1.33E-05	0.85	1.62	2.57E-04	0.65	1.56	22010014	11741821	38363493	22846617	36160817	21614214	40566170	24031488
RP_POS_742_57379a13_498	RP	POS	13.50	742.5738	PC O-34:3|PC O-16:1_18:2	184.0731(100), 742.5775(3)	2	4.56E-03	-0.67	1.08	3.46E-01	-0.17	0.64	2.70E-03	-0.76	1.21	1.85E-02	-0.59	0.87	27509150	10782359	21305605	8127407	22076231	8286829	20534980	7973334
RP_POS_211_1442a4_68	RP	POS	4.68	211.1442	Cyclo(Leu-Pro)	211.1448(100), 86.097(20), 70.0659(15), 183.1483(10)	2	1.14E-06	0.74	1.23	3.47E-01	0.20	0.60	5.74E-05	0.84	1.41	9.83E-05	0.64	1.28	4120346	2757407	7838989	5280349	7339098	4350402	8338879	6074308
RP_POS_774_59814a14_235	RP	POS	14.24	774.5981	PC 35:1	184.0732(100), 774.5886(3)	2	3.13E-02	-0.47	0.89	3.48E-01	0.18	0.63	1.13E-01	-0.38	0.68	1.69E-02	-0.56	0.97	5594907	2723488	4399800	2417749	4171632	2269888	4627969	2559625
RP_POS_146_06006a2_489	RP	POS	2.49	146.0601	3-Formylindole	118.065(100), 146.06(70), 100.1126(25)	2	1.71E-03	-0.55	1.15	3.48E-01	-0.20	1.02	3.52E-03	-0.65	1.20	1.34E-02	-0.45	1.06	4099296	731387	3567188	996310	3661257	810023	3473119	1153832
RP_POS_552_40198a11_315	RP	POS	11.32	552.4020	LPC 20:0	184.0728(100), 552.4073(32), 534.3874(6), 104.1073(90), 86.0969(15)	2	6.53E-04	-0.90	1.58	3.48E-01	-0.14	0.96	3.90E-04	-0.98	1.50	2.19E-03	-0.83	1.34	1978283	868918	1377404	508550	1425353	519035	1329455	498433
HILIC_NEG_154_06221a6_747	HILIC	NEG	6.75	154.0622	Histidine	154.062(100), 93.0454(60), 137.0364(40), 110.0723(15)	2	6.65E-01	-0.07	0.95	3.54E-01	-0.20	0.84	3.66E-01	-0.17	0.99	9.08E-01	0.02	0.96	2658371	423550	2616877	592206	2672017	646174	2561737	533692
RP_POS_330_26373a7_561	RP	POS	7.56	330.2637	CAR 11:0	85.0287(100), 330.2617(45)	2	4.65E-03	-0.66	1.24	3.66E-01	-0.16	0.55	3.15E-03	-0.74	1.23	1.83E-02	-0.58	1.10	1410131	667980	1024556	526669	1072474	516049	976638	537985
RP_POS_290_1387a4_214	RP	POS	4.21	290.1387	Benzoylecgonine	168.1011(100), 290.1392(90), 105.0335(20)	2	2.60E-01	-0.16	0.48	3.66E-01	-0.20	0.58	1.57E-02	-0.26	0.96	8.05E-01	-0.06	0.32	33304786	19176695	27011705	44093191	31030982	60079390	22992428	16899557
RP_NEG_762_50958a12_956	RP	NEG	12.96	762.5096	PE 38:6|PE 16:0_22:6	255.2321(100), 327.2347(65), 762.5117(18)	2	8.83E-01	0.03	0.70	3.68E-01	0.19	0.57	6.15E-01	0.12	0.57	7.23E-01	-0.07	0.34	2221924	1394956	2265595	1621868	2118604	1078662	2412586	2026571

Supplementary table 1: Metabolomics results (in asceding order according to p-value from progressive ALD vs non-progressive ALD comparison, with molecular features with ID_level of 1-2 first)

								all_ALD_vs_control			Prog_ALD_vs_non-prog_ALD			Prog_ALD_vs_control_ALD			Non-prog_ALD_vs_control			Healthy_control		all_ALD		Non-prog_ALD		Progressive_ALD	
								t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA								
Feature_ID	RP_HILIC	POS_NEG	Average.Rt	Average.Mz	Metabolite.name	curated_MSMS	ID_level	p	d	VIP	p	d	VIP	p	d	VIP	p	d	VIP	Mean	SD	Mean	SD	Mean	SD	Mean	SD
RP_NEG_502_29468a10_519	RP	NEG	10.52	502.2947	LPE 20:3	305.2496(100), 502.299(15), 196.0373(10), 78.9581(5), 314.0472(3)	2	1.57E-05	0.76	1.33	3.71E-01	-0.18	0.54	1.05E-03	0.67	1.22	2.26E-05	0.85	1.44	2189551	785199	3004883	1081984	3102270	1041137	2907496	1123365
RP_NEG_315_25494a9_606	RP	NEG	9.61	315.2549	FA 18:0;2O	315.2517(100)	2	1.07E-05	0.63	1.31	3.71E-01	0.19	1.15	4.22E-04	0.72	1.30	6.28E-04	0.53	1.34	1101285	174914	1332073	394960	1296549	319982	1367598	458483
RP_NEG_452_27863a10_388	RP	NEG	10.39	452.2786	LPE 16:0	255.2332(100), 452.2818(5)	2	4.27E-01	0.14	0.98	3.71E-01	-0.19	0.85	8.35E-01	0.05	0.70	2.23E-01	0.24	0.83	2050234	648451	2164708	860126	2242051	748494	2087365	960355
RP_POS_261_13089a2_881	RP	POS	2.88	261.1309	2-(4-oxoquinazolin-3(4H)-yl)ethyl isobutyrate [M+Na]+ Fragment	261.1308(100)	2	3.25E-02	0.32	1.11	3.74E-01	-0.20	1.10	1.83E-01	0.23	1.13	3.85E-02	0.42	1.12	752016	837212	1220018	1571878	1360692	1754650	1079344	1368518
RP_POS_228_2321a10_19	RP	POS	10.19	228.2321	Myristamide	228.2326(100)	2	7.08E-03	0.33	0.70	3.75E-01	0.20	0.92	6.19E-02	0.43	0.79	2.52E-04	0.23	1.26	5671005	1585307	7899559	7635445	7215211	2040035	8583907	10614721
RP_POS_522_3551a10_503	RP	POS	10.50	522.3551	LPC 18:1 (0:0/18:1)	184.0735(100), 522.3544(3.5), 504.3395(0.8)	2	4.28E-04	0.70	1.45	3.77E-01	0.17	0.94	1.00E-03	0.78	1.36	2.13E-03	0.61	1.39	5663874	19053947	71440087	20707991	69597550	15586719	73282625	24829799
RP_POS_264_19577a4_03	RP	POS	4.03	264.1958	O-desmethylvenlafaxine	58.066(100), 264.1947(35), 246.183(30), 107.0489(3), 201.1271(5)	2	9.26E-01	-0.01	0.49	3.77E-01	-0.20	0.93	2.77E-01	-0.11	0.80	6.93E-01	0.09	0.67	36252955	10352400	35915512	31033306	38678759	41189861	33152266	15283953
RP_POS_130_04987a0_526	RP	POS	0.53	130.0499	L-5-Oxoproline	84.0445(100), 130.0499(35)	2	1.46E-01	0.22	0.77	3.78E-01	-0.20	0.83	5.38E-01	0.12	0.53	8.08E-02	0.31	0.86	3962044	638049	4210061	1265301	4322335	1199232	4097787	1330700
RP_NEG_283_26535a11_611	RP	NEG	11.61	283.2654	FA 18:0 (Stearic acid)	283.2652(100)	2	6.84E-02	-0.34	0.87	3.79E-01	-0.18	1.00	3.04E-02	-0.43	0.92	2.71E-01	-0.25	0.80	35684798	9731904	31832770	11639142	32862751	13268862	30802788	9771194
RP_POS_205_09669a2_489	RP	POS	2.49	205.0967	Tryptophan	188.0713(100), 146.06(50), 144.0813(8), 159.0923(6)	2	1.95E-03	-0.53	1.14	3.79E-01	-0.18	1.04	4.61E-03	-0.62	1.18	1.47E-02	-0.44	1.05	214906042	36924841	187939500	52878667	192619124	42932474	183259877	61330924
RP_POS_188_07024a2_489	RP	POS	2.49	188.0702	Desethyl atrazine	146.06(100), 188.0713(45)	2	2.03E-03	-0.54	1.14	3.80E-01	-0.18	1.03	4.68E-03	-0.63	1.18	1.44E-02	-0.44	1.05	140834135	24720587	122982071	34681411	126042652	27984289	119921489	40347371
RP_NEG_464_31503a11_092	RP	NEG	11.09	464.3150	LPE O-18:1	464.3122(100), 78.9574(37), 140.011(28), 196.0376(42), 267.2686(25)	2	2.43E-01	-0.25	0.84	3.84E-01	-0.17	1.11	1.58E-01	-0.34	0.96	4.78E-01	-0.17	0.81	1383779	509829	1263932	465748	1304678	455965	1223187	476420
RP_POS_748_52667a13_248	RP	POS	13.25	748.5267	PE P-38:6|PE P-16:0 22:6	385.2754(100), 364.262(30), 266.283(15), 607.5018(5)	2	5.87E-01	-0.09	0.89	3.86E-01	0.19	0.57	9.69E-01	0.01	0.67	2.30E-01	-0.18	0.54	4062683	1229143	3899582	2059318	3719612	1285516	4079553	2617150
RP_POS_283_26343a10_223	RP	POS	10.22	283.2634	FA 18:1 (Petroselinic acid)	57.0706(100), 69.0707(75), 71.0851(73), 83.0861(70), 97.1011(60), 247.2419(57), 265.253(40), 283.2611(13)	2	4.39E-01	0.14	0.87	3.86E-01	0.18	0.81	2.75E-01	0.23	0.76	8.28E-01	0.04	0.80	13532845	1569967	13803898	2105300	13620425	2049973	13987371	2164242
RP_POS_830_56531a13_206	RP	POS	13.21	830.5653	PC 38:5|PC 16:0_22:5 AND PC 18:1 20:4	146.9817(100), 86.0968(60), 647.4933(60), 771.4937(38), 830.5549(31), 625.5184(8)	2	2.86E-04	0.66	1.16	3.89E-01	0.18	0.92	1.16E-03	0.75	1.14	1.76E-03	0.57	1.22	28128006	5046313	32350098	6474490	31789156	4800968	32911039	7810383
RP_POS_796_62048a14_574	RP	POS	14.57	796.6205	PC O-38:4	184.0735(100), 796.6392(3)	2	1.21E-03	-0.76	1.24	3.90E-01	-0.15	0.51	6.60E-04	-0.83	1.36	6.71E-03	-0.68	1.12	7402895	3209518	5255040	2508968	5472167	2736897	5037913	2265279
RP_NEG_745_552a12_329	RP	NEG	12.33	745.5520	SM 34:2;2O|SM 18:2;2O/16:0 [M+HCOO]-	685.5215(100), 168.0421(90), 78.9574(70)	2	2.23E-05	-0.95	1.66	3.94E-01	-0.15	0.55	2.55E-05	-1.02	1.61	1.46E-04	-0.87	1.63	18773203	3901374	15157995	3350073	15445213	3080113	14870777	3608263
RP_POS_132_10172a1_457	RP	POS	1.46	132.1017	Leucine	86.097(100), 132.1024(4), 69.0707(2)	2	3.99E-01	0.14	0.65	3.97E-01	-0.18	0.58	8.20E-01	0.05	0.50	2.17E-01	0.23	0.46	48056445	9970087	50038594	15372099	51347192	13942726	48729996	16719180
RP_POS_130_04988a1_13	RP	POS	1.13	130.0499	L-5-Oxoproline	84.045(100), 130.0495(25)	2	1.49E-12	0.96	1.58	3.98E-01	0.17	0.98	1.25E-07	1.05	1.66	4.09E-08	0.87	1.76	1318412	247380	1950368	676330	1892827	584263	2007910	758986
RP_POS_758_5683a14_259	RP	POS	14.26	758.5683	PC 34:2	184.0733(100), 758.5762(3)	2	9.45E-01	-0.01	0.33	4.03E-01	0.18	0.57	7.34E-01	0.08	0.19	6.17E-01	-0.10	0.76	3714471	1846936	3686687	2270330	3495610	2042959	3877763	2483102
RP_POS_314_23242a6_778	RP	POS	6.78	314.2324	CAR 10:1	85.0287(100), 314.2295(50)	2	8.13E-02	-0.28	0.76	4.07E-01	-0.18	1.10	2.50E-02	-0.37	0.89	3.89E-01	-0.19	0.61	12811109	8019099	9389338	13248868	10495408	16019797	8283267	9773264
RP_POS_327_07709a9_047	RP	POS	9.05	327.0771	Triphenylphosphate	327.0796(100), 233.0359(8), 153.0699(3)	2	4.99E-03	-0.61	0.97	4.08E-01	-0.16	0.72	2.49E-03	-0.69	1.17	2.96E-02	-0.53	0.80	7013783	434494	6759470	396830	6792496	447817	6726444	339700
RP_POS_665_51068a14_775	RP	POS	14.78	665.5107	DG 38:5	665.5103(100)	2	3.53E-01	0.11	0.69	4.09E-01	0.19	0.50	3.73E-01	0.21	0.50	7.05E-01	0.02	0.70	2035861	1147348	2654761	6315848	2128198	944917	3181324	8895798
RP_POS_301_17847a9_141	RP	POS	9.14	301.1785	Adrenosterone	301.1745(100)	2	3.27E-04	-0.62	1.04	4.09E-01	-0.17	0.68	4.74E-04	-0.71	1.19	7.63E-03	-0.53	1.10	6143161	238114	5939639	338394	5967726	341576	5911553	336264
RP_NEG_279_23267a10_979	RP	NEG	10.98	279.2327	FA 18:2 (Linoleic acid)	279.2349(100)	2	1.96E-02	0.41	1.43	4.11E-01	-0.17	1.32	1.20E-01	0.32	1.18	1.40E-02	0.50	1.36	12552057	4667778	15046064	6404274	15576262	6183556	14515865	6637501
RP_POS_326_7095a5_652	RP	POS	5.65	326.7095	Midazolam	326.0836(100), 291.1169(12.5)	2	5.52E-07	0.60	1.30	4.12E-01	-0.18	1.20	9.44E-04	0.51	1.37	1.90E-04	0.69	1.40	16097	28028	333009	590096	381740	639785	284279	537924
RP_POS_166_08618a2_202	RP	POS	2.20	166.0862	Phenylalanine	120.0814(100), 166.0852(3)	1	2.93E-01	0.16	0.69	4.16E-01	0.18	0.79	2.44E-01	0.25	0.71	6.39E-01	0.08	0.88	136273962	20951880	141771171	36442441	138786555	27143424	144755788	43911971
HILIC_NEG_267_07355a2_387	HILIC	NEG	2.39	267.0736	Inosine	135.0308(100), 267.0735(20)	2	7.28E-07	0.61	1.09	4.18E-01	0.18	0.73	4.25E-04	0.70	1.10	1.63E-04	0.52	1.41	832259	706355	2721892	3391594	2445132	2690788	2998652	3980441
RP_NEG_552_36853a10_868	RP	NEG	10.87	552.3685	LPC O-18:1 [M+HCOO]-	492.3474(100), 78.9574(23), 168.0421(15), 403.2585(12)	2	1.18E-02	-0.62	1.11	4.20E-01	-0.14	1.01	7.08E-03	-0.69	1.24	3.69E-02	-0.55	1.02	5279083	1958924	4296888	1380586	4408323	1507995	4184953	1245519
HILIC_POS_585_27112a0_629	HILIC	POS	0.63	585.2711	Bilirubin	299.137(100), 585.2726(15)	2	8.95E-01	-0.03	0.61	4.21E-01	0.16	0.87	8.28E-01	0.05	0.11	6.18E-01	-0.11	0.26	5149821	3229515	5063813	3134634	4810107	2571050	5317518	3620874
RP_POS_478_29291a10_214	RP	POS	10.21	478.2929	LPE 18:2	337.2718(100), 81.075(11), 60.0813(10)	2	1.31E-01	0.30	1.05	4.26E-01	-0.16	0.80	3.59E-01	0.22	0.75	6.58E-02	0.38	1.04	10213853	4844408	11753397	5229000	12172810	4236385	11333983	6077577
RP_POS_360_27429a7_451	RP	POS	7.45	360.2743	3-Hydroxydodecanoyl carnitine	85.0287(100), 360.274(75), 60.0815(22), 145.0492(7)	1	6.31E-03	0.47	1.20	4.28E-01	0.17	0.98	6.98E-03	0.55	1.13	5.22E-02	0.38	1.13	366625	189970	488198	272773	466468	268116	509928	278350
RP_POS_349_18338a3_84	RP	POS	3.84	349.1834	Hydroquinide	349.1806(100)	2	9.85E-01	-0.01	1.17	4.29E-01	-0.12	1.13	8.15E-01	-0.07	0.92	8.47E-01	0.06	0.96	1042639	3307351	1031017	1703008	1166495	1826131	895539	1577165
RP_NEG_277_21768a10_735	RP	NEG	10.74	277.2177	FA 18:3 (alfa-Linolenic acid)	277.2188(100)	2	1.71E-04	0.56	1.44	4.30E-01	-0.17	1.08	5.42E-03	0.47	1.27	1.26E-03	0.65	1.47	1728649	856666	2618103	1707427	2753729	1877494	2482477	1525642
RP_POS_357_27878a9_306	RP	POS	9.31	357.2788	Ursodeoxycholic acid	357.279(100)	1	2.67E-02	0.35	1.34	4.36E-01	-0.17	0.58	1.17E-01	0.27	0.89	3.95E-02	0.44	1.34	915513	682452	1288614	1134211	1377452	1305738	1199776	937051
RP_POS_605_42249a10_446	RP	POS	10.45	605.4225	DG 34:7	605.4208(100)	2	5.45E-02	-0.39	0.74	4.41E-01	-0.15	0.47	3.03E-02	-0.47	0.92	1.83E-01	-0.31	0.62	10260635	2544909	9239521	2596078	9441009	2911231	9038033	2249148
SCFA_Butyric acid	SCFA	SCFA			FA 04:0 (Butyric acid)	targeted_SCFA_analysis	1	1.06E-04	0.68	1.46	4.41E-01	0.26	0.86	1.13E-02	0.83	1.65	9.16E-04	0.57	1.26	58021	16579	95665	60482	89560	43544	103628	77652
RP_POS_548_37103a10_752	RP	POS	10.75	548.3710	LPC 20:2	184.0733(100), 548.3658(40), 530.3571(8), 104.1076(85)	2	1.66E-01	0.29	1.02	4.42E-01	-0.15	0.86	3.76E-01	0.22	0.71	9.51E-02	0.37	0.99	8480351	3845579	9564763	3651667	9847076	3046809	9282449	4182795
RP_NEG_854_59344a13_875	RP	NEG	13.88	854.5934	PC 38:4|PC 18:0_20:4 [M+HCOO]-	303.2314(100), 283.2654(60), 794.5798(35)	2	6.43E-01	-0.10	0.51	4.43E-01	0.15	0.80	9.10E-01	-0.03	0.49	4.40E-01	-0.18	0.37	47166926	13343749	45946327	11385913	45066393	9225503	46826260	13237584
RP_POS_772_58472a13_42	RP	POS	13.42	772.5847	PC 35:2	184.0375(100), 772.5782(3)	2	5.78E-06	-1.07	1.81	4.44E-01	0.13	0.62	3.81E-05	-1.00	1.70	4.52E-06	-1.13	1.66	12361109	4429692	7949428	3420103	7685940	3360279	8212916	3492817
RP_POS_768_55292a12_749	RP	POS	12.75	768.5529	PC 35:4	184.0732(100), 768.5555(2)	2	2.81E-07	-1.24	2.28	4.52E-01	-0.12	0.94	2.92E-07	-1.30	2.15	1.12E-06	-1.18	2.06	6690765	2363296	3933603	1713930	4063282	1545202	3803923	1874324
RP_POS_393_20926a4_2	RP	POS	4.20	393.2093	Octaethylene glycol	393.2081(100)	2	9.80E-01	-0.01	1.20	4.53E-01	-0.12	1.11	8.20E-01	-0.07	0.93	8.61E-01	0.05	1.00	858259	2781646	845127	1423761	952673	1527502	737582	1318595
RP_POS_778_53705a12_264	RP	POS	12.26	778.5371	PC 36:6	184.0732(100), 778.5347(2)	2	9.73E-08	0.80	1.42	4.55E-01	0.16	0.49	6.90E-06	0.88	1.53	3.99E-05	0.73	1.36	2076262	1164581	3832540	2268510	3661847	2123924	4003233	2413874
RP_POS_482_32401a10_932	RP	POS	10.93	482.3240	LPE 18:0	341.3073(100), 482.3236(3), 62.0607(25)	2	4.86E-02	0.35	1.09	4.60E-01	0.16	1.03	5.73E-02	0.43	0.90	1.44E-01	0.27	0.97	11637003	3349306	13126806	4474901	12794057	3623624	13459555	5205913
RP_POS_271_1156a4_569	RP	POS	4.57	271.1156	7-Prenyl-theophylline [M+Na]+	271.1138(100)	2	1.38E-01	0.21	0.45	4.61E-01	-0.16	0.57	3.59E-01	0.13	0.48	1.72E-01	0.29	0.78	5017487	299581	5145602	673770	5195594	832572	5095609	467889
RP_POS_241_06731a4_851	RP	POS	4.85	241.0673	Triacetin [M+Na]+	241.0692(100), 181.0459(55), 159.0647(15)	2	5.71E-01	0.10	0.53	4.66E-01	-0.15	0.54	8.97E-01	0.03	0.46	4.09E-01	0.18	0.55	127014501	37011469	131591705	46574044	135009565	49969992	128173845	43147548
HILIC_NEG_243_06212a1_415	HILIC	NEG	1.42	243.0621	Uridine	99.9255(100), 110.025(60), 200.0576(12), 140.035(8)	2	7.77E-01	0.05	0.85	4.67E-01	-0.16	0.66	8.89E-01	-0.03	0.62	5.40E-01	0.13	0.90	973097	315535	993117	429201	1024523	440275	961711	419918
RP_POS_526_29272a10_209	RP	POS	10.21	526.2927	LPE 22:6	385.2761(100), 93.0701(20)	2	2.82E-02	0.35	1.13	4.70E-01	-0.16	0.48	1.55E-01	0.27	0.79	3.05E-02	0.42	1.02	5383130	1794742	6372059	3098304	6597502	3186539	6146617	3022768
RP_NEG_462_2998a10_799	RP	NEG	10.80	462.2998	LPE O-18:2	462.2972(100), 78.9573(50), 140.0109(32), 401.2463(8)	2	2.20E-02	0.36	0.69	4.71E-01	0.16	0.74	1.75E-02	0.44	1.04	1.56E-01	0.28	0.52	876008	285856	1040460	492855	1004744	525076	1076177	460936
RP_POS_521_41681a13_623	RP	POS	13.62	521.4168	DG 27:0 [M+Na]+	521.4131(100)	2	8.98E-01	0.02	0.37	4.72E-01	0.16	0.51	6.60E-01	0.10	0.29	6.01E-01	-0.06	0.20	7970697	876494	8003579	2039391	7855666	1097773	8151491	2674576
RP_NEG_512_30035a9_796	RP	NEG	9.80	512.3004	LPC 14:0 [M+HCOO]-	227.1999(100), 452.2813(20)	2	1.08E-03	0.49	0.99	4.75E-01	-0.16	0.52	3.00E-02	0.42	0.88	1.82E-03	0.57	1.01	2813005	951238	3649756	1832976	3781555	1756298	3517958	1915238
HILIC_POS_269_08807a2_457	HILIC	POS	2.46	269.0881	Inosine	137.0452(100)	1	1.27E-08	0.69	1.17	4.77E-01	0.16	0.68	1.23E-04	0.76	1.19	9.46E-06	0.61	1.61	616313	556925	4680200	6498685	4215373	5123935	5145027	7657157
RP_POS_205_09686a2_893	RP	POS	2.89	205.0969	Tryptophan	188.0694(100), 146.0603(50)	2	1.27E-03	-0.55	1.19	4.78E-01	-0.15	1.06	4.17E-03	-0.63	1.19	8.30E-03	-0.48	1.14	195531238	33166336	170266727	47475128	173656253	39143306	166877201	54755166
RP_POS_280_26343a9_476	RP	POS	9.48	280.2634	Isomer of Linoleamide	95.0861(100), 263.2354(85), 81.0701(80), 245.2251(78), 280.2631(77(	1	3.51E-01	-0.26	0.87	4.78E-01	-0.11	0.49	2.74E-01	-0.32	0.69	4.81E-01	-0.21	0.56	51073097	93184363	34857843	48288913	38302393	50397795	31413294	46336534
RP_POS_508_37546a10_864	RP	POS	10.86	508.3755	LPC O-18:1	104.1074(100), 508.3809(20), 184.0729(15), 86.0969(11), 125.0001(5)	2	2.16E-01	-0.29	0.80	4.79E-01	-0.13	1.07	1.55E-01	-0.36	0.85	3.75E-01	-0.22	0.72	13762126	5211367	12500057	4011929	12786176	4147950	12213938	3891924
RP_POS_794_60358a14_273	RP	POS	14.27	794.6036	PC O-38:5	184.0732(100), 794.6079(2)	2	1.84E-01	-0.25	0.45	4.79E-01	-0.15	0.45	1.14E-01	-0.32	0.77	4.34E-01	-0.17	0.36	9099459	3799126	8009789	4537374	8332886	4997720	7686692	4050362
RP_POS_327_00729a8_121	RP	POS	8.12	327.0073	Tris(1-chloro-2-propyl)phosphate	98.9848(100), 174.9912(15), 251.0011(3), 327.0083(1)	2	8.82E-01	-0.03	0.47	4.81E-01	0.14	0.54	8.46E-01	0.04	0.45	6.68E-01	-0.10	0.26	2697591	549557	2680901	564614	2640853	630144	2720949	493688
RP_POS_833_64868a14_816	RP	POS	14.82	833.6487	SM 42:3;2O [M+Na]+	650.5846(100), 774.5735(60), 833.6593(45)	2	6.84E-03	-0.62	1.12	4.81E-01	-0.13	0.43	5.93E-03	-0.69	1.15	2.12E-02	-0.56	0.98	3700607	1729577	2747557	1393262	2846328	1341976	2648785	1449540
HILIC_NEG_128_03552a4_083	HILIC	NEG	4.08	128.0355	Pyroglutamic acid	128.0348(100), 99.9254(70)	2	1.61E-06	0.75	1.31	4.85E-01	0.15	0.75	7.34E-05	0.82	1.29	7.19E-05	0.68	1.36	3026358	935988	4225100	1656981	4108585	1403447	4341614	1884102
RP_POS_697_52405a12_209	RP	POS	12.21	697.5241	SM 32:1;2O|SM 16:1;2O/16:0	514.4564(100), 638.4449(75), 697.5195(45), 86.0968(55), 146.9816(50)	2	1.70E-02	-0.53	1.07	4.87E-01	0.13	0.51	4.59E-02	-0.46	0.96	1.60E-02	-0.60	0.99	6677836	2350756	5533015	2030298	5390854	2207390	5675177	1847845
RP_NEG_498_29034a9_329	RP	NEG	9.33	498.2903	BA 24:1;O3;T	498.2869(100)	2	3.58E-01	0.14	0.37	4.88E-01	-0.15	0.57	7.42E-01	0.06	0.25	2.46E-01	0.22	0.57	763407	930596	985977	1761165	1108915	1738962	863039	1792170
RP_POS_689_55872a12_472	RP	POS	12.47	689.5587	SM 33:1;2O|SM 17:1;2O/16:0	184.0732(100), 689.5507(1)	2	4.03E-07	-1.14	1.94	5.00E-01	-0.11	0.45	2.87E-07	-1.20	1.99	4.87E-06	-1.09	1.73	7770546	2542305	4830612	2141337	4975905	2343282	4685318	1931365
RP_POS_269_08749a0_71	RP	POS	0.71	269.0875	Inosine	137.0454(100)	2	5.73E-09	0.72	1.33	5.01E-01	0.15	0.82	5.32E-05	0.79	1.42	1.13E-05	0.64	1.44	1813541	2525401	11765200	15151157	10737561	12675315	12792838	17348009
HILIC_POS_316_24817a0_739	HILIC	POS	0.74	316.2482	AC 10:0 (Decanoylcarnitine)	85.0288(100), 316.2486(40)	1	3.38E-01	-0.16	0.43	5.01E-01	-0.14	0.74	1.91E-01	-0.24	0.49	6.82E-01	-0.09	0.40	40185602	26760107	34311483	38476920	36916730	45113134	31706236	30693876
RP_NEG_566_34497a10_62	RP	NEG	10.62	566.3450	LPC 18:1 [M+HCOO]-	281.2505(100), 506.3257(15)	2	5.42E-03	0.61	1.35	5.03E-01	-0.13	0.95	2.66E-02	0.55	1.10	3.18E-03	0.67	1.38	221223504	60554526	256125688	53763647	259755428	45130398	252495948	61452496
RP_POS_286_20123a5_18	RP	POS	5.18	286.2012	CAR 08:1	85.0287(100), 286.2001(60), 227.1275(15), 60.0815(10), 144.1012(2)	2	9.80E-01	0.00	0.50	5.03E-01	-0.14	0.52	7.14E-01	-0.08	0.47	7.45E-01	0.07	0.28	8390101	5705101	8358390	7606952	8871245	7591542	7845535	7664468
RP_NEG_476_27872a10_214	RP	NEG	10.21	476.2787	LPE 18:2	279.2348(100), 476.2775(5), 214.0468(2)	2	1.17E-01	0.31	1.06	5.04E-01	-0.14	0.74	3.04E-01	0.24	0.77	6.77E-02	0.38	1.04	6116442	2901782	7067016	3061822	7272964	2479517	6861068	3564585
RP_POS_811_66663a14_816	RP	POS	14.82	811.6666	SM 42:3;2O	184.0735(100), 811.5959(5)	2	5.48E-03	-0.65	1.16	5.08E-01	-0.12	0.41	5.05E-03	-0.71	1.23	1.57E-02	-0.59	0.96	10023574	4435843	7520757	3441475	7750180	3274154	7291335	3619629
RP_POS_228_19582a7_801	RP	POS	7.80	228.1958	Isomer of myristic acid	95.0857(100), 175.1473(70), 109.1013(60), 193.1584(44), 83.086(38), 81.0705(37)	2	1.40E-01	0.27	0.61	5.11E-01	-0.14	0.41	3.14E-01	0.20	0.48	1.31E-01	0.33	0.57	1696132	1203389	2089921	1558830	2193009	1746071	1986833	1356111
RP_POS_792_58734a13_501	RP	POS	13.50	792.5873	PC O-38:6|PC O-18:2 20:4	184.0732(100), 792.5884(2)	2	3.83E-01	0.16	0.41	5.11E-01	0.14	0.66	2.76E-01	0.23	0.51	6.63E-01	0.09	0.46	14305680	5008874	15247256	6026510	14848928	6152628	15645585	5932977
RP_NEG_592_36322a10_754	RP	NEG	10.75	592.3632	LPC 20:2 [M+HCOO]-	307.2629(100), 532.3364(35), 224.0686(10)	2	5.48E-02	0.40	1.08	5.13E-01	-0.13	0.85	1.68E-01	0.33	0.81	3.24E-02	0.46	1.08	3933779	1783412	4642689	1753524	4758257	1446189	4527121	2023295
RP_POS_703_57452a12_767	RP	POS	12.77	703.5745	SM 34:1;2O|SM 18:1;2O/16:0	184.0731(100), 703.5678(1)	2	5.04E-02	-0.40	0.78	5.13E-01	0.13	0.46	1.39E-01	-0.34	0.63	4.02E-02	-0.47	0.79	65151616	20742593	56707781	20821581	55336844	20669004	58078718	21092198
RP_POS_280_26337a9_618	RP	POS	9.62	280.2634	Isomer of Linoleamide	95.0856(100), 263.2366(95), 81.0705(85), 280.2633(83), 245.2274(81)	2	3.81E-01	-0.24	0.85	5.13E-01	-0.10	0.44	3.06E-01	-0.30	0.67	5.07E-01	-0.19	0.56	44356405	80386491	31211959	42202231	33989529	43397983	28434388	41222256
RP_POS_224_12646a0_621	RP	POS	0.62	224.1265	4-Hydroxybenzoylcholine	224.1285(100), 165.0546(35)	2	1.44E-04	-0.71	1.45	5.16E-01	-0.13	0.96	2.69E-04	-0.78	1.53	1.93E-03	-0.65	1.25	3256972	1031004	2362769	1246849	2444270	1238463	2281268	1262397

Supplementary table 1: Metabolomics results (in asceding order according to p-value from progressive ALD vs non-progressive ALD comparison, with molecular features with ID_level of 1-2 first)

								all_ALD_vs_control			Prog_ALD_vs_non-prog_ALD			Prog_ALD_vs_control_ALD			Non-prog_ALD_vs_control			Healthy_control		all_ALD		Non-prog_ALD		Progressive_ALD	
								t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA								
Feature_ID	RP_HILIC	POS_NEG	Average.Rt	Average.Mz	Metabolite.name	curated_MSMS	ID_level	p	d	VIP	p	d	VIP	p	d	VIP	p	d	VIP	Mean	SD	Mean	SD	Mean	SD	Mean	SD
RP_POS_372_15863a4_998	RP	POS	5.00	372.1586	Trazodone	176.0813(100), 372.1578(95), 148.051(20)	2	1.79E-02	0.33	0.87	5.17E-01	0.14	0.61	4.08E-02	0.41	0.98	1.06E-01	0.26	0.58	16272740	27347849	35474317	63734652	31314203	55372877	39634432	71453740
RP_POS_206_08124a4_894	RP	POS	4.89	206.0812	Indolelactic acid	160.076(100), 188.0697(95), 206.0813(80), 118.0655(65), 130.0658(55), 146.0604(50), 170.0596(25)	1	2.88E-02	0.32	0.70	5.22E-01	-0.14	0.46	1.64E-01	0.25	0.58	4.11E-02	0.39	0.77	4956957	1583391	5926814	3368122	6144005	3518983	5709624	3231175
RP_POS_468_30829a9_797	RP	POS	9.80	468.3083	isomer of LPC 14:0	184.0735(100), 468.3025(5)	1	2.07E-03	0.47	0.96	5.24E-01	-0.14	0.46	4.01E-02	0.40	0.86	3.20E-03	0.54	0.97	5328266	1816484	6821623	3463392	7043898	3280413	6599348	3656914
RP_POS_641_51044a14_987	RP	POS	14.99	641.5104	DG 36:3 [M+Na]+	641.5031(100)	2	1.60E-02	-0.36	0.88	5.27E-01	0.14	0.40	2.11E-01	-0.29	0.60	7.28E-04	-0.43	1.22	13052776	6599062	8773886	13011373	7944179	5911730	9603593	17484085
RP_POS_619_43799a10_66	RP	POS	10.66	619.4380	DG 35:7	619.4352(100)	2	5.86E-01	-0.13	0.35	5.27E-01	0.12	0.38	7.81E-01	-0.07	0.65	4.72E-01	-0.19	0.33	17563798	1216923	17434626	952030	17374055	1060831	17495197	835684
RP_POS_316_24829a7_242	RP	POS	7.24	316.2483	CAR 10:0 (Decanoylcarnitine)	85.0288(100), 316.2482(60), 257.173(12)	1	4.31E-01	-0.13	0.82	5.29E-01	-0.14	1.12	2.49E-01	-0.20	0.65	7.80E-01	-0.06	0.72	37688743	24173527	33212645	37097010	35565302	44188674	30859988	28574935
RP_NEG_524_27887a10_209	RP	NEG	10.21	524.2789	LPE 22:6	327.2359(100), 214.0472(17), 524.2744(13), 78.9581(6)	2	3.26E-02	0.34	1.11	5.29E-01	-0.14	0.40	1.51E-01	0.27	0.76	3.79E-02	0.41	1.01	3233949	1093302	3811236	1826935	3926993	1876613	3695480	1787309
RP_POS_468_30856a9_952	RP	POS	9.95	468.3086	LPC 14:0	184.0731(100), 468.3103	1	1.81E-03	0.47	0.97	5.29E-01	-0.14	0.46	3.65E-02	0.40	0.86	3.00E-03	0.54	0.98	45344790	15652041	58388159	29867795	60280060	28389760	56496259	31449849
RP_NEG_804_57751a13_722	RP	NEG	13.72	804.5775	PC 34:1|PC 16:0_18:1 [M+HCOO]-	281.2505(100), 255.2333(40), 744.5633(20)	2	5.35E-10	1.18	1.89	5.32E-01	0.11	0.82	7.32E-09	1.23	1.91	2.15E-08	1.12	1.91	87874739	17784332	115791326	21319888	114449050	19892324	117133601	22780913
RP_POS_725_5556a12_767	RP	POS	12.77	725.5556	SM 34:1;2O|SM 18:1;2O/16:0	542.4913(100), 666.4796(65), 725.5598(45), 502.4989(5), 86.0967(55), 146.9816(40)	2	3.07E-02	-0.44	0.86	5.34E-01	0.12	0.40	9.36E-02	-0.38	0.71	2.70E-02	-0.50	0.86	20749412	6408338	17839364	6594740	17426994	6621366	18251734	6609025
RP_POS_217_14339a6_035	RP	POS	6.04	217.1434	(2R)-2-[(2R,5S)-5-[(2S)-2-hydroxybutyl]oxolan-2-yl]propanoic acid	125.0957(100), 97.1012(65), 217.105(50), 107.0857(25), 135.0811(20), 83.086(17), 203.1276(80)	2	5.99E-01	0.08	0.72	5.38E-01	-0.14	0.71	9.34E-01	0.02	0.75	4.33E-01	0.15	0.66	987881	129009	1004473	216055	1017872	215788	991073	217673
RP_POS_254_24776a10_363	RP	POS	10.36	254.2478	Palmitoleamide	254.246(100), 83.0862(35), 219.2116(31), 97.1012(30), 69.0703(28), 237.2218(25)	1	3.23E-04	0.48	0.87	5.39E-01	0.14	0.77	1.60E-02	0.55	0.87	7.08E-05	0.41	1.36	20340429	7779324	30005944	22246795	28628435	9999780	31383453	29934463
RP_POS_176_07071a5_352	RP	POS	5.35	176.0707	3-Indoleacetic acid	130.0655(100), 176.07(15)	1	5.82E-01	-0.12	0.39	5.48E-01	0.12	0.55	8.13E-01	-0.06	0.40	4.29E-01	-0.18	0.64	11947198	6025911	11280733	5557720	10944113	4747168	11617354	6296032
RP_POS_137_04588a1_786	RP	POS	1.79	137.0459	Hypoxanthine	137.0456(100), 90.9482(30), 104.9641(28)	1	2.08E-10	0.77	1.44	5.49E-01	0.13	0.78	2.29E-05	0.83	1.49	8.95E-07	0.70	1.64	18962	15981	5941841	8361684	5437496	6817378	6446187	9709102
RP_POS_370_29498a8_445	RP	POS	8.45	370.2950	CAR 14:1	85.029(100), 370.2926(65)	2	6.13E-02	0.32	1.04	5.50E-01	-0.13	1.47	1.52E-01	0.25	0.88	8.56E-02	0.38	0.98	9632693	5652766	12088475	8206654	12583107	9680527	11593843	6470001
RP_POS_223_09589a7_494	RP	POS	7.49	223.0959	Diethyl-phthalate	149.0227(100), 177.0534(35), 223.0945(30)	2	7.36E-01	0.07	0.40	5.54E-01	0.12	0.40	5.89E-01	0.13	0.38	9.47E-01	0.02	0.38	14571521	2424680	14733926	2144592	14606123	2049113	14861728	2249493
RP_POS_338_34174a11_668	RP	POS	11.67	338.3417	13-Docosenamide	338.3423(100), 83.086(50), 97.1011(48), 69.0707(45), 321.3165(32), 95.0856(30), 81.0704(28), 71.0881(25),	2	9.34E-01	-0.02	0.69	5.62E-01	-0.12	0.34	7.36E-01	-0.08	0.39	8.53E-01	0.04	0.45	300408471	155545546	297747518	159339634	307053555	162156516	288441480	157559220
RP_POS_181_07202a2_801	RP	POS	2.80	181.0720	Paraxanthine	181.0714(100), 124.05(10)	1	6.79E-01	-0.08	0.44	5.63E-01	-0.12	0.34	5.35E-01	-0.14	0.44	9.28E-01	-0.02	0.45	22872361	22954693	20868889	26076092	22386445	24443731	19351332	27777796
HILIC_NEG_204_06667a0_701	HILIC	NEG	0.70	204.0667	Indolelactic acid	99.9254(100), 117.929(80), 158.061(35), 204.0672(30), 186.0561(15)	2	1.83E-03	0.44	0.71	5.63E-01	-0.13	0.55	3.42E-02	0.37	0.69	6.69E-03	0.50	0.88	401583	123922	518135	292733	535164	300445	501106	286837
RP_NEG_852_57751a13_206	RP	NEG	13.21	852.5775	PC 38:5|PC 16:0_22:5 AND PC 18:1_20:4 [M+HCOO]-	303.2311(100), 329.2491(85), 281.25(62), 255.2327(60), 792.5487(47)	2	6.08E-05	0.75	1.29	5.64E-01	0.11	0.59	5.13E-04	0.81	1.25	2.05E-04	0.70	1.44	18740458	3477253	21940162	4186753	21696824	2999299	22183500	5128245
RP_POS_264_19583a4_245	RP	POS	4.25	264.1958	Tramadol	58.0657(100), 264.1949(15)	2	7.50E-02	0.24	0.64	5.66E-01	-0.13	0.80	9.29E-02	0.17	0.99	1.83E-01	0.30	0.62	8515547	6466223	12401100	18383475	13466898	24667614	11335303	8484803
RP_POS_673_52698a11_854	RP	POS	11.85	673.5270	SM 32:2;2O|SM 18:2;2O/14:0	184.0735(100), 673.5216(1)	2	2.07E-05	-0.92	1.68	5.67E-01	-0.10	0.35	3.36E-05	-0.98	1.62	1.29E-04	-0.87	1.51	8740001	2638617	6265067	2408024	6403758	2327003	6126376	2502259
RP_POS_476_27728a10_053	RP	POS	10.05	476.2773	LPE 18:3	335.2592(100), 475.3276(45), 62.0608(40)	2	8.14E-03	0.44	0.97	5.69E-01	0.12	0.92	2.20E-02	0.50	1.03	3.17E-02	0.37	1.04	2551975	1609965	3581253	2510618	3437109	2033129	3725397	2925582
RP_POS_758_57062a13_16	RP	POS	13.16	758.5706	PC 34:2|PC 16:1_18:1	184.0731(100), 758.5703(3)	1	5.08E-02	-0.39	0.71	5.74E-01	0.11	0.45	1.31E-01	-0.33	0.70	4.88E-02	-0.44	0.79	883410931	108139484	838762607	116184921	832183905	119875550	845341309	113202860
HILIC_NEG_137_02422a0_6	HILIC	NEG	0.60	137.0242	Salicylic acid	93.0344(100), 137.0243(35)	2	9.12E-02	0.20	1.01	5.74E-01	-0.13	0.55	4.16E-01	0.13	0.58	1.22E-01	0.26	0.46	519567	497048	2456543	11324196	3097669	11569911	1815417	11153036
HILIC_NEG_131_04617a6_199	HILIC	NEG	6.20	131.0462	L-Asparagine	114.0195(100), 113.0327(60), 70.0292(45), 95.0236(25)	2	5.75E-01	-0.09	1.23	5.75E-01	0.12	0.77	9.04E-01	-0.02	1.09	3.98E-01	-0.15	1.17	624896	118232	608091	213206	596048	189079	620135	236209
RP_NEG_311_29678a12_128	RP	NEG	12.13	311.2968	FA 20:0 (Arachidic acid)	311.297(100)	2	3.85E-02	-0.44	0.82	5.80E-01	-0.11	0.77	2.83E-02	-0.49	0.86	1.09E-01	-0.39	0.73	1126993	283106	1006545	265703	1021340	294739	991750	235200
RP_POS_250_1800Sa4_057	RP	POS	4.06	250.1801	N,O-Didesmethylvenlafaxine	250.181(100), 232.1693(90), 201.1271(35)	2	6.69E-01	0.06	0.82	5.82E-01	-0.12	0.51	9.90E-01	0.00	0.71	5.95E-01	0.12	0.92	12712287	4620417	13245028	9360119	13765324	12681721	12724732	3953874
RP_POS_778_53485a12_761	RP	POS	12.76	778.5349	PC 34:3 [M+Na]+	146.9817(100), 86.0968(55), 595.4709(45), 719.4662(25), 573.4848(13), 184.0727(65)	2	2.26E-03	0.53	0.91	5.84E-01	0.11	0.42	4.74E-03	0.58	1.05	1.74E-02	0.47	0.87	15464081	7387793	20773023	10549162	20191767	10199307	21354279	10960173
RP_POS_135_04413a4_201	RP	POS	4.20	135.0441	Caffeic acid	135.0439(100), 107.0502(1)	2	5.41E-01	-0.12	0.41	5.87E-01	0.11	0.42	7.72E-01	-0.07	0.27	4.21E-01	-0.18	0.42	4418869	878341	4307432	934303	4256382	898592	4358483	975127
RP_NEG_616_36328a10_679	RP	NEG	10.68	616.3633	LPC 22:4 [M+HCOO]-	331.2642(100), 556.3359(40), 224.0689(15)	2	3.07E-08	1.01	1.81	5.90E-01	-0.10	0.69	8.41E-06	0.95	1.65	4.73E-08	1.06	1.91	1466780	684728	2407240	890388	2455594	758768	2358886	1010575
RP_NEG_830_59357a14	RP	NEG	14.00	830.5936	PC 36:2|PC 18:0_18:2 [M+HCOO]-	279.2348(100), 283.2654(35), 770.5653(22)	2	1.62E-02	-0.53	0.95	5.91E-01	0.10	0.44	4.59E-02	-0.48	0.90	1.46E-02	-0.58	0.95	92634970	30139630	77804413	26451668	76371481	25825761	79237346	27248864
RP_POS_280_26428a10_59	RP	POS	10.59	280.2643	Linoleamide	95.0861(100), 263.2354(85), 81.0701(80), 245.2251(78), 280.2631(77)	1	2.48E-04	0.63	1.13	5.96E-01	-0.11	0.37	4.91E-03	0.57	0.98	5.14E-04	0.68	1.42	267038186	110285312	363730128	158490893	372192861	152033407	355267396	166804254
RP_NEG_327_23331a10_908	RP	NEG	10.91	327.2333	FA 22:6 (Docosahexaenoic acid)	327.2354(100), 283.2422(90), 59.0125(60)	2	8.19E-04	0.46	1.51	5.97E-01	0.12	0.65	8.36E-03	0.52	1.19	1.16E-02	0.40	1.41	34948557	14373270	50139335	36270685	48207895	31469336	52070774	40743602
RP_POS_319_07315a8_805	RP	POS	8.81	319.0732	Fenofibric acid	233.036(100), 138.994(20), 121.028(10)	2	7.67E-02	0.22	0.55	5.98E-01	-0.12	0.89	3.39E-02	0.16	0.96	2.22E-01	0.28	0.42	26937156	30571846	53423095	138156730	60771980	189699101	46074211	49680328
RP_POS_524_37073a10_823	RP	POS	10.82	524.3707	LPC 18:0	184.0733(100), 524.373(4), 506.3576(1)	2	8.68E-01	-0.04	0.81	6.07E-01	-0.10	1.02	7.35E-01	-0.09	0.47	9.70E-01	0.01	0.76	76633060	27043115	75762690	20826831	76840482	19377230	74684897	22327522
RP_POS_832_58173a13_652	RP	POS	13.65	832.5817	PC 38:4 [M+Na]+	146.9822(100), 86.0971(50), 649.5156(45), 832.5833(30), 773.5108(25), 627.528(10)	2	1.30E-05	0.93	1.62	6.09E-01	-0.09	0.47	9.10E-05	0.88	1.61	2.52E-05	0.97	1.45	4576992	2097768	6614203	2001430	6717349	2064161	6511056	1952106
HILIC_NEG_104_03526a6_129	HILIC	NEG	6.13	104.0353	Serine	74.0242(100), 72.0078(85), 104.0355(40)	2	4.48E-01	-0.11	1.17	6.09E-01	-0.11	0.78	4.10E-01	-0.17	1.20	7.39E-01	-0.05	1.23	434664	100427	414031	204989	424593	172207	403470	234554
RP_POS_181_07196a3_128	RP	POS	3.13	181.0720	Theophylline	181.0714(100), 124.05(10)	1	5.99E-01	-0.11	0.42	6.21E-01	-0.10	0.30	4.99E-01	-0.16	0.41	8.02E-01	-0.06	0.46	24004588	25066833	21287511	26081356	22586103	24554396	19988919	27712756
RP_POS_301_14124a9_441	RP	POS	9.44	301.1412	Enterodiol	301.1396(100)	2	9.55E-01	-0.01	0.20	6.21E-01	-0.10	0.81	7.89E-01	-0.06	0.37	8.56E-01	0.04	0.32	23196939	1508878	23179068	1642412	23260808	1448457	23097328	1827134
RP_POS_723_53973a12_326	RP	POS	12.33	723.5397	SM 34:2;2O|SM 18:2;2O/16:0	540.4738(100), 664.4639(60), 723.552(35), 500.4831(5), 60.0815(85), 86.0968(55), 146.9818(45)	2	2.70E-05	-0.93	1.58	6.25E-01	-0.09	0.38	4.70E-05	-0.98	1.55	1.23E-04	-0.89	1.52	17957657	4538358	13797057	3950766	13991695	3761828	13602418	4160167
RP_POS_784_58533a13_398	RP	POS	13.40	784.5853	PC 36:3	184.0735(100), 784.587(2)	2	5.40E-01	0.14	0.48	6.25E-01	-0.09	0.34	7.08E-01	0.09	0.46	4.47E-01	0.19	0.62	230433572	66764797	238443952	54138646	241106816	52587814	235781088	56052233
HILIC_NEG_173_10446a6_934	HILIC	NEG	6.93	173.1045	Arginine	131.0821(100), 173.1049(3)	2	4.80E-02	0.26	1.10	6.32E-01	-0.11	0.79	2.38E-01	0.21	0.95	7.07E-02	0.32	1.17	1034788	283150	1227747	826753	1267611	823202	1187882	836710
RP_POS_293_09753a0_622	RP	POS	0.62	293.0975	Ethylenediaminetetraacetic acid EDTA	160.0599(100), 132.0647(40), 293.0956(20)	2	1.30E-04	-0.54	1.19	6.37E-01	0.10	1.09	7.01E-03	-0.48	1.18	1.25E-03	-0.59	1.31	344120143	76564293	253987961	183489614	245274050	184551764	262701873	183874061
RP_POS_466_32883a11_091	RP	POS	11.09	466.3288	LPE O-18:1	293.3134(100), 466.3249(50), 312.3251(40), 448.3138(30), 86.0604(17)	2	2.48E-01	-0.26	0.81	6.42E-01	-0.09	1.17	2.09E-01	-0.30	0.87	3.86E-01	-0.21	0.75	1729807	680119	1573120	589020	1600719	606868	1545520	575436
RP_POS_832_58038a13_871	RP	POS	13.87	832.5804	PC 38:4 [M+Na]+	184.0732(100), 810.5858(10), 146.982(50), 86.0969(30)	2	4.04E-01	-0.18	0.56	6.47E-01	0.09	0.71	5.79E-01	-0.14	0.55	3.18E-01	-0.23	0.43	72485785	20863863	69027981	18023057	68197476	14970895	69858486	20754639
RP_POS_177_10231a1_38	RP	POS	1.38	177.1023	Cotinine	177.1026(100), 80.05(7), 98.0601(4), 105.9347(25), 102.0558(21)	2	2.99E-05	0.70	1.22	6.49E-01	0.09	0.64	5.38E-04	0.75	1.16	2.46E-04	0.65	1.32	1548913	1218458	2806941	1854286	2721814	1524741	2892069	2146462
RP_NEG_788_54688a12_835	RP	NEG	12.84	788.5469	PC 33:2|PC 15:0_18:2 [M+HCOO]-	279.2347(100), 241.2187(40), 728.5233(20)	2	1.53E-11	-1.61	2.70	6.50E-01	-0.06	0.84	8.98E-12	-1.64	2.57	3.57E-11	-1.58	2.33	4142222	1106158	2207653	780576	2243306	848076	2172000	713587
RP_POS_314_2324Sa6_93	RP	POS	6.93	314.2325	CAR 10:1	85.0287(100), 314.2295(55)	2	1.01E-01	-0.32	0.78	6.53E-01	-0.09	0.55	1.13E-01	-0.37	0.63	1.84E-01	-0.28	0.86	4264808	1712469	3673122	1845631	3756655	1608975	3589589	2068619
RP_POS_175_11873a0_512	RP	POS	0.51	175.1187	Arginine	175.1188(100), 60.0564(58), 70.0657(50), 116.071(45), 130.0979(20), 158.0928(20)	1	3.93E-04	0.43	1.15	6.55E-01	-0.10	1.11	1.90E-02	0.38	1.12	5.99E-03	0.48	1.23	2599035	574173	3712283	2877674	3841634	2986902	3582932	2788421
RP_POS_572_37091a10_678	RP	POS	10.68	572.3709	LPC 22:4	184.0733(100), 572.3646(25), 554.3591(5), 104.1076(90)	2	2.71E-07	0.95	1.73	6.60E-01	-0.09	0.65	3.78E-05	0.90	1.55	3.17E-07	0.99	1.87	3113946	1601976	5111163	2028865	5200994	1662158	5021331	2353158
RP_NEG_255_23318a11_162	RP	NEG	11.16	255.2332	FA 16:0 (Palmitic acid)	255.2333(100)	2	1.37E-01	0.26	1.05	6.62E-01	-0.09	1.01	2.90E-01	0.21	0.91	1.39E-01	0.31	1.04	10526365	2451524	11350402	3344242	11497585	3423933	11203219	3290689
RP_NEG_474_26349a10_052	RP	NEG	10.05	474.2635	LPE 18:3	277.2187(100), 474.2629(17), 196.0374(13), 78.9574(5), 214.0472(3)	2	7.18E-03	0.44	0.98	6.62E-01	0.09	0.73	2.33E-02	0.49	0.97	2.57E-02	0.39	1.01	1613306	1025964	2285009	1628497	2213316	1354091	2356702	1874586
RP_POS_361_19992a6_798	RP	POS	6.80	361.1999	Cortisone	361.2028(100), 163.1108(50)	1	1.22E-01	0.28	1.39	6.67E-01	0.09	0.38	1.06E-01	0.32	0.92	2.87E-01	0.23	1.27	1663070	350644	1784397	464106	1764314	503061	1804479	425784
RP_POS_643_52563a11_838	RP	POS	11.84	643.5256	DG 36:2	643.5267(100)	2	3.11E-01	-0.35	0.85	6.68E-01	-0.03	0.38	2.90E-01	-0.37	0.63	3.39E-01	-0.33	0.71	3725506	9070868	2063702	1886235	2145228	2059932	1982176	1712159
RP_NEG_233_15483a9_107	RP	NEG	9.11	233.1548	FA 15:4	233.1547(100)	2	1.20E-01	0.31	0.62	6.71E-01	-0.09	0.57	2.13E-01	0.27	0.52	1.27E-01	0.36	0.66	1375937	80108	1401903	83554	1405475	90835	1398330	76340
RP_POS_356_27927a8_084	RP	POS	8.08	356.2793	CAR 13:1	85.0289(100), 356.2804(75)	2	4.91E-02	-0.37	0.73	6.80E-01	-0.09	0.26	8.02E-02	-0.41	0.63	8.66E-02	-0.33	0.85	2805312	1246859	2271661	1486055	2333462	1113532	2209860	1792774
RP_NEG_747_56763a12_77	RP	NEG	12.77	747.5676	SM 34:1;2O [M+HCOO]-	687.5526(100), 168.0422(90), 78.9574(70)	2	6.60E-02	-0.38	0.78	6.82E-01	0.08	0.27	1.39E-01	-0.34	0.66	6.60E-02	-0.42	0.73	19181533	5643149	17031042	5622379	16798901	5606800	17263183	5685176
RP_NEG_552_33093a10_39	RP	NEG	10.39	552.3309	LPC 17:1 [M+HCOO]-	267.2311(100), 492.3061(40), 224.0688(10)	2	8.45E-04	0.58	1.20	6.86E-01	0.08	0.86	3.76E-03	0.62	1.15	4.48E-03	0.54	1.13	2527326	936737	3261859	1306827	3208562	1154120	3315156	1453497
RP_POS_522_35614a10_619	RP	POS	10.62	522.3561	LPC 18:1 (18:1/0:0)	184.0733(100), 522.3521(30), 504.3383(6), 104.1077(80)	2	1.88E-03	0.64	1.41	6.90E-01	-0.08	0.90	1.20E-02	0.60	1.17	1.37E-03	0.68	1.45	642570021	211946767	783412433	210869915	791883872	166949297	774940994	248638666
RP_NEG_719_53613a12_212	RP	NEG	12.21	719.5361	SM 32:1;2O [M+HCOO]-	659.5084(100), 168.0419(70), 78.9579(60)	2	1.57E-02	-0.55	1.08	6.92E-01	0.07	0.36	3.10E-02	-0.51	1.02	1.96E-02	-0.59	1.02	9356178	2901327	7935443	2395881	7839715	2617002	8031172	2174909
HILIC_POS_162_11221a4_832	HILIC	POS	4.83	162.1122	Carnitine	162.1135(100), 103.0395(25), 60.0815(20)	1	1.27E-02	0.43	1.02	6.92E-01	-0.08	0.60	7.43E-02	0.38	0.65	1.21E-02	0.47	0.90	1634011394	449777697	########	648622698	1922026229	558316812	1870206254	732748959
HILIC_POS_290_13861a0_815	HILIC	POS	0.82	290.1386	Benzoylecgonine	168.101(100), 290.1383(80), 105.0342(10)	2	2.55E-01	0.15	0.53	6.95E-01	-0.09	0.32	2.24E-01	0.10	0.65	4.02E-01	0.19	0.48	25629873	23169226	34892575	69925189	37660295	96455687	32124855	23654125
RP_POS_834_59906a13_712	RP	POS	13.71	834.5991	PC 40:6|PC 18:0_22:6	184.0735(100), 834.5901(2)	2	2.55E-02	-0.47	1.06	7.03E-01	0.08	0.62	7.03E-02	-0.43	0.82	2.40E-02	-0.50	1.08	52296554	18601535	43650946	18179607	42951716	16536842	44350177	19831191
HILIC_POS_193_09724a0_67	HILIC	POS	0.67	193.0972	trans-3-Hydroxycotinine	193.0967(100), 134.0603(10)	2	3.81E-10	0.87	1.55	7.03E-01	0.08	0.47	1.69E-06	0.91	1.56	1.38E-06	0.83	1.83	2373358	3323212	9315459	8338632	8994888	7850491	9636030	8868183
RP_POS_295_1889a9_271	RP	POS	9.27	295.1889	Cinchonine	295.1871(100), 277.2146(5)	2	6.77E-01	-0.09	0.62	7.05E-01	-0.07	0.37	5.91E-01	-0.13	0.27	8.26E-01	-0.05	0.54	2354727	367035	2324170	334602	2336923	337973	2311418	334133
RP_POS_278_21146a5_275	RP	POS	5.28	278.2115	Venlafaxine	278.113(25), 58.0657(100), 121.0646(10)	2	6.95E-01	0.06	0.98	7.09E-01	0.08	0.54	5.95E-01	0.10	0.64	9.32E-01	0.02	0.86	51434856	21637735	53745595	44598410	52066106	44134648	55425083	45442326
HILIC_POS_264_19559a0_623	HILIC	POS	0.62	264.1956	Tramadol	58.0658(100), 264.1966(15)	2	2.75E-02	0.26	0.92	7.10E-01	-0.09	0.51	1.34E-01	0.21	0.72	1.07E-01	0.30	0.81	50682	255102	1847580	8018984	2147794	9033989	1547366	6937121
RP_POS_428_37332a9_66	RP	POS	9.66	428.3733	CAR 18:0 (Octadecanoylcarnitine)	85.0289(100), 428.3723(55)	1	1.49E-02	0.47	0.79	7.20E-01	-0.07	0.54	5.00E-02	0.43	0.83	1.87E-02	0.50	0.95	2169652	687330	2533545	793045	2562199	769360	2504891	822853
RP_NEG_562_31641a9_896	RP	NEG	9.90	562.3164	LPC 18:3 [M+HCOO]-	277.2187(100), 502.2986(16)	2	1.77E-01	0.25	0.71	7.23E-01	-0.07	0.68	3.26E-01	0.21	0.78	1.71E-01	0.29	0.75	922447	678064	1121691	835280	1151515	809490	1091867	867488
RP_POS_259_19034a9_529	RP	POS	9.53	259.1903	Dibutyladipate	129.054(100), 111.044(95), 101.0597(62), 185.1172(50)	2	1.87E-02	-0.45	0.76	7.33E-01	-0.07	0.36	2.10E-02	-0.49	0.90	6.13E-02	-0.42	0.63	14822955	438317	14599883	500056	14617058	536052	14582707	466113

Supplementary table 1: Metabolomics results (in asceding order according to p-value from progressive ALD vs non-progressive ALD comparison, with molecular features with ID_level of 1-2 first)

							all_ALD_vs_control			Prog_ALD_vs_non-prog_ALD			Prog_ALD_vs_control_ALD			Non-prog_ALD_vs_control			Healthy_control		all_ALD		Non-prog_ALD		Progressive_ALD	
							t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA								
Feature_ID	RP_HILIC	POS_NEG	Average.Rt	Average.Mz	Metabolite.name	curated_MSMS	ID_level	p	d	VIP	p	d	VIP	p	d	VIP	p	d	VIP	Mean	SD	Mean	SD	Mean	SD	Mean	SD
RP_POS_137_04588a1_043	RP	POS	1.04	137.0459	Hypoxanthine	137.0455(100), 118.9426(10), 110.0345(1), 90.9483(35)	2	1.92E-12	0.86	1.65	7.36E-01	0.07	0.80	2.32E-06	0.90	1.66	1.39E-07	0.82	1.80	439489	248933	5144824	5840917	4946302	5181871	5343347	6480483
RP_POS_392_27905a8_113	RP	POS	8.11	392.2791	CAR 16:4	392.2112(100), 85.0287(55)	2	7.15E-01	0.06	0.93	7.40E-01	-0.07	0.83	9.15E-01	0.02	0.54	5.66E-01	0.10	1.07	646880	330891	675482	515795	692767	382496	658196	624984
RP_NEG_528_31067a10_684	RP	NEG	10.68	528.3107	LPE 22:4	331.2644(100), 196.0375(20), 528.3052(19), 78.9581(7), 213.6675(5)	2	4.31E-15	1.05	1.86	7.43E-01	0.07	0.24	1.47E-07	1.08	1.76	4.39E-12	1.02	2.09	528511	249574	1279950	719757	1256173	540359	1303726	868061
RP_POS_162_11258a0_532	RP	POS	0.53	162.1126	Carnitine	162.112(100), 103.0398(17), 60.0815(14)	1	4.28E-03	0.43	0.75	7.44E-01	-0.07	0.58	5.98E-02	0.39	0.68	4.65E-03	0.46	1.22	57941749	9420896	65258198	18722540	65875206	15243603	64641190	21796247
RP_POS_508_33942a10_389	RP	POS	10.39	508.3394	LPC 17:1	184.0736(100), 508.3387(30), 490.3309(8), 104.1069(80)	2	4.84E-04	0.59	1.22	7.47E-01	0.07	0.80	3.77E-03	0.62	1.15	2.35E-03	0.55	1.18	6163829	2422772	8208925	3634819	8090973	3095735	8326878	4132975
RP_NEG_480_31073a10_825	RP	NEG	10.83	480.3107	LPE 18:0	283.2652(100), 480.3055(4), 214.0472(2), 196.0375(1.5)	2	3.58E-01	0.17	0.99	7.50E-01	-0.07	0.94	5.36E-01	0.14	0.67	3.12E-01	0.21	0.92	1466967	525073	1570032	614795	1589799	543705	1550266	683554
RP_POS_138_05482a0_59	RP	POS	0.59	138.0548	Trigonelline	138.0541(100), 94.066(2)	2	3.43E-01	0.16	0.41	7.55E-01	0.07	0.41	3.61E-01	0.19	0.49	5.07E-01	0.12	0.57	3272951	2314067	3784983	3479730	3675755	3149115	3894211	3810891
RP_POS_202_18037a0_709	RP	POS	0.71	202.1804	4-Hydroxy-1-(2-hydroxyethyl)-2,2,6,6-tetramethylpiperidine	202.1808(100), 102.092(25), 62.067(10)	2	7.86E-01	-0.05	0.52	7.58E-01	-0.06	0.39	6.90E-01	-0.09	0.40	9.24E-01	-0.02	0.53	2517635	1089386	2455993	1172567	2492434	1274507	2419553	1072759
RP_POS_232_15433a1_769	RP	POS	1.77	232.1543	CAR 04:0	85.0288(100), 232.1552(55), 173.0817(20), 60.0815(6)	2	2.16E-05	0.54	0.89	7.58E-01	-0.07	0.80	7.08E-03	0.51	0.92	2.68E-04	0.57	1.12	2064631	829454	3570267	3082336	3665876	2739915	3474658	3416093
RP_POS_235_18044a3_588	RP	POS	3.59	235.1804	Lidocaine	86.0966(100), 235.1806(30)	2	5.15E-03	-0.98	1.94	7.59E-01	0.01	0.29	5.43E-03	-0.97	1.47	4.96E-03	-0.98	1.43	20065082	33880888	2014217	3331720	1911146	3189974	2117288	3497090
HILIC_POS_104_10756a1_472	HILIC	POS	1.47	104.1076	Choline	104.1071(100), 60.0815(10)	1	1.83E-01	0.22	0.77	7.59E-01	-0.07	0.76	3.65E-01	0.19	0.31	1.79E-01	0.25	0.48	493867570	124397242	532838667	189251515	538681304	174174145	526996031	204833870
RP_POS_348_28735a10_06	RP	POS	10.06	348.2874	NAE 20:4	348.2853(100), 60.0816(7), 229.3589(3)	2	2.96E-01	-0.29	0.97	7.61E-01	-0.05	0.36	2.76E-01	-0.32	0.72	3.54E-01	-0.27	0.62	6273951	9626486	4390550	5036950	4544924	5072329	4236175	5048004
RP_NEG_526_29449a10_455	RP	NEG	10.46	526.2945	LPE 22:5	329.2492(100), 196.0373(24), 526.298(24), 78.9574(9), 214.0502(5)	2	1.55E-14	1.04	1.81	7.63E-01	0.06	0.46	1.16E-07	1.07	1.74	6.06E-11	1.01	1.97	2340255	877228	4833635	2417566	4760098	1947424	4907173	2829317
RP_POS_120_0807a1_451	RP	POS	1.45	120.0807	Indoline	120.0814(100), 103.0546(16)	2	2.11E-01	0.20	0.64	7.64E-01	0.07	0.37	2.79E-01	0.24	0.61	3.18E-01	0.17	0.77	11711349	2585834	12488764	4132979	12363926	3258360	12613601	4884968
RP_POS_286_20123a5_543	RP	POS	5.54	286.2012	CAR 08:1 (Octenoyl-L-carnitine)	85.287(100), 286.2004(55), 60.0815(14), 227.128(11)	1	3.33E-01	0.17	0.75	7.72E-01	-0.06	0.73	5.07E-01	0.14	0.49	3.27E-01	0.20	0.90	1063170	444287	1160851	622774	1179040	617832	1142662	633419
RP_POS_766_53497a12_834	RP	POS	12.83	766.5350	PC 33:2 [M+Na]+	146.982(100), 766.5388(45), 86.097(40), 583.4727(35), 707.4636(25), 561.4822(13), 184.0732(16)	2	1.08E-09	-1.53	2.55	7.72E-01	-0.04	0.65	8.69E-10	-1.54	2.42	2.18E-09	-1.51	2.18	5598485	1653919	3132237	1055330	3163116	1153644	3101559	957782
RP_POS_207_09889a5_341	RP	POS	5.34	207.0989	p-methoxycinnamic acid ethyl ester	207.978(100)	2	8.74E-01	0.03	0.36	7.74E-01	0.06	0.22	7.82E-01	0.06	0.18	9.96E-01	0.00	0.23	503348	168743	508964	186619	503573	189878	514355	185071
RP_POS_528_30847a10_456	RP	POS	10.46	528.3085	LPE 22:5	387.2857(100), 528.3135(6), 62.0608(50)	2	1.82E-13	1.02	1.78	7.85E-01	0.06	0.48	2.05E-07	1.05	1.72	3.14E-10	0.99	1.92	3929779	1554351	7880602	3913990	7773118	3209279	7988086	4541830
HILIC_NEG_124_00751a5_262	HILIC	NEG	5.26	124.0075	Taurine	124.0074(100), 79.9569(60)	2	1.26E-04	0.48	1.11	7.90E-01	0.06	0.76	4.99E-03	0.51	1.16	5.96E-03	0.45	1.26	1428645	392639	2173114	1747362	2126127	1655556	2220102	1850267
RP_POS_337_23535a10_16	RP	POS	10.16	337.2354	8-hydroxy-8-(3-octyloxiran-2-yl)octanoic acid	337.236(100)	2	4.76E-02	-0.44	0.79	7.97E-01	0.05	0.45	7.95E-02	-0.42	0.70	5.64E-02	-0.47	0.85	2303486	426936	2133210	360784	2123865	376286	2142555	348164
RP_POS_701_55817a12_326	RP	POS	12.33	701.5582	SM 34:2;2O|SM 18:2;2O/16:0	184.0732(100), 701.5657(1)	2	1.09E-04	-0.77	1.30	8.05E-01	0.05	0.46	8.84E-04	-0.75	1.24	2.14E-04	-0.79	1.36	54398915	12108276	43952049	13091718	43627078	12210424	44277020	14034743
RP_POS_132_10216a0_712	RP	POS	0.71	132.1022	Isoleucine	86.0971(100), 131.9745(10), 113.9642(30)	1	6.06E-01	0.09	0.65	8.06E-01	-0.05	0.62	7.71E-01	0.06	0.46	5.47E-01	0.12	0.31	160933478	28469498	164269687	40055047	165262736	36055529	163276639	44040243
RP_POS_180_06563a3_625	RP	POS	3.63	180.0656	Hippuric acid	105.0335(100), 95.0497(1), 77.0394(0.5)	1	2.15E-02	-0.50	0.88	8.09E-01	0.05	0.78	5.35E-02	-0.47	0.76	2.14E-02	-0.52	1.08	14629099	12569778	8682900	11514323	8402188	9951182	8963611	12987616
RP_POS_424_34186a9_11	RP	POS	9.11	424.3419	CAR 18:2	85.0289(100), 424.3397(70)	2	1.14E-04	0.64	1.05	8.09E-01	0.05	0.16	9.12E-04	0.67	1.13	1.39E-03	0.62	1.16	5288946	1931920	7124655	2971845	7052386	2886054	7196923	3082857
HILIC_NEG_118_05093a5_743	HILIC	NEG	5.74	118.0509	Threonine	74.0243(100), 72.0078(60), 117.9291(45),	2	2.85E-01	-0.20	1.01	8.09E-01	0.05	0.68	4.67E-01	-0.17	0.87	2.37E-01	-0.22	0.88	1367000	383063	1277592	479347	1265930	358191	1289253	579360
RP_POS_737_50073a10_467	RP	POS	10.47	737.5007	DG 44:11	737.4964(100)	2	1.59E-01	-0.30	0.99	8.12E-01	-0.05	0.68	1.89E-01	-0.32	0.81	2.16E-01	-0.27	0.81	3189125	469781	3054471	444621	3065133	381121	3043808	503909
RP_POS_794_6048a13_71	RP	POS	13.71	794.6048	PC O-38:5|PC O-18:1_20:4	184.0735(100), 794.6074(3)	2	3.01E-05	-0.89	1.38	8.13E-01	0.04	0.51	1.11E-04	-0.86	1.41	9.85E-05	-0.91	1.38	41457806	9241474	32944335	8804584	32734176	9398958	33154494	8257898
HILIC_POS_137_04573a1_385	HILIC	POS	1.39	137.0457	Hypoxanthine	137.0464(100)	1	1.85E-15	0.99	1.68	8.15E-01	-0.05	0.63	1.76E-07	0.96	1.63	1.71E-09	1.01	2.13	13278742	6945242	73969884	63907985	75479832	59482359	72459935	68622217
RP_POS_287_10013a3_743	RP	POS	3.74	287.1001	(4R)-3-methylidene-4-[(E)-3-methyl-4-(4-methyl-5-oxooxolan-2-yl)but-2-enyl]oxolan-2-one	287.0972(100)	2	7.37E-02	-0.37	0.66	8.29E-01	-0.04	0.26	1.06E-01	-0.39	0.63	1.08E-01	-0.34	0.73	2670017	1728836	2028013	1742726	2066033	1479249	1989993	1986213
RP_POS_279_09348a7_822	RP	POS	7.82	279.0935	Triphenylphosphine oxide	279.0936(100), 219.0576(10), 201.046(3)	2	8.16E-02	-0.36	0.68	8.37E-01	-0.04	0.53	9.47E-02	-0.38	0.74	1.39E-01	-0.34	0.69	2323279	102584	2286458	100409	2288542	102412	2284373	99361
RP_POS_315_07913a0_62	RP	POS	0.62	315.0791	Altenuene [M+Na]+	315.0771(100)	2	5.19E-08	-0.74	1.36	8.39E-01	0.04	1.10	3.54E-05	-0.72	1.46	3.77E-05	-0.76	1.43	38518270	6155492	26992060	16672075	26650092	17360393	27334027	16123489
RP_POS_744_55316a12_832	RP	POS	12.83	744.5532	PC 33:2|PC 15:0 18:2	184.0735(100), 744.5581(3)	2	2.61E-10	-1.57	2.61	8.55E-01	-0.02	0.84	2.27E-10	-1.58	2.46	4.21E-10	-1.55	2.26	16783209	5094784	8746595	3304584	8807646	3560758	8685545	3062158
RP_POS_153_05492a4_29	RP	POS	4.29	153.0549	Vanillin	111.0443(100), 125.0599(90), 153.0543(60), 93.0339(35), 65.0394(20)	2	7.84E-01	0.05	0.36	8.60E-01	-0.04	0.35	8.74E-01	0.03	0.20	7.49E-01	0.07	0.37	1142092	402451	1165528	464208	1173771	485133	1157285	447083
RP_POS_288_21689a5_995	RP	POS	6.00	288.2169	CAR 08:0 (Octanoylcarnitine)	85.0289(100), 288.2181(65), 229.1446(15), 60.087(10)	1	7.19E-01	-0.06	0.55	8.61E-01	-0.04	0.87	6.99E-01	-0.07	0.33	8.48E-01	-0.04	0.62	21320913	16124078	19849249	29217768	20365653	28634752	19332845	30071327
RP_POS_357_27878a9_935	RP	POS	9.94	357.2788	Deoxycholic acid	357.2788(100)	2	6.63E-02	0.28	1.07	8.64E-01	-0.04	0.36	1.31E-01	0.26	0.64	1.38E-01	0.30	1.21	5847692	5418303	8392201	9792397	8561535	10876975	8222866	8681701
RP_POS_647_45959a13_458	RP	POS	13.46	647.4596	DG 37:7	647.4604(100)	2	4.63E-01	-0.16	0.72	8.67E-01	0.03	0.12	5.47E-01	-0.14	0.51	4.63E-01	-0.17	0.49	18032271	15822888	15704894	14362217	15462123	14656257	15947665	14206691
RP_NEG_802_56183a13_163	RP	NEG	13.16	802.5618	PC 34:2|PC 16:1_18:1 [M+HCOO]-	279.2347(100), 255.2332(40), 742.5426(20)	2	1.97E-01	-0.27	0.51	8.68E-01	0.03	0.12	2.67E-01	-0.25	0.50	2.21E-01	-0.29	0.54	154183146	15830139	150015761	15234768	149760145	15820413	150271377	14782226
RP_POS_171_11302a2_883	RP	POS	2.88	171.1130	fragment of Levetiracetam	126.0915(100), 154.0866(10), 171.1126(2)	2	1.62E-01	0.16	0.73	8.72E-01	-0.04	0.21	3.23E-01	0.14	0.86	3.23E-01	0.18	0.45	16475	26850	4226907	29857357	4712029	33239450	3741785	26377551
RP_NEG_838_59821a13_713	RP	NEG	13.71	838.5982	PC O-38:5|PC O-18:1_20:4 [M+HCOO]-	303.2313(100), 778.5822(32), 492.3481(14), 474.341(6)	2	3.75E-06	-0.97	1.51	8.73E-01	-0.03	0.45	9.50E-06	-0.98	1.59	2.86E-05	-0.95	1.46	8330119	1790423	6455357	1758573	6483591	1859715	6427123	1669762
HILIC_POS_288_21689a0_864	HILIC	POS	0.86	288.2169	AC 08:0 (Octanoylcarnitine)	85.0289(100), 288.217(40), 229.1458(10), 60.0815(8)	2	5.26E-01	-0.10	0.23	8.82E-01	-0.03	0.53	5.52E-01	-0.12	0.21	6.51E-01	-0.09	0.42	30269778	24328954	26588313	38714828	27166255	37577880	26010372	40193103
RP_NEG_301_21786a10_704	RP	NEG	10.70	301.2179	FA 20:5 (Eicosapentaenoic acid)	301.2179(100), 257.228(35), 59.0125(25)	2	2.55E-07	0.70	1.55	8.85E-01	-0.03	0.46	1.17E-04	0.68	1.42	8.10E-05	0.71	1.56	3033004	1632654	5947949	4508959	6013395	4582137	5882502	4480136
RP_POS_128_10689a5_058	RP	POS	5.06	128.1069	N-Cyclohexylformahide	83.0857(100), 128.1064(90), 55.055(45)	2	1.22E-02	-0.38	1.11	8.86E-01	0.03	1.08	5.09E-02	-0.37	1.08	3.65E-02	-0.40	1.16	1131158	263199	957633	495400	950475	502092	964791	493608
RP_NEG_271_22827a9_674	RP	NEG	9.67	271.2283	FA 16:0;O	271.2284(100)	2	3.04E-02	0.40	0.91	8.89E-01	-0.03	0.65	7.75E-02	0.39	0.78	4.24E-02	0.42	1.01	4892522	679177	5215608	828369	5227275	769506	5203940	891053
RP_POS_312_21686a6_182	RP	POS	6.18	312.2169	CAR 10:2	85.0287(100), 312.2154(60)	2	3.99E-01	-0.14	0.63	8.89E-01	0.03	0.66	5.72E-01	-0.12	0.46	3.89E-01	-0.15	0.76	966026	603165	842337	994441	828383	834103	856292	1141001
RP_POS_834_60022a13_433	RP	POS	13.43	834.6002	PC 40:6	184.0732(100), 834.5837(2)	2	5.46E-01	0.13	0.71	8.94E-01	0.03	0.08	5.53E-01	0.15	0.42	6.08E-01	0.12	0.56	3311247	2245781	3579447	1918492	3553717	1785956	3605176	2060424
RP_NEG_436_28381a10_706	RP	NEG	10.71	436.2838	LPE O-16:1	436.2795(100), 78.9574(40), 40.0107(35), 375.2247(7)	2	2.26E-01	0.21	0.74	9.00E-01	0.03	1.05	2.77E-01	0.23	1.02	3.28E-01	0.20	0.68	1888692	568081	2043162	770161	2033457	760557	2052866	787250
RP_POS_265_11829a3_744	RP	POS	3.74	265.1183	Phenylacetylglutamine	130.0502(100), 84.0447(15), 91.0546(14), 136.0754(14), 147.0768(13)	2	6.04E-02	-0.39	0.68	9.16E-01	-0.02	0.26	1.02E-01	-0.40	0.63	7.55E-02	-0.38	0.79	15156074	10009048	11272449	9795410	11376815	7812471	11168083	11523946
HILIC_POS_329_15283a0_665	HILIC	POS	0.67	329.1528	Tiapride	256.0634(100), 329.1509(20)	2	4.92E-01	0.09	0.33	9.17E-01	-0.02	0.81	4.60E-01	0.08	0.35	6.40E-01	0.11	0.41	32998445	12021384	35606228	31273429	35936748	41612805	35275709	15625812
RP_POS_171_11292a3_143	RP	POS	3.14	171.1129	fragment of Levetiracetam	126.0916(100), 154.0867(15), 171.1128(2)	2	1.60E-01	0.16	0.74	9.23E-01	-0.02	0.19	3.22E-01	0.15	0.86	3.25E-01	0.17	0.45	112525	127697	5310251	36748375	5666173	39465870	4954328	34214512
HILIC_NEG_135_03123a1_359	HILIC	NEG	1.36	135.0312	Hypoxanthine	134.8954(100), 92.0248(40),	1	6.84E-12	0.84	1.41	9.29E-01	-0.02	0.63	6.71E-06	0.85	1.39	1.67E-07	0.83	1.93	399889	202553	4344143	5059150	4298956	4520376	4389331	5592350
RP_POS_856_58093a13_71	RP	POS	13.71	856.5809	PC 40:6 [M+Na]+	146.9816(100), 86.0967(75), 673.5201(65), 797.5168(35), 856.577(30), 651.5269(7)	2	2.08E-03	-0.63	1.23	9.34E-01	-0.02	0.68	5.46E-03	-0.64	1.10	4.90E-03	-0.62	1.26	17370979	5516717	13724735	5632727	13772096	5359139	13677375	5947922
RP_NEG_391_28635a9_932	RP	NEG	9.93	391.2864	ST 24:1;O4	391.2819(100), 345.2812(4)	2	7.31E-02	0.28	1.12	9.39E-01	-0.02	0.32	1.24E-01	0.28	0.68	1.56E-01	0.29	1.23	2783687	2643468	3959113	4494025	3993984	4976631	3924242	4004416
HILIC_POS_181_07201a0_589	HILIC	POS	0.59	181.0720	Theobromine	181.0721(100)	1	4.06E-01	-0.16	0.41	9.42E-01	-0.02	0.78	4.80E-01	-0.17	0.25	4.46E-01	-0.15	0.40	1106868	1011130	928487	1161614	936978	924536	919996	1367961
RP_POS_400_3421a9_256	RP	POS	9.26	400.3421	CAR 16:0 (Palmitoylcarnitine)	85.0289(100), 400.3445(60), 341.2653(3)	1	5.15E-11	1.10	1.74	9.42E-01	0.01	0.52	7.54E-09	1.11	1.85	2.41E-08	1.10	1.79	8173107	2510079	12619895	3837374	12591921	3952736	12647869	3758414
RP_POS_279_15955a9_441	RP	POS	9.44	279.1596	Di-n-butyl phthalate	149.0228(100), 57.0705(30)	2	2.42E-01	0.22	0.37	9.46E-01	-0.01	0.79	3.38E-01	0.22	0.56	2.70E-01	0.23	0.44	13701354	827864	13907389	950514	13913898	867211	13900881	1035979
RP_NEG_836_58185a13_511	RP	NEG	13.51	836.5819	PC O-38:6|PC O-18:2_20:4 [M+HCOO]-	303.2352(100), 776.5573(40), 490.333(12), 224.0689(6), 472.514(4)	2	9.67E-02	0.30	1.04	9.52E-01	-0.01	0.32	1.47E-01	0.30	0.77	1.58E-01	0.29	1.19	3286584	846390	3599760	1104045	3596203	1092166	3606494	1126848
HILIC_POS_177_10228a0_539	HILIC	POS	0.54	177.1023	Cotinine	130.0504(100), 72.0816(10)	2	6.12E-06	0.77	1.47	9.52E-01	0.01	0.77	2.17E-04	0.78	1.24	4.24E-05	0.77	1.78	15551735	42281610	62686699	61845171	62312468	54823660	63060931	68715271
HILIC_POS_522_35626a1_248	HILIC	POS	1.25	522.3563	LPC 18:1	184.0744(100), 104.1074(70), 522.3516(25)	2	4.36E-05	0.72	1.34	9.56E-01	0.01	0.74	8.20E-04	0.73	1.23	1.48E-04	0.72	1.47	128351678	57139722	183922757	77856149	183489140	66200812	184356375	88678827
HILIC_POS_286_20114a0_973	HILIC	POS	0.97	286.2011	AC 08:1 (Octenoylcarnitine)	85.0288(100), 286.1991(40), 227.1266(10)	2	9.37E-01	-0.01	0.42	9.60E-01	-0.01	0.32	9.29E-01	-0.02	0.19	9.63E-01	-0.01	0.31	17516222	12770829	17296540	15794118	17375515	13935305	17217565	17600959
RP_POS_160_13316a0_62	RP	POS	0.62	160.1332	NAE 6:0	160.1331(100), 101.0597(30), 132.0647(25), 60.0811(20)	2	4.97E-02	0.33	0.60	9.69E-01	-0.01	0.41	1.10E-01	0.32	0.57	8.93E-02	0.33	0.66	7676440	2388600	8781542	3595630	8795479	3500403	8767606	3723943
RP_POS_209_09201a1_959	RP	POS	1.96	209.0920	Kynurenine	94.066(100), 192.0655(70), 146.0603(50), 136.0753(40), 150.0549(22), 174.0555(21), 209.1368(17), 120.044(16), 74.0241(15)	1	9.00E-03	-0.45	1.32	9.69E-01	-0.01	1.05	4.05E-02	-0.45	1.41	1.47E-02	-0.44	1.09	4261031	927291	3693314	1339991	3698496	1090184	3688132	1561807
RP_POS_209_0919a1_27	RP	POS	1.27	209.0919	Kynurenine	94.0658(100), 192.065(80), 146.0603(50), 136.0754(45), 174.0556(20), 120.044(20)	2	1.17E-02	-0.42	1.31	9.69E-01	0.01	0.98	5.69E-02	-0.42	1.37	1.49E-02	-0.43	1.07	6543839	1394390	5711957	2073637	5703938	1624119	5719976	2459634
RP_POS_260_18573a4_181	RP	POS	4.18	260.1857	CAR 06:0	85.0289(100), 201.111(15), 260.1852(65)	1	1.46E-01	0.19	0.54	9.71E-01	-0.01	0.89	2.97E-01	0.19	0.46	2.44E-01	0.20	0.60	4479197	3117743	5991977	8766753	6024268	8434849	5959685	9172328
RP_POS_639_49524a14_158	RP	POS	14.16	639.4952	DG 36:4 [M+Na]+	639.4892(100)	2	4.71E-05	-0.78	1.41	9.74E-01	0.01	0.13	1.18E-03	-0.78	1.20	3.01E-05	-0.79	1.56	4358980	2523025	2020048	2916362	2010306	1784217	2029790	3741696
RP_NEG_878_59351a13_715	RP	NEG	13.72	878.5935	PC 40:6|PC 18:0_22:6 [M+HCOO]-	283.2655(100), 327.2355(82), 818.5672(42)	2	2.83E-03	-0.64	1.26	9.78E-01	-0.01	0.61	6.93E-03	-0.64	1.11	5.32E-03	-0.63	1.28	12537726	4211780	9888858	3962111	9900055	3726800	9877662	4222289
RP_POS_647_51154a11_755	RP	POS	11.76	647.5115	SM 30:1;2O	184.0732(100), 647.438(3)	2	1.05E-03	-0.68	1.28	9.83E-01	0.00	0.08	2.10E-03	-0.68	1.23	3.42E-03	-0.68	1.11	3008272	1095287	2238521	1078025	2236187	1169611	2240855	989944
HILIC_NEG_178_05095a0_972	HILIC	NEG	0.97	178.0510	Hippuric acid	134.0613(100), 178.0513(35)	2	2.74E-02	-0.48	1.20	9.84E-01	0.00	0.35	4.79E-02	-0.48	0.86	3.74E-02	-0.48	1.28	3228058	3024747	1864608	2702452	1869985	2449670	1859230	2958817
RP_POS_183_08109a8_099	RP	POS	8.10	183.0811	Benzophenone	105.0334(100), 183.0797(30)	2	3.66E-01	0.16	0.52	9.90E-01	0.00	0.43	4.29E-01	0.16	0.39	4.53E-01	0.16	0.44	953261	335737	1021796	462784	1021219	480373	1022373	449388
RP_POS_372_31073a8_758	RP	POS	8.76	372.3107	CAR 14:0 (Myristoylcarnitine)	85.0289(100), 372.3084(55)	1	8.20E-07	0.80	1.42	9.96E-01	0.00	1.23	1.79E-05	0.80	1.49	7.04E-05	0.80	1.39	2668655	1220323	4236890	2018220	4235953	2155767	4237827	1892674
RP_POS_454_29248a10_516	RP	POS	10.52	454.2925	LPE 16:0	313.2715(100), 454.2939(3), 62.0608(22)	2	3.06E-01	0.17	1.01	1.00E+00	0.00	0.64	4.12E-01	0.17	0.79	3.67E-01	0.17	0.73	13923437	2981231	14631808	4424308	14631687	4072751	14631929	4791783
HILIC_NEG_185_96243a0_927	HILIC	NEG	0.927	185.9624				2.51E-02	-0.46	0.90	7.75E-08	-0.99	2.78	4.05E-05	-0.96	1.73	8.91E-01	0.03	0.25	9259307	2722957	7988111	2679166	9338422	2196344	6637801	2440764
RP_POS_815_54254a12_719	RP	POS	12.72	815.5425				3.20E-01	-0.19	0.90	2.23E-07	-1.01	2.89	9.39E-04	-0.69	1.39	1.33E-01	0.31	0.89	1262636	347916	1189013	401195	1384856	366288	993169	335794

Supplementary table 1: Metabolomics results (in asceding order according to p-value from progressive ALD vs non-progressive ALD comparison, with molecular features with ID_level of 1-2 first)

								all_ALD_vs_control			Prog_ALD_vs_non-prog_ALD			Prog_ALD_vs_control_ALD			Non-prog_ALD_vs_control			Healthy_control		all_ALD		Non-prog_ALD		Progressive_ALD	
								t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA								
Feature_ID	RP_HILIC	POS_NEG	Average.Rt	Average.Mz	Metabolite.name	curated_MSMS	ID_level	p	d	VIP	p	d	VIP	p	d	VIP	p	d	VIP	Mean	SD	Mean	SD	Mean	SD	Mean	SD
RP_NEG_516_29498a9_311	RP	NEG	9.31	516.2950	adduct of glycochenodeoxycholic acid	448.3027(100), 516.295(30), 74.0234(30)		1.26E-05	0.57	1.01	6.56E-07	1.08	2.91	4.78E-07	1.11	1.58	6.60E-01	0.03	0.55	1023753	1184072	2948146	3683681	1136232	1026734	4760059	4434152
RP_NEG_241_08723a7_928	RP	NEG	7.93	241.0872	Unknown	59.0125(100), 167.0854(70), 220.9839(45), 241.0872(40)	4	1.16E-02	0.51	1.34	1.33E-06	0.92	2.77	6.98E-05	0.97	1.46	7.84E-01	0.05	1.01	2687704	7194284	6535019	7391871	3073661	4088760	9996378	8320194
RP_POS_792_55078a13_116	RP	POS	13.12	792.5508				3.86E-17	1.18	2.03	2.61E-06	0.88	2.71	8.34E-14	1.62	2.30	1.62E-10	0.74	2.06	3832488	454985	5165148	1090586	4665638	557138	5664658	1258341
HILIC_NEG_167_00179a0_923	HILIC	NEG	0.923	167.0018				1.02E-03	-0.62	1.18	2.62E-06	-0.90	2.41	4.84E-07	-1.07	1.93	3.99E-01	-0.17	0.41	313210	84045	251396	100168	296276	94141	206516	85434
RP_POS_506_2402a9_303	RP	POS	9.30	506.2402				2.19E-05	0.54	0.98	2.91E-06	1.03	2.77	2.13E-06	1.06	1.47	6.73E-01	0.03	0.53	293007	349076	911661	1261071	325235	313182	1498088	1553430
HILIC_NEG_205_02945a0_927	HILIC	NEG	0.927	205.0295				1.50E-03	-0.64	1.20	3.43E-06	-0.87	2.39	2.57E-06	-1.07	1.80	3.17E-01	-0.21	0.43	264104	63272	220607	66527	250092	58383	191121	61312
HILIC_POS_130_04999a6_374	HILIC	POS	6.374	130.0500				8.26E-11	0.82	1.37	3.58E-06	0.97	2.49	3.69E-09	1.31	1.80	2.13E-05	0.33	1.38	401113	164754	940433	701025	620370	274350	1260497	841767
HILIC_NEG_109_01061a0_921	HILIC	NEG	0.921	109.0106				3.24E-03	-0.65	1.26	3.80E-06	-0.82	2.38	1.13E-05	-1.06	1.86	2.93E-01	-0.24	0.62	298106	105924	233259	92928	274292	87716	192226	79481
RP_POS_508_23563a9_303	RP	POS	9.30	508.2356				1.22E-05	0.56	1.00	4.64E-06	1.01	2.72	2.02E-06	1.06	1.48	3.90E-01	0.06	0.58	89891	125455	315955	444483	113332	110013	518577	550702
RP_POS_810_09253a13_873	RP	POS	13.87	810.0925				8.85E-05	0.63	1.13	4.84E-06	0.92	2.65	1.31E-07	1.09	1.70	2.78E-01	0.18	0.66	2396410	752065	3141164	1229377	2601917	942420	3680411	1253788
HILIC_NEG_127_00108a0_926	HILIC	NEG	0.926	127.0011				5.11E-03	-0.58	1.17	5.15E-06	-0.85	2.37	1.42E-05	-1.00	1.75	4.72E-01	-0.15	0.37	494093	119592	423088	119614	475228	107881	370947	108261
RP_POS_535_258a9_302	RP	POS	9.30	535.2580				3.40E-05	0.53	0.96	5.56E-06	1.00	2.70	4.22E-06	1.03	1.44	6.77E-01	0.03	0.51	166959	215276	543132	788501	186280	185088	899984	980823
RP_POS_503_23114a9_301	RP	POS	9.30	503.2311				2.59E-05	0.53	0.98	6.36E-06	1.00	2.69	4.15E-06	1.03	1.44	5.90E-01	0.03	0.50	105160	130333	346583	502511	120489	115974	572676	626431
RP_POS_148_06046a0_543	RP	POS	0.54	148.0605				1.12E-10	0.80	1.25	7.33E-06	0.95	2.98	1.18E-08	1.28	1.73	1.78E-06	0.33	1.48	442788	274402	1503924	1418589	873715	480492	2134134	1739094
RP_POS_743_54504a12_973	RP	POS	12.97	743.5450				8.51E-14	0.92	1.90	7.35E-06	0.92	2.60	1.26E-10	1.38	2.11	2.42E-06	0.46	1.48	231434	157109	1395079	1329183	814825	759671	1975333	1518315
RP_POS_748_54736a12_19	RP	POS	12.19	748.5474				2.58E-14	0.94	1.69	9.68E-06	0.91	2.59	2.81E-10	1.40	1.98	7.78E-09	0.48	1.73	164728	86144	1101743	1047318	646412	486456	1557074	1247549
RP_NEG_532_29065a8_82	RP	NEG	8.82	532.2907				7.89E-05	0.49	0.94	1.01E-05	0.98	2.64	1.16E-05	0.99	1.38	9.53E-01	0.00	0.29	261277	381513	957120	1565533	265863	271446	1648378	1975588
HILIC_NEG_132_92355a0_926	HILIC	NEG	0.926	132.9236				4.05E-05	-0.83	1.48	1.02E-05	-0.80	2.25	5.19E-08	-1.23	2.04	3.98E-02	-0.42	0.82	1452156	334333	1144807	353426	1294417	328563	995197	314221
RP_NEG_146_04506a0_542	RP	NEG	0.54	146.0451				1.37E-10	0.81	1.25	1.05E-05	0.93	2.95	1.26E-08	1.28	1.73	3.92E-06	0.34	1.47	448241	310244	1464168	1341837	878493	475526	2049843	1646708
RP_POS_519_22754a8_815	RP	POS	8.82	519.2275				4.63E-04	0.43	0.88	1.87E-05	0.96	2.58	4.79E-05	0.92	1.30	3.69E-01	-0.05	0.55	183958	241713	594741	1058797	140628	150552	1048855	1349614
RP_POS_522_23578a8_815	RP	POS	8.82	522.2358				3.44E-04	0.44	0.89	2.06E-05	0.96	2.57	4.31E-05	0.92	1.30	4.75E-01	-0.04	0.36	138029	163785	436771	757500	113727	122651	759814	965043
RP_POS_393_73969a12_975	RP	POS	12.98	393.7397	Unknown	86.0969(95), 309.1511(90), 327.1637(75), 393.2073(70), 163.0143(20)	4	2.47E-24	1.37	2.21	2.28E-05	0.75	2.46	4.73E-17	1.75	2.48	1.44E-14	1.00	2.25	1267184	719372	4244481	1976616	3431543	1346413	5057419	2175366
HILIC_NEG_355_15808a0_927	HILIC	NEG	0.927	355.1581				1.47E-07	-1.11	1.85	2.38E-05	-0.71	2.18	2.48E-10	-1.46	2.39	3.83E-04	-0.75	1.37	313057	100781	189232	97980	229140	95683	149325	83611
HILIC_NEG_84_00858a0_926	HILIC	NEG	0.926	84.0086				7.09E-05	-0.81	1.46	2.46E-05	-0.77	2.18	1.34E-07	-1.20	2.10	4.36E-02	-0.43	0.87	351236	72327	287548	74254	317737	71216	257359	64871
RP_POS_472_30325a9_303	RP	POS	9.30	472.3033	Glycodeoxycholic acid [M+Na]+	472.3047(100), 98.0215(1)		7.20E-05	0.49	0.94	2.47E-05	0.94	2.56	2.06E-05	0.96	1.35	7.39E-01	0.02	0.55	3039859	3923409	11472633	19295939	3325857	3513354	19619408	24586024
RP_POS_405_74146a12_647	RP	POS	12.65	405.7415	Unknown	335.1653(95), 86.0969(60), 212.1168(65), 406.2035(35)		4.05E-04	0.65	1.16	2.76E-05	0.82	2.43	2.68E-06	1.06	1.64	1.70E-01	0.24	1.04	1588618	644500	2108058	799301	1783163	578446	2432953	860687
RP_NEG_613_36023a8_937	RP	NEG	8.94	613.3602	Unknown	613.3566(100), 75.0076(7)		5.14E-09	0.72	1.26	2.76E-05	0.91	2.45	2.06E-07	1.17	1.69	1.00E-05	0.26	1.53	684912	303750	1839248	1746302	1109717	511122	2568780	2194077
HILIC_NEG_255_08762a0_613	HILIC	NEG	0.613	255.0876				3.93E-05	-1.13	2.19	3.21E-05	-0.55	2.20	1.21E-06	-1.41	2.27	1.59E-03	-0.86	1.64	256694	191502	91704	99880	131940	105780	51469	75247
HILIC_NEG_383_19a0_927	HILIC	NEG	0.927	383.1900				8.33E-08	-1.10	1.82	3.47E-05	-0.71	2.14	1.70E-10	-1.45	2.33	2.91E-04	-0.74	1.38	204496	62766	124853	64888	150777	60573	98929	58875
HILIC_NEG_94_99465a0_926	HILIC	NEG	0.926	94.9947				1.38E-02	-0.52	1.05	3.56E-05	-0.77	2.18	9.54E-05	-0.90	1.58	5.58E-01	-0.13	0.26	849094	217120	737505	209539	821116	198591	653893	187093
HILIC_NEG_61_98754a0_925	HILIC	NEG	0.925	61.9875				1.63E-03	-0.65	1.22	3.61E-05	-0.77	2.14	7.63E-06	-1.03	1.77	2.14E-01	-0.26	0.57	3812079	1338937	2907530	1344058	3443372	1228029	2371689	1247326
RP_POS_787_60437a13_874	RP	POS	13.87	787.6044				1.17E-06	0.72	1.26	3.75E-05	0.85	2.41	1.88E-07	1.15	1.68	1.92E-02	0.29	1.07	21837007	8202893	33231848	16708783	26468603	9039657	39995093	19723061
HILIC_NEG_141_01675a0_926	HILIC	NEG	0.926	141.0168				5.88E-04	-0.73	1.32	3.91E-05	-0.75	2.14	2.65E-06	-1.10	1.87	1.04E-01	-0.35	0.74	258484	67263	208930	64041	234362	60245	183499	57766
HILIC_NEG_159_00731a0_927	HILIC	NEG	0.927	159.0073				3.46E-03	-0.58	1.17	4.24E-05	-0.78	2.19	1.31E-05	-0.97	1.71	3.67E-01	-0.19	0.48	639113	134674	554021	144871	611305	136067	496738	131120
RP_POS_755_53815a12_975	RP	POS	12.98	755.5382				2.88E-24	1.34	2.17	4.53E-05	0.73	2.39	3.11E-16	1.71	2.43	2.41E-14	0.98	2.21	5023013	2407678	15767393	7392969	12830614	5033708	18704173	8215098
HILIC_POS_214_05875a6_377	HILIC	POS	6.377	214.0588				6.51E-11	0.88	1.35	4.57E-05	0.83	2.18	1.36E-09	1.29	1.85	9.20E-05	0.46	1.26	367415	172177	780439	493218	583793	302456	977085	566653
HILIC_NEG_145_05052a0_926	HILIC	NEG	0.926	145.0505				1.36E-02	-0.47	0.97	4.83E-05	-0.79	2.17	5.06E-05	-0.87	1.61	7.13E-01	-0.08	0.41	196559	55365	166919	63217	191752	60877	142085	55764
HILIC_NEG_158_95026a0_926	HILIC	NEG	0.926	158.9503				2.16E-02	-0.48	0.90	4.92E-05	-0.76	2.21	2.49E-04	-0.86	1.48	6.48E-01	-0.10	0.36	2162393	1116689	1629263	1079519	2052934	950857	1205593	1041181
RP_POS_467_34717a9_304	RP	POS	9.30	467.3472				8.56E-05	0.48	0.92	4.94E-05	0.91	2.48	3.54E-05	0.94	1.31	5.77E-01	0.03	0.54	182339	268499	775993	1379751	214477	227719	1337510	1775092
HILIC_NEG_223_01962a0_927	HILIC	NEG	0.927	223.0196				5.20E-02	-0.38	0.98	5.44E-05	-0.79	2.14	3.81E-04	-0.78	1.38	9.58E-01	0.01	0.21	647979	136157	591909	147839	649623	142516	534196	130576
HILIC_NEG_117_01929a0_926	HILIC	NEG	0.926	117.0193				2.48E-01	-0.23	0.64	5.53E-05	-0.80	2.24	4.93E-03	-0.62	1.17	4.07E-01	0.17	0.38	247414	87927	226010	97091	263879	85936	188141	93456
HILIC_POS_64_01659a0_936	HILIC	POS	0.936	64.0166				4.39E-03	-0.57	1.15	5.58E-05	-0.77	2.13	2.21E-05	-0.96	1.65	3.76E-01	-0.19	0.39	3177636	698188	2750524	736751	3037672	686939	2463377	675666
HILIC_POS_102_06667a0_938	HILIC	POS	0.938	102.0667				1.50E-02	-0.50	0.98	5.82E-05	-0.76	2.18	1.51E-04	-0.88	1.50	5.72E-01	-0.12	0.29	3065697	1045798	2531749	1042261	2937144	921817	2126353	1004810
RP_NEG_564_22815a8_82	RP	NEG	8.82	564.2282				5.03E-04	0.43	0.98	6.02E-05	0.90	2.47	8.67E-05	0.88	1.29	7.82E-01	-0.02	1.09	219164	247914	626997	1053873	203800	239292	1050193	1349519
RP_NEG_844_53448a12_981	RP	NEG	12.98	844.5345	Unknown	112.9846(100)	4	1.05E-25	1.42	2.28	6.23E-05	0.69	2.35	5.61E-18	1.77	2.54	2.24E-15	1.08	2.29	747812	410539	2467535	1073008	2049459	777563	2885612	1168278
RP_NEG_255_08781a5_615	RP	NEG	5.62	255.0878	Unknown	211.0959(100), 255.0858(15)	4	5.45E-06	-1.16	2.14	6.27E-05	-0.58	2.29	8.89E-08	-1.45	2.26	5.49E-04	-0.87	1.63	3717300	2357448	1389079	1506265	1973704	1552018	804454	1215603
RP_POS_430_29501a8_815	RP	POS	8.82	430.2950				2.08E-04	0.45	0.92	6.52E-05	0.90	2.45	7.14E-05	0.90	1.28	9.81E-01	0.00	0.27	235779	341379	1041980	2015119	234118	267148	1849842	2607872
RP_POS_626_35291a8_932	RP	POS	8.93	626.3529				5.44E-05	0.57	1.05	6.54E-05	0.86	2.69	8.10E-06	1.00	1.54	1.84E-01	0.14	0.69	208361	263063	530472	612873	287983	260459	772961	755679
RP_NEG_448_30566a8_816	RP	POS	8.82	448.3057				1.91E-04	0.45	0.92	6.63E-05	0.90	2.44	6.84E-05	0.90	1.28	9.50E-01	0.00	0.32	453378	671473	2040002	3939699	462339	549753	3617664	5096799
HILIC_POS_61_04051a0_938	HILIC	POS	0.938	61.0405				1.85E-02	-0.48	0.96	6.65E-05	-0.76	2.17	1.85E-04	-0.86	1.46	6.35E-01	-0.10	0.25	48360374	16964561	39957372	17176130	46588760	15428018	33325983	16379573
HILIC_POS_105_04271a0_936	HILIC	POS	0.936	105.0427				5.27E-03	-0.57	1.13	6.88E-05	-0.75	2.11	3.10E-05	-0.95	1.63	3.64E-01	-0.20	0.36	943328	207092	820709	208396	901021	199961	740396	186001
HILIC_NEG_241_01036a0_928	HILIC	NEG	0.928	241.0104				1.34E-01	-0.31	0.93	6.96E-05	-0.76	2.11	2.48E-03	-0.69	1.21	7.70E-01	0.07	0.16	1162314	236917	1089660	228286	1177590	219549	1001730	203253
HILIC_NEG_255_02582a0_928	HILIC	NEG	0.928	255.0258				2.95E-02	-0.42	1.00	7.42E-05	-0.78	2.08	1.77E-04	-0.81	1.49	8.77E-01	-0.03	0.23	447394	92356	404226	103693	444026	100222	364426	91907
RP_POS_834_59906a13_327	RP	POS	13.33	834.5991				1.54E-02	0.41	0.83	7.59E-05	0.82	2.42	2.37E-04	0.82	1.33	9.69E-01	0.01	0.31	4447135	1688604	5400352	2425313	4461753	1571902	6338951	2759631
RP_POS_239_09129a5_617	RP	POS	5.62	239.0913	Unknown	193.0846(100), 179.0706(95), 239.0901(65)	4	6.94E-06	-1.15	2.11	7.91E-05	-0.57	2.27	1.33E-07	-1.44	2.22	5.81E-04	-0.87	1.61	5286117	3341434	2036617	2096400	2839424	2133182	1233809	1736004
RP_NEG_180_10265a7_559	RP	NEG	7.56	180.1027	Unknown	180.1009(100), 92.9186(55), 136.9082(25)	4	4.13E-02	-0.41	1.12	8.07E-05	-0.76	2.35	6.36E-04	-0.79	1.72	8.72E-01	-0.03	0.42	842149	386189	677054	396573	828665	336401	525443	397083
RP_POS_776_57916a12_716	RP	POS	12.72	776.5792				7.71E-14	1.00	1.63	8.25E-05	0.79	2.31	6.20E-11	1.39	2.00	4.70E-07	0.61	1.62	981672	306115	1852670	887386	1510594	562867	2194746	1017522
RP_POS_832_58417a12_925	RP	POS	12.93	832.5842				1.51E-01	0.29	0.73	8.46E-05	-0.76	2.26	6.84E-01	-0.09	0.49	3.05E-03	0.67	1.23	2526547	917362	2799285	933725	3154964	875532	2443606	858338
RP_POS_377_76468a12_972	RP	POS	12.97	377.7647				1.35E-17	1.12	1.94	9.53E-05	0.76	2.27	7.59E-13	1.49	2.24	7.51E-09	0.74	1.82	121994	149629	685905	503328	494228	355322	877582	557329
RP_POS_828_54968a12_737	RP	POS	12.74	828.5497				2.01E-06	-1.02	1.66	9.69E-05	-0.67	2.25	5.55E-09	-1.35	2.25	2.09E-03	-0.68	1.21	18742550	5726388	12571720	5414190	14622435	5599100	10521005	4392346
RP_NEG_528_26459a8_664	RP	NEG	8.66	528.2646				9.06E-06	0.53	1.01	9.90E-05	0.88	2.31	2.41E-05	0.96	1.35	2.44E-06	0.09	1.68	327506	309342	4978169	9922496	1095360	973626	8860978	12930794
RP_NEG_776_54681a12_974	RP	NEG	12.97	776.5468	Unknown	253.2186(100), 716.5328(20), 281.2506(18), 227.2003(7), 224.0687(3)	4	1.63E-24	1.37	2.21	1.07E-04	0.69	2.27	7.17E-17	1.72	2.47	3.16E-14	1.03	2.20	8943970	4249507	26763794	11807275	22302798	8620947	31224791	12912577
RP_NEG_874_56213a12_637	RP	NEG	12.64	874.5621				5.91E-06	-0.92	1.67	1.13E-04	-0.70	2.24	1.06E-08	-1.27	2.16	7.83E-03	-0.57	1.12	2687971	682241	1985533	708348	2251524	736898	1719542	571267
RP_POS_412_28439a8_816	RP	POS	8.82	412.2844				3.03E-04	0.44	0.91	1.13E-04	0.87	2.38	1.22E-04	0.87	1.26	9.95E-01	0.00	0.38	99305	134181	420868	829435	99121	101273	742615	1080944
RP_NEG_254_62338a10_423	RP	NEG	10.42	254.6234				3.70E-05	0.61	1.06	1.33E-04	0.81	2.22	4.66E-06	1.02	1.49	9.27E-02	0.21	0.80	249755	221211	504285	443159	337199	234578	671370	533654
RP_POS_718_53705a12_652	RP	POS	12.65	718.5371				1.26E-04	0.72	1.21	1.38E-04	0.74	2.21	1.74E-06	1.09	1.67	5.60E-02	0.35	0.75	548603	478139	967574	579158	752191	434670	1182957	627760
RP_POS_846_52197a12_648	RP	POS	12.65	846.5220				9.49E-04	0.62	1.18	1.49E-04	0.75	2.20	2.01E-05	0.99	1.51	1.68E-01	0.24	0.79	1191758	466556	1538544	564457	1328789	376855	1748298	641807
HILIC_NEG_191_01344a0_927	HILIC	NEG	0.927	191.0134				1.01E-02	-0.52	1.11	1.61E-04	-0.72	2.01	8.57E-05	-0.88	1.53	4.68E-01	-0.16	0.30	572474	123346	504997	128295	552052	123712	457942	115896
RP_POS_414_29956a9_303	RP	POS	9.30	414.2996	fragment of glycochenodeoxycholic acid	414.2977(100), 76.0397(50), 339.2651(35), 201.1645(30)		2.69E-04	0.44	0.90	1.63E-04	0.85	2.35	1.41E-04	0.87	1.23	7.40E-01	0.01	0.54	2485881	3215531	10568920	20719997	2717953	2837691	18419887	27084210
RP_POS_279_08383a5_618	RP	POS	5.62	279.0838				1.41E-05	-1.13	2.07	1.82E-04	-0.54	2.16	4.01E-07	-1.40	2.14	7.60E-04	-0.87	1.60	1026156	691983	383394	417597	535534	419581	231254	359233
HILIC_NEG_115_92058a0_924	HILIC	NEG	0.924	115.9206				4.48E-05	-0.85	1.54	1.90E-04	-0.68	1.96	2.31E-07	-1.19	1.99	1.80E-02	-0.51	0.92	57826180	11206515	47703324	11125467	51743341	10862038	43663308	9939041
RP_NEG_548_23315a9_311	RP	NEG	9.31	548.2332	adduct of glycochenodeoxycholic acid	548.2355(100), 115.9192(40)		2.93E-04	0.44	0.90	1.94E-04	0.84	2.32	1.62E-04	0.86	1.21	6.84E-01	0.02	0.55	512585	661267	2109091	4108122	569937	547386	3648246	5381769
RP_NEG_528_26501a11_393	RP	NEG	11.39	528.2650	Glycine conjugated sterol	448.3024(100), 528.269(75), 74.0234(25)	3	2.19E-04	0.44	1.03	2.17E-04	0.84	2.21	1.66E-04	0.86	1.25	4.50E-01	0.02	0.75	50156	69295	332054	725718	62060	69064	602048	954224
HILIC_POS_198_08466a6_377	HILIC	POS	6.377	198.0847				2.10E-10	0.87	1.31	2.22E-04	0.76	2.01	3.25E-09	1.25	1.81	1.24E-04	0.49	1.25	1234923	489420	2302965	1279859	1839407	864099	2766523	1457496
RP_POS_483_34271a8_815	RP	POS	8.82	483.3427				1.26E-04	0.46	0.97	2.23E-04	0.83	2.31	1.12E-04	0.88	1.26	2.63E-01	0.05	0.80	99316	153654	510887	999704	140189	169477	881586	1307688
RP_NEG_385_16937a6_699	RP	NEG	6.70	385.1694				4.49E-07	0.62	1.10	2.28E-04	0.81	2.17	6.42E-06	1.02	1.49	3.66E-04	0.21	1.14	1444696	1270914	5805050	7823798	2920126	2306315	8689973	10068192
RP_POS_809_58661a13_886	RP	POS	13.89	809.5866				2.99E-07	0.75	1.37	2.31E-04	0.77	2.18	3.76E-07	1.13	1.70	2.84E-03	0.36	1.30	9589129	3210521	14441415	6856301	11944424	3596252	16938407	8325841
HILIC_POS_171_18552a6_378	HILIC	POS	6.378	171.1855				4.43E-03	0.62	0.93	2.31E-04	0.67	1.97	1.30E-04	0.96	1.45	1.81E-01	0.29	0.56	6074760	1578314	7007302	1399381	6503534	1052875	7511071	1526444
RP_POS_435_1987a9_274	RP	POS	9.27	435.1987				6.83E-02	0.35	0.68	2.35E-04	0.74	2.14	3.11E-03	0.72	1.10	9.13E-01	-0.02	0.19	348381	254333	447476	287412	342927	151439	552026	348792
HILIC_NEG_528_26385a2_819	HILIC	NEG	2.819	528.2639				2.10E-04	0.46	1.06	2.36E-04	0.82	2.03	1.06E-04	0.88	1.19	4.15E-01	0.05	0.41	60552	146026	307985	594446	89185	166443	526786	767163
RP_NEG_800_54694a12_651	RP	NEG	12.65	800.5469				3.48E-03	0.54	1.11	2.44E-04	0.73	2.15	9.96E-05	0.91	1.40	3.18E-01	0.18	0.68	11624528	3751941	14074309	4598473	12416658	2985719	15731961	5310477
HILIC_POS_466_31595a2_257	HILIC	POS	2.257	466.3160				2.42E-03	0.41	0.93	2.47E-04	0.81	2.06	2.89E-04	0.82	1.12	9.45E-01	0.01	0.07	182307	409213	587528	1090851	188648	392400	986408	1387630
RP_NEG_530_3028a10_376	RP	NEG	10.38	530.3028	Unknown	255.2334(100), 480.3058(20)		3.99E-01	0.17	1.04	2.51E-04	-0.71	2.18	4.30E-01	-0.18	0.71	1.53E-02	0.53	1.22	3064658	488288	3148915	485155	3322258	397595	2975572	506114

Supplementary table 1: Metabolomics results (in asceding order according to p-value from progressive ALD vs non-progressive ALD comparison, with molecular features with ID_level of 1-2 first)

								all_ALD_vs_control			Prog_ALD_vs_non-prog_ALD			Prog_ALD_vs_control_ALD			Non-prog_ALD_vs_control			Healthy_control		all_ALD		Non-prog_ALD		Progressive_ALD	
								t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA								
Feature_ID	RP_HILIC	POS_NEG	Average.Rt	Average.Mz	Metabolite.name	curated_MSMS	ID_level	p	d	VIP	p	d	VIP	p	d	VIP	p	d	VIP	Mean	SD	Mean	SD	Mean	SD	Mean	SD
RP_POS_182_11761a7_562	RP	POS	7.56	182.1176	Unknown	90.9482(100), 104.964(45), 107.9506(40), 102.9475(35), 71.93(28), 72.9374(26)		4.73E-02	-0.40	1.09	2.63E-04	-0.71	2.18	1.30E-03	-0.76	1.63	8.21E-01	-0.05	0.42	1445426	654003	1173807	673508	1413744	549200	933871	705247
HILIC_NEG_85_0038a0_926	HILIC	NEG	0.926	85.0038				6.69E-02	-0.39	0.83	2.66E-04	-0.69	1.91	1.36E-03	-0.74	1.28	8.53E-01	-0.04	0.08	14414556	3461971	13116626	3248509	14271632	3295951	11961620	2781217
HILIC_NEG_464_30185a2_143	HILIC	NEG	2.143	464.3019				1.82E-03	0.42	0.93	2.73E-04	0.80	2.05	2.36E-04	0.82	1.14	8.45E-01	0.02	0.14	108827	228407	345527	623963	119353	249549	571702	787359
HILIC_NEG_298_03687a0_725	HILIC	NEG	0.725	298.0369				1.80E-10	0.78	1.45	2.80E-04	0.77	2.07	4.65E-08	1.17	1.69	1.41E-04	0.39	1.23	35479	57383	385613	486036	211647	295734	559580	572766
RP_POS_562_29688a10_264	RP	POS	10.26	562.2969				2.76E-05	0.68	1.45	2.88E-04	0.74	2.26	1.95E-06	1.05	1.84	4.02E-02	0.31	1.22	297990	187058	496985	304157	388553	197665	605417	351915
RP_NEG_608_31805a10_376	RP	NEG	10.38	608.3181	Unknown	112.9847(100)		7.49E-01	0.06	0.96	3.06E-04	-0.72	2.14	1.99E-01	-0.29	0.76	4.65E-02	0.42	1.05	9504143	1152015	9580218	1211955	10007566	996033	9152870	1266040
RP_POS_738_53973a13_289	RP	POS	13.29	738.5397				1.17E-07	0.78	1.37	3.07E-04	0.74	2.09	1.45E-07	1.15	1.78	1.66E-03	0.41	1.08	141482	203069	454568	419477	305222	247911	603915	498531
RP_POS_822_52136a12_982	RP	POS	12.98	822.5214				2.21E-21	1.24	2.02	3.15E-04	0.68	2.13	5.21E-15	1.58	2.39	1.80E-10	0.90	1.88	683150	431863	2563282	1455401	2050835	1169285	3075729	1541578
RP_NEG_199_80447a0_564	RP	NEG	0.56	199.8045				4.18E-06	-0.81	1.27	3.29E-04	-0.70	2.32	4.82E-08	-1.16	1.84	1.02E-02	-0.46	0.94	53195314	7249007	45122695	9889787	48589585	8524547	41655804	10020713
RP_NEG_627_37616a9_253	RP	NEG	9.25	627.3762	Unknown	627.3838(100)		5.45E-10	0.75	1.25	3.47E-04	0.78	2.11	6.91E-07	1.14	1.58	1.44E-12	0.36	2.09	407494	250478	3197672	4040634	1748149	1008643	4647196	5261301
HILIC_NEG_172_99106a0_723	HILIC	NEG	0.723	172.9911				3.55E-10	0.76	1.44	3.58E-04	0.76	2.06	5.78E-08	1.15	1.69	3.52E-04	0.38	1.15	14217	14587	109301	134925	61888	86367	156714	157269
RP_POS_1002_66528a10_502	RP	POS	10.50	1002.6653				5.50E-01	-0.12	0.93	3.61E-04	-0.71	2.10	3.44E-02	-0.47	0.97	2.73E-01	0.24	0.80	2123731	415395	2072071	443630	2226477	403725	1917665	431256
RP_POS_220_9955a3_001	RP	POS	3.00	220.9955				6.61E-11	0.80	1.43	3.67E-04	0.76	2.09	3.01E-08	1.18	1.74	7.79E-05	0.42	1.19	161212	104970	800833	862231	498168	541997	1103497	1010617
HILIC_NEG_300_03079a0_724	HILIC	NEG	0.724	300.0308				3.40E-10	0.77	1.44	3.69E-04	0.76	2.04	7.93E-08	1.15	1.66	1.68E-04	0.39	1.21	810269	1252405	8228931	10487691	4545116	6348068	11912745	12419147
RP_POS_778_53461a12_651	RP	POS	12.65	778.5346				9.94E-04	0.57	1.14	3.82E-04	0.72	2.07	3.90E-05	0.93	1.45	1.98E-01	0.21	0.85	12954055	4683357	16574971	6545505	14286434	4256438	18863507	7599723
RP_POS_222_01918a3_001	RP	POS	3.00	222.0192	Unknown	90.948(100), 222.1122(70), 171.9812(70), 105.9347(65) 55.935(65), 189.9921(60), 72.938(55), 149.9609(50)		1.08E-11	0.85	1.49	3.85E-04	0.75	2.08	1.22E-08	1.22	1.78	1.13E-05	0.48	1.34	402132	224170	1325081	1159257	919259	713248	1730903	1367608
RP_NEG_480_30746a10_376	RP	NEG	10.38	480.3075				2.63E-01	0.23	1.00	3.95E-04	-0.69	2.12	5.97E-01	-0.12	0.66	1.05E-02	0.57	1.16	1764882	392126	1855143	396324	1992236	361203	1718050	385392
HILIC_POS_352_24622a0_936	HILIC	POS	0.936	352.2462				9.80E-04	-0.66	1.23	4.09E-04	-0.67	1.88	7.23E-06	-1.00	1.67	1.30E-01	-0.33	0.64	608585	127853	516889	134904	563452	133922	470325	120040
HILIC_NEG_183_9826a0_725	HILIC	NEG	0.725	183.9826				1.03E-10	0.79	1.47	4.18E-04	0.75	2.03	4.24E-08	1.17	1.70	7.25E-05	0.42	1.28	18455	23648	136307	159765	80708	98594	191905	188525
RP_POS_218_99495a3	RP	POS	3.00	218.9950	Unknown	219.1728(100), 190.9995(80), 129.0543(60), 111.0443(55), 101.0599(50)		1.44E-11	0.83	1.46	4.20E-04	0.75	2.07	1.67E-08	1.20	1.77	2.11E-05	0.46	1.29	296811	188519	1414904	1443415	913041	907290	1916768	1694763
RP_NEG_241_92035a2_997	RP	NEG	3.00	241.9204	Unknown	157.862(95), 125.8727(50)	4	1.94E-13	0.96	1.61	4.32E-04	0.72	2.05	4.66E-10	1.31	1.92	1.28E-06	0.60	1.50	862039	853625	3578876	2944397	2559721	2003509	4598031	3373733
RP_POS_506_24136a9_451	RP	POS	9.45	506.2414				3.91E-05	0.50	1.02	4.34E-04	0.79	2.08	7.74E-05	0.89	1.37	6.16E-02	0.11	0.87	134835	128793	468470	745833	205505	208739	731435	969119
HILIC_NEG_216_98085a0_724	HILIC	NEG	0.724	216.9809				3.73E-10	0.77	1.45	4.34E-04	0.75	2.03	9.74E-08	1.14	1.65	1.30E-04	0.39	1.24	377041	332270	2143037	2494638	1276469	1490697	3009605	2969636
RP_NEG_448_30771a8_331	RP	NEG	8.33	448.3077				1.22E-06	0.59	0.98	4.41E-04	0.78	2.06	1.03E-05	0.97	1.35	9.52E-03	0.20	1.00	799056	708084	3608792	5323080	1747080	2343609	5470503	6684513
HILIC_NEG_98_93896a0_927	HILIC	NEG	0.927	98.9390				9.23E-05	-0.78	1.46	4.56E-04	-0.66	1.88	6.44E-07	-1.11	1.87	3.18E-02	-0.45	0.87	2122456	397045	1776453	425420	1922112	413851	1630793	388697
RP_POS_798_56085a12_715	RP	POS	12.72	798.5609				5.67E-16	1.10	1.76	4.92E-04	0.68	2.05	6.31E-12	1.44	2.08	1.04E-08	0.76	1.82	270448	147515	711669	397443	575555	281504	847782	449546
HILIC_NEG_115_00371a0_927	HILIC	NEG	0.927	115.0037				9.18E-01	-0.02	0.61	4.96E-04	-0.70	2.01	9.21E-02	-0.37	0.65	1.08E-01	0.33	0.64	247127	65172	245713	74718	271159	64904	220267	75800
HILIC_NEG_100_93339a0_928	HILIC	NEG	0.928	100.9334				3.53E-04	-0.72	1.38	4.97E-04	-0.66	1.88	3.21E-06	-1.05	1.75	6.63E-02	-0.39	0.73	45556039	8563219	38837189	9044061	41914842	8695947	35759536	8385069
HILIC_NEG_383_15366a0_603	HILIC	NEG	0.603	383.1537				5.95E-03	0.42	0.92	5.01E-04	0.75	1.86	4.33E-04	0.79	1.34	7.46E-01	0.04	0.18	77734	62543	123369	119009	82277	60618	164461	146610
RP_POS_275_63443a10_375	RP	POS	10.38	275.6344				3.60E-01	0.17	0.95	5.12E-04	-0.71	2.02	3.81E-01	-0.19	0.64	8.60E-03	0.52	1.12	485526	77870	501043	97062	534043	81241	468042	101054
RP_NEG_411_20331a9_303	RP	NEG	9.30	411.2033				1.22E-01	0.32	0.63	5.19E-04	0.68	2.02	8.67E-03	0.66	1.04	9.07E-01	-0.02	0.19	778189	580071	963354	577588	765014	328405	1161694	697059
RP_POS_342_24582a11_299	RP	POS	11.30	342.2458				9.95E-01	0.00	0.67	5.19E-04	-0.74	2.34	1.44E-02	-0.37	1.31	1.21E-01	0.37	0.78	289324	292268	289727	407224	431116	525344	148338	135143
RP_NEG_243_91692a2_995	RP	NEG	3.00	243.9169				1.28E-13	0.96	1.61	5.22E-04	0.71	2.02	4.43E-10	1.31	1.93	1.11E-06	0.60	1.51	540405	516524	2245942	1843162	1616912	1272426	2874971	2106478
RP_POS_367_31839a11_61	RP	POS	11.61	367.3184				5.80E-02	0.32	0.72	5.42E-04	0.74	2.07	3.55E-03	0.69	0.97	7.25E-01	-0.05	0.54	499671	217387	596632	326248	484272	144364	708992	410418
RP_POS_385_75302a12_976	RP	POS	12.98	385.7530				1.73E-18	1.15	1.87	5.70E-04	0.67	2.04	1.43E-12	1.49	2.20	2.75E-10	0.82	1.91	184832	244282	1104870	784611	838989	553713	1370752	890463
HILIC_POS_495_37915a1_021	HILIC	POS	1.021	495.3792				2.06E-03	0.42	0.87	5.80E-04	0.76	1.93	4.00E-04	0.80	1.10	7.01E-01	0.04	0.19	283824	746777	1040172	2009284	349975	775796	1730370	2565694
RP_NEG_626_27393a10_376	RP	NEG	10.38	626.2739				3.84E-01	0.17	0.92	5.97E-04	-0.68	2.05	4.54E-01	-0.17	0.65	1.82E-02	0.51	1.07	1354570	231936	1396465	245359	1478868	217765	1314062	245665
HILIC_NEG_152_99689a0_927	HILIC	NEG	0.927	152.9969				4.13E-01	-0.16	0.78	6.05E-04	-0.68	1.87	2.60E-02	-0.50	0.87	4.27E-01	0.17	0.30	398173	82847	384190	85583	412897	79174	355483	82754
RP_NEG_510_25403a10_414	RP	NEG	10.41	510.2540				4.85E-05	0.59	1.04	6.08E-04	0.72	2.01	1.73E-06	0.95	1.64	1.44E-01	0.23	0.66	568601	415037	1056605	891879	757109	740228	1356101	936022
HILIC_POS_371_24084a0_936	HILIC	POS	0.936	371.2408				9.07E-05	-0.82	1.49	6.14E-04	-0.63	1.82	1.06E-06	-1.13	1.83	1.91E-02	-0.51	1.10	2776997	492128	2354785	480256	2515688	460360	2193882	448589
HILIC_NEG_209_00429a0_927	HILIC	NEG	0.927	209.0043				2.81E-01	-0.22	0.86	6.20E-04	-0.67	1.91	1.49E-02	-0.56	0.96	6.08E-01	0.11	0.22	1213334	249895	1158007	250308	1241809	235283	1074206	238530
HILIC_NEG_130_99248a0_927	HILIC	NEG	0.927	130.9925				1.54E-01	-0.30	0.92	6.40E-04	-0.66	1.85	6.50E-03	-0.63	1.09	8.97E-01	0.03	0.05	1611391	326988	1516337	312637	1620760	303412	1411914	288386
RP_POS_414_30035a8_329	RP	POS	8.33	414.3004				2.71E-06	0.56	0.95	6.44E-04	0.76	2.00	2.05E-05	0.94	1.30	1.24E-02	0.18	0.96	214377	183485	1018923	1590341	478097	685774	1559749	2010665
RP_POS_389_26825a9_044	RP	POS	9.04	389.2683				6.64E-06	0.56	0.99	6.44E-04	0.76	2.02	3.20E-05	0.93	1.37	1.35E-02	0.18	1.04	364733	158150	755104	779625	489251	286645	1020957	1000815
HILIC_POS_315_12683a6_128	HILIC	POS	6.128	315.1268				4.06E-02	-0.34	1.01	6.57E-04	-0.72	1.77	1.35E-03	-0.70	1.18	9.09E-01	0.02	0.97	399302	68907	365739	105778	401176	76719	330302	118985
RP_NEG_516_29504a9_46	RP	NEG	9.46	516.2950				1.45E-04	0.46	0.88	6.64E-04	0.77	2.03	1.91E-04	0.84	1.23	1.60E-01	0.08	0.83	365871	332333	1142291	1891527	498523	515139	1790058	2472316
RP_POS_779_53833a12_647	RP	POS	12.65	779.5383				2.57E-03	0.56	1.09	6.72E-04	0.68	1.99	1.16E-04	0.90	1.39	2.14E-01	0.22	0.83	6783807	2687701	8596759	3282253	7496400	2187098	9697119	3809439
HILIC_NEG_288_61975a4_126	HILIC	NEG	4.126	288.6198				1.11E-03	0.42	0.97	6.75E-04	0.76	1.96	3.75E-04	0.80	1.09	5.98E-01	0.04	0.21	80120	180523	304315	591824	103084	206957	505546	763013
RP_POS_586_3075a10_376	RP	POS	10.38	586.3075				3.76E-01	0.18	0.87	6.86E-04	-0.66	2.03	5.22E-01	-0.15	0.58	2.09E-02	0.51	1.10	1089998	179409	1122441	176434	1181102	152869	1063779	180281
HILIC_POS_371_24008a1_843	HILIC	POS	1.843	371.2401				1.95E-05	0.66	1.19	6.98E-04	0.70	1.83	2.04E-06	1.01	1.54	4.40E-02	0.30	0.70	2150315	798824	3066540	1474275	2575011	1074901	3558069	1656156
HILIC_NEG_305_02322a0_928	HILIC	NEG	0.928	305.0232				3.20E-02	-0.43	1.04	7.23E-04	-0.66	1.83	8.68E-04	-0.76	1.28	6.27E-01	-0.10	0.36	445975	88080	406257	91197	436438	83524	376075	89266
HILIC_NEG_201_994a0_726	HILIC	NEG	0.726	201.9940				2.21E-11	0.83	1.50	7.25E-04	0.71	1.96	2.28E-08	1.19	1.74	2.07E-05	0.48	1.39	54840	42524	233481	229301	156975	147159	309988	269499
RP_NEG_131_0704a4_436	RP	NEG	4.44	131.0704				2.46E-08	0.68	1.27	7.32E-04	0.74	2.01	2.63E-06	1.05	1.49	8.17E-05	0.31	1.23	811071	430232	3046880	3634213	1823951	1605233	4269810	4588641
RP_NEG_532_30115a10_378	RP	NEG	10.38	532.3012				4.01E-01	0.17	0.93	7.33E-04	-0.67	2.00	4.71E-01	-0.16	0.66	2.19E-02	0.50	1.07	852969	141567	877491	145546	925628	127933	829353	147322
RP_POS_211_14409a4_835	RP	POS	4.84	211.1441				3.44E-07	0.63	1.13	7.59E-04	0.74	1.98	6.79E-06	1.00	1.51	1.71E-03	0.26	1.08	1367255	1164140	4757753	5929564	2768850	2671212	6746655	7471862
RP_NEG_624_34003a8_857	RP	NEG	8.86	624.3400				1.27E-02	0.41	0.72	7.75E-04	0.71	1.97	6.51E-04	0.76	1.13	7.31E-01	0.05	0.44	524964	896002	1066763	1420121	595205	898698	1538322	1677252
RP_NEG_297_24396a10_659	RP	NEG	10.66	297.2440				6.89E-11	0.89	1.74	7.79E-04	0.69	2.03	1.15E-08	1.23	1.88	8.95E-06	0.54	1.61	5770117	1265716	8678148	3414243	7544191	2116667	9812104	4055556
RP_NEG_383_15396a7_368	RP	NEG	7.37	383.1540				5.17E-02	0.29	0.95	7.80E-04	0.73	2.18	3.80E-03	0.66	1.48	5.55E-01	-0.07	0.28	5602839	4490025	7897884	8537671	5038301	3713773	10757467	10806986
HILIC_NEG_291_00748a0_929	HILIC	NEG	0.929	291.0075				2.26E-01	-0.25	0.90	8.08E-04	-0.65	1.86	9.84E-03	-0.58	1.04	7.69E-01	0.07	0.11	913875	181706	869111	173148	926005	182432	812217	143824
RP_NEG_480_30966a10_504	RP	NEG	10.50	480.3097				8.89E-01	0.03	0.89	8.08E-04	-0.67	2.03	1.82E-01	-0.31	0.79	8.40E-02	0.36	0.96	6934896	806044	6958292	859606	7240791	707175	6675793	911022
HILIC_POS_185_03258a6_129	HILIC	POS	6.129	185.0326				1.26E-02	-0.41	1.10	8.32E-04	-0.70	1.75	4.92E-04	-0.76	1.31	7.41E-01	-0.05	1.00	5139389	723681	4698313	1164971	5081673	831144	4314953	1323360
RP_POS_250_01358a3_003	RP	POS	3.00	250.0136				1.60E-12	0.88	1.53	8.40E-04	0.70	1.97	8.44E-09	1.23	1.81	2.17E-06	0.53	1.44	1559964	1048159	6278501	5669747	4408300	3619544	8148702	6686474
RP_NEG_221_15494a9_398	RP	NEG	9.40	221.1549				8.47E-02	-0.42	0.86	8.44E-04	-0.58	2.04	5.93E-03	-0.71	1.34	6.13E-01	-0.13	0.48	847604	73403	822907	52120	839960	53285	805853	45338
RP_POS_1019_63129a10_502	RP	POS	10.50	1019.6313				2.86E-01	-0.20	0.87	8.72E-04	-0.68	1.97	1.41E-02	-0.54	1.07	4.79E-01	0.14	0.81	3051675	469185	2943643	567430	3128817	494148	2758468	579969
HILIC_NEG_143_05215a0_724	HILIC	NEG	0.724	143.0522				2.07E-10	0.78	1.45	9.04E-04	0.71	1.97	1.25E-07	1.13	1.63	5.02E-05	0.42	1.30	79301	55874	385121	424833	245616	258373	524625	508109
RP_POS_284_67719a10_375	RP	POS	10.38	284.6772				3.70E-01	0.17	1.04	9.12E-04	-0.68	2.03	4.25E-01	-0.17	0.70	1.34E-02	0.51	1.29	593571	107321	614337	129680	656510	112890	572164	132677
RP_NEG_269_21277a10_123	RP	NEG	10.12	269.2128	Unknown	269.2101(100), 59.0125(85), 197.1898(30)	4	1.76E-12	0.89	1.67	9.19E-04	0.69	1.98	9.55E-09	1.23	1.84	1.09E-06	0.54	1.65	1329804	188739	2053331	858818	1771815	531965	2334846	1022480
RP_NEG_365_23138a10_656	RP	NEG	10.66	365.2314				1.12E-09	0.83	1.70	9.38E-04	0.69	2.06	3.65E-08	1.18	1.85	1.05E-04	0.49	1.48	663049	152157	979653	398715	849372	260698	1109934	467535
RP_POS_253_02148a3	RP	POS	3.00	253.0215				1.25E-11	0.84	1.52	9.43E-04	0.70	1.95	1.58E-08	1.19	1.79	2.69E-05	0.49	1.27	234888	186259	1120010	1127375	752221	767146	1487799	1305111
RP_POS_507_32281a10_374	RP	POS	10.37	507.3228				2.18E-01	0.23	1.00	9.47E-04	-0.67	1.96	5.98E-01	-0.11	0.64	7.90E-03	0.57	1.18	393680	103990	421446	126411	462403	121512	380489	118732
HILIC_NEG_117_05568a0_723	HILIC	NEG	0.723	117.0557				1.70E-08	0.68	1.39	9.54E-04	0.72	2.01	1.61E-06	1.04	1.47	5.10E-04	0.32	1.09	10534389	8458682	67421089	91803222	37321873	50080241	97520304	112564318
RP_NEG_160_8412a0_548	RP	NEG	0.55	160.8412				4.13E-01	-0.15	0.44	9.86E-04	-0.68	2.13	2.11E-02	-0.49	0.83	3.41E-01	0.19	0.61	6197568	1561827	5917296	1984653	6558322	1809212	5276269	1961179
RP_NEG_546_28064a10_635	RP	NEG	10.64	546.2806				1.32E-01	0.27	0.80	9.90E-04	0.68	2.18	5.62E-03	0.61	1.07	7.25E-01	-0.07	0.66	971949	261512	1058899	334642	950656	272516	1167142	357883
RP_POS_472_30341a8_33	RP	POS	8.33	472.3034				2.69E-06	0.56	0.96	9.97E-04	0.73	1.94	2.68E-05	0.93	1.29	8.38E-03	0.20	1.03	118185	112431	601560	954603	288194	417802	914925	1210855
HILIC_NEG_189_05757a0_723	HILIC	NEG	0.723	189.0576				6.37E-11	0.80	1.47	9.98E-04	0.70	1.98	6.41E-08	1.15	1.67	2.89E-05	0.45	1.35	21875	18454	118511	129452	76383	81515	160639	153593
HILIC_NEG_71_04948a0_723	HILIC	NEG	0.723	71.0495				2.63E-08	0.67	1.39	1.02E-03	0.72	2.01	2.07E-06	1.03	1.45	6.87E-04	0.31	1.07	89489	76170	609432	852757	331267	464399	887597	1046734
RP_NEG_164_83536a0_55	RP	NEG	0.55	164.8354				9.64E-02	-0.29	0.80	1.02E-03	-0.68	2.15	2.18E-03	-0.63	1.07	7.81E-01	0.05	0.55	2275394	506644	2083067	708305	2311260	654083	1854875	692486
RP_POS_791_54138a12_971	RP	POS	12.97	791.5414				3.27E-19	1.54	2.45	1.02E-03	0.52	1.92	2.36E-18	1.80	2.59	2.29E-14	1.28	2.38	2210821	1086136	5188988	1561266	4684876	1244102	5693100	1690688
RP_POS_240_09941a10_375	RP	POS	10.38	240.0994				5.11E-01	0.12	0.96	1.03E-03	-0.68	2.00	2.91E-01	-0.22	0.68	2.10E-02	0.46	1.16	1104302	146820	1125630	191373	1187254	167623	1064005	195312
HILIC_POS_243_13365a1_72	HILIC	POS	1.72	243.1337				1.40E-03	0.58	1.15	1.04E-03	0.66	1.84	1.03E-04	0.91	1.35	1.37E-01	0.25	0.61	159304	307571	382595	390406	255883	237404	509306	467779
RP_POS_659_4754a10_377	RP	POS	10.38	659.4754				5.93E-01	0.12	0.97	1.05E-03	0.62	1.96	8.70E-02	0.43	0.95	4.15E-01	-0.19	0.84	987790	212496	1010208	179968	952303	150178	1068112	189847
RP_POS_716_55865a13_271	RP	POS	13.27	716.5587				1.15E-09	0.78	1.33	1.06E-03	0.70	1.91	2.02E-07	1.12	1.66	8.10E-05	0.43	1.30	279333	201596	844896	782911	590871	463025	1098921	944630
RP_POS_414_0452a0_553	RP	POS	0.55	414.0452				6.13E-03	0.37	0.70	1.07E-03	0.73	2.00	1.14E-03	0.73	1.11	9.70E-01	0.00	0.62	472573	85830	551494	239082	473328	94120	629660	306855
RP_NEG_1035_66504a10_375	RP	NEG	10.38	1035.6650				1.27E-01	0.30	1.03	1.08E-03	-0.65	1.97	8.90E-01	-0.03	0.66	4.45E-03	0.62	1.21	5930021	2029266	6584946	2246372	7305096	2118652	5864795	2155985
RP_NEG_185_04305a2_988	RP	NEG	2.99	185.0431				2.68E-13	0.92	1.56	1.10E-03	0.67	1.90	1.19E-09	1.26	1.89	3.82E-06	0.59	1.40	264106	181588	981611	813713	719940	593791	1243282	919480

Supplementary table 1: Metabolomics results (in asceding order according to p-value from progressive ALD vs non-progressive ALD comparison, with molecular features with ID_level of 1-2 first)

								all_ALD_vs_control			Prog_ALD_vs_non-prog_ALD			Prog_ALD_vs_control_ALD			Non-prog_ALD_vs_control			Healthy_control		all_ALD		Non-prog_ALD		Progressive_ALD	
								t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA								
Feature_ID	RP_HILIC	POS_NEG	Average.Rt	Average.Mz	Metabolite.name	curated_MSMS	ID_level	p	d	VIP	p	d	VIP	p	d	VIP	p	d	VIP	Mean	SD	Mean	SD	Mean	SD	Mean	SD
RP_POS_322_07068a3_003	RP	POS	3.00	322.0707				4.71E-06	0.55	1.08	1.11E-03	0.72	1.94	1.27E-05	0.91	1.39	7.69E-02	0.19	0.57	122447	230748	1275938	2353867	517138	1519406	2034737	2776833
RP_POS_1013_65375a10_502	RP	POS	10.50	1013.6538				6.47E-01	-0.09	0.92	1.12E-03	-0.66	2.02	5.96E-02	-0.42	0.94	2.37E-01	0.24	0.83	15567390	1775098	15395180	2038673	16047342	1779909	14743018	2088332
RP_NEG_612_2644a10_376	RP	NEG	10.38	612.2644				2.90E-01	0.20	1.00	1.13E-03	-0.66	1.91	5.65E-01	-0.13	0.62	1.02E-02	0.53	1.25	2124985	260514	2183622	298861	2279207	252874	2088036	312837
HILIC_NEG_68_995a0_927	HILIC	NEG	0.927	68.9950				1.25E-02	-0.50	1.10	1.14E-03	-0.63	1.77	2.01E-04	-0.82	1.48	3.97E-01	-0.19	0.40	400606	75412	360635	78303	385650	80633	335620	67891
RP_NEG_1035_66479a10_503	RP	NEG	10.50	1035.6648				8.20E-01	0.05	0.92	1.15E-03	-0.65	2.02	2.21E-01	-0.28	0.78	8.23E-02	0.37	0.97	44540337	7360813	44887900	7796077	47377385	6659921	42398416	8111439
HILIC_NEG_448_3074a0_992	HILIC	NEG	0.992	448.3074				2.39E-03	0.41	0.85	1.17E-03	0.72	1.84	5.83E-04	0.77	1.07	5.99E-01	0.05	0.27	580400	1290916	1861764	3448593	744874	1495022	2978654	4387186
HILIC_NEG_243_06223a3_277	HILIC	NEG	3.277	243.0622				9.82E-05	0.58	0.92	1.17E-03	0.69	1.74	2.45E-05	0.93	1.39	7.66E-02	0.24	0.71	458687	67461	530832	132276	488326	80705	573339	158589
HILIC_POS_295_18622a1_04	HILIC	POS	1.04	295.1862				5.84E-06	0.58	1.27	1.18E-03	0.71	1.76	1.53E-05	0.94	1.37	3.00E-02	0.23	0.70	147240	233214	580136	817444	316890	457731	843381	999563
RP_POS_302_21466a8_097	RP	POS	8.10	302.2147				7.71E-13	0.96	1.72	1.21E-03	0.66	2.00	5.75E-10	1.29	1.96	2.41E-06	0.63	1.54	207485	144350	595420	415234	462991	304260	727849	469034
RP_POS_417_33597a9_229	RP	POS	9.23	417.3360				5.31E-08	0.65	1.11	1.24E-03	0.72	1.91	1.17E-05	1.01	1.41	2.58E-11	0.29	1.98	73350	47426	648299	973572	332265	213063	964332	1290659
RP_POS_472_30341a9_451	RP	POS	9.45	472.3034				2.64E-04	0.44	0.85	1.25E-03	0.73	1.93	4.25E-04	0.80	1.18	1.24E-01	0.07	0.85	892341	873526	3442648	6583863	1307855	1539860	5577440	8712478
HILIC_NEG_242_10832a0_723	HILIC	NEG	0.723	242.1083				6.83E-07	0.60	1.28	1.28E-03	0.71	1.93	1.14E-05	0.95	1.35	6.81E-03	0.24	0.84	17527	33201	191829	324507	87960	172106	295698	401398
RP_POS_365_30182a11_257	RP	POS	11.26	365.3018				5.45E-05	0.59	1.34	1.30E-03	0.69	1.90	3.35E-05	0.93	1.46	4.47E-02	0.24	1.00	854327	546071	1489876	1167318	1116306	596498	1863445	1453429
RP_POS_399_32559a9_234	RP	POS	9.23	399.3256				1.10E-08	0.69	1.16	1.31E-03	0.71	1.90	6.10E-06	1.04	1.45	7.12E-12	0.33	2.05	90388	59071	683149	946471	377438	226284	988860	1252182
RP_NEG_448_30728a9_46	RP	NEG	9.46	448.3073				3.06E-04	0.43	0.82	1.33E-03	0.73	1.92	4.69E-04	0.80	1.16	1.36E-01	0.07	0.86	3574796	3385350	12681256	23682691	5040534	5427395	20321977	31378102
RP_POS_876_54926a12_545	RP	POS	12.55	876.5493				1.35E-02	-0.49	1.19	1.36E-03	-0.63	1.88	1.60E-04	-0.80	1.59	4.38E-01	-0.17	0.62	728227	330540	553553	356718	665978	385380	441127	287714
RP_POS_413_78531a14_754	RP	POS	14.75	413.7853				3.38E-03	0.51	0.87	1.42E-03	0.66	1.88	1.89E-04	0.84	1.23	2.83E-01	0.18	0.48	913521	749439	1423960	1039752	1096601	743973	1751318	1188291
RP_POS_537_30505a10_499	RP	POS	10.50	537.3051				1.16E-04	0.61	1.19	1.43E-03	0.66	1.89	1.25E-05	0.94	1.72	7.51E-02	0.28	0.81	316996	164891	481245	285278	391500	206724	570990	324431
RP_POS_337_27118a11_097	RP	POS	11.10	337.2712				1.11E-01	0.28	1.07	1.54E-03	0.67	1.85	1.02E-02	0.61	1.02	7.45E-01	-0.05	0.77	981814	469592	1149732	629208	951147	305557	1348316	791226
RP_POS_568_33685a10_396	RP	POS	10.40	568.3369				4.33E-02	0.41	1.06	1.54E-03	-0.62	1.86	6.72E-01	0.09	0.54	1.14E-03	0.72	1.30	2229139	856328	2593312	898262	2872870	797186	2313753	913901
RP_POS_826_53473a12_406	RP	POS	12.41	826.5347				3.20E-01	-0.21	0.81	1.59E-03	-0.61	1.84	2.28E-02	-0.52	1.00	7.08E-01	0.09	0.43	2062574	1323996	1797651	1212506	2174478	1292387	1420823	1005130
RP_POS_1020_13263a10_499	RP	POS	10.50	1020.1326				7.69E-01	-0.06	0.95	1.59E-03	-0.64	1.95	9.21E-02	-0.38	0.88	1.96E-01	0.26	0.90	2904945	455803	2876664	521787	3038690	446422	2714638	545170
RP_NEG_288_03061a3_001	RP	NEG	3.00	288.0306				1.80E-06	0.57	1.11	1.61E-03	0.70	1.89	1.52E-05	0.92	1.38	2.52E-02	0.22	0.68	80078	184533	1911647	3596447	786571	2152095	3036724	4349489
RP_POS_290_0444a3_002	RP	POS	3.00	290.0444				3.33E-06	0.55	1.14	1.62E-03	0.70	1.90	2.76E-05	0.90	1.37	2.44E-02	0.20	0.68	63190	136752	1985962	3895484	765059	2130437	3206865	4804005
RP_NEG_205_83928a15_552	RP	NEG	15.55	205.8393				1.48E-01	-0.31	0.54	1.62E-03	-0.60	2.14	5.95E-03	-0.62	1.13	9.60E-01	-0.01	0.15	5058702	267611	4980620	240918	5055620	276509	4905620	171263
RP_POS_651_37079a9_234	RP	POS	9.23	651.3708				4.33E-08	0.66	1.12	1.62E-03	0.70	1.86	1.29E-05	1.01	1.41	1.16E-11	0.31	2.03	104865	67376	908674	1350555	480632	301485	1336715	1794550
HILIC_NEG_224_06192a1_193	HILIC	NEG	1.193	224.0619				2.31E-08	0.75	1.35	1.64E-03	0.67	1.70	8.50E-07	1.08	1.65	2.11E-04	0.41	1.58	1253002	3477946	8213789	9940646	5102618	5500076	11324960	12232943
RP_POS_797_02637a12_96	RP	POS	12.96	797.0264				1.48E-19	1.34	2.13	1.66E-03	0.56	1.86	3.83E-16	1.62	2.41	1.31E-11	1.06	2.05	186766	215239	826252	430331	693114	364745	959390	452697
HILIC_NEG_185_04303a0_722	HILIC	NEG	0.722	185.0430				2.71E-08	0.67	1.35	1.70E-03	0.69	1.98	3.22E-06	1.02	1.43	3.08E-04	0.33	1.14	53344	44073	291211	388482	169971	207043	412452	481717
RP_POS_765_98688a10_375	RP	POS	10.38	765.9869				2.54E-01	0.21	0.95	1.72E-03	-0.65	1.90	5.69E-01	-0.12	0.65	1.03E-02	0.53	1.11	1495725	485156	1617508	619771	1808402	581784	1426614	602686
RP_POS_771_96429a10_374	RP	POS	10.37	771.9643				2.83E-01	0.21	0.96	1.74E-03	-0.63	1.90	6.19E-01	-0.11	0.65	1.86E-02	0.52	1.07	445443	198297	490261	219012	557679	216769	422843	201612
HILIC_POS_659_41449a1_228	HILIC	POS	1.228	659.4145				1.20E-02	0.50	0.90	1.74E-03	-0.61	1.67	3.69E-01	0.19	0.35	3.35E-04	0.80	1.39	343402	186154	443474	200427	505163	193698	381785	189412
RP_POS_524_29938a10_375	RP	POS	10.38	524.2994				2.10E-01	0.24	0.97	1.74E-03	-0.64	1.93	7.03E-01	-0.08	0.66	8.91E-03	0.55	1.15	2757585	711987	2948869	835158	3205893	771949	2691844	823704
RP_POS_1013_65259a10_375	RP	POS	10.38	1013.6526				1.07E-01	0.29	1.03	1.75E-03	-0.64	1.90	9.00E-01	-0.03	0.65	3.61E-03	0.62	1.22	2046055	872038	2355023	1091226	2690773	1054637	2019273	1031277
RP_POS_1041_68689a10_506	RP	POS	10.51	1041.6869				1.81E-02	0.47	1.17	1.76E-03	-0.61	1.85	4.37E-01	0.17	0.65	4.99E-04	0.78	1.36	11670630	5298174	14322989	5548621	16029294	5184188	12616685	5420804
RP_POS_430_74789a12_734	RP	POS	12.73	430.7479				1.25E-04	-0.84	1.36	1.76E-03	-0.56	1.81	1.57E-06	-1.12	1.91	1.72E-02	-0.56	0.99	1959496	702878	1377666	632567	1572625	693219	1182707	500325
HILIC_NEG_224_06194a1_296	HILIC	NEG	1.296	224.0619				5.19E-05	0.58	1.10	1.77E-03	0.67	1.67	2.79E-05	0.92	1.45	5.52E-02	0.25	0.82	486846	287329	829783	638271	631817	385147	1027750	771217
HILIC_NEG_244_00462a0_616	HILIC	NEG	0.616	244.0046				3.25E-08	0.69	1.44	1.77E-03	0.68	1.81	1.93E-06	1.03	1.48	7.61E-04	0.35	1.21	148102	66288	346542	314722	248887	184125	444197	383089
RP_NEG_201_80153a0_564	RP	NEG	0.56	201.8015				1.63E-03	-0.56	0.98	1.78E-03	-0.63	2.11	5.11E-05	-0.88	1.44	1.89E-01	-0.25	0.76	11844908	1676013	10628734	2228451	11313818	1903205	9943650	2335231
HILIC_NEG_213_04958a6_093	HILIC	NEG	6.093	213.0496				2.30E-01	-0.18	0.94	1.78E-03	-0.67	1.67	9.07E-03	-0.52	1.06	3.65E-01	0.15	1.04	214932	30923	205404	56871	222889	48094	187918	59981
HILIC_NEG_243_10449a0_723	HILIC	NEG	0.723	243.1045				4.62E-07	0.60	1.30	1.79E-03	0.69	1.92	1.06E-05	0.95	1.35	5.26E-03	0.26	0.86	47159	120545	760516	1308746	354195	730487	1166837	1609362
RP_POS_326_03061a3_86	RP	POS	3.86	326.0306				1.64E-02	0.36	0.67	1.79E-03	0.68	1.83	2.16E-03	0.70	1.12	9.07E-01	0.01	0.48	625418	810330	1154263	1629465	646506	758070	1662020	2064866
HILIC_NEG_144_92342a0_926	HILIC	NEG	0.926	144.9234				5.12E-07	-0.87	1.56	1.84E-03	-0.61	1.70	6.11E-09	-1.18	2.00	2.91E-03	-0.57	1.08	47275634	6409501	39280130	9102254	42068052	8913495	36492207	8490008
HILIC_POS_432_31088a1_021	HILIC	POS	1.021	432.3109				4.37E-03	0.38	0.81	1.86E-03	0.70	1.80	1.44E-03	0.72	0.98	7.41E-01	0.03	0.17	486976	1157615	1651439	3453224	574226	1163911	2728651	4513319
RP_POS_432_31104a9_451	RP	POS	9.45	432.3110				4.24E-04	0.42	0.80	1.86E-03	0.71	1.87	7.01E-04	0.77	1.12	1.12E-01	0.07	0.87	582966	585906	2370446	4803000	866931	1012553	3873961	6400763
RP_POS_236_03358a3_003	RP	POS	3.00	236.0336				7.82E-12	0.87	1.52	1.88E-03	0.65	1.87	1.25E-08	1.20	1.80	8.29E-06	0.55	1.37	1005533	742972	3425360	2926629	2525579	2022876	4325142	3400123
RP_POS_794_50818a12_646	RP	POS	12.65	794.5082				2.57E-04	0.61	1.26	1.88E-03	0.64	1.82	3.08E-05	0.93	1.48	7.30E-02	0.28	0.83	775270	373643	1111056	579342	932891	395796	1289222	675787
HILIC_NEG_540_33002a1_126	HILIC	NEG	1.126	540.3300				2.38E-02	0.41	0.64	1.96E-03	-0.63	1.65	6.33E-01	0.10	0.35	5.43E-04	0.73	1.26	1648139	382164	1840306	482803	1987332	460426	1693279	463515
RP_POS_172_09648a0_708	RP	POS	0.71	172.0965				1.01E-04	0.54	1.03	1.99E-03	0.67	1.83	3.36E-05	0.88	1.40	1.16E-01	0.21	0.55	189664	134814	351990	325898	252287	222381	451693	380586
RP_POS_991_67139a10_502	RP	POS	10.50	991.6714				1.98E-01	0.25	1.02	2.02E-03	-0.62	1.93	7.58E-01	-0.07	0.66	9.38E-03	0.56	1.17	228750475	65772381	246769168	75203124	269608672	70190754	223929665	73723259
HILIC_NEG_279_61429a1_729	HILIC	NEG	1.729	279.6143				1.00E-03	0.45	0.97	2.02E-03	0.68	1.70	4.01E-04	0.79	1.10	3.07E-01	0.11	0.36	131784	96513	234281	251937	156701	121425	311862	318139
HILIC_NEG_176_99821a0_927	HILIC	NEG	0.927	176.9982				7.23E-02	-0.36	0.97	2.07E-03	-0.61	1.75	3.25E-03	-0.66	1.14	7.97E-01	-0.06	0.13	1558665	294342	1447694	309582	1541497	293335	1353892	299392
HILIC_POS_250_1284a1_039	HILIC	POS	1.039	250.1284				3.55E-05	0.53	1.24	2.10E-03	0.68	1.68	6.77E-05	0.86	1.25	6.80E-02	0.19	0.60	284522	383194	964872	1435512	525667	786630	1404077	1775101
HILIC_NEG_213_99434a0_618	HILIC	NEG	0.618	213.9943				1.20E-08	0.70	1.45	2.14E-03	0.66	1.79	1.55E-06	1.04	1.48	2.97E-04	0.37	1.25	181313	76987	445647	408975	320941	239208	570353	498976
RP_POS_791_54236a12_813	RP	POS	12.81	791.5424				2.68E-02	0.41	0.80	2.14E-03	-0.62	1.92	5.95E-01	0.10	0.60	1.33E-03	0.72	1.24	1256153	604568	1549740	730228	1770643	788391	1328836	596825
HILIC_NEG_234_8201a0_996	HILIC	NEG	0.996	234.8201				5.66E-03	-0.42	0.69	2.16E-03	-0.66	1.64	4.09E-04	-0.75	1.14	5.40E-01	-0.09	0.43	645745	99859	573068	186784	629669	136129	516466	213118
RP_NEG_145_06091a0_529	RP	NEG	0.53	145.0609				3.66E-01	-0.14	0.64	2.17E-03	-0.66	1.78	1.70E-02	-0.47	0.87	2.89E-01	0.19	0.64	6863256	1183331	6596615	2056239	7217289	1821287	5975942	2106952
RP_NEG_429_30151a9_971	RP	NEG	9.97	429.3015				4.32E-04	0.49	0.89	2.17E-03	0.67	1.89	2.67E-04	0.82	1.18	1.51E-01	0.15	0.76	1047233	337282	1419439	838601	1162565	371516	1676313	1071527
HILIC_NEG_315_04205a6_344	HILIC	NEG	6.344	315.0421				1.73E-02	0.46	0.94	2.19E-03	0.61	1.75	9.32E-04	0.77	1.17	4.25E-01	0.16	0.40	2897535	627441	3219190	701708	3007294	566231	3431086	763274
RP_POS_453_29739a9_972	RP	POS	9.97	453.2974	Steroid, unknown	453.3004(100)	3	8.95E-05	0.53	0.96	2.21E-03	0.67	1.87	1.09E-04	0.87	1.25	5.90E-02	0.20	0.87	1990529	643141	2823285	1714992	2299506	808104	3347064	2174742
HILIC_NEG_540_32996a1_253	HILIC	NEG	1.253	540.3300				7.52E-02	0.32	0.72	2.22E-03	-0.63	1.66	9.96E-01	0.00	0.31	3.17E-03	0.63	1.05	11139541	2611250	12180229	3445264	13217880	3556227	11142578	3022877
RP_POS_431_31564a9_972	RP	POS	9.97	431.3156				8.75E-05	0.53	0.95	2.23E-03	0.67	1.87	1.14E-04	0.87	1.24	5.48E-02	0.20	0.87	4861497	1546398	6876501	4152438	5608824	1898068	8144179	5287260
RP_POS_414_30026a9_451	RP	POS	9.45	414.3003				3.35E-04	0.43	0.81	2.24E-03	0.69	1.85	7.03E-04	0.77	1.12	5.41E-02	0.08	0.94	263600	261072	1086130	2171077	418502	455358	1753757	2899371
RP_NEG_465_25021a8_564	RP	NEG	8.56	465.2502				1.76E-02	-0.59	1.10	2.26E-03	-0.53	1.81	7.23E-04	-0.85	1.67	2.31E-01	-0.33	0.75	1633145	1356266	996713	932408	1280537	1170635	712889	470876
HILIC_NEG_259_00095a0_929	HILIC	NEG	0.929	259.0010				2.72E-01	-0.22	0.89	2.29E-03	-0.61	1.70	1.62E-02	-0.52	0.94	6.95E-01	0.09	0.15	1184436	211155	1136007	226139	1203891	229700	1068122	202866
HILIC_POS_191_04037a6_128	HILIC	POS	6.128	191.0404				4.89E-02	-0.34	1.00	2.30E-03	-0.64	1.60	2.87E-03	-0.66	1.17	9.13E-01	-0.02	0.98	869309	86989	829771	123949	867088	93857	792454	139244
RP_NEG_397_22391a9_544	RP	NEG	9.54	397.2239				2.35E-08	0.70	1.23	2.33E-03	0.66	1.83	5.50E-07	1.02	1.59	3.34E-03	0.37	0.95	1205686	1049919	4391292	4994879	2888286	3667015	5894297	5687664
RP_POS_434_32614a9_857	RP	POS	9.86	434.3261				3.18E-02	0.31	0.66	2.34E-03	0.68	1.85	5.77E-03	0.64	1.03	7.26E-01	-0.03	0.62	150717	265407	316247	599918	132643	145703	499852	798200
RP_POS_522_79785a10_375	RP	POS	10.38	522.7979				3.90E-01	0.17	0.95	2.39E-03	-0.62	1.89	5.08E-01	-0.14	0.70	2.85E-02	0.47	1.03	1400718	384027	1470529	434773	1600502	410056	1340555	423427
RP_NEG_475_3071a9_971	RP	NEG	9.97	475.3071				2.47E-04	0.50	0.91	2.39E-03	0.67	1.88	2.14E-04	0.83	1.19	1.03E-01	0.17	0.79	1960317	603619	2675172	1565223	2200296	695672	3150048	2001416
HILIC_POS_414_30017a1_021	HILIC	POS	1.021	414.3002				6.90E-03	0.37	0.83	2.45E-03	0.67	1.76	1.86E-03	0.71	0.97	7.17E-01	0.04	0.16	250176	669210	815963	1685709	304463	644689	1327464	2188984
RP_POS_518_31934a10_376	RP	POS	10.38	518.3193	LPC 16:0 [M+Na]+	459.2449(60), 313.2737(50), 518.3217(50), 86.0972(40), 104.107(2), 146.9823(100)		1.85E-01	0.26	1.00	2.49E-03	-0.61	1.89	8.31E-01	-0.05	0.63	7.92E-03	0.56	1.20	58036062	10919761	61101830	12185999	64733609	10597371	57470050	12680909
HILIC_POS_534_29486a1_171	HILIC	POS	1.171	534.2949				6.23E-02	0.35	0.59	2.49E-03	-0.61	1.62	8.32E-01	0.04	0.36	2.20E-03	0.66	1.13	544283	206835	627901	245450	700983	234417	554818	236367
RP_POS_828_55182a12_321	RP	POS	12.32	828.5518				3.13E-01	0.17	0.84	2.56E-03	-0.63	1.78	4.27E-01	-0.14	0.60	2.40E-02	0.49	0.83	677131	378634	763959	532115	922383	586514	605536	420536
RP_POS_205_19521a9_512	RP	POS	9.51	205.1952				2.46E-08	0.70	1.23	2.57E-03	0.65	1.81	4.08E-07	1.02	1.62	4.38E-03	0.37	0.93	261559	215626	900596	1001085	602468	768192	1198723	1119504
RP_POS_421_21954a9_513	RP	POS	9.51	421.2195				2.82E-08	0.69	1.23	2.63E-03	0.65	1.80	5.37E-07	1.01	1.61	4.46E-03	0.36	0.94	553025	484860	2073082	2409421	1357073	1824721	2789091	2711684
RP_NEG_778_56183a13_58	RP	NEG	13.58	778.5618				2.99E-02	0.42	0.89	2.64E-03	0.60	1.76	2.03E-03	0.72	1.17	5.46E-01	0.12	0.33	2277814	1030658	2759665	1168437	2412638	899843	3106692	1304939
HILIC_POS_204_08662a1_039	HILIC	POS	1.039	204.0866				4.38E-07	0.61	1.31	2.65E-03	0.66	1.66	1.83E-05	0.94	1.36	1.47E-03	0.27	0.96	44742	55603	378306	610708	195272	309802	561340	767588
RP_POS_195_08783a3_778	RP	POS	3.78	195.0878				7.42E-02	0.28	0.56	2.68E-03	0.65	1.76	7.43E-03	0.60	0.99	7.19E-01	-0.05	0.58	41485600	48375992	63494421	86917083	37524135	48618924	89464707	107345673
RP_POS_756_54956a13_575	RP	POS	13.58	756.5496				1.30E-02	0.48	0.95	2.69E-03	0.60	1.75	7.78E-04	0.78	1.26	3.46E-01	0.19	0.40	2972271	1422189	3733412	1579670	3265444	1265407	4201380	1730162
RP_POS_339_28687a11_173	RP	POS	11.17	339.2869				3.15E-04	0.56	1.09	2.73E-03	0.64	1.77	1.66E-04	0.88	1.25	5.21E-02	0.24	0.89	945223	396109	1316039	701971	1105456	281711	1526621	908692
RP_POS_754_99414a10_375	RP	POS	10.38	754.9941				8.44E-02	0.29	0.94	2.74E-03	-0.63	1.78	9.11E-01	-0.02	0.58	3.06E-03	0.61	1.19	267455	112245	312404	163416	360619	163747	2641289	149658
RP_POS_770_46606a10_374	RP	POS	10.37	770.4661				4.28E-02	0.37	1.07	2.77E-03	-0.61	1.82	7.28E-01	0.07	0.67	1.82E-03	0.68	1.24	261912	119775	315221	147342	358657	149603	2717842	132780
RP_POS_416_26428a9_512	RP	POS	9.51	416.2643				5.16E-08	0.68	1.21	2.78E-03	0.65	1.79	7.72E-07	1.00	1.58	5.87E-03	0.35	0.91	169565	168515	680571	826906	436136	625073	925006	932121
HILIC_NEG_134_89479a6_412	HILIC	NEG	6.412	134.8948				6.02E-01	0.10	0.36	2.83E-03	-0.60	1.79	3.58E-01	-0.20	0.36	7.26E-02	0.40	0.77	11966943	7140530	12743475	7709107	15010762	7730484	10476188	7058480
HILIC_NEG_99_92568a0_725	HILIC	NEG	0.725	99.9257				6.63E-11	0.86	1.54	2.84E-03	0.62	1.73	2.74E-08	1.17	1.74	1.79E-05	0.55	1.47	628620	154343	1025211	485795	881617	338760	1168806	565661
RP_POS_445_3674a12_358	RP	POS	12.36	445.3674				1.42E-01	-0.26	1.15	2.84E-03	-0.62	1.77	9.59E-03	-0.57	1.33	8.05E-01	0.05	0.42	3600099	568800	3414303	741474	3632702	599912	3195903	808425

Supplementary table 1: Metabolomics results (in asceding order according to p-value from progressive ALD vs non-progressive ALD comparison, with molecular features with ID_level of 1-2 first)

								all_ALD_vs_control			Prog_ALD_vs_non-prog_ALD			Prog_ALD_vs_control_ALD			Non-prog_ALD_vs_control			Healthy_control		all_ALD		Non-prog_ALD		Progressive_ALD	
								t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA								
Feature_ID	RP_HILIC	POS_NEG	Average.Rt	Average.Mz	Metabolite.name	curated_MSMS	ID_level	p	d	VIP	p	d	VIP	p	d	VIP	p	d	VIP	Mean	SD	Mean	SD	Mean	SD	Mean	SD
RP_POS_519_32245a10_375	RP	POS	10.38	519.3225				2.01E-01	0.25	1.00	2.86E-03	-0.60	1.86	8.18E-01	-0.05	0.63	9.66E-03	0.55	1.19	15052620	2867150	15827101	3177835	16761276	2770446	14892926	3308626
RP_POS_445_36655a12_428	RP	POS	12.43	445.3666				1.73E-01	-0.27	1.02	2.87E-03	-0.59	1.79	1.45E-02	-0.57	1.19	9.12E-01	0.02	0.38	6252891	1338067	5872964	1402339	6285207	1194348	5460722	1483224
RP_POS_478_32712a10_505	RP	POS	10.51	478.3271				5.72E-01	-0.11	0.55	2.92E-03	-0.60	1.72	5.72E-02	-0.41	0.86	4.04E-01	0.19	0.47	1257216	402610	1209919	432013	1336626	440428	1083213	387735
RP_NEG_261_0748a7_839	RP	NEG	7.84	261.0748				1.85E-02	-0.50	1.17	2.94E-03	-0.56	1.75	6.18E-04	-0.79	1.43	3.44E-01	-0.22	0.84	730735	530472	472931	490652	616863	522241	328999	413978
HILIC_POS_151_04778a6_129	HILIC	POS	6.129	151.0478				3.64E-02	-0.35	1.08	2.99E-03	-0.63	1.60	1.97E-03	-0.66	1.18	8.54E-01	-0.03	1.03	1476248	281309	1335620	435374	1463259	349479	1207981	477060
HILIC_NEG_181_05098a1_076	HILIC	NEG	1.076	181.0510				2.15E-03	0.49	0.95	3.03E-03	0.63	1.74	3.07E-04	0.80	1.18	2.42E-01	0.18	0.49	284045	113125	371364	190577	315309	123009	427419	227677
RP_NEG_195_81055a0_565	RP	NEG	0.57	195.8106				7.64E-06	-0.77	1.21	3.08E-03	-0.59	1.98	4.00E-07	-1.07	1.68	9.09E-03	-0.48	0.97	81377646	10831710	69507558	15589848	74056318	13810867	64958799	16064863
RP_POS_497_39624a13_923	RP	POS	13.92	497.3962				1.87E-01	0.31	0.51	3.09E-03	-0.54	1.80	8.83E-01	0.04	0.38	1.72E-02	0.58	0.97	4398990	1346618	4748010	1048139	5054376	825854	4441643	1160183
HILIC_POS_152_03162a6_129	HILIC	POS	6.129	152.0316				2.61E-02	-0.36	1.10	3.17E-03	-0.63	1.59	1.58E-03	-0.67	1.20	7.87E-01	-0.05	1.09	1030442	183954	930172	300620	1017822	234591	842523	334482
HILIC_NEG_157_90067a0_943	HILIC	NEG	0.943	157.9007				4.02E-08	0.82	1.41	3.19E-03	0.60	1.59	8.89E-08	1.12	1.77	5.99E-04	0.52	1.48	825296	171984	1096923	343854	996678	262174	1197168	386834
RP_POS_267_19305a9_053	RP	POS	9.05	267.1931				9.00E-08	0.70	1.30	3.20E-03	0.64	1.74	5.78E-06	1.02	1.49	1.04E-04	0.38	1.45	884569	112865	1119503	363510	1012463	170541	1226543	463150
RP_POS_329_16251a10_822	RP	POS	10.82	329.1625				2.12E-07	0.93	1.78	3.22E-03	0.57	1.86	5.48E-08	1.21	1.94	2.31E-04	0.64	1.60	227644	219817	508566	295522	422462	222979	594671	334064
HILIC_NEG_118_92419a0_925	HILIC	NEG	0.925	118.9242				2.89E-06	-0.95	1.68	3.22E-03	-0.54	1.66	7.73E-08	-1.22	1.95	1.11E-03	-0.68	1.33	3313377	629625	2638906	655681	2829272	622494	2448541	638085
RP_POS_222_01859a1_361	RP	POS	1.36	222.0186				8.84E-09	0.69	1.26	3.23E-03	0.64	1.80	1.50E-06	1.01	1.50	6.87E-04	0.37	1.05	75641	42281	1250019	1867437	704335	1225569	1795703	2221732
RP_POS_593_33289a8_601	RP	POS	8.60	593.3329				4.59E-04	0.43	0.79	3.27E-03	0.66	1.86	7.51E-04	0.76	1.06	1.48E-01	0.10	0.67	162134	215465	573996	1077675	255979	366150	892014	1416335
RP_POS_781_05286a12_965	RP	POS	12.97	781.0529				9.92E-18	1.32	2.11	3.31E-03	0.53	1.71	5.98E-15	1.58	2.35	2.97E-11	1.06	2.01	1621498	848078	3888936	1553701	3438314	1284876	4339557	1676880
RP_POS_550_39172a11_282	RP	POS	11.28	550.3917				2.09E-04	0.50	1.12	3.33E-03	0.64	1.72	1.60E-04	0.82	1.35	1.25E-01	0.18	0.70	257110	142225	435340	393409	320417	227777	550264	483595
RP_NEG_650_35107a13_182	RP	NEG	13.18	650.3511				6.39E-01	-0.10	0.31	3.35E-03	-0.56	2.01	1.03E-01	-0.38	0.83	4.43E-01	0.18	0.49	4254238	643931	4193936	580613	4361873	567666	4025999	548908
HILIC_NEG_273_97845a0_729	HILIC	NEG	0.729	273.9785				8.16E-14	0.98	1.67	3.38E-03	0.60	1.72	4.93E-10	1.28	1.97	7.19E-07	0.68	1.64	150221	76587	386199	247511	314464	190459	457935	277483
HILIC_NEG_117_05566a0_925	HILIC	NEG	0.925	117.0557				1.07E-06	0.58	1.30	3.42E-03	0.65	1.90	3.30E-05	0.91	1.27	2.47E-03	0.26	0.94	272594	233814	1627924	2580653	874285	1307252	2381563	3253832
HILIC_NEG_165_0192a0_927	HILIC	NEG	0.927	165.0192				3.58E-01	0.16	0.47	3.45E-03	-0.61	1.86	4.97E-01	-0.14	0.34	1.95E-02	0.47	0.82	1069857	399687	1151425	527574	1303567	479433	999284	534092
HILIC_NEG_199_978a0_726	HILIC	NEG	0.726	199.9780				5.23E-15	1.04	1.75	3.48E-03	0.58	1.75	1.58E-10	1.34	2.04	2.82E-08	0.75	1.85	1030219	502997	2560853	1480413	2132664	1087188	2989042	1694644
RP_NEG_952_79413a0_49	RP	NEG	0.49	952.7941				2.19E-05	-0.64	1.09	3.52E-03	0.61	1.74	7.07E-02	-0.33	0.65	1.91E-07	-0.95	1.59	941871	210808	695864	408747	578182	365490	813545	419180
HILIC_POS_104_57923a1_471	HILIC	POS	1.471	104.5792				6.05E-01	0.10	0.37	3.53E-03	-0.59	1.69	3.33E-01	-0.19	0.52	1.02E-01	0.40	0.66	564304	324001	599016	343129	698296	404800	499736	232164
RP_POS_676_48987a11_909	RP	POS	11.91	676.4899				1.50E-05	0.54	1.36	3.55E-03	0.65	1.90	1.24E-04	0.87	1.33	5.69E-03	0.22	1.00	211310	252051	725270	1050239	418468	407943	1032071	1367480
HILIC_NEG_128_92851a0_927	HILIC	NEG	0.927	128.9285				1.03E-03	-0.68	1.32	3.56E-03	-0.55	1.62	3.93E-05	-0.95	1.56	6.35E-02	-0.40	0.75	1037518	210685	888576	211988	949511	198031	827641	209765
RP_POS_252_06531a0_782	RP	POS	0.78	252.0653				2.03E-03	0.38	1.07	3.64E-03	0.65	1.78	5.55E-04	0.71	1.11	6.19E-01	0.06	0.44	364301	165279	606749	711470	401544	484255	811954	838016
RP_POS_1032_76379a0_491	RP	POS	0.49	1032.7638				6.81E-02	-0.30	0.59	3.67E-03	0.62	1.74	9.78E-01	0.01	0.15	7.44E-04	-0.61	1.21	357915	147948	293850	227296	228587	182849	359113	249510
HILIC_NEG_323_01358a0_929	HILIC	NEG	0.929	323.0136				2.38E-02	-0.43	1.09	3.68E-03	-0.58	1.64	1.01E-03	-0.72	1.31	5.05E-01	-0.14	0.42	635202	99098	586561	115425	619627	107738	553494	114362
HILIC_POS_467_3479a1_021	HILIC	POS	1.021	467.3479				1.02E-02	0.35	0.83	3.70E-03	0.65	1.73	2.87E-03	0.68	0.93	7.58E-01	0.03	0.14	351827	959461	1121531	2414269	419772	985723	1823290	3130441
RP_POS_798_02966a13_107	RP	POS	13.11	798.0297				2.94E-03	0.41	0.98	3.71E-03	0.63	1.76	8.38E-05	0.73	1.36	5.58E-01	0.10	0.78	543187	128338	660822	314230	570890	291850	750754	312753
RP_POS_754_53717a12_325	RP	POS	12.33	754.5372				6.14E-04	0.50	1.07	3.81E-03	0.63	1.76	2.51E-04	0.81	1.24	1.45E-01	0.19	0.70	1292226	861356	2129362	1822053	1604456	1044737	2654269	2248050
HILIC_NEG_257_10077a0_721	HILIC	NEG	0.721	257.1008				2.24E-05	0.50	1.21	3.81E-03	0.65	1.87	1.68E-04	0.83	1.16	2.43E-02	0.18	0.68	5944	10017	170102	368459	63595	175029	276610	469583
HILIC_NEG_206_9729a5_429	HILIC	NEG	5.429	206.9729				8.81E-02	-0.27	0.55	3.82E-03	-0.62	1.61	4.75E-03	-0.58	0.96	8.02E-01	0.04	0.53	517310	29052	504923	50262	519283	42066	490564	53979
RP_NEG_181_05008a3_115	RP	NEG	3.12	181.0501				3.98E-03	0.50	0.80	3.91E-03	0.59	1.70	3.26E-04	0.80	1.20	2.39E-01	0.21	0.51	2355798	978333	3007592	1344196	2623783	1022398	3391402	1518114
RP_NEG_195_1024a7_839	RP	NEG	7.84	195.1024				2.07E-02	-0.50	1.20	4.00E-03	-0.54	1.71	8.46E-04	-0.77	1.42	3.31E-01	-0.23	0.89	1073999	831040	679780	746434	892011	802558	467549	624240
RP_POS_168_98039a11_211	RP	POS	11.21	168.9804				4.89E-02	-0.40	0.81	4.00E-03	-0.57	1.71	4.46E-03	-0.68	1.09	5.82E-01	-0.11	0.78	5412281	476684	5215146	497485	5356803	384195	5073488	558100
RP_POS_770_60443a13_97	RP	POS	13.97	770.6044				4.62E-01	-0.15	0.53	4.01E-03	-0.58	1.75	4.43E-02	-0.43	0.81	5.34E-01	0.14	0.43	3067138	1518755	2835429	1602384	3290541	1664396	2380318	1412355
RP_POS_626_35352a8_826	RP	POS	8.83	626.3535				4.20E-02	0.34	0.64	4.02E-03	0.61	1.69	5.06E-03	0.65	0.98	7.96E-01	0.04	0.50	257845	493427	491989	721805	285300	421940	698677	887367
RP_POS_350_30484a11_274	RP	POS	11.27	350.3048				1.68E-10	0.90	1.77	4.09E-03	0.59	1.73	1.19E-08	1.19	1.90	2.12E-05	0.60	1.60	200983	125844	463033	302433	377045	225835	549021	344540
RP_POS_245_07646a0_708	RP	POS	0.71	245.0765				5.85E-02	0.29	0.51	4.17E-03	0.62	1.70	4.29E-03	0.60	1.00	8.96E-01	-0.02	0.69	2310812	358320	2486438	663593	2298268	505412	2674607	749664
RP_NEG_918_5495a12_958	RP	NEG	12.96	918.5495				3.30E-07	-0.96	1.65	4.18E-03	-0.54	1.71	1.96E-08	-1.23	2.02	3.30E-04	-0.69	1.38	6035673	948468	4875347	1144921	5199124	1023132	4551570	1178007
RP_POS_351_25034a10_53	RP	POS	10.53	351.2503				4.15E-06	0.56	1.12	4.22E-03	0.63	1.84	3.03E-05	0.88	1.38	2.43E-02	0.25	0.95	369196	193089	943823	1138125	620276	728895	1267371	1368271
HILIC_POS_159_07652a6_376	HILIC	POS	6.376	159.0765				1.00E-07	0.74	1.19	4.28E-03	0.60	1.68	5.69E-07	1.04	1.55	1.58E-03	0.44	1.04	1951951	647040	3056579	1579998	2609450	1167039	3503708	1809349
RP_NEG_162_8383a0_549	RP	NEG	0.55	162.8383				1.50E-01	-0.27	0.53	4.32E-03	-0.58	1.82	9.29E-03	-0.56	0.98	9.14E-01	0.02	0.47	6731821	1741835	6189161	2086685	6776860	1970218	5601463	2052007
RP_POS_222_01857a1_586	RP	POS	1.59	222.0186				5.23E-08	0.65	1.22	4.34E-03	0.63	1.73	3.73E-06	0.96	1.43	2.30E-03	0.34	0.97	212016	100851	1977322	2991534	1130279	2015379	2824365	3543330
HILIC_NEG_341_00436a0_931	HILIC	NEG	0.931	341.0044				2.45E-02	-0.46	1.06	4.38E-03	-0.55	1.62	1.05E-03	-0.74	1.30	4.07E-01	-0.19	0.50	632147	120282	575657	119534	609284	122115	542030	107929
RP_POS_856_58228a13_294	RP	POS	13.29	856.5823				2.86E-04	0.60	1.11	4.40E-03	0.59	1.67	1.00E-04	0.90	1.37	4.15E-02	0.30	0.84	1110551	731112	1763781	1140613	1440114	645243	2087448	1413652
HILIC_NEG_142_92879a0_925	HILIC	NEG	0.925	142.9288				1.25E-06	-0.97	1.75	4.46E-03	-0.52	1.58	2.49E-08	-1.23	2.07	7.62E-04	-0.71	1.42	2186885	392643	1745530	420971	1863730	424704	1627330	386217
RP_POS_422_76144a12_957	RP	POS	12.96	422.7614				1.17E-09	-1.04	1.82	4.51E-03	-0.54	1.72	1.30E-10	-1.31	2.18	2.68E-05	-0.77	1.54	3701185	531714	2854025	785606	3074307	738813	2633743	775936
RP_NEG_1085_68042a10_512	RP	NEG	10.51	1085.6804				1.60E-02	0.47	1.11	4.55E-03	-0.57	1.66	3.96E-01	0.18	0.61	4.94E-04	0.75	1.36	2246321	737805	2629715	829102	2862031	750156	2397400	846150
RP_POS_833_52869a12_953	RP	POS	12.95	833.5287				1.93E-10	-1.16	2.00	4.55E-03	-0.51	1.73	1.00E-11	-1.41	2.34	2.47E-06	-0.90	1.66	2085860	485333	1287635	633515	1465069	612002	1110200	609980
HILIC_NEG_141_92377a0_925	HILIC	NEG	0.925	141.9238				1.83E-07	-1.12	1.88	4.56E-03	-0.49	1.66	5.89E-09	-1.36	2.18	5.24E-05	-0.88	1.54	187964	63884	110535	59941	127322	57821	93749	57800
RP_POS_780_04431a13_025	RP	POS	13.03	780.0443				1.54E-15	1.08	1.76	4.57E-03	0.56	1.69	5.72E-12	1.36	2.10	1.49E-07	0.80	1.57	244604	192900	813603	524076	666763	452092	960444	553647
HILIC_NEG_174_83954a3_03	HILIC	NEG	3.03	174.8395				6.48E-02	-0.24	1.19	4.60E-03	-0.63	1.54	3.45E-03	-0.56	1.36	6.43E-01	0.07	1.00	2363532	84990	2309727	246752	2378845	206722	2240609	265579
RP_NEG_383_15402a7_66	RP	NEG	7.66	383.1540				1.70E-05	0.57	1.08	4.61E-03	0.62	1.78	6.21E-05	0.88	1.25	1.66E-02	0.26	0.82	524006	379819	1104922	1113005	790447	606040	1419398	1390587
RP_POS_351_24969a10_403	RP	POS	10.40	351.2497				1.51E-01	0.27	0.69	4.64E-03	0.58	1.74	1.44E-02	0.56	0.91	8.96E-01	-0.02	0.56	1284557	329885	1387469	401831	1274885	316258	1500053	447600
HILIC_NEG_134_89471a1_21	HILIC	NEG	1.21	134.8947				1.42E-04	0.55	1.04	4.65E-03	0.61	1.60	6.31E-05	0.85	1.39	7.68E-02	0.25	0.83	4220295	835953	5138692	1803532	4632059	1243516	5645326	2121715
RP_POS_916_65485a11_15	RP	POS	11.15	916.6549				7.69E-04	0.44	1.14	4.78E-03	-0.62	1.81	2.89E-01	0.13	0.62	3.65E-04	0.75	1.35	373636	73050	464321	229365	528635	275093	400008	148905
RP_NEG_239_09262a7_84	RP	NEG	7.84	239.0926				1.99E-02	-0.50	1.19	4.85E-03	-0.53	1.68	8.56E-04	-0.77	1.41	3.20E-01	-0.24	0.89	23778995	18113508	15105789	16505336	19702639	17714357	10508939	13910031
RP_POS_532_3736a11_171	RP	POS	11.17	532.3736				8.59E-06	-1.11	1.80	4.88E-03	-0.44	1.78	3.51E-07	-1.32	2.05	4.84E-04	-0.89	1.48	1316804	535851	800106	365087	901968	419670	698245	268326
RP_POS_257_14951a5_025	RP	POS	5.03	257.1495				4.43E-04	0.59	1.24	4.89E-03	0.58	1.74	3.63E-05	0.88	1.48	9.16E-02	0.30	0.84	299340	423653	662000	646998	481966	539383	842033	699053
RP_NEG_193_81514a0_564	RP	NEG	0.56	193.8151				2.84E-02	-0.35	0.77	4.94E-03	-0.60	1.83	1.01E-03	-0.65	1.23	8.01E-01	-0.05	0.72	4455357	582734	4135566	999917	4413182	929064	3857950	999812
RP_POS_395_2417a12_981	RP	POS	12.98	395.2417				5.53E-17	1.15	1.89	4.94E-03	0.54	1.65	8.43E-13	1.42	2.18	8.32E-09	0.88	1.84	193302	180387	738757	461585	610500	393816	867013	491739
HILIC_NEG_286_01492a0_928	HILIC	NEG	0.928	286.0149				1.30E-08	0.69	1.35	5.06E-03	0.61	1.85	1.80E-06	1.00	1.46	7.73E-04	0.39	1.05	56984	61914	346391	457750	218990	312290	473792	541014
RP_POS_764_55731a12_946	RP	POS	12.95	764.5573				2.13E-01	0.23	1.14	5.07E-03	-0.58	1.64	7.73E-01	-0.06	0.52	2.01E-02	0.52	1.13	2677401	1334458	3037331	1616750	3485363	1734997	2589299	1364271
RP_POS_878_58411a14_752	RP	POS	14.75	878.5841				3.69E-03	0.50	0.98	5.14E-03	0.58	1.68	4.64E-04	0.79	1.15	2.20E-01	0.20	0.52	1244171	993906	1925077	1441047	1524917	1015700	2325237	1684391
RP_POS_490_15332a4_587	RP	POS	4.59	490.1533				8.01E-01	-0.04	0.69	5.16E-03	0.61	1.64	2.48E-01	0.26	0.63	1.56E-02	-0.34	1.16	19661702	5764448	19307739	9627107	16617066	4753230	21998413	12242782
RP_POS_292_64673a10_374	RP	POS	10.37	292.6467				5.71E-01	0.11	0.97	5.18E-03	-0.57	1.83	4.15E-01	-0.18	0.75	6.19E-02	0.39	0.99	2365060	345746	2406598	398889	2516775	364113	2296421	405118
RP_POS_381_27661a11_41	RP	POS	11.41	381.2766				6.74E-08	0.69	1.49	5.20E-03	0.61	1.64	8.65E-06	0.99	1.51	5.20E-05	0.39	1.53	356792	272434	994485	1002828	714362	482707	1274609	1280119
RP_NEG_203_0202a0_525	RP	NEG	0.53	203.0202				5.86E-01	-0.08	0.65	5.22E-03	-0.61	1.64	4.35E-02	-0.39	0.77	2.15E-01	0.22	0.78	1205407	199618	1177313	374050	1280530	344217	1074095	377431
RP_NEG_307_0806a7_839	RP	NEG	7.84	307.0806				1.77E-02	-0.51	1.19	5.24E-03	-0.53	1.65	7.40E-04	-0.78	1.42	2.99E-01	-0.25	0.87	1051182	758842	680287	693980	871955	750305	488618	578891
RP_POS_546_35522a10_396	RP	POS	10.40	546.3552				7.28E-03	0.52	1.16	5.27E-03	-0.55	1.65	2.57E-01	0.25	0.71	2.07E-04	0.80	1.40	8829750	3648121	10950161	4059378	12069473	3632932	9830848	4187880
HILIC_NEG_315_04214a5_429	HILIC	NEG	5.429	315.0421				5.05E-01	0.15	0.72	5.32E-03	0.53	1.75	9.46E-02	0.41	0.67	6.19E-01	-0.12	0.33	9734853	1826115	9975672	1562687	9545245	1398780	10406098	1612184
RP_POS_219_17447a10_407	RP	POS	10.41	219.1745				2.66E-01	-0.23	0.61	5.35E-03	0.55	1.61	8.43E-01	0.05	0.33	2.55E-02	-0.50	0.82	1496251	119509	1469006	118531	1436385	109009	1501627	119713
RP_NEG_556_29852a10_328	RP	NEG	10.33	556.2985				9.07E-03	-0.62	1.25	5.37E-03	-0.49	1.70	9.59E-04	-0.86	1.37	1.19E-01	-0.37	0.92	1244444	231933	1122368	177407	1171221	149654	1073514	190582
RP_POS_616_85449a0_493	RP	POS	0.49	616.8545				1.91E-01	-0.21	0.58	5.39E-03	0.60	1.71	6.54E-01	0.09	0.38	2.04E-03	-0.51	1.13	1719770	321552	1615507	551467	1463283	400719	1767731	637630
RP_POS_811_57617a11_162	RP	POS	11.16	811.5762				9.33E-03	0.31	0.95	5.41E-03	-0.63	1.75	9.48E-01	-0.01	0.70	1.96E-03	0.62	1.25	617096	44400	729402	416763	844466	488818	614337	291487
RP_POS_742_53693a13_288	RP	POS	13.29	742.5369				5.71E-01	0.10	0.30	5.47E-03	0.58	1.68	1.01E-01	0.39	0.60	2.75E-01	-0.19	0.53	912198	858089	1017837	1069867	721351	585178	1314323	1338194
RP_POS_478_38901a15_435	RP	POS	15.44	478.3890				7.09E-01	-0.09	0.39	5.53E-03	-0.51	1.77	1.55E-01	-0.34	0.65	5.32E-01	0.17	0.40	10341445	4736219	9999366	3571702	10982121	4105146	9016611	2636513
HILIC_POS_202_08626a0_5	HILIC	POS	0.5	202.0863				1.32E-01	0.25	0.52	5.55E-03	-0.59	1.48	7.70E-01	-0.05	0.11	9.94E-03	0.54	0.85	616719	403976	762711	642885	939132	699986	586289	530599
HILIC_NEG_127_05118a6_093	HILIC	NEG	6.093	127.0512				3.12E-01	-0.16	0.93	5.56E-03	-0.60	1.52	2.07E-02	-0.46	0.95	4.52E-01	0.14	1.11	426936	92607	404063	154517	446404	140817	361722	157322
HILIC_NEG_337_02905a0_929	HILIC	NEG	0.929	337.0291				1.18E-01	-0.31	0.91	5.64E-03	-0.55	1.60	9.32E-03	-0.58	1.04	8.87E-01	-0.03	0.27	356204	71708	332601	77819	353887	72476	311315	77831
RP_POS_208_00293a1_583	RP	POS	1.58	208.0029				1.12E-07	0.63	1.22	5.65E-03	0.61	1.68	7.63E-06	0.94	1.40	2.40E-03	0.33	0.97	169726	55927	1289309	1954602	751492	1283086	1827125	2341430
RP_POS_801_98657a10_326	RP	POS	10.33	801.9866				5.29E-04	-0.84	1.50	5.76E-03	-0.46	1.72	4.31E-05	-1.07	1.69	1.25E-02	-0.61	1.17	2365960	787885	1800905	569895	1956455	525249	1645355	575260
RP_POS_584_29944a10_296	RP	POS	10.30	584.2994				5.12E-01	0.13	0.78	5.78E-03	-0.56	1.72	4.86E-01	-0.15	0.51	6.35E-02	0.41	0.98	323110	149876	343679	164884	388652	158997	298706	159751
RP_NEG_261_97763a2_998	RP	NEG	3.00	261.9776				6.62E-14	0.94	1.53	5.91E-03	0.57	1.62	1.71E-09	1.23	1.86	1.21E-06	0.66	1.47	608091	386751	2290937	1862742	1782852	1458767	2799022	2087004
HILIC_NEG_157_03674a1_818	HILIC	NEG	1.818	157.0367				3.86E-03	0.46	0.85	5.95E-03	0.59	1.66	4.96E-04	0.75	1.19	3.06E-01	0.16	0.60	308954	106512	386984	183896	336822	137257	437145	210597

Supplementary table 1: Metabolomics results (in asceding order according to p-value from progressive ALD vs non-progressive ALD comparison, with molecular features with ID_level of 1-2 first)

								all_ALD_vs_control			Prog_ALD_vs_non-prog_ALD			Prog_ALD_vs_control_ALD			Non-prog_ALD_vs_control			Healthy_control		all_ALD		Non-prog_ALD		Progressive_ALD	
								t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA								
Feature_ID	RP_HILIC	POS_NEG	Average.Rt	Average.Mz	Metabolite.name	curated_MSMS	ID_level	p	d	VIP	p	d	VIP	p	d	VIP	p	d	VIP	Mean	SD	Mean	SD	Mean	SD	Mean	SD
HILIC_NEG_226_99448a0_929	HILIC	NEG	0.929	226.9945				6.45E-02	-0.38	1.02	6.02E-03	-0.54	1.60	3.84E-03	-0.65	1.14	6.27E-01	-0.11	0.38	1323802	252943	1226761	253279	1295550	260254	1157972	228517
RP_POS_345_17273a10_821	RP	POS	10.82	345.1727				3.83E-09	1.02	1.89	6.04E-03	0.52	1.85	4.06E-09	1.28	2.03	9.94E-06	0.76	1.76	1422353	1076885	3058951	1550650	2637006	1203466	3480895	1745403
RP_POS_191_0004a1_358	RP	POS	1.36	191.0004				4.71E-08	0.65	1.20	6.08E-03	0.60	1.68	5.70E-06	0.95	1.42	1.13E-03	0.35	1.05	38571	15964	1100056	1793701	610655	1169403	1589457	2155012
RP_POS_930_78479a0_49	RP	POS	0.49	930.7848				8.15E-06	-0.71	1.15	6.13E-03	0.57	1.65	2.56E-02	-0.42	0.77	1.20E-07	-0.99	1.62	820052	199780	586825	344433	493461	308938	680190	355609
RP_NEG_197_80746a0_564	RP	NEG	0.56	197.8075				8.72E-06	-0.74	1.16	6.17E-03	-0.56	1.78	1.61E-06	-1.02	1.57	7.33E-03	-0.46	0.99	105387688	13311902	90586550	20438971	96128107	16969485	85044993	22212474
RP_POS_566_41052a11_538	RP	POS	11.54	566.4105				1.57E-07	-1.46	2.54	6.19E-03	-0.31	1.62	2.09E-08	-1.62	2.36	1.50E-06	-1.31	2.17	1419913	724154	558200	335164	648910	328360	467489	319921
HILIC_NEG_394_05457a6_093	HILIC	NEG	6.093	394.0546				1.51E-01	-0.22	0.96	6.20E-03	-0.59	1.49	1.12E-02	-0.52	0.99	6.61E-01	0.07	1.09	147755	31628	136250	56617	151591	47155	120909	61421
RP_POS_340_16956a10_822	RP	POS	10.82	340.1696				1.44E-09	1.05	1.93	6.20E-03	0.52	1.83	1.46E-09	1.31	2.07	4.37E-06	0.79	1.78	1476986	1112626	3219745	1579912	2791269	1248613	3648220	1763371
RP_POS_190_99989a1_584	RP	POS	1.58	190.9999				1.40E-07	0.63	1.18	6.25E-03	0.60	1.66	6.01E-06	0.93	1.40	4.89E-03	0.33	0.93	53318	29491	1313627	2221543	710404	1575756	1916850	2597230
RP_POS_389_33591a10_383	RP	POS	10.38	389.3359				6.79E-02	-0.35	0.95	6.26E-03	0.56	1.65	7.57E-01	-0.07	0.59	2.63E-03	-0.62	1.20	2083456	315313	1959140	369287	1859239	319501	2059040	391255
RP_POS_343_1777a10_821	RP	POS	10.82	343.1777				8.06E-09	1.01	1.88	6.30E-03	0.52	1.83	6.03E-09	1.27	2.02	1.66E-05	0.75	1.73	4061285	3094324	8613808	4352747	7435457	3418597	9792158	4874318
HILIC_POS_597_36407a0_504	HILIC	POS	0.504	597.3641				4.02E-02	0.31	0.83	6.31E-03	0.60	1.47	6.66E-03	0.61	1.06	9.24E-01	0.01	0.05	342972	803770	776281	1525046	360858	863452	1191705	1897696
RP_POS_621_44031a10_832	RP	POS	10.83	621.4403				3.64E-10	1.20	2.07	6.33E-03	0.48	1.73	1.97E-10	1.44	2.13	1.95E-07	0.96	2.00	299039	162129	556278	190825	504591	141139	607965	219543
RP_POS_355_26041a11_273	RP	POS	11.27	355.2604				7.98E-10	0.86	1.75	6.40E-03	0.56	1.70	8.68E-08	1.14	1.83	2.15E-05	0.57	1.67	1978773	1381941	4760048	3382804	3843849	2353950	5676246	3983225
RP_POS_829_55212a12_957	RP	POS	12.96	829.5521				1.29E-09	-1.08	1.94	6.44E-03	-0.51	1.65	1.31E-10	-1.33	2.24	1.09E-05	-0.83	1.61	52700672	7731029	40672440	10473719	43494239	9886666	37850641	10374972
HILIC_NEG_229_98845a0_727	HILIC	NEG	0.727	229.9885				1.36E-13	0.98	1.68	6.54E-03	0.55	1.62	9.26E-10	1.26	1.96	4.12E-07	0.71	1.69	842204	423032	2059390	1267019	1717789	977495	2400992	1431709
RP_POS_251_04604a10_284	RP	POS	10.28	251.0460				3.37E-01	-0.20	0.68	6.59E-03	0.54	1.60	7.66E-01	0.07	0.46	3.09E-02	-0.47	0.95	1003287	64667	990578	64090	973325	51143	1007832	71245
RP_POS_223_09645a7_844	RP	POS	7.84	223.0965	Unknown	223.0948(100)	4	6.23E-03	-0.60	1.30	6.66E-03	-0.50	1.61	3.12E-04	-0.85	1.49	1.40E-01	-0.35	0.99	27130613	12457396	20082777	11010406	23038904	11479800	17126649	9762800
HILIC_NEG_162_98238a0_927	HILIC	NEG	0.927	162.9824				9.20E-02	-0.34	0.97	6.70E-03	-0.54	1.56	5.68E-03	-0.61	1.10	7.66E-01	-0.07	0.41	657789	123524	614173	130398	649153	134198	579194	117679
RP_POS_311_15125a10_822	RP	POS	10.82	311.1513				2.32E-09	1.03	1.89	6.75E-03	0.52	1.83	3.07E-09	1.28	2.04	6.94E-06	0.77	1.74	1254997	969944	2759894	1414479	2380046	1106103	3139742	1588839
HILIC_POS_169_05852a6_129	HILIC	POS	6.129	169.0585				7.90E-02	-0.30	1.04	6.78E-03	-0.57	1.49	5.91E-03	-0.58	1.05	9.52E-01	-0.01	0.86	21744044	4745749	19801250	6981927	21672636	5965768	17929865	7466723
HILIC_POS_103_63889a1_471	HILIC	POS	1.471	103.6389				6.10E-01	0.10	0.29	6.78E-03	-0.54	1.58	3.95E-01	-0.17	0.55	1.24E-01	0.37	0.61	585514	326288	619833	339986	711302	401431	528363	235200
HILIC_POS_326_03983a2_981	HILIC	POS	2.981	326.0398				7.87E-10	0.93	1.60	6.80E-03	0.54	1.67	2.43E-08	1.20	1.78	6.77E-06	0.66	1.50	841652	380565	1515751	732649	1318734	512202	1712767	861938
RP_POS_122_05782a1_855	RP	POS	1.86	122.0578				8.44E-07	0.59	0.97	6.86E-03	0.60	1.60	1.43E-05	0.89	1.44	1.26E-02	0.29	0.75	111468	177108	1047211	1759163	574797	1248680	1519626	2058592
RP_POS_1061_65332a10_324	RP	POS	10.32	1061.6533				3.96E-03	-0.71	1.37	6.88E-03	-0.46	1.79	3.81E-04	-0.94	1.52	5.70E-02	-0.48	1.02	5892145	2406965	4492884	1706694	4949078	1628166	4036689	1676130
RP_POS_389_19781a11_277	RP	POS	11.28	389.1978				2.36E-11	0.97	1.84	6.92E-03	0.54	1.67	4.81E-09	1.24	1.95	1.15E-06	0.70	1.74	418925	223942	882294	483392	752673	349986	1011915	561539
RP_POS_760_82007a0_495	RP	POS	0.50	760.8201				5.66E-04	-0.56	0.97	6.94E-03	0.56	1.58	1.25E-01	-0.28	0.55	2.42E-05	-0.85	1.34	2262916	358104	1958016	568117	1806298	563931	2109734	535824
RP_POS_998_76965a0_49	RP	POS	0.49	998.7697				1.65E-02	-0.40	0.76	6.95E-03	0.57	1.61	5.75E-01	-0.11	0.27	2.56E-04	-0.68	1.28	469064	161000	376926	246098	311163	210564	442688	263062
RP_POS_421_255a13_292	RP	POS	13.29	421.2550				2.18E-01	-0.26	0.67	6.96E-03	0.52	1.78	9.98E-01	0.00	0.91	2.91E-02	-0.52	0.79	1578407	594610	1430089	554062	1282128	573585	1578051	496544
RP_POS_313_14688a10_822	RP	POS	10.82	313.1469				2.44E-09	1.06	1.93	7.02E-03	0.51	1.80	1.60E-09	1.31	2.07	5.41E-06	0.81	1.78	429146	351453	964846	479550	836724	387346	1092969	530180
RP_POS_502_29034a10_63	RP	POS	10.63	502.2903				1.87E-02	0.42	1.06	7.02E-03	0.56	1.93	1.78E-03	0.70	1.22	4.36E-01	0.14	0.86	4630983	1347422	5344726	1763579	4873445	1396151	5816006	1970123
HILIC_NEG_243_96837a0_93	HILIC	NEG	0.93	243.9684				1.88E-02	0.43	0.76	7.05E-03	-0.55	1.88	4.91E-01	0.15	0.26	2.91E-04	0.70	1.36	218331	59457	249494	75323	269621	58768	229368	84751
RP_POS_402_77249a13_069	RP	POS	13.07	402.7725				9.86E-01	0.00	0.55	7.14E-03	-0.54	1.66	2.03E-01	-0.28	0.94	2.28E-01	0.27	0.76	3618290	886716	3615013	961331	3870893	963118	3359133	897752
RP_POS_854_81024a0_494	RP	POS	0.49	854.8102				8.98E-03	-0.39	0.73	7.16E-03	0.58	1.63	6.13E-01	-0.10	0.24	3.99E-05	-0.68	1.36	6761107	759689	6228004	1484795	5832148	1174380	6623860	1659897
HILIC_NEG_257_98428a0_929	HILIC	NEG	0.929	257.9843				5.11E-01	0.13	0.70	7.25E-03	-0.55	1.72	4.98E-01	-0.15	0.31	5.64E-02	0.40	0.70	243775	76059	254370	87491	277621	78458	231119	90592
HILIC_NEG_353_99582a7_369	HILIC	NEG	7.369	353.9958				9.39E-01	-0.02	0.44	7.27E-03	-0.54	1.76	1.97E-01	-0.29	0.61	2.54E-01	0.25	0.45	445145	17313	444870	18254	449718	17954	440022	17404
HILIC_POS_368_21997a2_225	HILIC	POS	2.225	368.2200				1.74E-01	-0.28	0.88	7.34E-03	-0.53	1.49	1.67E-02	-0.55	1.04	9.32E-01	-0.02	0.50	1251979	352776	1153749	344692	1245192	346981	1062305	320295
HILIC_POS_566_32043a1_198	HILIC	POS	1.198	566.3204				1.80E-01	0.29	0.56	7.40E-03	-0.52	1.43	8.96E-01	0.03	0.06	1.79E-02	0.55	1.04	1276025	549130	1424713	500132	1557333	439468	1292093	525684
RP_POS_416_36465a12_743	RP	POS	12.74	416.3647				8.05E-01	0.04	0.80	7.48E-03	0.59	1.59	1.39E-01	0.33	1.21	7.71E-02	-0.25	0.74	898169	337595	919019	597079	759701	345473	1078337	741033
RP_POS_372_1951a10_821	RP	POS	10.82	372.1951				2.51E-09	1.03	1.89	7.53E-03	0.51	1.84	4.99E-09	1.28	2.02	4.53E-06	0.77	1.78	808057	599953	1733922	865889	1504196	645753	1963648	995052
RP_POS_512_2674a9_944	RP	POS	9.94	512.2674				4.72E-04	0.46	0.83	7.59E-03	0.59	1.58	5.54E-04	0.76	1.12	1.30E-01	0.16	0.61	537953	340144	966674	1032831	691333	567994	1242016	1295342
RP_NEG_865_09442a9_304	RP	NEG	9.30	865.0944				1.86E-02	-0.41	0.73	7.60E-03	-0.55	1.60	6.22E-04	-0.69	1.24	5.00E-01	-0.14	0.31	1738628	153735	1655938	209519	1711286	211195	1600589	194517
HILIC_POS_123_04765a0_765	HILIC	POS	0.765	123.0477				3.35E-05	0.49	1.17	7.64E-03	0.60	1.45	3.44E-04	0.79	1.12	1.26E-02	0.19	0.78	49340	34065	393518	789918	182531	361318	604506	1019448
RP_POS_255_12279a7_844	RP	POS	7.84	255.1228				1.75E-02	-0.52	1.21	7.79E-03	-0.50	1.60	1.04E-03	-0.77	1.39	2.57E-01	-0.27	0.91	13791479	10696638	8582118	9502410	11086091	10028518	6078145	8310687
RP_POS_358_07092a7_844	RP	POS	7.84	358.0709				1.45E-02	-0.53	1.21	7.81E-03	-0.50	1.59	8.17E-04	-0.78	1.40	2.37E-01	-0.28	0.92	1433427	1067723	896030	964124	1150010	1015386	642050	845805
RP_POS_241_10696a7_844	RP	POS	7.84	241.1070				2.09E-02	-0.51	1.19	7.82E-03	-0.50	1.60	1.31E-03	-0.76	1.37	2.79E-01	-0.26	0.90	3059994	2444822	1907469	2144035	2472214	2269377	1342724	1867251
RP_POS_429_37338a12_232	RP	POS	12.23	429.3734				6.74E-02	-0.33	0.87	7.82E-03	-0.55	1.58	4.02E-03	-0.61	1.19	7.75E-01	-0.06	0.24	1375291	280918	1261596	356474	1355419	342829	1167772	348201
HILIC_NEG_180_97351a5_428	HILIC	NEG	5.428	180.9735				1.39E-01	-0.32	0.83	7.83E-03	-0.51	1.43	1.66E-02	-0.57	0.92	7.96E-01	-0.06	0.43	397133	28017	388728	26003	395572	24049	381884	26308
RP_POS_122_05779a2_25	RP	POS	2.25	122.0578				2.00E-06	0.57	0.96	8.05E-03	0.59	1.56	3.17E-05	0.86	1.40	1.42E-02	0.28	0.76	105695	153097	921324	1596913	500370	1083523	1342279	1901747
RP_POS_856_58337a12_751	RP	POS	12.75	856.5834				3.49E-01	0.19	0.72	8.08E-03	-0.52	1.55	7.63E-01	-0.07	0.46	5.44E-02	0.46	0.84	764211	496092	858860	483762	985761	505825	731960	429072
RP_POS_325_1124a0_548	RP	POS	0.55	325.1124				3.32E-03	0.37	0.69	8.08E-03	0.60	1.68	3.13E-03	0.67	1.02	3.76E-01	0.07	0.80	3373037	586612	4151935	2386023	3517504	883092	4786366	3146604
RP_POS_825_5556a10_463	RP	POS	10.46	825.5556				6.07E-01	-0.11	0.63	8.19E-03	-0.51	1.64	1.02E-01	-0.37	0.83	5.49E-01	0.15	0.64	783140	241292	758303	220643	816152	243789	700455	179158
RP_POS_830_5556a12_954	RP	POS	12.95	830.5556				1.08E-09	-1.14	2.03	8.19E-03	-0.48	1.63	7.62E-11	-1.38	2.29	3.89E-06	-0.90	1.71	15484561	2704194	11323878	3333223	12196241	3208100	10451516	3256147
RP_POS_263_08887a7_844	RP	POS	7.84	263.0889	C14H14O5 similar to methyl 2-((4-methyl-2-oxo-2H-chromen-7-yl)oxy)propanoate (ALDH2 inhibitor)	263.0868(100)	3	1.77E-02	-0.53	1.21	8.22E-03	-0.49	1.60	1.16E-03	-0.77	1.38	2.44E-01	-0.28	0.91	15432619	12264530	9497393	10625315	12278943	11183806	6715843	9339770
HILIC_POS_172_09676a3_999	HILIC	POS	3.999	172.0968				1.13E-05	0.61	1.05	8.24E-03	0.57	1.67	2.46E-05	0.89	1.40	1.63E-02	0.32	0.79	424844	310795	859597	774932	656020	541288	1063174	914180
RP_POS_790_53442a12_671	RP	POS	12.67	790.5344				3.41E-04	0.60	1.07	8.25E-03	0.55	1.58	6.48E-05	0.87	1.37	5.33E-02	0.33	1.18	1500895	490846	1928520	742981	1733708	570748	2123332	843862
RP_POS_532_33722a10_73	RP	POS	10.73	532.3372				1.35E-06	-1.16	1.95	8.27E-03	-0.41	1.79	6.84E-08	-1.37	2.11	8.24E-05	-0.96	1.58	6027189	2219095	3638876	1620976	4062930	1716580	3214822	1412488
RP_NEG_197_80789a1_453	RP	NEG	1.45	197.8079				4.19E-01	0.15	0.55	8.32E-03	-0.54	1.79	5.80E-01	-0.12	0.62	4.89E-02	0.42	0.75	18767676	6084779	19817703	7113028	21675891	6894686	17959516	6902140
RP_POS_811_54388a13_276	RP	POS	13.28	811.5439				4.18E-01	-0.18	0.47	8.38E-03	0.50	1.63	7.75E-01	0.07	0.89	8.10E-02	-0.43	0.76	953737	558046	864430	470143	741716	475939	987144	435119
HILIC_POS_593_33301a0_5	HILIC	POS	0.5	593.3330				3.73E-03	0.40	0.99	8.39E-03	0.58	1.65	2.02E-03	0.69	0.96	3.10E-01	0.11	0.43	224077	373892	556021	907557	316595	437631	795447	1164310
RP_POS_352_24496a10_385	RP	POS	10.39	352.2450				5.57E-01	-0.12	0.98	8.46E-03	0.53	1.74	5.24E-01	0.15	0.69	5.83E-02	-0.38	1.05	11848734	1900462	11615940	2053213	11078861	1510429	12153019	2376409
RP_POS_485_35934a12_428	RP	POS	12.43	485.3593				4.62E-02	-0.38	1.29	8.47E-03	-0.54	1.57	4.58E-03	-0.64	1.29	5.83E-01	-0.11	0.63	2492355	467240	2290171	552181	2434290	460159	2146051	601577
HILIC_NEG_312_83673a3_956	HILIC	NEG	3.956	312.8367				2.53E-01	0.20	0.94	8.51E-03	-0.55	1.45	7.33E-01	-0.07	0.22	2.17E-02	0.48	1.04	1218792	430618	1327690	559361	1473406	547942	1181973	537197
RP_POS_181_08603a7_843	RP	POS	7.84	181.0860				1.82E-02	-0.52	1.20	8.53E-03	-0.49	1.59	1.20E-03	-0.77	1.37	2.51E-01	-0.27	0.91	11490341	8999932	7147131	7884944	9201531	8267206	5092732	6975202
RP_POS_820_58307a13_876	RP	POS	13.88	820.5831				1.30E-02	0.50	0.97	8.62E-03	0.52	1.55	6.23E-04	0.76	1.31	2.79E-01	0.24	0.69	4685755	1686392	5575777	1770476	5115199	1817582	6036356	1611402
RP_POS_792_04407a12_816	RP	POS	12.82	792.0441				3.02E-02	0.40	0.81	8.69E-03	-0.54	1.68	4.77E-01	0.14	0.52	3.26E-03	0.67	1.12	1033104	582754	1310117	706649	1494092	789152	1126143	563081
HILIC_NEG_276_992a0_93	HILIC	NEG	0.93	276.9920				5.04E-01	-0.13	0.83	8.74E-03	-0.52	1.47	7.67E-02	-0.40	0.67	5.68E-01	0.13	0.27	702126	129778	684271	134039	719071	131495	649471	128597
RP_POS_991_67065a10_375	RP	POS	10.38	991.6707				8.67E-02	0.32	1.03	8.83E-03	-0.53	1.65	7.95E-01	0.05	0.63	6.38E-03	0.59	1.20	7817987	4633030	9536605	5513072	10965990	5412943	8107221	5285698
RP_POS_421_7709a14_746	RP	POS	14.75	421.7709				3.42E-05	0.60	1.04	8.84E-03	0.56	1.57	4.61E-05	0.88	1.30	1.94E-02	0.32	0.89	978925	658453	1768356	1410504	1400742	940435	2135970	1690986
RP_POS_817_55908a12_956	RP	POS	12.96	817.5591				7.36E-08	-1.03	1.88	8.87E-03	-0.48	1.60	3.95E-09	-1.27	2.15	8.03E-05	-0.79	1.52	8043150	1994345	5454021	2328051	6057308	2248583	4850735	2269662
HILIC_NEG_117_91902a0_924	HILIC	NEG	0.924	117.9190				2.32E-04	-0.75	1.41	8.93E-03	-0.49	1.48	1.26E-05	-1.00	1.65	1.88E-02	-0.50	0.92	1656600	327707	1392275	335727	1479204	320908	1305346	330637
RP_POS_504_34174a10_775	RP	POS	10.78	504.3417				3.52E-03	-0.67	1.21	8.95E-03	-0.47	1.70	2.09E-04	-0.91	1.53	7.48E-02	-0.44	0.88	3698728	1003344	3097949	808718	3307492	868131	2888406	691474
RP_POS_245_12845a5_215	RP	POS	5.22	245.1285				2.22E-04	0.44	0.81	9.05E-03	0.59	1.54	6.87E-04	0.73	1.14	1.16E-01	0.14	0.61	157986	154646	1106217	2460768	464458	1341734	1747976	3097349
RP_POS_287_13309a10_198	RP	POS	10.20	287.1331				1.28E-02	-0.60	1.29	9.06E-03	-0.46	1.76	1.59E-03	-0.83	1.36	1.30E-01	-0.37	0.95	769626	303558	618719	221131	675882	202101	561557	226457
RP_POS_374_32639a10_959	RP	POS	10.96	374.3264				1.24E-05	0.53	0.98	9.27E-03	0.58	1.65	1.51E-04	0.82	1.20	1.05E-02	0.25	0.94	199382	189097	693245	1028633	425801	559295	960690	1295755
HILIC_POS_141_10233a0_559	HILIC	POS	0.559	141.1023				4.57E-10	0.79	1.26	9.27E-03	0.56	1.51	1.23E-06	1.07	1.48	7.31E-07	0.52	1.56	338553	349501	1356452	1373491	999350	745002	1713553	1730947
RP_POS_279_23154a11_259	RP	POS	11.26	279.2315				8.01E-02	-0.39	0.63	9.36E-03	-0.50	1.65	3.69E-03	-0.64	1.37	5.92E-01	-0.14	0.60	1123613	1124438	727867	971283	980540	1247628	475194	468151
RP_POS_321_23984a10_662	RP	POS	10.66	321.2398				9.85E-03	0.44	1.28	9.48E-03	0.54	1.68	1.10E-03	0.71	1.40	3.36E-01	0.17	0.96	8743920	1481309	9638183	2132306	9089245	1709395	10187120	2376817
RP_NEG_357_28125a11_419	RP	NEG	11.42	357.2813	FA 24:5 (Tetracosapentaenoic acid)	357.2808(100)	3	4.77E-08	0.72	1.55	9.61E-03	0.56	1.53	4.95E-06	1.00	1.56	9.12E-05	0.45	1.49	386592	325185	1039423	967431	789303	558338	1289544	1204795
RP_POS_964_77942a0_491	RP	POS	0.49	964.7794				6.65E-03	-0.44	0.80	9.73E-03	0.55	1.52	3.92E-01	-0.17	0.34	1.19E-04	-0.72	1.27	643614	185086	521413	292732	446385	255118	596440	310741
HILIC_POS_358_25897a1_046	HILIC	POS	1.046	358.2590				1.43E-06	0.65	1.21	9.78E-03	0.56	1.59	1.64E-05	0.93	1.49	2.63E-03	0.37	0.99	398886	172632	684959	476146	562350	303224	807567	579165
RP_POS_377_24228a11_272	RP	POS	11.27	377.2423				1.45E-08	0.82	1.73	9.79E-03	0.54	1.64	3.83E-07	1.09	1.79	8.59E-05	0.55	1.63	422708	343226	1010315	747035	818331	522367	1202298	882850
RP_POS_788_55511a13_105	RP	POS	13.11	788.5551				4.92E-01	-0.17	0.52	9.86E-03	-0.46	1.56	1.17E-01	-0.40	0.65	8.07E-01	0.06	0.40	503879	562890	429443	402829	532508	428605	326379	349962
RP_POS_828_80743a0_494	RP	POS	0.49	828.8074				1.19E-02	-0.41	0.91	9.90E-03	0.55	1.57	4.97E-01	-0.14	0.28	2.18E-04	-0.68	1.32	1576561	268671	1412015	429112	1302271	370813	1521760	458203

Supplementary table 1: Metabolomics results (in asceding order according to p-value from progressive ALD vs non-progressive ALD comparison, with molecular features with ID_level of 1-2 first)

							all_ALD_vs_control			Prog_ALD_vs_non-prog_ALD			Prog_ALD_vs_control_ALD			Non-prog_ALD_vs_control			Healthy_control		all_ALD		Non-prog_ALD		Progressive_ALD	
							t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA								
Feature_ID	RP_HILIC	POS_NEG	Average.Rt	Average.Mz	Metabolite.name	curated_MSMS	ID_level	p	d	VIP	p	d	VIP	p	d	VIP	p	d	VIP	Mean	SD	Mean	SD	Mean	SD	Mean	SD
HILIC_NEG_286_01495a0_712	HILIC	NEG	0.712	286.0150				2.19E-09	0.73	1.31	9.92E-03	0.56	1.73	3.79E-06	1.01	1.49	4.01E-06	0.45	1.46	67573	95983	487214	621912	326971	341138	647456	782728
HILIC_POS_357_68613a1_919	HILIC	POS	1.919	357.6861				1.16E-01	-0.24	1.01	1.01E-02	-0.56	1.40	7.90E-03	-0.52	1.05	8.51E-01	0.03	1.24	674113	137125	619730	242775	681603	222969	557857	248102
HILIC_POS_657_39923a1_223	HILIC	POS	1.223	657.3992				1.80E-01	0.29	0.54	1.01E-02	-0.50	1.38	8.61E-01	0.04	0.07	2.06E-02	0.54	0.98	764956	398620	872863	362371	965223	324472	780503	377642
RP_POS_605_27783a10_198	RP	POS	10.20	605.2778				2.39E-02	-0.53	1.23	1.01E-02	-0.46	1.81	2.95E-03	-0.76	1.32	2.14E-01	-0.30	0.91	560656	199637	470669	152062	509410	143307	431929	152046
RP_POS_529_29218a10_629	RP	POS	10.63	529.2922				1.57E-03	0.54	1.15	1.02E-02	0.53	1.84	1.89E-04	0.81	1.40	1.24E-01	0.27	1.01	433848	184004	571604	265739	503862	220050	639345	291356
RP_POS_375_32016a10_385	RP	POS	10.39	375.3202				4.94E-02	-0.42	1.08	1.03E-02	0.50	1.61	4.96E-01	-0.17	0.63	2.31E-03	-0.66	1.35	1115210	301995	993161	286575	919981	204774	1066342	336252
RP_POS_786_82269a0_494	RP	POS	0.49	786.8227				2.47E-03	-0.45	0.80	1.03E-02	0.55	1.56	3.58E-01	-0.18	0.32	2.35E-05	-0.73	1.36	8508001	904735	7770039	1759821	7321965	1485152	8218112	1908332
RP_NEG_606_36053a10_827	RP	NEG	10.83	606.3605				4.96E-11	0.85	1.78	1.03E-02	0.54	1.65	1.23E-08	1.12	1.92	8.77E-05	0.58	1.59	146785	157786	592951	555445	451617	475526	734286	597028
RP_POS_429_37189a13_84	RP	POS	13.84	429.3719				7.32E-03	-0.56	0.95	1.03E-02	-0.49	1.51	5.42E-04	-0.81	1.36	1.54E-01	-0.32	0.57	2904698	979237	2353945	942502	2593530	908124	2114360	923534
RP_NEG_384_9368a12_889	RP	NEG	12.89	384.9368				3.09E-02	0.40	0.84	1.03E-02	0.53	1.52	1.91E-03	0.66	1.30	5.16E-01	0.13	0.54	2095809	417054	2294913	520184	2162687	502779	2427139	508171
RP_POS_922_79694a0_493	RP	POS	0.49	922.7969				3.61E-01	-0.14	0.59	1.03E-02	0.56	1.63	4.77E-01	0.15	0.45	7.68E-03	-0.42	1.04	3611814	489690	3492026	978803	3242512	732662	3741541	1127746
RP_POS_300_21698a7_727	RP	POS	7.73	300.2170				2.18E-01	0.21	0.82	1.03E-02	0.54	1.68	3.31E-02	0.48	1.20	7.19E-01	-0.06	0.27	1031289	72992	1051844	103769	1025357	71608	1078332	123272
RP_POS_718_57379a13_467	RP	POS	13.47	718.5738				6.72E-05	0.50	0.95	1.04E-02	0.57	1.59	3.97E-04	0.78	1.17	2.04E-02	0.21	0.76	625450	258237	1112125	1087828	832877	528516	1391374	1397290
HILIC_NEG_113_92606a0_924	HILIC	NEG	0.924	113.9261				2.50E-04	-0.78	1.49	1.04E-02	-0.47	1.47	1.21E-05	-1.02	1.71	1.60E-02	-0.54	1.03	2577393	539993	2150718	508830	2279949	516294	2021488	471655
RP_POS_817_05078a12_806	RP	POS	12.81	817.0508				5.06E-02	-0.44	1.01	1.04E-02	-0.47	1.51	5.52E-03	-0.68	1.19	3.94E-01	-0.21	0.63	1016058	484762	826158	400247	927764	401353	724552	376181
RP_NEG_622_33478a10_73	RP	NEG	10.73	622.3348				1.26E-07	-1.19	1.99	1.04E-02	-0.42	1.80	5.26E-09	-1.40	2.19	1.81E-05	-0.98	1.65	1500743	464155	933148	393992	1033187	408622	833108	355291
RP_POS_808_58264a13_877	RP	POS	13.88	808.5826				1.97E-01	0.33	0.81	1.05E-02	0.44	1.56	4.68E-02	0.55	0.95	6.75E-01	0.11	0.22	20554492	22497510	26116782	14670131	22393948	12635815	29839616	15712069
HILIC_NEG_564_33032a1_229	HILIC	NEG	1.229	564.3303				1.18E-01	-0.39	0.86	1.07E-02	-0.45	1.39	2.14E-02	-0.61	1.12	5.24E-01	-0.16	0.41	5193958	2418451	4459746	1676328	4883720	1601085	4035773	1657463
RP_POS_705_59076a13_073	RP	POS	13.07	705.5908				2.55E-01	-0.23	0.49	1.08E-02	0.51	1.74	9.18E-01	0.02	0.76	2.73E-02	-0.48	0.89	640714	450264	534740	462151	417868	411096	651612	484407
HILIC_POS_171_07648a6_13	HILIC	POS	6.13	171.0765				5.93E-01	-0.09	0.92	1.08E-02	-0.54	1.43	7.35E-02	-0.36	0.78	3.56E-01	0.18	0.89	2907094	799166	2808925	1161560	3102532	1102176	2515318	1155535
RP_POS_205_98705a15_422	RP	POS	15.42	205.9871				8.83E-01	0.03	0.65	1.09E-02	-0.53	1.52	3.44E-01	-0.24	0.55	7.80E-02	0.29	0.77	86730667	7368657	86961317	8715523	89192473	2701596	84730161	11662460
RP_POS_546_35413a10_512	RP	POS	10.51	546.3541				8.37E-03	0.52	1.12	1.09E-02	-0.50	1.51	2.19E-01	0.27	0.70	4.06E-04	0.77	1.32	42862096	14547795	51104394	15747076	55077608	14371216	47131180	16194207
HILIC_NEG_121_02934a0_927	HILIC	NEG	0.927	121.0293				2.87E-01	0.19	0.49	1.12E-02	-0.53	1.71	7.49E-01	-0.07	0.18	2.33E-02	0.46	0.82	253159	93551	274926	117154	304412	103700	245441	123298
RP_POS_591_31775a6_112	RP	POS	6.11	591.3178				4.45E-04	0.42	0.81	1.12E-02	0.58	1.66	1.81E-03	0.71	1.04	2.51E-02	0.13	0.91	293920	424660	1497224	3235926	671461	1038701	2322987	4322687
RP_NEG_554_30267a10_198	RP	NEG	10.20	554.3027				4.31E-02	-0.49	1.16	1.12E-02	-0.45	1.68	6.34E-03	-0.71	1.23	2.93E-01	-0.26	0.87	1835798	695153	1558225	510563	1686615	478624	1429835	513758
RP_NEG_654_30365a10_031	RP	NEG	10.03	654.3037				8.40E-02	0.38	1.02	1.12E-02	-0.48	1.54	5.44E-01	0.14	0.55	1.05E-02	0.62	1.11	1418433	970958	1755926	841306	1967389	826508	1544464	809729
HILIC_NEG_590_34821a1_17	HILIC	NEG	1.17	590.3482				2.59E-04	0.72	1.35	1.15E-02	-0.49	1.40	2.73E-02	0.48	0.84	9.14E-06	0.97	1.75	277587	117237	372449	127453	404405	114995	340494	132333
HILIC_POS_496_33929a1_171	HILIC	POS	1.171	496.3393				9.01E-02	0.32	0.83	1.15E-02	-0.52	1.43	7.85E-01	0.06	0.15	7.51E-03	0.57	1.00	81227841	29966228	92273103	36179543	101340749	35687315	83205456	34687854
RP_POS_299_62543a10_032	RP	POS	10.03	299.6254				1.02E-01	0.35	1.00	1.15E-02	-0.48	1.54	6.24E-01	0.11	0.56	1.37E-02	0.60	1.07	1368712	973408	1691229	880624	1911794	901968	1470664	808699
RP_POS_401_26575a10_667	RP	POS	10.67	401.2658				8.01E-05	0.52	1.09	1.16E-02	0.56	1.58	2.46E-04	0.79	1.24	3.70E-02	0.24	0.94	392513	193471	678434	612980	523985	365338	832883	759607
HILIC_NEG_221_06674a5_435	HILIC	NEG	5.435	221.0667				1.05E-03	0.42	0.95	1.16E-02	0.56	1.42	8.94E-04	0.70	1.02	2.35E-01	0.14	0.55	191922	157974	397667	546304	260211	352086	535123	663674
RP_POS_779_54333a13_018	RP	POS	13.02	779.5433				8.37E-14	1.05	1.72	1.17E-02	0.50	1.55	1.88E-10	1.30	1.99	1.39E-07	0.79	1.71	381909	270570	1064214	653433	900582	533909	1227846	723161
HILIC_POS_633_39838a1_259	HILIC	POS	1.259	633.3984				1.27E-01	-0.35	0.72	1.17E-02	-0.46	1.40	1.77E-02	-0.59	1.17	6.26E-01	-0.12	0.31	1367101	634023	1176146	501128	1301477	520219	1050814	452435
HILIC_POS_130_05009a6_129	HILIC	POS	6.129	130.0501				2.60E-01	-0.19	0.98	1.19E-02	-0.53	1.42	2.51E-02	-0.46	0.91	6.90E-01	0.08	1.00	45020294	12496810	41767036	18302088	46331319	17087860	37202753	18500224
RP_POS_338_16592a7_822	RP	POS	7.82	338.1659				8.38E-01	0.05	0.35	1.19E-02	0.48	1.62	2.41E-01	0.28	0.84	4.28E-01	-0.19	0.55	936943	56035	939193	47096	927454	46358	950932	45288
HILIC_POS_84_04503a6_129	HILIC	POS	6.129	84.0450				3.02E-01	-0.17	0.98	1.20E-02	-0.53	1.42	2.93E-02	-0.44	0.91	6.29E-01	0.09	0.98	1261139	343234	1178976	506712	1305234	478912	1052719	506818
HILIC_POS_590_32074a1_185	HILIC	POS	1.185	590.3207				9.39E-01	-0.01	0.39	1.21E-02	-0.51	1.41	2.00E-01	-0.27	0.55	2.67E-01	0.24	0.41	442316	211805	438883	243306	499425	244919	378342	228338
RP_POS_202_14374a6_99	RP	POS	6.99	202.1437				5.15E-01	0.13	0.59	1.21E-02	0.50	1.65	1.11E-01	0.38	0.89	5.70E-01	-0.12	0.29	476864	321035	519818	326611	438386	257023	601250	368691
HILIC_NEG_355_01974a0_93	HILIC	NEG	0.93	355.0197				4.27E-01	-0.16	0.85	1.22E-02	-0.50	1.53	5.69E-02	-0.41	0.77	6.80E-01	0.09	0.15	475158	94299	459609	99803	484421	105381	434796	88108
RP_NEG_672_85962a0_493	RP	NEG	0.49	672.8596				2.05E-03	-0.47	0.85	1.23E-02	0.54	1.55	3.06E-01	-0.20	0.39	1.75E-05	-0.74	1.38	11552465	1058021	10693228	1965822	10204352	1612408	11182104	2172594
RP_POS_288_6337a10_198	RP	POS	10.20	288.6337				2.13E-02	-0.55	1.23	1.23E-02	-0.44	1.73	3.03E-03	-0.77	1.31	1.79E-01	-0.33	0.93	5388529	1962276	4488949	1453389	4849754	1335871	4128145	1489149
HILIC_NEG_564_33057a1_105	HILIC	NEG	1.105	564.3306				1.63E-01	-0.34	0.76	1.24E-02	-0.44	1.37	3.30E-02	-0.56	1.03	6.32E-01	-0.12	0.33	798559	398912	690996	278353	760050	266700	621941	275103
RP_POS_510_35535a10_729	RP	POS	10.73	510.3554				3.32E-07	-1.20	2.01	1.24E-02	-0.39	1.79	1.92E-08	-1.40	2.16	2.23E-05	-1.00	1.66	26266052	8770785	16086955	6740759	17758978	6952004	14414931	6145500
RP_POS_513_84949a11_128	RP	POS	11.13	513.8495				1.45E-01	0.30	0.87	1.25E-02	-0.50	1.69	7.95E-01	0.05	0.56	2.78E-02	0.55	1.06	292229	730229	511529	727408	692558	870820	330499	493797
RP_POS_718_83563a0_495	RP	POS	0.50	718.8356				4.83E-05	-0.59	0.99	1.25E-02	0.53	1.53	8.06E-02	-0.33	0.59	1.03E-06	-0.86	1.51	11527421	1112660	10228347	2360347	9643415	2090628	10813280	2487406
HILIC_POS_101_07129a6_129	HILIC	POS	6.129	101.0713				3.42E-01	-0.17	0.97	1.25E-02	-0.53	1.42	3.75E-02	-0.43	0.86	6.29E-01	0.10	0.91	869321	220337	822289	299879	896549	286359	748029	297379
RP_POS_534_29584a10_375	RP	POS	10.38	534.2958				3.35E-01	0.20	0.99	1.26E-02	-0.49	1.70	8.67E-01	-0.04	0.58	4.94E-02	0.45	1.13	1200930	372112	1273501	350100	1360173	313469	1186829	366126
RP_POS_496_33994a11_254	RP	POS	11.25	496.3399				6.64E-01	0.08	1.11	1.26E-02	-0.52	1.61	3.52E-01	-0.18	0.68	1.19E-01	0.34	1.02	1713920	639759	1774909	821480	1978237	873877	1571582	717911
RP_POS_1009_66394a11_135	RP	POS	11.14	1009.6639				2.19E-02	0.28	0.94	1.27E-02	-0.56	1.58	9.64E-01	0.00	0.57	6.86E-03	0.56	1.17	691598	78167	795544	425699	901332	517780	689755	274231
RP_POS_254_95401a15_48	RP	POS	15.48	254.9540				6.21E-01	-0.12	0.51	1.27E-02	-0.45	1.46	1.82E-01	-0.34	0.94	6.80E-01	0.11	0.26	1984815	114299	1973925	83050	1994447	80774	1953402	80940
HILIC_NEG_373_01025a0_931	HILIC	NEG	0.931	373.0103				6.66E-01	-0.09	0.77	1.28E-02	-0.50	1.52	1.45E-01	-0.34	0.56	4.75E-01	0.16	0.27	496185	98882	487472	98707	511853	92293	463091	99769
RP_NEG_554_34717a10_73	RP	NEG	10.73	554.3472				2.83E-07	-1.19	1.98	1.30E-02	-0.40	1.79	1.51E-08	-1.39	2.16	2.40E-05	-0.99	1.64	12017512	3966194	7367836	3165794	8147958	3291071	6587714	2859347
HILIC_POS_204_12309a3_117	HILIC	POS	3.117	204.1231				1.17E-08	0.85	1.54	1.31E-02	0.51	1.53	1.12E-07	1.11	1.79	1.09E-04	0.60	1.27	17133221	9170763	32241256	18255451	27738896	14422153	36743617	20590189
HILIC_NEG_128_03555a6_093	HILIC	NEG	6.093	128.0356				4.04E-01	-0.14	0.91	1.31E-02	-0.52	1.41	4.36E-02	-0.41	0.80	5.55E-01	0.12	0.91	210067	54397	199746	76445	218558	74967	180934	73925
RP_POS_320_90628a15_426	RP	POS	15.43	320.9063				2.01E-03	-0.40	0.75	1.32E-02	-0.55	1.92	1.31E-03	-0.68	1.24	2.90E-01	-0.13	0.49	5096230	186995	4885002	582617	5028935	380167	4741068	706404
RP_POS_548_30023a10_327	RP	POS	10.33	548.3002				1.57E-03	-0.77	1.45	1.32E-02	-0.42	1.70	1.87E-04	-0.98	1.59	2.40E-02	-0.56	1.12	6780706	1949891	5520994	1410516	5867655	1320358	5174332	1425172
RP_POS_496_33984a11_163	RP	POS	11.16	496.3398				5.09E-01	-0.12	0.99	1.33E-02	-0.51	1.52	8.20E-02	-0.38	0.90	5.25E-01	0.13	0.87	2538286	759994	2430684	904127	2652812	839499	2208557	919848
HILIC_POS_360_27429a1_026	HILIC	POS	1.026	360.2743				1.82E-05	0.63	1.19	1.33E-02	0.53	1.55	3.37E-05	0.89	1.43	1.08E-02	0.36	0.87	650784	303763	1024262	637692	867016	445871	1181509	756531
RP_POS_299_19543a10_824	RP	POS	10.82	299.1954				1.13E-10	0.91	1.77	1.33E-02	0.51	1.66	1.11E-08	1.16	1.94	1.39E-05	0.66	1.66	469689	451908	1406933	1058385	1146737	863153	1667130	1174742
RP_POS_692_83264a0_496	RP	POS	0.50	692.8326				6.73E-05	-0.63	1.17	1.34E-02	0.52	1.49	4.90E-02	-0.37	0.72	2.59E-06	-0.89	1.62	2917216	400511	2504537	689115	2335374	640144	2673700	700904
HILIC_POS_595_34863a0_504	HILIC	POS	0.504	595.3486				2.84E-04	0.54	1.09	1.34E-02	0.53	1.32	3.22E-04	0.80	1.40	4.08E-02	0.27	0.87	214152	420124	639228	855498	427766	500336	850690	1066347
RP_NEG_195_8111a1_454	RP	NEG	1.45	195.8111				7.14E-01	-0.07	0.40	1.34E-02	-0.50	1.65	1.41E-01	-0.32	0.72	4.09E-01	0.18	0.57	16952238	5443179	16535445	5986379	18004212	5826225	15066679	5835866
HILIC_NEG_241_9742a1_3	HILIC	NEG	1.3	241.9742				4.22E-07	0.86	1.47	1.34E-02	0.49	1.38	5.20E-07	1.11	1.61	2.53E-04	0.61	1.34	1866818	289905	2236146	429177	2130571	320805	2341722	496469
RP_POS_145_04935a0_549	RP	POS	0.55	145.0494				2.88E-03	0.37	0.71	1.35E-02	0.56	1.60	3.59E-03	0.65	1.01	2.62E-01	0.09	0.90	1605154	236596	1924550	963723	1685606	407198	2163493	1262597
HILIC_NEG_229_08878a0_713	HILIC	NEG	0.713	229.0888				3.48E-05	0.49	1.00	1.36E-02	0.56	1.68	7.04E-04	0.77	1.04	1.47E-04	0.22	1.19	24422	54477	238681	486165	117976	149521	359386	652262
RP_POS_807_96405a10_325	RP	POS	10.33	807.9641				4.47E-04	-0.86	1.54	1.36E-02	-0.41	1.72	5.03E-05	-1.06	1.69	8.26E-03	-0.65	1.22	1693898	722945	1168580	513329	1294240	486841	1042921	512983
RP_NEG_986_7937a0_49	RP	NEG	0.49	986.7937				3.43E-03	-0.51	0.92	1.39E-02	0.51	1.53	2.26E-01	-0.25	0.56	6.67E-05	-0.76	1.37	724298	237632	562409	331397	481426	276788	643393	363172
RP_POS_411_759a13_588	RP	POS	13.59	411.7590				4.88E-02	-0.37	0.78	1.40E-02	-0.50	1.44	2.66E-03	-0.62	1.10	5.89E-01	-0.12	0.43	1705112	566100	1462007	678868	1627634	718441	1296380	599156
RP_POS_1087_67004a10_31	RP	POS	10.31	1087.6700				6.45E-01	0.10	0.80	1.40E-02	-0.48	1.76	5.70E-01	-0.14	0.50	1.42E-01	0.34	0.87	4268638	2726805	4519171	2448794	5116549	2144773	3921792	2605230
RP_NEG_182_04524a0_714	RP	NEG	0.71	182.0452				1.59E-03	0.37	1.11	1.40E-02	0.56	1.70	4.49E-03	0.65	1.40	1.74E-02	0.09	0.96	124676	85193	2643680	7753882	724200	1718948	4563161	10535577
RP_NEG_590_34711a10_518	RP	NEG	10.52	590.3471				1.39E-02	0.48	1.00	1.42E-02	-0.49	1.44	2.79E-01	0.23	0.63	8.68E-04	0.72	1.22	11703401	3465987	13540214	3850114	14477072	3593747	12603356	3904231
RP_NEG_504_31015a10_325	RP	NEG	10.33	504.3102				2.34E-02	-0.52	1.17	1.44E-02	-0.45	1.68	3.49E-03	-0.74	1.26	2.07E-01	-0.30	0.86	3609918	988166	3159305	796778	3352953	702122	2965657	844490
RP_NEG_213_14952a8_782	RP	NEG	8.78	213.1495				3.66E-07	0.75	1.69	1.44E-02	0.51	1.82	9.79E-07	1.00	1.74	1.67E-03	0.49	1.51	539212	506378	1285921	1049162	1030761	860016	1541080	1162519
HILIC_NEG_132_92365a6_093	HILIC	NEG	6.093	132.9237				2.40E-01	-0.22	0.79	1.44E-02	-0.50	1.35	3.08E-02	-0.47	0.78	8.74E-01	0.03	0.73	1416004	325695	1333540	390005	1428229	361782	1238852	397654
RP_POS_472_94687a10_708	RP	POS	10.71	472.9469				2.11E-01	-0.25	0.79	1.46E-02	0.49	1.43	9.85E-01	0.00	0.54	2.27E-02	-0.49	1.23	503925	162199	461663	171313	420104	152564	503221	180262
HILIC_POS_414_32086a0_857	HILIC	POS	0.857	414.3209				4.05E-10	0.90	1.57	1.47E-02	0.50	1.50	5.87E-09	1.15	1.96	5.16E-05	0.66	1.34	244481	126916	488234	276574	421215	244502	555253	292575
RP_POS_269_22601a11_598	RP	POS	11.60	269.2260				5.01E-01	-0.10	0.57	1.47E-02	-0.54	1.60	7.46E-02	-0.37	0.74	2.75E-01	0.17	0.64	1597896	303105	1542851	615572	1692287	474199	1393416	703671
HILIC_POS_184_07373a1_303	HILIC	POS	1.303	184.0737				4.02E-01	0.17	0.40	1.49E-02	-0.49	1.31	7.46E-01	-0.07	0.22	6.67E-02	0.41	0.68	968652	300698	1020461	306171	1094467	293825	946455	303124
RP_POS_204_12276a0_644	RP	POS	0.64	204.1228				2.19E-09	0.91	1.60	1.51E-02	0.49	1.43	2.95E-08	1.16	1.82	2.65E-05	0.66	1.43	100345344	29038109	149933949	55369613	136551356	44467282	163316543	62058992
RP_POS_559_51782a14_005	RP	POS	14.01	559.5178				3.14E-01	0.24	0.60	1.51E-02	-0.44	1.67	9.17E-01	0.03	0.59	7.86E-02	0.46	0.77	15999089	3163370	16613861	2273137	17162338	2321170	16065384	2106655
HILIC_NEG_175_04192a0_927	HILIC	NEG	0.927	175.0419				3.59E-01	0.13	0.22	1.52E-02	-0.53	1.45	4.21E-01	-0.13	0.67	4.26E-02	0.40	0.80	307984	97457	332334	200544	380688	217359	283980	170997
RP_NEG_394_01221a2_884	RP	NEG	2.88	394.0122				6.66E-07	-0.79	1.50	1.53E-02	-0.50	1.64	1.54E-06	-1.04	1.70	5.78E-04	-0.55	1.39	825744	129518	656146	219409	709119	162740	603172	255053
HILIC_NEG_231_93166a6_094	HILIC	NEG	6.094	231.9317				6.91E-01	-0.06	0.88	1.53E-02	-0.52	1.38	1.05E-01	-0.33	0.65	2.96E-01	0.20	0.78	1249825	253674	1225911	399129	1321988	367463	1129834	409867
RP_POS_417_33597a10_092	RP	POS	10.09	417.3360				9.42E-07	0.69	1.13	1.54E-02	0.51	1.52	3.84E-06	0.95	1.46	3.21E-03	0.44	0.98	610042	175708	874640	406273	776688	319384	972591	460323
RP_POS_282_11905a0_709	RP	POS	0.71	282.1191				1.24E-02	0.39	0.88	1.54E-02	0.52	1.46	1.44E-03	0.65	1.27	4.50E-01	0.13	0.67	616712	80199	667772	141545	633698	122388	701845	152087
RP_NEG_526_31641a10_112	RP	NEG	10.11	526.3164				9.99E-09	-1.21	2.07	1.55E-02	-0.41	1.62	2.43E-10	-1.41	2.32	6.66E-06	-1.00	1.71	1402667	409573	838207	399054	934291	448100	742123	319537
RP_NEG_221_06644a0_71	RP	NEG	0.71	221.0664				3.35E-06	0.56	1.04	1.55E-02	0.54	1.70	6.52E-05	0.83	1.29	1.07E-02	0.29	0.85	575985	551993	2625310	4067432	1644030	2771691	3606591	4876294
RP_NEG_586_31592a10_032	RP	NEG	10.03	586.3159				1.06E-01	0.35	0.99	1.56E-02	-0.46	1.47	6.02E-01	0.12	0.54	1.55E-02	0.58	1.08	13386445	10091489	16675127	8988052	18832829	8923701	14517424	8607264

Supplementary table 1: Metabolomics results (in asceding order according to p-value from progressive ALD vs non-progressive ALD comparison, with molecular features with ID_level of 1-2 first)

								all_ALD_vs_control			Prog_ALD_vs_non-prog_ALD			Prog_ALD_vs_control_ALD			Non-prog_ALD_vs_control			Healthy_control		all_ALD		Non-prog_ALD		Progressive_ALD	
								t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA								
Feature_ID	RP_HILIC	POS_NEG	Average.Rt	Average.Mz	Metabolite.name	curated_MSMS	ID_level	p	d	VIP	p	d	VIP	p	d	VIP	p	d	VIP	Mean	SD	Mean	SD	Mean	SD	Mean	SD
RP_POS_480_30835a10_627	RP	POS	10.63	480.3084				6.43E-03	0.49	1.22	1.57E-02	0.50	1.83	1.24E-03	0.74	1.28	1.71E-01	0.25	1.00	29830240	11465595	36870138	14662252	33342993	10781898	40397282	17108830
RP_POS_430_7482a12_957	RP	POS	12.96	430.7482				2.68E-11	-1.11	2.00	1.57E-02	-0.46	1.50	1.84E-11	-1.34	2.29	1.32E-06	-0.88	1.68	11923276	1518641	9173081	2349414	9736431	2264644	8609732	2318588
RP_POS_367_18271a10_823	RP	POS	10.82	367.1827				2.23E-12	0.95	1.79	1.58E-02	0.49	1.62	2.87E-09	1.20	1.98	2.12E-06	0.71	1.72	150682	133317	486811	362609	399802	298677	573820	401243
RP_POS_289_63089a10_198	RP	POS	10.20	289.6309				2.07E-02	-0.55	1.23	1.59E-02	-0.43	1.69	3.06E-03	-0.76	1.30	1.74E-01	-0.33	0.92	1886027	694246	1565262	527219	1691527	493525	1438997	534312
HILIC_NEG_157_90068a3_677	HILIC	NEG	3.677	157.9007				4.61E-01	0.16	0.35	1.59E-02	0.46	1.77	1.02E-01	0.39	0.83	7.90E-01	-0.06	0.25	1597135	930605	1732611	788028	1543919	793543	1921303	743152
HILIC_NEG_194_9884a0_928	HILIC	NEG	0.928	194.9884				3.59E-02	-0.45	1.08	1.59E-02	-0.46	1.40	3.42E-03	-0.68	1.19	3.44E-01	-0.22	0.42	1214232	236095	1112983	214440	1164310	223459	1061655	193899
RP_NEG_348_00562a2_887	RP	NEG	2.89	348.0056				2.05E-07	-0.83	1.55	1.60E-02	-0.49	1.62	7.57E-07	-1.08	1.72	2.01E-04	-0.59	1.48	897664	139029	706531	234388	762786	171258	650277	274242
RP_POS_218_13808a1_423	RP	POS	1.42	218.1381				2.43E-02	-0.43	0.97	1.60E-02	-0.49	1.45	1.93E-03	-0.67	1.14	3.77E-01	-0.19	0.84	4362831	1053082	3848999	1215115	4139576	1192316	3558422	1178646
RP_POS_757_6217a13_673	RP	POS	13.67	757.6217				8.54E-08	-1.32	2.24	1.60E-02	-0.35	1.41	7.52E-09	-1.49	2.29	2.55E-06	-1.14	1.92	2383610	924688	1243088	637628	1395564	622725	1090612	621453
RP_POS_307_09714a7_667	RP	POS	7.67	307.0971	Unknown	307.0947(100)	4	8.70E-05	-0.74	1.15	1.61E-02	-0.47	1.57	9.51E-06	-0.98	1.55	1.07E-02	-0.51	0.90	1230642	72540	1165790	85756	1186293	77968	1145288	89003
RP_POS_1009_62012a10_123	RP	POS	10.12	1009.6201				5.32E-05	0.48	1.73	1.61E-02	0.54	1.49	5.10E-04	0.75	1.44	2.50E-02	0.21	1.39	115460	45936	478792	856775	272480	476976	685104	1081080
RP_NEG_884_80939a0_489	RP	NEG	0.49	884.8094				9.35E-07	-0.69	1.20	1.63E-02	0.51	1.55	1.18E-02	-0.44	0.92	2.27E-07	-0.95	1.59	1453809	259217	1062856	600582	919546	576905	1206165	595001
RP_POS_379_28143a10_961	RP	POS	10.96	379.2814				2.21E-05	0.51	1.00	1.63E-02	0.54	1.51	3.17E-04	0.78	1.15	9.68E-03	0.24	0.95	3485387	2357394	10391855	15029442	6778423	8203313	14005286	19037781
RP_POS_532_27985a10_124	RP	POS	10.12	532.2799				9.24E-19	1.12	2.01	1.63E-02	0.48	1.53	1.72E-10	1.36	2.07	5.56E-12	0.88	2.03	126360	86253	584081	407825	486405	280211	681757	487902
HILIC_NEG_100_93347a4_019	HILIC	NEG	4.019	100.9335				7.90E-02	-0.33	0.79	1.64E-02	-0.49	1.41	1.07E-02	-0.57	1.01	6.79E-01	-0.08	0.24	24259981	3966759	22745385	4768721	23882824	4062166	21607947	5177255
RP_POS_410_76151a13_071	RP	POS	13.07	410.7615				7.82E-01	-0.05	0.54	1.64E-02	-0.49	1.41	1.86E-01	-0.30	1.14	3.82E-01	0.19	0.41	4932500	1044681	4872339	1127397	5140926	1047783	4603751	1150181
RP_POS_807_56879a13_293	RP	POS	13.29	807.5688				1.96E-02	-0.41	0.85	1.65E-02	0.50	1.46	4.55E-01	-0.16	0.64	5.80E-04	-0.66	1.18	55868771	8636414	51257142	11816567	48441352	9813642	54072933	13023961
RP_POS_762_96265a10_123	RP	POS	10.12	762.9627				1.88E-07	0.62	1.80	1.66E-02	0.53	1.49	2.77E-05	0.89	1.59	7.82E-04	0.36	1.44	66604	30317	366804	533696	239153	339033	494456	653666
HILIC_NEG_129_03648a0_927	HILIC	NEG	0.927	129.0365				6.67E-02	0.28	0.47	1.66E-02	-0.52	1.52	9.29E-01	0.02	0.44	4.10E-03	0.54	1.08	1911195	706391	2251628	1346523	2571924	1309680	1931332	1318569
RP_POS_572_29913a10_303	RP	POS	10.30	572.2991				1.79E-01	0.28	0.69	1.66E-02	-0.47	1.69	8.58E-01	0.04	0.31	1.91E-02	0.51	0.95	655585	214216	714526	209768	764468	173457	664584	231788
HILIC_POS_199_14436a0_568	HILIC	POS	0.568	199.1444				8.90E-05	0.46	0.89	1.70E-02	0.54	1.37	7.86E-04	0.73	1.14	2.43E-02	0.19	0.68	66652	113661	2200428	5217859	952649	2692520	3448207	6676873
HILIC_POS_591_31738a1_146	HILIC	POS	1.146	591.3174				2.81E-03	0.41	0.92	1.71E-02	0.53	1.56	3.06E-03	0.68	0.93	1.56E-01	0.15	0.74	524860	1216000	1672139	3088461	933195	1322152	2411083	4050852
HILIC_POS_510_35641a1_264	HILIC	POS	1.264	510.3564				4.76E-06	-0.93	1.76	1.72E-02	-0.44	1.37	1.89E-07	-1.15	2.18	1.13E-03	-0.71	1.37	9213077	2616829	6488554	2701715	7128146	2855946	5848961	2399210
HILIC_POS_568_33966a1_187	HILIC	POS	1.187	568.3397				9.14E-01	0.02	0.39	1.72E-02	-0.49	1.35	2.90E-01	-0.22	0.45	2.30E-01	0.26	0.44	13815626	6513071	13963799	7413361	15718052	7577023	12209545	6880824
RP_POS_862_79767a0_491	RP	POS	0.49	862.7977				6.00E-06	-0.69	1.17	1.73E-02	0.50	1.52	1.72E-02	-0.44	0.84	4.76E-07	-0.94	1.55	1226839	265305	897852	504240	778602	472738	1017102	511080
RP_NEG_636_2608a10_199	RP	NEG	10.20	636.2608				5.08E-02	-0.46	1.15	1.74E-02	-0.43	1.63	8.56E-03	-0.68	1.19	3.15E-01	-0.25	0.87	1413032	495882	1221227	377966	1310486	355001	1131968	382553
RP_POS_363_16211a10_943	RP	POS	10.94	363.1621				9.63E-06	0.78	1.59	1.75E-02	0.47	1.48	3.60E-06	1.02	1.67	2.38E-03	0.55	1.44	722797	443530	1194137	601497	1051952	487944	1336321	672036
RP_POS_271_65808a10_198	RP	POS	10.20	271.6581				3.74E-02	-0.49	1.19	1.77E-02	-0.43	1.70	6.14E-03	-0.71	1.24	2.54E-01	-0.28	0.89	997022	378804	840484	287290	908147	269612	772820	291069
RP_POS_161_98155a15_628	RP	POS	15.63	161.9816				3.66E-01	0.18	0.65	1.78E-02	-0.48	1.39	7.75E-01	-0.06	0.42	5.83E-02	0.42	0.70	9725622	3654698	10416137	3969731	11350905	3840516	9481369	3912330
HILIC_POS_154_05872a5_591	HILIC	POS	5.591	154.0587				1.54E-01	0.29	0.51	1.78E-02	-0.47	1.58	8.20E-01	0.05	0.54	1.86E-02	0.52	0.93	2996643	1784974	3525560	1846893	3960301	1726038	3090818	1877957
RP_POS_185_11481a13_641	RP	POS	13.64	185.1148				1.19E-01	0.33	0.71	1.79E-02	-0.46	1.68	6.60E-01	0.10	0.20	1.79E-02	0.56	1.09	7496618	3807039	8706083	3588338	9550079	3610625	7862086	3394816
RP_NEG_554_29889a10_328	RP	NEG	10.33	554.2989				1.14E-03	-0.75	1.38	1.79E-02	-0.42	1.55	1.36E-04	-0.96	1.57	2.17E-02	-0.54	1.07	4591511	844805	4021669	673029	4179942	632089	3863396	681557
RP_POS_546_79639a10_326	RP	POS	10.33	546.7964				1.63E-03	-0.76	1.45	1.79E-02	-0.41	1.69	2.48E-04	-0.96	1.57	2.19E-02	-0.56	1.14	3531944	1049565	2855455	770763	3036788	679841	2674121	819136
RP_POS_508_37546a11_094	RP	POS	11.09	508.3755				3.21E-04	-0.93	1.65	1.79E-02	-0.37	1.84	4.33E-05	-1.11	1.70	4.35E-03	-0.74	1.33	2040421	850368	1410925	535326	1536799	530388	1285051	515122
HILIC_POS_532_2807a1_342	HILIC	POS	1.342	532.2807				2.39E-17	1.14	1.88	1.80E-02	0.46	1.28	1.01E-10	1.37	2.12	1.39E-11	0.91	2.23	151712	94243	457828	263045	395757	183011	519899	313753
RP_NEG_706_85394a0_49	RP	NEG	0.49	706.8539				1.07E-02	-0.39	0.73	1.80E-02	0.51	1.48	5.25E-01	-0.13	0.28	9.17E-05	-0.64	1.28	1743780	286050	1550949	543024	1423025	418377	1678874	622359
RP_POS_163_05981a0_551	RP	POS	0.55	163.0598				1.55E-03	0.39	0.72	1.80E-02	0.54	1.55	3.45E-03	0.66	1.03	1.15E-01	0.12	0.94	648072	106533	821736	502072	702429	200821	941043	663263
RP_POS_184_06007a0_716	RP	POS	0.72	184.0601				5.70E-03	0.32	1.14	1.81E-02	0.54	1.69	1.01E-02	0.59	1.38	2.78E-03	0.05	1.57	26765	35659	1862303	6494508	312721	640757	3411886	8939076
RP_POS_276_63242a10_375	RP	POS	10.38	276.6324				9.55E-01	0.01	0.97	1.81E-02	-0.48	1.68	3.09E-01	-0.23	0.76	2.45E-01	0.25	0.93	1912647	272097	1915815	294328	1984923	272204	1846707	301966
RP_NEG_740_84741a0_49	RP	NEG	0.49	740.8474				5.14E-01	-0.10	0.67	1.83E-02	0.52	1.58	4.38E-01	0.16	0.52	3.12E-02	-0.36	1.02	8161315	952215	8001460	1769497	7586161	1421491	8416759	1988345
HILIC_NEG_200_85857a1_004	HILIC	NEG	1.004	200.8586				1.01E-01	-0.27	0.68	1.84E-02	-0.50	1.48	1.07E-02	-0.52	0.87	9.26E-01	-0.02	0.07	1285731	216293	1200873	339163	1280319	308332	1121428	352791
HILIC_POS_202_84023a2_967	HILIC	POS	2.967	202.8402				4.81E-05	0.63	1.18	1.85E-02	0.50	1.36	5.70E-05	0.88	1.29	1.12E-02	0.38	0.95	274285	312619	609284	559847	477793	392173	740774	666460
RP_NEG_1083_66467a10_324	RP	NEG	10.32	1083.6647				1.35E-02	-0.60	1.26	1.86E-02	-0.41	1.66	2.06E-03	-0.80	1.34	1.17E-01	-0.39	0.96	19920394	8503167	15726486	6198648	17176086	5923237	14276886	6185260
HILIC_NEG_182_04585a0_926	HILIC	NEG	0.926	182.0459				3.28E-02	0.26	0.73	1.86E-02	0.54	1.42	2.11E-02	0.53	0.95	9.09E-01	-0.01	0.19	121312	227316	359209	1026051	115748	192948	602669	1403158
RP_NEG_632_32227a10_198	RP	NEG	10.20	632.3223				3.56E-02	-0.50	1.18	1.91E-02	-0.42	1.62	6.18E-03	-0.71	1.23	2.36E-01	-0.29	0.88	5545369	1888650	4758550	1410750	5087212	1310090	4429888	1443699
RP_POS_237_14616a8_784	RP	POS	8.78	237.1462				1.26E-07	0.75	1.63	1.91E-02	0.49	1.82	9.20E-07	1.00	1.72	9.80E-04	0.51	1.48	980108	275336	1427961	629886	1281076	517062	1574846	700161
HILIC_POS_593_33301a1_134	HILIC	POS	1.134	593.3330				3.60E-03	0.48	0.98	1.91E-02	0.50	1.36	1.43E-03	0.73	1.22	1.34E-01	0.23	0.78	340456	974409	1030188	1526430	672860	959246	1387516	1877977
HILIC_POS_58_06563a3_7	HILIC	POS	3.7	58.0656				8.28E-04	0.53	1.12	1.92E-02	0.50	1.38	2.61E-04	0.78	1.43	8.90E-02	0.28	0.71	1944544	929545	2739627	1609222	2364605	1275032	3114648	1821898
HILIC_POS_542_3233a1_263	HILIC	POS	1.263	542.3233				1.74E-01	0.28	0.54	1.93E-02	-0.46	1.26	8.15E-01	0.05	0.15	2.83E-02	0.51	0.90	13062776	5571602	14614839	5441321	15880012	5513595	13349667	5114078
RP_POS_806_46277a10_324	RP	POS	10.32	806.4628				4.58E-04	-0.85	1.48	1.95E-02	-0.39	1.41	6.30E-05	-1.04	1.63	7.75E-03	-0.65	1.18	814484	402782	521630	294102	589889	271117	453371	302892
HILIC_POS_114_06653a1_344	HILIC	POS	1.344	114.0665				1.61E-01	-0.33	0.82	1.96E-02	-0.43	1.39	3.77E-02	-0.54	0.83	6.42E-01	-0.11	0.44	6817202	3115266	5959056	2443572	6526648	2019746	5391465	2706862
RP_POS_590_32166a10_193	RP	POS	10.19	590.3217				6.63E-01	-0.08	0.99	1.96E-02	-0.49	1.43	1.19E-01	-0.32	0.79	4.41E-01	0.16	0.93	1350391	543586	1298940	675358	1455540	679091	1142340	640557
RP_POS_278_88852a15_459	RP	POS	15.46	278.8885				8.62E-01	0.04	0.37	1.96E-02	-0.42	1.64	5.08E-01	-0.17	0.48	3.20E-01	0.25	0.47	24383787	7495871	24634018	5492278	25907411	5231846	23360625	5501307
RP_POS_314_2327a7_727	RP	POS	7.73	314.2327				5.87E-02	0.33	0.84	1.97E-02	0.49	1.48	9.98E-03	0.57	1.30	6.51E-01	0.08	0.32	3214346	258802	3326676	364537	3241989	282663	3411364	417075
RP_POS_390_17505a0_706	RP	POS	0.71	390.1751				1.02E-12	0.89	1.51	1.98E-02	0.49	1.44	2.45E-08	1.14	1.75	2.22E-06	0.64	1.48	50640	46277	259490	248097	201916	194929	317064	282132
RP_POS_298_12088a10_031	RP	POS	10.03	298.1209				1.34E-01	0.34	0.99	1.98E-02	-0.44	1.46	6.27E-01	0.12	0.56	2.35E-02	0.56	1.02	373660	288403	459889	243719	516321	240715	403458	235728
HILIC_POS_116_10729a0_871	HILIC	POS	0.871	116.1073				9.58E-02	-0.37	0.71	2.00E-02	-0.44	1.28	1.16E-02	-0.59	1.10	5.39E-01	-0.15	0.23	2270863	1302090	1836760	1104647	2092594	1231815	1580925	902469
RP_POS_279_64697a10_198	RP	POS	10.20	279.6470				1.72E-02	-0.58	1.26	2.00E-02	-0.41	1.64	2.93E-03	-0.78	1.31	1.31E-01	-0.38	0.96	1133728	447796	921918	319615	995820	300549	848017	323908
RP_POS_394_2081a9_967	RP	POS	9.97	394.2081				7.82E-07	0.73	1.17	2.01E-02	0.49	1.44	1.55E-08	0.97	1.93	1.16E-02	0.49	0.76	729119	693513	1714948	1425807	1385321	1567390	2044575	1195360
RP_POS_127_0389a0_55	RP	POS	0.55	127.0389				1.78E-03	0.39	0.72	2.02E-02	0.53	1.53	3.76E-03	0.65	0.99	1.31E-01	0.12	0.95	902430	131937	1110958	609467	968789	259166	1253128	801288
HILIC_NEG_588_33142a1_16	HILIC	NEG	1.16	588.3314				1.05E-01	0.36	0.65	2.02E-02	-0.44	1.23	5.75E-01	0.14	0.23	1.36E-02	0.58	1.08	859795	344226	971899	299864	1041158	259596	902640	323252
RP_NEG_593_47961a11_359	RP	NEG	11.36	593.4796				9.39E-02	-0.31	0.57	2.03E-02	-0.48	1.44	3.58E-03	-0.55	1.23	7.63E-01	-0.07	0.65	3199275	1972330	2478041	2414732	3037225	2885144	1918857	1678890
RP_POS_766_57135a13_684	RP	POS	13.68	766.5714				6.10E-07	-1.11	1.78	2.03E-02	-0.39	1.35	4.84E-08	-1.31	2.01	5.22E-05	-0.92	1.48	3012720	1256802	1585597	1089250	1836858	1077260	1334337	1052527
RP_POS_746_50861a13_381	RP	POS	13.38	746.5086				5.34E-01	-0.13	0.94	2.03E-02	-0.45	1.36	9.61E-02	-0.36	0.83	7.06E-01	0.09	0.71	1456151	816567	1354181	754434	1528820	895349	1179541	534850
RP_NEG_305_24933a11_199	RP	NEG	11.20	305.2493				2.53E-12	0.92	1.70	2.03E-02	0.48	1.58	5.56E-08	1.16	1.81	9.12E-08	0.68	1.80	825345	510884	2260259	1620623	1884946	1092201	2635572	1956034
RP_NEG_224_97958a0_713	RP	NEG	0.71	224.9796				9.56E-01	0.01	0.91	2.07E-02	-0.52	1.46	1.70E-01	-0.25	0.88	1.03E-01	0.27	1.19	2479574	228868	2483676	632129	2629100	572254	2338253	660829
HILIC_POS_127_08677a1_355	HILIC	POS	1.355	127.0868				2.63E-06	0.56	1.30	2.07E-02	0.52	1.28	1.27E-04	0.82	1.17	3.18E-03	0.30	0.89	141168	29471	583358	885765	378492	539870	788223	1099117
RP_NEG_541_26648a7_01	RP	NEG	7.01	541.2665				2.77E-02	-0.49	0.92	2.07E-02	-0.44	1.36	2.68E-03	-0.70	1.39	2.68E-01	-0.27	0.54	1508728	951920	1082527	827343	1272903	900425	892150	705856
HILIC_POS_242_07932a2_974	HILIC	POS	2.974	242.0793				5.08E-12	1.01	1.65	2.07E-02	0.46	1.54	6.61E-10	1.24	1.91	1.15E-06	0.78	1.55	13012609	6284734	26356616	13195004	23321082	11376540	29392150	14266702
RP_POS_280_0603a0_78	RP	POS	0.78	280.0603				1.48E-02	0.30	0.94	2.08E-02	0.52	1.43	7.40E-03	0.56	0.88	7.56E-01	0.03	0.59	1128873	509010	1823358	2659246	1209063	1699435	2437652	3260261
RP_POS_271_22675a10_292	RP	POS	10.29	271.2268				1.90E-01	-0.22	0.87	2.08E-02	0.49	1.41	8.88E-01	0.03	0.64	1.50E-02	-0.47	0.99	657776	63311	638272	95959	616225	87709	660320	99597
HILIC_NEG_222_83035a0_881	HILIC	NEG	0.881	222.8304				1.87E-01	0.26	0.77	2.09E-02	0.47	1.41	3.18E-02	0.49	0.90	9.13E-01	0.02	0.12	204842	66642	223386	73541	206485	64546	240287	78598
HILIC_NEG_158_84668a3_003	HILIC	NEG	3.003	158.8467				2.23E-01	0.22	0.72	2.10E-02	-0.49	1.37	8.86E-01	-0.02	0.26	5.14E-02	0.46	1.05	2541994	482108	2672013	626574	2816577	774765	2527450	387674
HILIC_POS_136_0482a5_591	HILIC	POS	5.591	136.0482				1.66E-01	0.28	0.52	2.10E-02	-0.46	1.54	8.24E-01	0.05	0.52	2.18E-02	0.51	0.91	1028804	597723	1200614	614598	1341589	571506	1059638	629279
RP_POS_300_6228a10_032	RP	POS	10.03	300.6228				8.79E-02	0.37	1.02	2.12E-02	-0.44	1.43	5.25E-01	0.15	0.58	1.35E-02	0.59	1.07	463867	338763	581159	307790	651683	304946	510636	297086
RP_POS_542_31909a10_325	RP	POS	10.33	542.3191				3.21E-02	-0.51	1.18	2.13E-02	-0.41	1.62	6.09E-03	-0.72	1.25	2.11E-01	-0.31	0.91	122428496	28944418	110124597	21608700	115072398	19351032	105176796	22781089
RP_POS_255_23143a10_824	RP	POS	10.82	255.2314				5.90E-09	0.83	1.68	2.17E-02	0.48	1.63	1.22E-07	1.07	1.84	1.36E-04	0.59	1.56	583800	491153	1467012	1105527	1214351	925667	1719672	1217449
RP_POS_367_21362a11_689	RP	POS	11.69	367.2136				1.06E-09	0.90	1.78	2.17E-02	0.47	1.49	4.29E-08	1.14	1.87	1.55E-05	0.67	1.66	272445	203203	638820	414345	544106	331219	733534	467819
HILIC_POS_517_33057a1_407	HILIC	POS	1.407	517.3306				1.84E-02	0.29	0.56	2.17E-02	0.53	1.51	1.68E-02	0.55	0.75	6.54E-01	0.02	0.18	142817	420565	694011	2183364	188929	498824	1199094	2976909
HILIC_POS_494_3241a1_339	HILIC	POS	1.339	494.3241				8.85E-17	1.09	1.78	2.18E-02	0.46	1.24	5.55E-10	1.32	2.01	4.32E-11	0.86	2.13	24459837	11924044	66481482	38451949	57675560	26457791	75287405	46141207
RP_POS_227_12498a0_552	RP	POS	0.55	227.1250				1.09E-04	-0.80	1.68	2.18E-02	-0.43	1.35	1.01E-05	-1.02	1.91	6.91E-03	-0.59	1.21	5565916	1646756	4167517	1636386	4540738	1584205	3794296	1617463
HILIC_NEG_128_0401a0_927	HILIC	NEG	0.927	128.0401				7.80E-02	0.27	0.52	2.18E-02	-0.50	1.49	9.11E-01	0.02	0.39	5.23E-03	0.52	1.02	462394	176986	542760	325069	616894	309427	468626	326397
RP_POS_156_04227a15_444	RP	POS	15.44	156.0423				3.13E-01	-0.20	1.42	2.19E-02	0.47	1.56	8.75E-01	0.04	0.75	4.55E-02	-0.43	1.44	2563572	776428	2399141	850300	2205321	775779	2592962	884463
HILIC_POS_100_05094a1_727	HILIC	POS	1.727	100.0509				6.14E-01	0.07	0.99	2.20E-02	-0.51	1.26	3.61E-01	-0.18	0.43	3.77E-02	0.33	0.79	441032	164193	464643	365974	548148	293846	381138	412348
RP_POS_781_55603a12_575	RP	POS	12.58	781.5560				2.14E-06	0.80	1.42	2.22E-02	0.46	1.40	5.78E-06	1.03	1.59	3.90E-04	0.56	1.35	7227800	2713316	10459729	4122764	9518110	2694839	11401349	5026888
HILIC_NEG_229_08868a0_927	HILIC	NEG	0.927	229.0887				3.76E-07	0.61	1.20	2.23E-02	0.50	1.51	2.57E-05	0.86	1.30	2.74E-03	0.36	0.97	33402	39738	220128	337507	143210	242048	297046	399357
RP_POS_518_31989a11_609	RP	POS	11.61	518.3199				6.49E-01	0.10	0.93	2.24E-02	-0.45	1.60	5.81E-01	-0.13	0.61	1.63E-01	0.32	0.98	1096879	346190	1128687	328437	1203263	310193	1054111	332224
RP_POS_417_74237a12_566	RP	POS	12.57	417.7424				5.99E-07	0.93	1.56	2.25E-02	0.44	1.44	7.99E-07	1.15	1.71	6.38E-05	0.71	1.62	655273	369197	1096831	456237	992855	304634	1200806	552890

Supplementary table 1: Metabolomics results (in asceding order according to p-value from progressive ALD vs non-progressive ALD comparison, with molecular features with ID_level of 1-2 first)

								all_ALD_vs_control			Prog_ALD_vs_non-prog_ALD			Prog_ALD_vs_control_ALD			Non-prog_ALD_vs_control			Healthy_control		all_ALD		Non-prog_ALD		Progressive_ALD	
								t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA								
Feature_ID	RP_HILIC	POS_NEG	Average.Rt	Average.Mz	Metabolite.name	curated_MSMS	ID_level	p	d	VIP	p	d	VIP	p	d	VIP	p	d	VIP	Mean	SD	Mean	SD	Mean	SD	Mean	SD
HILIC_NEG_165_05551a0_687	HILIC	NEG	0.687	165.0555				1.70E-04	0.47	1.12	2.25E-02	0.51	1.64	1.45E-03	0.72	0.97	5.80E-03	0.21	0.93	228271	96386	410438	437591	310042	164524	510835	582444
RP_POS_312_63242a10_292	RP	POS	10.29	312.6324				4.67E-01	-0.14	0.98	2.26E-02	-0.47	1.38	8.04E-02	-0.37	0.84	6.45E-01	0.10	0.87	1626653	526136	1544743	621416	1685683	618602	1403803	597486
RP_POS_587_46381a13_624	RP	POS	13.62	587.4638				1.87E-04	0.45	0.86	2.30E-02	0.51	1.35	1.67E-03	0.71	1.00	5.74E-03	0.20	0.85	276242	314007	997574	1783982	589674	673009	1405474	2374371
RP_POS_315_13431a7_11	RP	POS	7.11	315.1343				1.87E-02	0.33	0.91	2.31E-02	0.50	1.63	8.50E-03	0.58	1.01	5.33E-01	0.08	0.79	535358	297195	746211	712083	584249	407611	908173	897101
RP_POS_822_53815a13_295	RP	POS	13.30	822.5382				6.07E-02	-0.37	0.73	2.31E-02	0.45	1.38	5.00E-01	-0.15	0.55	7.80E-03	-0.60	1.04	5848419	1363150	5309959	1448696	4982680	1444454	5637238	1391126
RP_POS_828_60211a11_162	RP	POS	11.16	828.6021				3.08E-06	0.56	1.27	2.31E-02	-0.51	1.60	5.18E-03	0.31	1.16	1.03E-04	0.82	1.41	139888	54339	340391	396185	430297	482782	250485	259910
HILIC_NEG_195_81082a0_733	HILIC	NEG	0.733	195.8108				2.59E-06	0.57	1.10	2.32E-02	0.50	1.24	6.24E-05	0.82	1.24	8.07E-03	0.32	0.82	200324	98987	518528	618374	378493	441679	658564	733128
RP_NEG_526_31622a10_247	RP	NEG	10.25	526.3162				4.52E-08	-1.19	2.02	2.32E-02	-0.38	1.61	1.79E-09	-1.38	2.25	1.14E-05	-1.00	1.67	11615785	3391681	7251229	3082997	7948054	3451109	6554404	2510502
RP_NEG_676_30615a10_378	RP	NEG	10.38	676.3062				2.89E-01	-0.21	1.23	2.33E-02	-0.46	1.35	4.78E-02	-0.44	0.93	9.28E-01	0.02	1.36	1752571	184937	1711592	198847	1756466	196224	1666718	193064
RP_NEG_267_12448a8_867	RP	NEG	8.87	267.1245				2.37E-05	-1.04	1.77	2.33E-02	-0.36	1.42	2.14E-06	-1.22	1.92	6.80E-04	-0.86	1.44	10910017	5513259	5913757	3882256	6790296	4212465	5037218	3337448
RP_POS_440_81302a15_449	RP	POS	15.45	440.8130				7.19E-01	0.07	0.35	2.34E-02	-0.47	1.37	4.60E-01	-0.17	0.71	1.38E-01	0.30	0.55	1987133	191419	2001802	223634	2052254	192397	1951351	242556
HILIC_POS_203_13907a4_671	HILIC	POS	4.671	203.1391				1.61E-07	0.70	1.16	2.34E-02	0.49	1.48	5.96E-06	0.95	1.48	7.00E-04	0.46	1.14	2144190	978032	3957162	2776375	3329461	2031072	4584863	3262588
RP_POS_289_63144a10_328	RP	POS	10.33	289.6314				6.06E-03	-0.67	1.34	2.34E-02	-0.39	1.52	1.20E-03	-0.87	1.41	5.20E-02	-0.48	1.08	5146292	953692	4621067	673195	4772912	574557	4469222	733799
RP_POS_522_28308a10_124	RP	POS	10.12	522.2831				3.85E-16	1.02	1.89	2.35E-02	0.47	1.41	4.51E-09	1.25	1.94	3.04E-10	0.79	1.88	285968	238587	1779141	1509670	1437569	1027260	2120712	1819712
HILIC_NEG_134_89471a5_468	HILIC	NEG	5.468	134.8947				3.37E-01	0.22	0.55	2.35E-02	-0.42	1.42	9.69E-01	0.01	0.09	9.66E-02	0.43	0.90	10051414	6126976	11204501	4898084	12310201	5564632	10098800	3874518
RP_POS_284_09827a0_709	RP	POS	0.71	284.0983				1.11E-03	0.39	1.21	2.35E-02	-0.52	1.45	1.89E-02	0.13	1.42	4.57E-03	0.65	1.16	162343	130502	550401	1134713	809242	1531972	291560	343152
RP_POS_295_22372a10_514	RP	POS	10.51	295.2237				4.65E-01	-0.15	0.92	2.35E-02	0.45	1.49	7.72E-01	0.07	0.64	9.31E-02	-0.38	0.89	1038140	683263	937153	649160	790828	564922	1083478	698989
RP_POS_317_24707a10_853	RP	POS	10.85	317.2471				5.41E-02	-0.30	0.77	2.35E-02	-0.49	1.49	1.01E-02	-0.54	0.97	7.41E-01	-0.05	0.44	2033080	454559	1810830	807993	1993181	631069	1628480	923536
RP_POS_315_13382a7_304	RP	POS	7.30	315.1338				9.47E-02	0.22	0.79	2.37E-02	0.51	1.65	3.21E-02	0.48	0.85	7.35E-01	-0.03	0.63	805619	411456	1045593	1225756	767583	600312	1323603	1586666
RP_POS_482_32376a10_248	RP	POS	10.25	482.3238				1.47E-07	-1.17	1.99	2.39E-02	-0.38	1.60	6.93E-09	-1.36	2.20	2.29E-05	-0.98	1.62	24276555	7456937	15206503	6490092	16666818	7211732	13746187	5361068
RP_POS_454_38867a9_734	RP	POS	9.73	454.3887				1.25E-05	0.79	1.31	2.39E-02	0.45	1.35	4.35E-06	1.01	1.52	2.45E-03	0.56	1.22	387081	176106	570030	232144	517822	195387	622238	255231
RP_POS_237_22096a10_823	RP	POS	10.82	237.2210				4.24E-08	0.78	1.64	2.39E-02	0.47	1.58	4.22E-07	1.02	1.77	4.77E-04	0.55	1.53	148502	116268	343614	261457	284821	220670	402406	286994
RP_POS_1063_67041a10_316	RP	POS	10.32	1063.6704				8.55E-01	-0.04	0.87	2.41E-02	-0.42	1.75	3.18E-01	-0.25	0.68	4.79E-01	0.17	0.82	20223956	13289417	19750544	10686727	22150051	9392845	17351038	11435348
RP_POS_804_54102a12_692	RP	POS	12.69	804.5410				5.52E-03	0.55	1.22	2.42E-02	-0.45	1.38	1.32E-01	0.32	0.79	5.51E-04	0.77	1.32	6442410	2481055	7930790	2715326	8539472	2673493	7322107	2644388
RP_POS_520_77899a10_124	RP	POS	10.12	520.7790				1.72E-15	0.99	1.85	2.44E-02	0.47	1.40	9.42E-09	1.23	1.91	8.47E-10	0.76	1.83	135178	119494	932866	833792	745385	565349	1120347	1006605
RP_POS_814_53406a12_648	RP	POS	12.65	814.5341				1.93E-15	-1.67	2.94	2.44E-02	-0.31	1.36	7.88E-17	-1.83	2.97	3.66E-13	-1.52	2.43	1349572	390791	459513	364978	541347	409448	377679	296349
RP_POS_287_634a10_198	RP	POS	10.20	287.6340				4.23E-02	-0.49	1.18	2.44E-02	-0.40	1.68	8.68E-03	-0.69	1.20	2.46E-01	-0.28	0.89	999399	412337	833884	306064	902425	275252	765343	322353
RP_POS_360_16348a5_551	RP	POS	5.55	360.1635				8.90E-02	-0.26	0.74	2.45E-02	-0.49	1.34	1.35E-02	-0.51	0.88	9.16E-01	-0.02	0.72	1087392	184277	1007385	332886	1081930	280984	932839	365507
RP_NEG_124_99035a0_739	RP	NEG	0.74	124.9904				8.77E-08	0.65	1.14	2.46E-02	0.49	1.60	1.05E-05	0.89	1.44	1.62E-03	0.40	0.99	252080	387812	2386566	3648682	1568528	2756125	3204604	4235038
RP_POS_223_09445a5_877	RP	POS	5.88	223.0945	Unknown	223.0948(100)	4	7.71E-01	-0.06	0.58	2.46E-02	0.45	1.54	4.64E-01	0.17	0.70	2.05E-01	-0.28	0.64	11326891	2539576	11175096	2586137	10596907	2482307	11753284	2582365
RP_NEG_612_3316a10_294	RP	NEG	10.29	612.3316				7.30E-01	-0.06	0.96	2.47E-02	-0.47	1.36	1.49E-01	-0.30	0.74	4.04E-01	0.17	0.91	19029455	6441113	18540961	8318020	20399365	8260115	16682558	8032007
HILIC_POS_546_35638a1_092	HILIC	POS	1.092	546.3564				5.92E-03	0.52	1.06	2.49E-02	-0.45	1.27	1.67E-01	0.29	0.61	4.31E-04	0.75	1.51	2049668	842224	2559975	992293	2781401	923433	2338550	1018134
RP_NEG_478_29431a10_626	RP	NEG	10.63	478.2943				5.17E-03	0.51	1.28	2.50E-02	0.46	1.74	1.50E-03	0.74	1.28	1.12E-01	0.29	1.04	19231009	8969929	24844035	11158045	22347445	7772318	27340625	13357227
RP_POS_581_27795a10_375	RP	POS	10.38	581.2780				6.30E-01	0.09	0.94	2.51E-02	-0.46	1.61	5.40E-01	-0.14	0.69	1.27E-01	0.32	0.96	893265	127391	906205	143655	938224	130183	874185	150515
RP_NEG_528_26471a10_882	RP	NEG	10.88	528.2647				3.25E-03	0.35	1.06	2.51E-02	0.51	1.50	7.99E-03	0.60	1.09	6.83E-02	0.09	0.89	235778	187335	727609	1599669	366662	441803	1088556	2170031
HILIC_POS_341_24319a0_568	HILIC	POS	0.568	341.2432				9.62E-01	-0.01	1.17	2.51E-02	-0.47	1.30	1.99E-01	-0.25	1.01	2.89E-01	0.23	1.02	221564	108785	220410	147544	253309	160577	187511	126447
RP_POS_546_7962a10_198	RP	POS	10.20	546.7962				1.93E-02	-0.60	1.26	2.53E-02	-0.37	1.58	3.66E-03	-0.78	1.31	1.21E-01	-0.41	0.97	584423	399433	401121	258252	458604	261206	343637	244494
HILIC_NEG_197_80795a0_733	HILIC	NEG	0.733	197.8080				3.93E-05	0.50	1.15	2.54E-02	0.50	1.23	2.86E-04	0.75	1.11	3.70E-02	0.25	0.69	299382	120075	665755	828477	480831	581134	850678	989571
RP_POS_275_62561a9_984	RP	POS	9.98	275.6256				1.67E-18	1.13	1.97	2.54E-02	0.45	1.41	4.74E-10	1.35	2.02	2.30E-13	0.90	2.12	273590	111714	771300	439714	673039	279408	869560	541175
RP_POS_452_27649a10_139	RP	POS	10.14	452.2765				3.24E-17	1.06	1.90	2.56E-02	0.45	1.40	1.01E-09	1.28	1.98	2.98E-10	0.83	1.86	1825393	1069967	9096250	7018789	7533307	5098534	10659194	8279603
RP_POS_790_57117a13_587	RP	POS	13.59	790.5712				1.04E-02	-0.50	0.86	2.59E-02	-0.45	1.31	4.65E-04	-0.72	1.31	2.30E-01	-0.27	0.49	14985345	3939096	12802383	4414727	13782429	5015223	11822338	3502105
RP_NEG_165_0551a4_826	RP	NEG	4.83	165.0551				2.73E-02	0.33	0.72	2.61E-02	0.49	1.40	1.17E-02	0.58	0.86	4.86E-01	0.09	0.41	1343041	781307	1797444	1486157	1465929	762080	2128960	1912417
HILIC_NEG_224_82733a0_881	HILIC	NEG	0.881	224.8273				1.99E-01	0.25	0.77	2.62E-02	0.45	1.36	3.95E-02	0.48	0.88	8.98E-01	0.03	0.06	192113	64202	209463	70110	193940	59788	224985	76582
HILIC_POS_170_03275a5_591	HILIC	POS	5.591	170.0328				2.39E-01	0.24	0.54	2.62E-02	-0.44	1.42	9.41E-01	0.02	0.35	4.05E-02	0.46	0.82	787179	444720	895292	454795	995889	435132	794696	455966
RP_POS_631_14099a9_21	RP	POS	9.21	631.1410				4.00E-01	0.15	0.55	2.65E-02	0.47	1.32	9.54E-02	0.38	0.87	6.42E-01	-0.08	0.43	1790624	139955	1816686	182630	1776228	130178	1857145	217029
RP_POS_269_13846a8_87	RP	POS	8.87	269.1385	(E)-2-decylpent-2-enedioic acid	209.1155(100)	3	3.91E-05	-1.04	1.76	2.65E-02	-0.35	1.40	4.28E-06	-1.21	1.89	8.03E-04	-0.87	1.42	1786187	942248	964415	620816	1101591	677473	827239	530395
RP_NEG_850_81525a0_49	RP	NEG	0.49	850.8153				3.80E-07	-0.74	1.24	2.67E-02	0.47	1.45	6.72E-03	-0.50	0.95	3.98E-08	-0.97	1.66	1829811	287241	1397405	620210	1260629	553905	1534181	657404
RP_POS_794_81079a0_492	RP	POS	0.49	794.8108				1.72E-06	-0.69	1.20	2.67E-02	0.47	1.48	1.03E-02	-0.46	0.93	4.86E-07	-0.93	1.58	1759521	315182	1313332	686513	1161994	658237	1464670	687170
RP_POS_568_33972a10_296	RP	POS	10.30	568.3397				8.48E-01	-0.04	0.95	2.69E-02	-0.46	1.35	1.95E-01	-0.27	0.70	3.63E-01	0.20	0.92	51410557	20286973	50567238	25095737	56095989	25825990	45038487	23304108
HILIC_NEG_113_92614a1_049	HILIC	NEG	1.049	113.9261				8.60E-02	0.33	0.95	2.69E-02	0.45	1.32	1.25E-02	0.55	1.10	6.19E-01	0.10	0.22	1078956	262966	1175561	299950	1109499	281155	1241623	306304
RP_NEG_892_53381a12_696	RP	NEG	12.70	892.5338				2.13E-03	0.64	1.24	2.69E-02	-0.42	1.35	5.80E-02	0.42	0.85	2.01E-04	0.85	1.41	3653351	1272825	4487344	1262027	4765260	1198979	4209427	1273872
HILIC_NEG_144_92348a0_678	HILIC	NEG	0.678	144.9235				2.65E-01	-0.21	0.67	2.71E-02	0.46	1.36	9.29E-01	0.02	0.30	6.23E-02	-0.44	0.72	13107793	2007011	12629485	2342611	12112863	2746583	13146107	1731830
HILIC_POS_546_35394a1_211	HILIC	POS	1.211	546.3539				1.71E-03	0.58	1.14	2.72E-02	-0.45	1.28	8.73E-02	0.35	0.67	1.36E-04	0.80	1.46	16270131	6546929	20907216	8168864	22702529	7787593	19111902	8221804
RP_POS_148_09671a0_708	RP	POS	0.71	148.0967				1.92E-06	0.66	1.09	2.73E-02	0.48	1.33	6.21E-05	0.90	1.38	3.10E-04	0.42	1.19	2264174	569940	3137022	1425955	2821536	762910	3452509	1822920
RP_POS_519_32556a10_502	RP	POS	10.50	519.3256				9.77E-01	0.01	1.06	2.75E-02	-0.45	1.58	3.15E-01	-0.22	0.76	2.90E-01	0.23	1.22	50288492	4739960	50316548	5264765	51471597	5139288	49161500	5183257
RP_POS_266_97427a15_48	RP	POS	15.48	266.9743				4.70E-01	-0.16	0.66	2.76E-02	0.43	1.39	7.98E-01	0.06	0.17	1.27E-01	-0.37	1.01	1671039	85670	1658626	77875	1641550	81833	1675702	70434
RP_NEG_597_44775a11_158	RP	NEG	11.16	597.4478				3.90E-02	-0.50	0.77	2.77E-02	-0.39	1.40	5.92E-03	-0.69	1.22	2.46E-01	-0.30	0.58	945898	830760	607052	610004	740866	672288	473239	513118
RP_POS_975_63776a10_515	RP	POS	10.52	975.6378				7.08E-04	0.54	1.34	2.78E-02	0.47	1.74	5.97E-04	0.77	1.27	4.32E-02	0.30	1.04	241533	198718	413072	340693	338119	219926	488025	417946
RP_POS_744_58899a13_689	RP	POS	13.69	744.5890				9.42E-06	-0.99	1.56	2.78E-02	-0.38	1.31	7.66E-07	-1.18	1.87	6.01E-04	-0.80	1.24	10265504	3865631	6483914	3352037	7217901	3478204	5749927	3082896
RP_NEG_389_19415a10_824	RP	NEG	10.82	389.1942				1.06E-10	1.09	1.97	2.80E-02	0.42	1.57	5.36E-10	1.30	2.09	4.69E-07	0.89	1.83	243784	214253	613400	321123	543100	275872	683699	349504
RP_POS_1085_65271a10_312	RP	POS	10.31	1085.6527				8.33E-01	0.05	0.82	2.81E-02	-0.42	1.80	5.03E-01	-0.16	0.55	2.76E-01	0.26	0.75	1140567	448463	1159311	386445	1243812	354059	1074810	402240
RP_POS_564_30579a9_91	RP	POS	9.91	564.3058				1.25E-01	0.32	0.96	2.81E-02	-0.43	1.36	6.43E-01	0.10	0.55	2.36E-02	0.53	1.03	401329	334843	506879	327657	578522	342765	435237	298240
RP_POS_650_84888a0_495	RP	POS	0.50	650.8489				1.53E-06	-0.66	1.12	2.81E-02	0.47	1.43	1.57E-02	-0.43	0.83	4.86E-07	-0.90	1.54	11750463	969169	10228209	2480633	9686037	2340022	10770380	2521322
RP_POS_781_05304a12_808	RP	POS	12.81	781.0530				1.56E-01	0.24	0.55	2.82E-02	-0.47	1.33	9.71E-01	0.01	0.44	3.36E-02	0.47	0.92	516331	299271	614752	437680	710618	513727	518887	323055
RP_POS_507_32272a10_504	RP	POS	10.50	507.3227				1.02E-02	-0.50	0.92	2.82E-02	0.44	1.30	1.92E-01	-0.28	0.59	1.03E-03	-0.72	1.21	1538376	392681	1320610	436715	1225226	420173	1415995	436140
RP_POS_349_21094a10_945	RP	POS	10.95	349.2109				4.79E-05	0.72	1.61	2.84E-02	0.44	1.51	2.73E-05	0.94	1.62	5.22E-03	0.49	1.45	546584	449981	982666	618138	847550	477374	1117783	711930
RP_POS_542_32404a10_032	RP	POS	10.03	542.3240				1.04E-01	0.34	0.97	2.85E-02	-0.43	1.35	5.84E-01	0.12	0.56	1.90E-02	0.55	1.06	27258980	21983598	34612769	21621952	39328331	22471509	29897207	19854703
RP_POS_281_11304a3_034	RP	POS	3.03	281.1130				6.61E-05	0.47	1.14	2.87E-02	0.49	1.66	1.17E-03	0.72	1.30	4.49E-03	0.22	1.19	7313	8471	399094	940058	192645	439829	605543	1226794
RP_POS_283_15411a8_87	RP	POS	8.87	283.1541				2.59E-05	-1.05	1.77	2.87E-02	-0.35	1.38	2.78E-06	-1.22	1.91	5.98E-04	-0.87	1.44	7362510	3816148	3932648	2600230	4499162	2820508	3366135	2247250
RP_POS_551_4245a11_441	RP	POS	11.44	551.4245				9.86E-06	-1.27	2.19	2.88E-02	-0.26	1.29	2.40E-06	-1.40	2.00	5.61E-05	-1.14	1.90	1347790	774217	619653	339480	693528	322268	545778	343294
RP_NEG_1031_63354a10_124	RP	NEG	10.12	1031.6335				1.70E-12	0.87	1.79	2.89E-02	0.47	1.37	3.57E-07	1.10	1.75	1.89E-08	0.63	1.75	344741	299459	2617870	2792673	2007255	1740572	3228485	3459292
RP_POS_390_18442a10_943	RP	POS	10.94	390.1844				3.68E-05	0.76	1.56	2.91E-02	0.43	1.46	1.50E-05	0.98	1.61	3.47E-03	0.54	1.41	409343	354916	750205	444838	653419	357045	846992	503192
RP_NEG_153_01851a4_093	RP	NEG	4.09	153.0185				3.13E-04	0.48	0.85	2.91E-02	0.48	1.31	8.41E-04	0.72	1.16	4.38E-02	0.24	0.91	852418	608633	1599172	1704290	1227022	1045763	1971321	2119486
RP_POS_918_7074a0_5	RP	POS	0.50	918.7074				1.39E-02	0.42	0.96	2.91E-02	-0.46	1.49	2.96E-01	0.19	0.56	2.39E-03	0.65	1.33	406842	214936	530040	307838	596951	333931	463129	266111
RP_POS_291_1203a8_87	RP	POS	8.87	291.1203				3.04E-05	-1.05	1.78	2.91E-02	-0.34	1.37	3.48E-06	-1.22	1.90	6.23E-04	-0.88	1.44	7325158	3904812	3858874	2593978	4422638	2805889	3295109	2252358
RP_POS_279_64703a10_328	RP	POS	10.33	279.6470				2.76E-02	-0.54	1.07	2.92E-02	-0.38	1.27	6.43E-03	-0.73	1.16	1.61E-01	-0.35	0.74	2007611	386785	1839312	275887	1899255	236630	1779369	300755
RP_POS_1025_45825a0_487	RP	POS	0.49	1025.4583				2.27E-04	0.47	0.89	2.93E-02	-0.48	1.38	1.52E-01	0.23	0.68	1.10E-04	0.71	1.27	508178	43684	577430	165311	613312	170778	541547	153037
RP_POS_357_29956a10_959	RP	POS	10.96	357.2996				1.14E-04	0.46	0.95	2.94E-02	0.49	1.37	1.30E-03	0.71	1.04	1.03E-02	0.22	0.95	393813	317672	1336464	2286557	836534	1114307	1836394	2968441
RP_POS_569_4325a13_63	RP	POS	13.63	569.4325				1.93E-01	0.29	0.58	2.94E-02	0.42	1.28	4.49E-02	0.50	0.83	7.35E-01	0.08	0.66	2630507	1417336	2999414	1236786	2731176	1113156	3267651	1305579
RP_NEG_968_76837a0_493	RP	NEG	0.49	968.7684				9.61E-03	-0.50	0.92	2.94E-02	0.44	1.39	2.13E-01	-0.28	0.54	4.89E-04	-0.72	1.28	1300024	116387	1234633	131547	1206074	106825	1263192	147940
HILIC_NEG_182_04587a0_816	HILIC	NEG	0.816	182.0459				3.07E-03	0.35	1.03	2.94E-02	0.50	1.34	9.50E-03	0.60	1.09	6.77E-03	0.10	1.38	178189	101149	4142765	13059668	1274677	2739582	7010852	17896862
RP_POS_269_2265a10_854	RP	POS	10.85	269.2265				1.76E-02	-0.38	0.82	2.95E-02	-0.47	1.46	5.54E-03	-0.61	1.02	3.54E-01	-0.15	0.51	46851869	9408187	41328079	15645082	44729075	10980182	37927083	18717969
RP_POS_361_16687a10_943	RP	POS	10.94	361.1669				6.92E-06	0.79	1.62	2.95E-02	0.44	1.43	4.99E-06	1.01	1.68	1.36E-03	0.57	1.45	1968194	1149207	3220047	1593986	2874180	1276464	3565915	1805531
RP_NEG_511_29214a8_899	RP	NEG	8.90	511.2921				1.36E-01	-0.48	0.96	2.96E-02	-0.24	1.39	6.84E-02	-0.60	0.90	2.64E-01	-0.36	0.62	2552435	3317866	1641928	1033409	1865796	1038892	1418061	987970
RP_POS_684_84216a0_492	RP	POS	0.49	684.8422				4.92E-01	0.10	0.69	2.96E-02	0.48	1.53	1.02E-01	0.34	0.74	3.35E-01	-0.14	0.94	1805565	364187	1876195	797360	1703066	592626	2049324	933898
RP_POS_581_45367a12_257	RP	POS	12.26	581.4537				9.28E-02	-0.41	0.69	2.98E-02	-0.38	1.39	1.76E-02	-0.61	1.24	4.03E-01	-0.22	0.55	3251949	2859844	2316691	1992872	2748510	2249719	1884873	1606968
RP_POS_184_07294a10_198	RP	POS	10.20	184.0729				1.25E-01	-0.36	1.07	2.98E-02	-0.39	1.65	3.09E-02	-0.56	1.02	4.97E-01	-0.17	0.84	1693757	771366	1462097	578935	1587364	526701	1336831	606412
RP_NEG_680_31909a10_291	RP	NEG	10.29	680.3191				6.60E-01	-0.08	0.93	2.98E-02	-0.46	1.30	1.39E-01	-0.31	0.74	4.56E-01	0.15	0.86	1412029	403318	1372605	536337	1488597	517069	1256613	535132

Supplementary table 1: Metabolomics results (in asceding order according to p-value from progressive ALD vs non-progressive ALD comparison, with molecular features with ID_level of 1-2 first)

								all_ALD_vs_control			Prog_ALD_vs_non-prog_ALD			Prog_ALD_vs_control_ALD			Non-prog_ALD_vs_control			Healthy_control		all_ALD		Non-prog_ALD		Progressive_ALD	
								t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA								
Feature_ID	RP_HILIC	POS_NEG	Average.Rt	Average.Mz	Metabolite.name	curated_MSMS	ID_level	p	d	VIP	p	d	VIP	p	d	VIP	p	d	VIP	Mean	SD	Mean	SD	Mean	SD	Mean	SD
HILIC_NEG_498_29004a1_356	HILIC	NEG	1.356	498.2900				3.82E-02	0.29	0.74	2.99E-02	0.48	1.44	1.81E-02	0.53	0.75	6.80E-01	0.05	0.15	188589	677994	612428	1629046	257489	818152	967367	2106006
HILIC_NEG_61_98754a0_881	HILIC	NEG	0.881	61.9875				1.44E-01	0.29	0.70	2.99E-02	0.44	1.39	3.33E-02	0.51	0.83	7.10E-01	0.08	0.15	3768634	1690791	4283537	1760918	3902156	1378379	4664919	2016971
RP_NEG_650_28131a10_328	RP	NEG	10.33	650.2813				1.46E-03	-0.74	1.35	3.01E-02	-0.39	1.52	2.30E-04	-0.93	1.51	2.23E-02	-0.54	1.07	2077171	373426	1831119	299668	1895824	280607	1766414	306838
RP_POS_248_14882a0_71	RP	POS	0.71	248.1488				2.00E-08	0.69	1.17	3.03E-02	0.48	1.34	2.93E-05	0.93	1.31	1.71E-06	0.45	1.46	366090	354495	1701514	2121730	1240363	1085998	2162666	2735316
RP_POS_1053_6908a11_129	RP	POS	11.13	1053.6908				6.36E-04	0.41	1.08	3.04E-02	-0.49	1.52	1.49E-01	0.16	0.91	1.52E-03	0.65	1.28	246954	40944	354385	296766	418609	358525	290161	202432
RP_POS_353_2449a11_382	RP	POS	11.38	353.2449				9.80E-09	0.73	1.33	3.04E-02	0.47	1.27	4.78E-06	0.96	1.51	7.97E-05	0.49	1.31	356541	186390	857839	746599	696383	521665	1019296	894909
RP_POS_186_18484a9_04	RP	POS	9.04	186.1848				6.40E-02	0.44	0.74	3.04E-02	-0.39	1.29	3.45E-01	0.24	0.41	1.14E-02	0.63	1.04	864705	334210	987179	257305	1042647	234030	931711	269654
RP_POS_535_86243a11_127	RP	POS	11.13	535.8624				4.38E-06	0.55	1.24	3.05E-02	-0.48	1.52	7.58E-03	0.31	1.09	1.21E-04	0.79	1.40	289588	58204	501016	425078	592887	510093	409145	296058
RP_POS_313_63058a10_291	RP	POS	10.29	313.6306				4.79E-01	-0.13	1.01	3.06E-02	-0.46	1.31	8.18E-02	-0.35	0.84	6.24E-01	0.10	0.92	541813	168249	515416	221968	563218	224999	467614	210373
RP_POS_339_28903a10_962	RP	POS	10.96	339.2890				7.04E-05	0.48	0.98	3.07E-02	0.49	1.35	1.07E-03	0.72	1.05	6.17E-03	0.24	0.98	129859	109676	452797	757372	288590	371193	617003	982913
RP_POS_770_46136a10_501	RP	POS	10.50	770.4614				2.77E-02	-0.44	0.90	3.09E-02	-0.43	1.27	5.21E-03	-0.66	1.21	2.78E-01	-0.23	0.96	2080412	343263	1920615	361923	1998453	309966	1842776	395230
RP_POS_896_53857a12_74	RP	POS	12.74	896.5386				1.38E-04	-0.88	1.48	3.09E-02	-0.38	1.26	9.92E-06	-1.07	1.86	5.04E-03	-0.69	1.19	1202946	469271	822758	378102	904130	428476	741386	302879
RP_POS_679_49835a11_178	RP	POS	11.18	679.4984				1.02E-05	0.52	1.18	3.10E-02	-0.48	1.55	6.05E-03	0.28	1.20	3.06E-04	0.77	1.34	56770	29676	235153	380564	317317	473035	152989	234679
RP_POS_558_29468a10_324	RP	POS	10.32	558.2947				5.81E-02	-0.45	1.15	3.10E-02	-0.39	1.52	1.32E-02	-0.64	1.11	2.98E-01	-0.25	0.87	4107124	1583102	3514524	1197416	3771774	1084646	3257274	1259111
RP_POS_1039_67102a10_323	RP	POS	10.32	1039.6710				5.08E-02	-0.50	1.16	3.11E-02	-0.37	1.57	1.19E-02	-0.68	1.16	2.35E-01	-0.31	0.92	88142777	62285056	64495114	40806988	73255313	40046000	55734916	40051315
RP_POS_448_30518a8_668	RP	POS	8.67	448.3052				1.92E-01	0.18	0.64	3.12E-02	0.48	1.27	5.98E-02	0.42	0.88	5.87E-01	-0.06	0.34	519233	497498	716524	1220400	452630	598895	980419	1583778
HILIC_POS_183_00583a2_975	HILIC	POS	2.975	183.0058				3.87E-11	0.98	1.59	3.13E-02	0.43	1.50	1.58E-09	1.20	1.87	4.22E-06	0.77	1.49	1362144	647109	2641321	1308320	2360624	1176326	2922018	1383401
RP_NEG_558_31378a10_623	RP	NEG	10.62	558.3138				6.38E-02	0.37	1.22	3.14E-02	-0.43	1.29	4.92E-01	0.16	0.49	6.40E-03	0.59	1.60	1339595	243146	1433949	252541	1488119	213895	1379779	277699
RP_POS_257_22629a8_886	RP	POS	8.89	257.2263				1.18E-01	-0.51	0.98	3.14E-02	-0.23	1.39	5.96E-02	-0.62	0.93	2.30E-01	-0.39	0.65	1324370	1708487	832467	522689	944484	529596	720449	495886
RP_POS_766_53638a13_197	RP	POS	13.20	766.5364				1.00E-02	0.43	0.76	3.15E-02	0.46	1.30	3.65E-03	0.66	1.01	2.15E-01	0.20	0.68	1221102	668948	1633375	1021618	1413769	697618	1852981	1234347
RP_POS_593_33282a6_145	RP	POS	6.15	593.3328				3.18E-03	0.42	0.78	3.16E-02	0.47	1.40	3.85E-03	0.66	0.99	1.10E-01	0.19	0.69	403991	1194141	1423391	2643931	852784	1269611	1993997	3441949
HILIC_NEG_497_04599a7_623	HILIC	NEG	7.623	497.0460				6.29E-01	-0.10	0.23	3.16E-02	-0.43	1.21	1.57E-01	-0.31	0.60	6.27E-01	0.11	0.36	349835	16483	348216	16231	351691	17323	344741	14407
RP_NEG_594_30389a10_248	RP	NEG	10.25	594.3039				5.44E-09	-1.22	2.07	3.17E-02	-0.37	1.59	2.63E-10	-1.40	2.27	2.42E-06	-1.04	1.75	1198821	314909	753682	311559	820385	341364	686978	265536
RP_POS_287_13022a10_329	RP	POS	10.33	287.1302				3.32E-05	-0.89	1.65	3.18E-02	-0.39	1.36	6.30E-06	-1.09	1.74	1.31E-03	-0.70	1.43	3452946	613547	2893530	568841	3015251	499022	2771809	611968
HILIC_POS_148_09682a4_203	HILIC	POS	4.203	148.0968				2.55E-07	0.71	1.24	3.20E-02	0.46	1.41	2.07E-05	0.94	1.49	6.94E-05	0.49	1.44	3744443	1333315	5963412	3314847	5251464	1913528	6675360	4183857
RP_POS_284_63034a10_127	RP	POS	10.13	284.6303				1.86E-21	1.23	2.05	3.22E-02	0.41	1.35	1.15E-11	1.43	2.16	5.54E-14	1.02	2.15	238699	122467	832429	468101	732295	335190	932563	556680
RP_POS_896_78961a0_493	RP	POS	0.49	896.7896				7.93E-03	-0.48	0.92	3.25E-02	0.44	1.39	2.39E-01	-0.26	0.43	3.28E-04	-0.70	1.27	1041863	280570	873122	366570	794940	300676	951304	410620
RP_POS_748_52576a13_075	RP	POS	13.08	748.5258				5.98E-01	-0.11	0.64	3.27E-02	-0.41	1.31	1.54E-01	-0.32	0.61	7.09E-01	0.09	0.57	719780	853250	630179	761562	792441	859592	467917	615758
RP_POS_518_32239a10_503	RP	POS	10.50	518.3224				7.83E-01	0.05	1.10	3.27E-02	-0.44	1.57	4.48E-01	-0.17	0.73	2.09E-01	0.27	1.28	192184039	17857084	193219389	20085850	197492503	19397921	188946276	20039278
RP_POS_1015_66241a10_501	RP	POS	10.50	1015.6624				3.35E-01	-0.20	0.98	3.28E-02	-0.42	1.54	7.50E-02	-0.41	0.95	9.55E-01	0.01	0.75	2930353	528036	2826388	520120	2936941	504287	2715835	517033
HILIC_NEG_243_99753a0_882	HILIC	NEG	0.882	243.9975				2.06E-01	0.25	0.66	3.29E-02	0.43	1.39	4.88E-02	0.47	0.77	8.60E-01	0.04	0.07	139491	66586	157079	70774	142019	57477	172139	79710
RP_POS_300_63226a10_199	RP	POS	10.20	300.6323				2.62E-01	0.23	0.69	3.30E-02	-0.42	1.61	9.20E-01	0.02	0.33	4.83E-02	0.44	0.86	938712	301636	1007651	291840	1069664	262296	945637	308920
RP_POS_598_26404a10_376	RP	POS	10.38	598.2640				9.08E-01	-0.02	0.74	3.30E-02	-0.44	1.31	2.87E-01	-0.24	0.63	3.50E-01	0.20	0.69	614058	87987	611914	98323	632802	87798	591026	104562
HILIC_NEG_195_81104a0_882	HILIC	NEG	0.882	195.8110				4.17E-01	0.16	0.76	3.30E-02	0.43	1.34	8.89E-02	0.38	0.87	7.95E-01	-0.06	0.33	761696	139690	785420	151756	753199	149404	817642	148625
RP_POS_548_30035a10_198	RP	POS	10.20	548.3004				2.01E-02	-0.59	1.25	3.31E-02	-0.36	1.51	3.97E-03	-0.77	1.30	1.22E-01	-0.41	0.98	1011981	670989	705459	442062	799291	457903	611628	408879
RP_POS_516_30518a10_125	RP	POS	10.13	516.3052				6.28E-21	1.21	2.06	3.31E-02	0.41	1.33	1.81E-11	1.42	2.14	8.77E-14	1.01	2.14	11019593	5664615	36994391	20734025	32580684	14763110	41408098	24715721
HILIC_POS_290_15289a0_899	HILIC	POS	0.899	290.1529				3.29E-04	0.53	1.08	3.32E-02	0.46	1.26	5.34E-04	0.76	1.19	3.30E-02	0.30	0.73	218834	64202	283792	133432	255372	87928	312212	163070
RP_POS_274_17554a0_71	RP	POS	0.71	274.1755				7.72E-02	0.24	0.81	3.32E-02	-0.48	1.46	9.86E-01	0.00	0.90	2.08E-02	0.47	0.94	7271348	1644988	8243457	4617712	9225380	5451785	7261534	3375208
HILIC_POS_273_12112a3_697	HILIC	POS	3.697	273.1211				1.01E-02	0.31	0.84	3.34E-02	0.48	1.41	1.19E-02	0.56	0.90	3.93E-01	0.07	0.59	1315856	929016	2579272	4547946	1607544	2101612	3551000	5953648
HILIC_NEG_177_86018a2_978	HILIC	NEG	2.978	177.8602				5.72E-01	0.10	0.28	3.34E-02	0.45	1.29	1.31E-01	0.32	0.53	5.00E-01	-0.13	0.40	592945	168118	614389	233088	564969	202512	663808	252535
HILIC_POS_516_30615a1_34	HILIC	POS	1.34	516.3062				1.55E-17	1.13	1.84	3.35E-02	0.42	1.16	1.76E-10	1.34	2.07	3.95E-11	0.92	2.14	825900	402384	2251819	1254292	1985496	926838	2518142	1474728
HILIC_POS_245_0954a0_899	HILIC	POS	0.899	245.0954				9.41E-06	0.62	1.15	3.35E-02	0.46	1.23	7.63E-05	0.85	1.31	3.35E-03	0.40	0.99	380806	99252	515822	233069	466277	156629	565367	283212
RP_POS_310_20111a5_604	RP	POS	5.60	310.2011				6.59E-02	0.33	0.71	3.37E-02	0.44	1.27	1.64E-02	0.55	1.02	5.40E-01	0.11	0.50	471556	402822	636091	516802	526505	379234	745677	609338
HILIC_POS_480_30936a1_859	HILIC	POS	1.859	480.3094				4.26E-04	0.61	1.01	3.39E-02	0.44	1.33	3.40E-04	0.83	1.19	1.73E-02	0.39	0.98	1595496	830746	2289755	1176453	2040006	756047	2539504	1448250
RP_POS_430_24893a12_953	RP	POS	12.95	430.2489				1.49E-06	-0.91	1.56	3.41E-02	-0.41	1.41	4.65E-07	-1.11	1.82	3.28E-04	-0.70	1.48	1299367	311820	944185	376603	1023716	337840	864655	399387
RP_POS_209_11739a8_87	RP	POS	8.87	209.1174	Primin	209.1166(100), 153.0541(28)	3	3.39E-05	-1.04	1.78	3.42E-02	-0.33	1.34	4.21E-06	-1.21	1.89	6.41E-04	-0.88	1.45	2915744	1530214	1567512	1013763	1781489	1098093	1353535	881565
RP_POS_385_29306a10_443	RP	POS	10.44	385.2931				6.03E-01	-0.10	0.57	3.43E-02	0.43	1.33	6.04E-01	0.11	0.71	1.63E-01	-0.32	0.62	19844061	873106	19749688	934081	19552731	970699	19946645	861043
RP_POS_698_78564a6_136	RP	POS	6.14	698.7856				1.07E-05	0.52	1.16	3.48E-02	-0.47	1.45	1.47E-03	0.28	1.21	5.08E-04	0.76	1.22	72690	57807	802714	1570996	1135324	2017359	470105	831212
RP_NEG_294_98227a7_902	RP	NEG	7.90	294.9823				9.18E-01	-0.02	0.64	3.49E-02	-0.44	1.26	2.15E-01	-0.24	0.58	3.73E-01	0.20	0.74	14079954	794856	14062291	982896	14269226	1116071	13855356	786687
RP_POS_375_32004a10_27	RP	POS	10.27	375.3200				1.41E-01	-0.25	0.91	3.50E-02	0.45	1.24	8.93E-01	-0.03	0.77	1.01E-02	-0.48	0.94	1118803	78940	1092184	112034	1068616	91313	1115752	126046
RP_NEG_353_14334a10_835	RP	NEG	10.84	353.1433				1.52E-15	1.14	1.99	3.51E-02	0.41	1.44	2.46E-12	1.35	2.19	2.28E-08	0.94	1.82	1538010	1468708	5394155	3274327	4706513	3079468	6081797	3348599
RP_POS_287_07544a8_02	RP	POS	8.02	287.0754				1.08E-05	0.52	1.24	3.51E-02	0.47	1.62	3.23E-04	0.76	1.54	7.31E-03	0.28	0.86	186227	937617	14701569	31272380	8105440	19975734	21297699	38573558
RP_POS_274_18338a7_445	RP	POS	7.45	274.1834				3.88E-13	1.04	1.80	3.51E-02	0.42	1.59	2.45E-10	1.25	2.00	2.88E-07	0.83	1.66	702083	492212	1846040	1092260	1616626	970931	2075454	1166316
RP_POS_284_27005a7_999	RP	POS	8.00	284.2701				9.68E-01	0.01	0.87	3.52E-02	-0.41	1.39	4.01E-01	-0.20	0.77	3.77E-01	0.21	0.65	480561	240206	482459	214727	527525	221612	437393	199750
RP_POS_223_16919a11_151	RP	POS	11.15	223.1692				1.12E-02	-0.56	1.28	3.53E-02	-0.39	1.79	1.40E-03	-0.76	1.74	1.26E-01	-0.37	0.77	1276563	624143	952249	537599	1065053	568799	839445	484173
RP_POS_445_36612a13_123	RP	POS	13.12	445.3661				3.05E-01	-0.19	0.86	3.53E-02	-0.43	1.23	6.17E-02	-0.41	1.00	9.06E-01	0.02	0.78	916522	194094	873784	229693	921963	214202	825605	236589
RP_POS_538_34998a10_163	RP	POS	10.16	538.3500				1.96E-11	0.82	1.58	3.54E-02	0.45	1.30	1.08E-06	1.05	1.62	2.05E-07	0.59	1.63	59887	47414	522250	607607	394302	389935	650197	748631
RP_POS_990_7854a0_492	RP	POS	0.49	990.7854				2.75E-01	0.15	0.74	3.55E-02	0.47	1.51	5.99E-02	0.39	0.84	5.58E-01	-0.08	0.89	1776600	274706	1868323	681111	1725336	512019	2011311	795866
RP_NEG_1096_76135a0_49	RP	NEG	0.49	1096.7614				6.20E-07	-0.76	1.24	3.56E-02	0.44	1.44	4.54E-03	-0.54	1.02	7.50E-08	-0.97	1.61	1015500	208258	726750	399145	643147	359696	810353	422185
RP_POS_511_32394a9_957	RP	POS	9.96	511.3239				2.07E-05	0.58	0.94	3.56E-02	0.46	1.25	2.87E-05	0.81	1.31	2.79E-02	0.35	0.71	224566	154410	444439	415492	357416	371161	531463	442238
RP_POS_311_21945a10_579	RP	POS	10.58	311.2195				8.67E-01	0.04	0.44	3.58E-02	-0.40	1.30	5.07E-01	-0.16	0.34	3.41E-01	0.24	0.60	4020325	1528536	4070588	1254040	4332888	1285221	3808289	1176912
RP_NEG_195_8111a4_571	RP	NEG	4.57	195.8111				2.64E-02	-0.47	0.78	3.58E-02	-0.40	1.36	4.39E-03	-0.67	1.08	2.35E-01	-0.27	0.61	13196716	5245401	10794239	4926578	11824599	4728955	9763879	4950559
RP_POS_798_56366a12_279	RP	POS	12.28	798.5637				3.37E-02	0.37	1.04	3.59E-02	0.44	1.52	4.48E-03	0.59	1.20	4.45E-01	0.15	0.85	478732	265431	607510	365546	531075	349663	683945	368495
RP_POS_568_19092a11_014	RP	POS	11.01	568.1909				4.49E-01	0.16	0.54	3.61E-02	-0.42	1.28	8.07E-01	-0.05	0.32	1.18E-01	0.36	0.77	478772	142342	500801	142305	530523	147085	471080	132203
RP_POS_147_04408a0_71	RP	POS	0.71	147.0441				3.08E-01	0.18	0.89	3.62E-02	0.44	1.32	6.74E-02	0.40	1.22	8.07E-01	-0.05	0.58	1910041	400808	2002393	555593	1886342	464246	2118444	616973
HILIC_POS_120_0658a1_03	HILIC	POS	1.03	120.0658				1.27E-01	0.23	0.48	3.63E-02	0.46	1.19	3.96E-02	0.46	0.74	9.94E-01	0.00	0.68	3081967	1807344	3800257	3409523	3085062	2039424	4515453	4275956
RP_NEG_1059_66504a10_368	RP	NEG	10.37	1059.6650				8.07E-01	-0.06	0.98	3.63E-02	-0.39	1.52	3.19E-01	-0.25	0.75	5.59E-01	0.14	0.87	2073493	1077916	2022036	865222	2202644	768297	1841427	925011
HILIC_NEG_172_84219a3_03	HILIC	NEG	3.03	172.8422				7.93E-03	-0.37	1.33	3.63E-02	-0.46	1.16	2.22E-03	-0.60	1.45	3.86E-01	-0.14	1.28	2381887	103218	2297296	254843	2350491	219606	2244101	277874
RP_POS_241_01546a15_438	RP	POS	15.44	241.0155				3.80E-01	0.18	0.61	3.64E-02	-0.41	1.39	9.19E-01	-0.02	0.64	8.38E-02	0.39	0.84	2106331	292062	2158451	282484	2217353	257154	2099548	296671
RP_NEG_606_30359a9_984	RP	NEG	9.98	606.3036				8.45E-19	1.13	1.96	3.67E-02	0.42	1.31	2.97E-10	1.34	2.04	1.53E-12	0.93	2.04	377552	149172	1074613	611824	946802	423701	1202424	737180
HILIC_NEG_142_92889a1_049	HILIC	NEG	1.049	142.9289				2.00E-01	0.26	0.68	3.68E-02	0.42	1.45	4.24E-02	0.47	0.97	8.10E-01	0.05	0.15	1007029	352279	1100083	356543	1025912	335926	1174255	364371
RP_NEG_604_87225a0_495	RP	NEG	0.50	604.8723				1.01E-06	-0.69	1.16	3.74E-02	0.44	1.39	1.09E-02	-0.46	0.87	2.33E-07	-0.91	1.56	17203519	1182379	15390013	2831145	14802526	2586841	15977500	2966180
RP_NEG_206_78928a15_581	RP	NEG	15.58	206.7893				1.05E-01	-0.31	0.70	3.74E-02	-0.43	1.72	9.62E-03	-0.52	1.20	6.84E-01	-0.09	0.43	1030807	35831	1018292	42089	1027032	47536	1009552	34111
RP_POS_422_24435a10_284	RP	POS	10.28	422.2444				1.31E-01	-0.31	0.85	3.75E-02	0.41	1.39	6.35E-01	-0.11	0.46	2.22E-02	-0.52	1.02	1167086	103982	1134841	101185	1113857	93880	1155824	104756
RP_POS_965_63696a11_142	RP	POS	11.14	965.6370				1.20E-07	0.64	1.31	3.76E-02	-0.46	1.51	5.20E-04	0.41	1.29	3.02E-05	0.87	1.45	191368	96300	714996	906136	903350	1090904	526641	629641
RP_POS_369_29736a10_947	RP	POS	10.95	369.2974				4.58E-02	-0.44	1.04	3.80E-02	0.39	1.22	2.98E-01	-0.25	0.54	8.07E-03	-0.64	1.18	15700362	3328372	14358120	2858056	13767230	2733798	14949011	2884001
RP_POS_557_87524a11_121	RP	POS	11.12	557.8752				1.11E-05	0.54	1.23	3.81E-02	-0.46	1.46	9.30E-03	0.31	1.06	2.02E-04	0.77	1.37	334832	67842	496728	331816	565550	399889	427907	229942
RP_POS_831_49713a10_872	RP	POS	10.87	831.4971				7.88E-07	0.59	1.22	3.81E-02	-0.46	1.64	8.64E-04	0.36	1.32	1.10E-04	0.82	1.39	44786	21915	1008884	1827945	1388320	2258482	629448	1164646
HILIC_POS_257_14713a3_699	HILIC	POS	3.699	257.1471				1.85E-03	0.41	0.90	3.84E-02	0.46	1.37	2.55E-03	0.64	1.07	1.41E-01	0.18	0.57	14847614	10836656	26628262	31714963	20055208	20699326	33201316	38930315
RP_NEG_573_45459a11_525	RP	NEG	11.53	573.4546				1.50E-01	-0.38	0.63	3.84E-02	-0.34	1.25	3.75E-02	-0.55	1.02	4.69E-01	-0.21	0.53	2256990	2946636	1450318	1757971	1814967	2196066	1085669	1072346
HILIC_POS_140_06841a3_699	HILIC	POS	3.699	140.0684				3.49E-01	0.18	0.74	3.84E-02	0.42	1.26	8.30E-02	0.39	0.96	8.80E-01	-0.03	0.20	31950221	12177754	34361140	13702882	31532484	12259221	37189796	14586030
RP_POS_267_6478a10_375	RP	POS	10.38	267.6478				8.11E-01	0.05	0.85	3.85E-02	-0.42	1.47	4.91E-01	-0.16	0.70	2.49E-01	0.26	0.75	738873	117114	744590	118266	768993	109951	720187	122289
RP_POS_740_54968a11_175	RP	POS	11.18	740.5497				1.46E-06	0.57	1.24	3.85E-02	-0.46	1.53	1.22E-03	0.34	1.28	1.51E-04	0.80	1.39	34308	13074	241925	404480	325729	501419	158121	254545
RP_NEG_755_13904a9_304	RP	NEG	9.30	755.1390				1.35E-01	0.25	0.63	3.86E-02	0.44	1.21	2.61E-02	0.47	0.80	8.99E-01	0.02	0.27	1104657	79832	1133173	125396	1107296	107559	1159050	137235
HILIC_POS_352_24496a2_224	HILIC	POS	2.224	352.2450				9.27E-01	-0.02	0.65	3.87E-02	-0.42	1.25	2.90E-01	-0.23	0.55	3.88E-01	0.19	0.40	1904810	577872	1893832	631442	2023983	646537	1763681	594133
RP_POS_383_11526a0_548	RP	POS	0.55	383.1153				1.24E-04	0.49	0.92	3.90E-02	0.46	1.48	5.75E-04	0.72	1.11	3.40E-02	0.26	1.15	6825056	1185216	8669199	4160106	7810166	2860639	9528231	5027615
HILIC_POS_184_07355a1_167	HILIC	POS	1.167	184.0736				2.02E-01	0.28	0.66	3.90E-02	-0.40	1.24	7.42E-01	0.08	0.17	4.39E-02	0.48	0.84	1382050	627378	1542952	561628	1658496	534969	1427409	569079
RP_POS_813_55853a13_996	RP	POS	14.00	813.5585				2.27E-01	-0.27	0.71	3.91E-02	0.39	1.41	7.61E-01	-0.07	0.70	5.51E-02	-0.47	0.85	2218615	957654	1988620	815079	1821040	792634	2156201	810361

Supplementary table 1: Metabolomics results (in asceding order according to p-value from progressive ALD vs non-progressive ALD comparison, with molecular features with ID_level of 1-2 first)

								all_ALD_vs_control			Prog_ALD_vs_non-prog_ALD			Prog_ALD_vs_control_ALD			Non-prog_ALD_vs_control			Healthy_control		all_ALD		Non-prog_ALD		Progressive_ALD	
								t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA								
Feature_ID	RP_HILIC	POS_NEG	Average.Rt	Average.Mz	Metabolite.name	curated_MSMS	ID_level	p	d	VIP	p	d	VIP	p	d	VIP	p	d	VIP	Mean	SD	Mean	SD	Mean	SD	Mean	SD
RP_POS_936_72302a0_498	RP	POS	0.50	936.7230				1.61E-01	0.25	0.69	3.93E-02	-0.43	1.40	8.83E-01	0.03	0.44	2.57E-02	0.46	1.12	367269	129429	407998	174447	443841	174627	372155	168428
RP_POS_795_57465a13_297	RP	POS	13.30	795.5747				1.38E-01	-0.32	0.66	3.93E-02	0.40	1.26	6.13E-01	-0.12	0.59	2.83E-02	-0.52	0.95	3347652	1305871	2954391	1208627	2706148	1188797	3202635	1188430
HILIC_POS_166_08627a4_496	HILIC	POS	4.496	166.0863				1.74E-01	0.24	0.64	3.94E-02	-0.44	1.37	9.21E-01	0.02	0.26	5.32E-02	0.45	0.76	1387734	849620	1650735	1187151	1895763	1490279	1405708	709900
RP_POS_429_37354a13_124	RP	POS	13.12	429.3735				1.30E-01	-0.27	1.07	3.94E-02	-0.43	1.23	2.87E-02	-0.49	1.22	7.55E-01	-0.06	0.79	4382885	726392	4140437	923096	4330177	769850	3950697	1027356
RP_POS_330_24615a8_699	RP	POS	8.70	330.2462				2.16E-02	0.41	1.06	3.95E-02	0.43	1.25	4.75E-03	0.62	1.15	3.01E-01	0.19	0.69	1979724	911192	2452917	1207959	2204727	1018313	2701107	1336203
HILIC_NEG_198_90411a0_881	HILIC	NEG	0.881	198.9041				1.27E-01	0.30	0.71	3.96E-02	0.42	1.36	3.17E-02	0.51	0.83	6.41E-01	0.09	0.23	1051623	579657	1237288	620579	1109793	497150	1364783	705523
HILIC_NEG_187_94209a6_093	HILIC	NEG	6.093	187.9421				8.09E-02	-0.31	1.04	3.96E-02	-0.43	1.21	1.40E-02	-0.52	0.97	6.37E-01	-0.09	1.16	446442	102569	406108	137843	434389	126315	377827	144227
RP_POS_793_55548a12_651	RP	POS	12.65	793.5555				1.17E-12	-1.54	2.67	3.97E-02	-0.30	1.28	6.87E-14	-1.69	2.73	1.71E-10	-1.39	2.21	2216920	706675	881470	636997	1012197	701976	750744	540523
RP_POS_491_83658a11_136	RP	POS	11.14	491.8366				2.36E-05	0.51	1.16	3.99E-02	-0.46	1.48	2.55E-02	0.28	0.99	2.42E-04	0.74	1.35	222819	42729	354400	288383	413602	337674	295198	216450
RP_POS_535_2876a8_888	RP	POS	8.89	535.2876				1.24E-01	-0.50	0.98	4.00E-02	-0.22	1.37	6.49E-02	-0.61	0.91	2.35E-01	-0.39	0.64	708624	911127	450514	281049	508062	283152	392966	269548
RP_POS_597_44818a11_52	RP	POS	11.52	597.4482				1.29E-01	-0.42	0.67	4.00E-02	-0.33	1.25	3.75E-02	-0.58	1.00	3.85E-01	-0.25	0.53	2276137	3016327	1409356	1652917	1748672	1969530	1070040	1185754
RP_NEG_1028_77051a0_489	RP	NEG	0.49	1028.7705				8.75E-09	-0.76	1.33	4.01E-02	0.44	1.46	1.31E-03	-0.54	1.17	8.21E-08	-0.98	1.63	1954526	249738	1407197	772255	1249151	762459	1565243	756708
RP_POS_552_33093a10_822	RP	POS	10.82	552.3309				2.78E-03	-0.80	1.46	4.04E-02	-0.32	1.62	6.12E-04	-0.96	1.52	1.85E-02	-0.64	1.15	385231	243793	240205	139752	268767	143665	211643	130979
RP_POS_251_12784a8_87	RP	POS	8.87	251.1278				3.15E-05	-1.05	1.79	4.04E-02	-0.32	1.32	4.35E-06	-1.21	1.88	5.33E-04	-0.90	1.48	5502110	2664173	3145189	1740685	3501013	1881800	2789364	1523892
RP_POS_490_20676a7_364	RP	POS	7.36	490.2068				1.66E-04	0.53	1.74	4.05E-02	-0.45	1.21	5.48E-02	0.31	1.54	1.33E-04	0.75	1.31	341750	254947	633527	600065	756168	650046	510885	523688
RP_POS_199_14418a1_858	RP	POS	1.86	199.1442				4.86E-03	0.34	0.64	4.05E-02	0.47	1.26	1.03E-02	0.57	0.91	1.74E-01	0.10	0.42	591880	1074970	2713055	7133930	1244037	3075111	4182073	9432079
HILIC_POS_144_10202a5_185	HILIC	POS	5.185	144.1020				8.07E-05	0.53	1.10	4.07E-02	0.45	1.52	5.89E-04	0.76	1.07	8.30E-03	0.31	0.89	1629933	553087	2358253	1496654	2051182	856140	2665323	1897432
RP_NEG_636_3504a10_822	RP	NEG	10.82	636.3504				1.19E-02	-0.61	1.30	4.10E-02	-0.36	1.73	2.43E-03	-0.79	1.34	8.80E-02	-0.43	1.02	4182070	1290472	3532737	945521	3725379	919482	3340095	940787
RP_POS_534_29608a10_503	RP	POS	10.50	534.2961				1.24E-01	0.33	1.04	4.10E-02	-0.40	1.32	5.94E-01	0.13	0.65	2.17E-02	0.53	1.19	8285248	2263256	8995603	2140981	9431851	1953252	8559355	2248903
RP_POS_550_63068a10_818	RP	POS	10.82	550.6307				9.21E-02	-0.34	0.73	4.12E-02	0.41	1.50	5.68E-01	-0.14	0.49	8.14E-03	-0.55	1.11	1558656	267312	1465164	271475	1409715	185311	1520612	329069
HILIC_POS_494_32355a1_198	HILIC	POS	1.198	494.3236				1.24E-15	1.05	1.72	4.12E-02	0.41	1.12	4.01E-09	1.26	1.92	1.05E-10	0.84	2.09	2372110	1123370	6145572	3631955	5403920	2478686	6887224	4402836
RP_POS_723_52484a11_174	RP	POS	11.17	723.5248				5.74E-05	0.50	1.15	4.13E-02	-0.45	1.50	1.81E-02	0.28	1.19	5.35E-04	0.73	1.32	238561	125701	477403	528483	585329	647490	369476	348243
RP_POS_414_77185a12_955	RP	POS	12.96	414.7719				8.76E-06	-0.86	1.41	4.14E-02	-0.39	1.27	1.35E-06	-1.05	1.74	1.40E-03	-0.66	1.12	2094125	427587	1655020	493706	1755418	483200	1554623	488275
RP_POS_231_08386a1_43	RP	POS	1.43	231.0839				8.21E-13	0.88	1.56	4.15E-02	0.43	1.28	2.45E-07	1.10	1.63	4.24E-08	0.66	1.65	76097	90089	852557	938703	661061	635017	1044053	1141151
HILIC_POS_104_08233a2_484	HILIC	POS	2.484	104.0823				6.61E-05	0.56	1.07	4.15E-02	0.44	1.17	1.32E-04	0.78	1.38	2.48E-02	0.34	1.03	642753	174487	857588	418345	772441	336164	942735	475179
RP_POS_123_0441a0_71	RP	POS	0.71	123.0441				1.79E-01	0.22	0.82	4.16E-02	0.44	1.38	4.02E-02	0.44	1.22	9.74E-01	0.01	0.52	1195690	259947	1277543	391960	1197809	320720	1357278	441095
RP_POS_441_29593a12_887	RP	POS	12.89	441.2959				9.98E-01	0.00	0.45	4.16E-02	-0.40	1.40	3.92E-01	-0.20	0.78	4.05E-01	0.20	0.37	19554750	7288184	19559087	6636335	20907444	6853475	18210731	6188718
RP_NEG_918_80426a0_489	RP	NEG	0.49	918.8043				2.25E-04	-0.55	1.01	4.17E-02	0.44	1.33	8.55E-02	-0.33	0.62	1.11E-05	-0.77	1.47	1188291	242137	942580	479896	845085	419434	1040075	519594
HILIC_POS_568_33844a1_072	HILIC	POS	1.072	568.3384				6.14E-01	-0.10	0.49	4.18E-02	-0.42	1.13	1.51E-01	-0.31	0.57	5.96E-01	0.12	0.20	1470946	659376	1400214	769107	1556333	778575	1244095	734305
RP_POS_162_05811a0_731	RP	POS	0.73	162.0581				1.31E-03	0.38	0.77	4.18E-02	0.47	1.21	8.01E-03	0.61	0.92	2.58E-04	0.14	1.33	107005	177398	1086906	2947989	481616	644838	1692196	4049089
HILIC_POS_160_13315a1_954	HILIC	POS	1.954	160.1332				9.03E-01	-0.02	0.27	4.19E-02	0.45	1.31	3.77E-01	0.20	0.38	8.72E-02	-0.24	0.66	784716	589883	767086	1001097	562635	521625	971538	1291295
RP_NEG_766_56116a10_509	RP	NEG	10.51	766.5612				4.51E-02	-0.36	1.10	4.19E-02	0.42	1.41	4.68E-01	-0.15	0.81	5.76E-03	-0.57	1.15	1144457	204496	1053135	263350	999717	253667	1106553	264483
RP_NEG_822_53113a12_382	RP	NEG	12.38	822.5311				6.46E-02	-0.39	1.21	4.19E-02	-0.40	1.23	8.66E-03	-0.59	1.42	4.25E-01	-0.19	0.54	1699252	843006	1378987	807324	1542864	887664	1215110	688544
RP_POS_744_55261a13_974	RP	POS	13.97	744.5526				6.32E-01	0.10	0.45	4.20E-02	0.41	1.26	2.19E-01	0.30	0.51	6.08E-01	-0.11	0.44	856650	868244	941734	872124	764504	643938	1118963	1028574
RP_POS_331_26227a11_38	RP	POS	11.38	331.2623				5.17E-10	0.85	1.61	4.21E-02	0.43	1.30	2.25E-07	1.06	1.73	1.39E-05	0.64	1.50	606427	288676	1223631	761165	1069160	604131	1378103	869998
RP_POS_327_2291a10_943	RP	POS	10.94	327.2291				1.92E-06	0.81	1.66	4.24E-02	0.41	1.44	2.91E-06	1.01	1.71	5.23E-04	0.61	1.53	5124255	2723070	8354123	4018715	7539690	3254628	9168556	4547906
RP_POS_584_2937a10_125	RP	POS	10.13	584.2937				4.55E-24	1.37	2.24	4.27E-02	0.37	1.28	5.66E-14	1.55	2.32	3.53E-16	1.18	2.32	225257	92965	601726	250240	551057	189529	652396	292159
HILIC_NEG_247_89224a0_881	HILIC	NEG	0.881	247.8922				1.99E-01	0.26	0.68	4.29E-02	0.41	1.35	5.34E-02	0.46	0.77	7.88E-01	0.06	0.12	1628262	825192	1847928	852199	1675614	691321	2020243	963736
HILIC_POS_140_06827a3_921	HILIC	POS	3.921	140.0683				2.13E-03	0.38	0.84	4.29E-02	0.46	1.34	6.59E-03	0.61	0.85	7.18E-02	0.15	0.58	891014	388651	1495315	1798964	1129084	783773	1861546	2377091
RP_POS_235_16524a0_551	RP	POS	0.55	235.1652				4.05E-03	0.34	0.78	4.30E-02	0.46	1.28	1.13E-02	0.58	0.95	6.66E-02	0.11	0.62	334098	176420	694460	1187544	452470	391612	936450	1605127
RP_POS_469_32837a11_155	RP	POS	11.16	469.3284				8.31E-02	-0.39	1.10	4.31E-02	-0.38	1.83	1.50E-02	-0.58	1.43	4.27E-01	-0.19	0.83	3884576	2200326	3119213	1882686	3499018	2010163	2739409	1681131
RP_POS_223_09438a13_013	RP	POS	13.01	223.0944				5.05E-01	0.14	0.55	4.33E-02	-0.40	1.21	7.78E-01	-0.07	0.26	1.20E-01	0.34	0.91	12698281	3226739	13139189	3249648	13794407	2817040	12483970	3538937
RP_POS_772_54767a12_45	RP	POS	12.45	772.5477				2.03E-03	0.60	1.01	4.34E-02	0.40	1.32	3.88E-04	0.80	1.26	5.31E-02	0.40	0.77	412209	340023	642359	381906	565427	349711	719291	400381
RP_POS_921_61694a9_303	RP	POS	9.30	921.6169				5.07E-02	0.24	0.84	4.37E-02	0.46	1.63	4.30E-02	0.47	0.93	9.42E-01	0.00	1.02	882210	769750	1807167	4481033	895019	785694	2719315	6184966
RP_POS_1049_65857a11_113	RP	POS	11.11	1049.6586				1.71E-02	0.29	0.97	4.38E-02	-0.46	1.31	6.50E-01	0.06	0.66	1.00E-02	0.51	1.14	948041	77421	1076299	511843	1179440	604279	973158	377426
RP_POS_315_16895a10_823	RP	POS	10.82	315.1690				4.91E-10	0.83	1.69	4.39E-02	0.42	1.46	1.51E-07	1.04	1.83	4.27E-05	0.62	1.59	126986	142226	451163	410592	368574	348572	533752	452978
HILIC_NEG_243_79901a0_881	HILIC	NEG	0.881	243.7990				1.56E-01	0.28	0.70	4.39E-02	0.41	1.33	3.92E-02	0.48	0.81	7.14E-01	0.08	0.16	134552	65109	153926	70340	139776	58840	168076	78266
RP_POS_553_4588a13_479	RP	POS	13.48	553.4588				7.57E-03	0.52	0.93	4.40E-02	0.40	1.38	1.25E-03	0.72	1.35	1.29E-01	0.32	0.56	8800593	3891771	11049185	4318066	10181880	4102598	11916491	4393797
HILIC_NEG_130_06213a5_548	HILIC	NEG	5.548	130.0621				1.25E-01	0.29	0.53	4.41E-02	-0.41	1.47	7.10E-01	0.08	0.51	1.75E-02	0.50	0.94	198786	127005	240761	150138	270916	136662	210606	158147
HILIC_NEG_538_31622a1_289	HILIC	NEG	1.289	538.3162				2.33E-15	1.08	1.76	4.41E-02	0.40	1.09	1.29E-09	1.28	1.99	2.57E-10	0.88	2.08	387829	200977	966570	533022	859276	384232	1073864	634740
RP_POS_741_47552a11_146	RP	POS	11.15	741.4755				3.70E-05	0.49	1.12	4.41E-02	-0.45	1.46	4.65E-03	0.26	1.25	9.62E-04	0.72	1.24	84352	44318	379995	680564	517422	870323	242568	373875
RP_NEG_774_84094a0_49	RP	NEG	0.49	774.8409				9.82E-01	0.00	0.68	4.42E-02	0.44	1.45	2.92E-01	0.22	0.62	1.65E-01	-0.23	0.93	1551262	342707	1549232	653331	1417896	518018	1680568	747562
HILIC_NEG_200_8587a4_848	HILIC	NEG	4.848	200.8587				1.51E-01	-0.24	0.48	4.43E-02	-0.43	1.12	2.36E-02	-0.46	0.83	8.97E-01	-0.03	0.23	4021484	754296	3767444	1133482	3994838	1096649	3540050	1134731
RP_NEG_999_64355a10_625	RP	NEG	10.63	999.6436				2.38E-03	0.57	1.30	4.44E-02	0.41	1.64	9.79E-04	0.77	1.31	4.92E-02	0.36	1.13	2177106	1136305	2949016	1381033	2671438	1007899	3226594	1637169
RP_POS_358_27725a9_131	RP	POS	9.13	358.2773				4.34E-01	0.14	0.61	4.46E-02	0.42	1.21	1.14E-01	0.35	0.74	7.34E-01	-0.07	0.43	1623685	760791	1752987	943864	1563778	800438	1942196	1042199
RP_POS_489_28226a10_565	RP	POS	10.57	489.2823				5.01E-01	0.13	0.63	4.47E-02	0.41	1.24	1.71E-01	0.34	0.61	7.01E-01	-0.07	0.23	572334	867839	694287	942409	504820	594539	883754	1169469
HILIC_NEG_308_9978a0_931	HILIC	NEG	0.931	308.9978				5.64E-01	-0.11	0.82	4.49E-02	-0.41	1.32	1.50E-01	-0.32	0.52	6.57E-01	0.10	0.18	700931	123639	685886	139636	713822	133968	657950	140905
RP_NEG_246_98051a6_83	RP	NEG	6.83	246.9805				4.97E-01	0.12	0.72	4.49E-02	0.42	1.41	1.38E-01	0.33	0.64	6.55E-01	-0.09	0.45	4294135	1925662	4578647	2407897	4096518	1979262	5060777	2705994
RP_POS_536_29614a10_367	RP	POS	10.37	536.2961				5.63E-01	-0.13	0.98	4.50E-02	-0.39	1.53	1.96E-01	-0.32	0.80	7.72E-01	0.07	0.83	1110529	442301	1059675	387559	1137208	339390	982142	419542
RP_POS_391_28421a9_293	RP	POS	9.29	391.2842				9.94E-01	0.00	0.37	4.50E-02	0.40	1.19	4.46E-01	0.20	0.43	3.20E-01	-0.20	0.52	471058	804165	469871	761792	316633	406839	623108	979315
RP_POS_548_50317a12_891	RP	POS	12.89	548.5032				7.66E-01	-0.05	0.70	4.51E-02	-0.43	1.50	2.34E-01	-0.27	0.53	3.39E-01	0.16	0.65	3531011	777136	3477673	1139478	3705908	838756	3249438	1346662
RP_NEG_557_45856a12_261	RP	NEG	12.26	557.4586				7.94E-02	-0.41	0.66	4.53E-02	-0.36	1.27	1.55E-02	-0.60	1.18	3.69E-01	-0.23	0.50	2740385	2203828	1977958	1682154	2314110	1874055	1641806	1405112
RP_POS_516_30591a9_985	RP	POS	9.99	516.3059	LPC 16:1 [M+Na]+	457.2347(55), 516.3019(45), 311.2558(40), 86.097(37), 104.107(3)		3.23E-13	0.94	1.77	4.54E-02	0.42	1.26	9.58E-08	1.15	1.79	4.78E-09	0.73	1.77	1135834	634429	3260197	2360778	2787368	1559118	3733026	2893645
RP_POS_274_1228a10_123	RP	POS	10.12	274.1228				2.37E-20	1.27	2.10	4.54E-02	0.38	1.29	5.24E-12	1.46	2.18	9.58E-15	1.08	2.24	769941	278813	1728703	708633	1586882	496795	1870524	852477
RP_NEG_181_08611a6_273	RP	NEG	6.27	181.0861				2.27E-01	-0.18	1.00	4.56E-02	-0.44	1.37	3.60E-02	-0.40	1.20	8.27E-01	0.04	0.96	1536345	57198	1518064	111578	1540313	105933	1495815	113672
HILIC_NEG_214_07687a0_699	HILIC	NEG	0.699	214.0769				4.98E-07	0.61	1.11	4.57E-02	0.44	1.43	1.40E-04	0.83	1.28	6.46E-05	0.39	1.26	65562	122187	508310	800930	347706	438663	668914	1025184
RP_POS_802_53448a12_578	RP	POS	12.58	802.5345				6.71E-06	0.81	1.46	4.57E-02	0.40	1.22	1.19E-05	1.00	1.57	4.70E-04	0.61	1.35	4843585	2120134	7130692	2825358	6565803	1964569	7695582	3408439
HILIC_POS_156_04214a3_921	HILIC	POS	3.921	156.0421				1.69E-02	0.30	0.77	4.57E-02	0.45	1.28	1.77E-02	0.53	0.82	4.08E-01	0.08	0.39	839320	359945	1200057	1347015	929552	621522	1470563	1769267
RP_POS_592_42346a10_833	RP	POS	10.83	592.4235				8.77E-10	1.16	2.03	4.58E-02	0.36	1.59	1.26E-09	1.34	2.10	2.68E-07	0.98	1.91	744335	540028	1578634	652176	1448572	549239	1708696	723298
RP_POS_774_56299a12_345	RP	POS	12.35	774.5630				6.19E-02	0.35	0.82	4.58E-02	0.41	1.36	1.30E-02	0.56	1.12	4.66E-01	0.15	0.67	1523951	607201	1769212	714931	1626749	636375	1911675	765696
RP_NEG_203_00162a3_93	RP	NEG	3.93	203.0016				2.54E-04	0.44	0.73	4.59E-02	-0.45	1.20	7.38E-02	0.22	0.68	1.01E-03	0.67	1.00	901946	2227810	5951207	12779967	8503014	15180168	3399399	9287711
RP_POS_300_19925a7_851	RP	POS	7.85	300.1993				3.50E-01	-0.20	1.02	4.60E-02	-0.39	1.70	8.01E-02	-0.40	1.03	9.83E-01	-0.01	0.70	1349084	686844	1220023	630859	1345709	699064	1094336	532126
RP_POS_351_28671a11_342	RP	POS	11.34	351.2867				1.63E-01	0.21	0.73	4.60E-02	0.44	1.28	4.26E-02	0.43	0.85	9.81E-01	0.00	0.65	1132632	117478	1174526	213733	1131894	161937	1217158	249727
RP_POS_215_16412a8_932	RP	POS	8.93	215.1641				1.24E-08	0.71	1.33	4.61E-02	0.43	1.23	2.64E-05	0.93	1.39	8.85E-07	0.50	1.50	370357	151221	812894	673830	678021	357147	947767	867572
HILIC_NEG_199_80501a0_733	HILIC	NEG	0.733	199.8050				5.17E-05	0.49	1.09	4.64E-02	0.45	1.13	5.46E-04	0.71	1.06	2.44E-02	0.27	0.70	133497	59187	297276	374769	222598	262081	371954	451334
HILIC_NEG_163_89758a6_276	HILIC	NEG	6.276	163.8976				1.08E-02	-0.51	0.82	4.65E-02	-0.39	1.23	1.73E-03	-0.71	1.14	1.49E-01	-0.32	0.65	4236979	1599499	3369633	1677389	3702704	1638847	3036562	1665074
RP_POS_565_56689a15_222	RP	POS	15.22	565.5669				6.46E-01	-0.09	0.74	4.66E-02	-0.41	1.33	2.34E-01	-0.29	1.01	5.63E-01	0.11	0.44	8173379	780260	8099004	833145	8265045	537434	7932962	1028264
RP_POS_277_14078a8_586	RP	POS	8.59	277.1408				1.64E-01	0.27	0.87	4.66E-02	0.40	1.21	5.85E-02	0.48	0.75	6.95E-01	0.07	0.42	910814	473606	1049020	510037	947146	269719	1150894	657005
RP_POS_644_49329a10_55	RP	POS	10.55	644.4933				4.80E-01	-0.15	0.42	4.66E-02	0.39	1.16	8.42E-01	0.05	0.45	1.24E-01	-0.35	0.64	869129	178168	843658	169386	810025	148996	877291	182922
RP_POS_987_63837a10_123	RP	POS	10.12	987.6384				8.07E-05	0.47	1.51	4.67E-02	0.45	1.27	1.80E-03	0.69	1.25	2.53E-03	0.24	1.39	170066	249591	2079144	4623686	1154826	2169707	3003461	6061519
RP_POS_365_19815a11_38	RP	POS	11.38	365.1982				8.84E-10	0.89	1.78	4.68E-02	0.41	1.36	1.60E-07	1.09	1.81	7.02E-06	0.68	1.69	750136	401668	1504687	877386	1330423	689426	1678952	1008979
RP_NEG_363_9559a4_567	RP	NEG	4.57	363.9559				3.90E-03	-0.65	1.02	4.68E-02	-0.36	1.29	5.45E-04	-0.83	1.44	5.26E-02	-0.47	0.74	997449	594221	643891	498812	742823	527082	544959	452676
RP_NEG_1083_66528a10_198	RP	NEG	10.20	1083.6653				3.80E-02	-0.55	1.23	4.72E-02	-0.32	1.45	1.05E-02	-0.71	1.19	1.58E-01	-0.38	0.99	1850320	1430116	1276245	863382	1447148	867676	1105342	832826
RP_POS_819_96564a10_313	RP	POS	10.31	819.9656				6.89E-01	-0.08	1.07	4.73E-02	-0.39	1.60	2.42E-01	-0.28	0.96	6.09E-01	0.11	0.84	402258	179535	387724	172935	421967	152161	353482	186754
RP_POS_544_33655a10_308	RP	POS	10.31	544.3366				2.39E-02	0.47	0.99	4.73E-02	-0.39	1.57	2.42E-01	0.28	0.59	2.64E-03	0.66	1.22	158221120	51840915	182585937	50592522	192605904	42100955	172565970	56515976
RP_POS_377_12958a0_707	RP	POS	0.71	377.1296				5.33E-13	0.89	1.55	4.75E-02	0.42	1.18	4.77E-07	1.10	1.66	1.23E-09	0.67	1.79	76112	70171	870085	952592	680855	571124	1059314	1197549
RP_POS_199_14407a2_25	RP	POS	2.25	199.1441				2.49E-02	0.27	0.54	4.75E-02	0.45	1.22	2.55E-02	0.50	0.83	5.53E-01	0.05	0.38	986352	1371339	2712688	7200352	1277566	3000166	4147809	9567862

Supplementary table 1: Metabolomics results (in asceding order according to p-value from progressive ALD vs non-progressive ALD comparison, with molecular features with ID_level of 1-2 first)

								all_ALD_vs_control			Prog_ALD_vs_non-prog_ALD			Prog_ALD_vs_control_ALD			Non-prog_ALD_vs_control			Healthy_control		all_ALD		Non-prog_ALD		Progressive_ALD	
								t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA								
Feature_ID	RP_HILIC	POS_NEG	Average.Rt	Average.Mz	Metabolite.name	curated_MSMS	ID_level	p	d	VIP	p	d	VIP	p	d	VIP	p	d	VIP	Mean	SD	Mean	SD	Mean	SD	Mean	SD
HILIC_NEG_245_89449a0_881	HILIC	NEG	0.881	245.8945				1.88E-01	0.26	0.69	4.76E-02	0.40	1.33	5.18E-02	0.46	0.77	7.56E-01	0.06	0.14	11374423	5598566	12908407	5864448	11748343	4779718	14068472	6625197
RP_POS_331_28378a10_864	RP	POS	10.86	331.2838				3.37E-01	-0.21	0.55	4.77E-02	0.38	1.18	9.29E-01	-0.02	0.31	6.03E-02	-0.40	0.87	484997	746086	343187	632718	217247	291331	469127	831620
RP_NEG_203_0817a2_891	RP	NEG	2.89	203.0817				2.22E-05	-0.86	1.55	4.77E-02	-0.37	1.40	9.41E-06	-1.05	1.65	8.92E-04	-0.67	1.40	4378090	1074878	3353498	1122315	3575432	905086	3131563	1274828
HILIC_NEG_478_29453a1_767	HILIC	NEG	1.767	478.2945				4.98E-04	0.62	1.01	4.78E-02	0.40	1.25	3.57E-04	0.82	1.19	1.61E-02	0.42	1.00	337427	183649	485851	244025	437530	170654	534171	293980
HILIC_NEG_243_89899a0_881	HILIC	NEG	0.881	243.8990				1.92E-01	0.26	0.69	4.79E-02	0.40	1.33	5.27E-02	0.46	0.77	7.67E-01	0.06	0.13	29330435	14205185	33189065	14930726	30238458	12239770	36139672	16817349
HILIC_NEG_197_90608a0_881	HILIC	NEG	0.881	197.9061				1.83E-01	0.27	0.68	4.81E-02	0.40	1.32	5.06E-02	0.47	0.77	7.35E-01	0.07	0.14	148239	74363	168788	76773	153633	62786	183944	86588
RP_POS_732_54834a10_459	RP	POS	10.46	732.5483				3.37E-01	-0.16	0.36	4.82E-02	-0.43	1.34	1.53E-02	-0.37	1.00	8.28E-01	0.05	0.41	1132489	186025	1091111	274588	1145582	356675	1036640	138070
RP_POS_363_1962a11_38	RP	POS	11.38	363.1962				1.02E-09	0.88	1.72	4.83E-02	0.41	1.31	1.86E-07	1.08	1.78	8.24E-06	0.68	1.62	215099	122724	446048	271126	392543	213664	499553	311488
HILIC_POS_375_32129a1_117	HILIC	POS	1.117	375.3213				9.19E-03	-0.57	1.03	4.83E-02	-0.37	1.22	1.89E-03	-0.76	1.29	9.29E-02	-0.39	0.69	5460934	1630654	4585155	1446034	4870088	1349828	4300222	1495653
RP_POS_617_47498a11_603	RP	POS	11.60	617.4750				4.48E-02	-0.40	0.66	4.84E-02	-0.40	1.23	3.49E-03	-0.60	1.17	4.01E-01	-0.20	0.58	1254352	809480	911074	865776	1081996	1030388	740151	626985
HILIC_POS_189_0731a2_225	HILIC	POS	2.225	189.0731				5.10E-01	-0.13	0.75	4.85E-02	-0.40	1.20	1.42E-01	-0.33	0.64	7.56E-01	0.07	0.31	4388199	1111648	4236353	1172885	4467226	1130527	4005481	1180052
RP_POS_526_43097a10_66	RP	POS	10.66	526.4310				8.05E-01	-0.05	0.35	4.87E-02	0.41	1.22	4.52E-01	0.15	0.36	2.75E-01	-0.25	0.60	11990732	757972	11951370	849916	11784081	933712	12118660	728371
RP_NEG_554_34747a10_668	RP	NEG	10.67	554.3475				1.18E-05	-0.91	1.59	4.89E-02	-0.36	1.42	1.06E-06	-1.09	1.86	1.14E-03	-0.73	1.23	8821216	2859192	6013256	2835115	6570577	3030050	5455935	2534698
RP_POS_599_44495a11_441	RP	POS	11.44	599.4450				8.44E-06	-1.29	2.22	4.89E-02	-0.23	1.17	2.47E-06	-1.40	2.00	3.96E-05	-1.17	1.96	1330305	784564	585428	336559	651558	319258	519298	343518
HILIC_NEG_157_90102a0_708	HILIC	NEG	0.708	157.9010				6.48E-06	0.72	1.44	4.91E-02	-0.41	1.09	8.85E-03	0.52	0.93	4.24E-07	0.93	1.92	798803	228315	1065177	381683	1140156	332030	990198	415475
RP_NEG_207_83682a15_552	RP	NEG	15.55	207.8368				7.35E-01	0.07	0.50	4.92E-02	-0.39	1.18	5.85E-01	-0.13	0.31	2.34E-01	0.27	0.68	5226441	321516	5248665	319407	5311350	296754	5185981	331725
HILIC_POS_398_32581a0_618	HILIC	POS	0.618	398.3258				2.93E-07	0.86	1.59	4.93E-02	0.39	1.20	1.35E-07	1.06	2.00	4.14E-04	0.67	1.28	682912	476072	1302599	717443	1161864	700133	1443333	713685
RP_POS_192_13853a15_382	RP	POS	15.38	192.1385				2.83E-01	-0.24	0.45	4.93E-02	-0.37	1.76	7.87E-02	-0.43	0.85	8.10E-01	-0.06	0.44	3617860	2024828	3189510	1651717	3513504	1701490	2865516	1550070
HILIC_NEG_161_91367a0_881	HILIC	NEG	0.881	161.9137				2.54E-01	0.23	0.77	4.94E-02	0.40	1.35	7.23E-02	0.43	0.76	8.82E-01	0.03	0.15	1395926	420861	1495483	438617	1409410	363372	1581556	491464
RP_POS_144_1387a7_136	RP	POS	7.14	144.1387				7.51E-01	0.07	0.39	4.95E-02	-0.38	1.23	6.28E-01	-0.12	0.24	2.92E-01	0.26	0.60	1574072	739419	1620257	621924	1742173	629939	1498341	595244
HILIC_POS_249_10707a1_232	HILIC	POS	1.232	249.1071				7.70E-10	-1.31	2.41	4.95E-02	-0.32	1.06	6.29E-10	-1.47	2.27	2.60E-08	-1.14	2.64	5870275	1507443	3580988	1440539	3864114	1031732	3297862	1721799
HILIC_NEG_249_89191a0_881	HILIC	NEG	0.881	249.8919				1.87E-01	0.27	0.72	4.96E-02	0.39	1.33	5.34E-02	0.47	0.77	7.26E-01	0.07	0.17	347764	172301	394555	173087	360604	141479	428505	195347
RP_POS_510_35522a10_547	RP	POS	10.55	510.3552				2.56E-05	-0.88	1.56	4.96E-02	-0.36	1.39	2.19E-06	-1.06	1.82	2.11E-03	-0.70	1.20	2355282	828960	1579457	818474	1739862	883962	1419053	720813
HILIC_POS_152_02191a1_232	HILIC	POS	1.232	152.0219				9.83E-10	-1.18	2.09	4.97E-02	-0.35	1.08	3.11E-09	-1.36	2.09	7.89E-08	-1.01	2.40	2557537	339977	2037877	390277	2114515	279021	1961240	466800
RP_POS_236_87883a0_252	RP	POS	0.25	236.8788				7.91E-02	0.33	0.97	4.97E-02	0.40	1.67	1.68E-02	0.53	1.36	5.37E-01	0.12	0.58	696532	420549	857227	507772	757780	459248	956675	538364
RP_POS_652_49902a11_189	RP	POS	11.19	652.4990				4.45E-05	0.49	1.14	4.97E-02	-0.44	1.46	6.31E-03	0.26	1.22	1.03E-03	0.71	1.26	73724	41259	261265	433909	346666	551080	175864	248642
HILIC_POS_346_0094a6_3	HILIC	POS	6.3	346.0094				6.20E-01	-0.10	0.35	4.98E-02	-0.39	1.08	1.92E-01	-0.30	0.51	6.67E-01	0.10	0.19	28718187	8635720	27840788	8771834	29557603	8510152	26123973	8776249
RP_POS_237_14597a8_931	RP	POS	8.93	237.1460				7.15E-09	0.72	1.35	5.01E-02	0.43	1.23	2.01E-05	0.94	1.40	1.06E-06	0.51	1.48	1338999	471394	2769033	2142210	2347904	1195436	3190162	2735100
HILIC_POS_248_14923a4_251	HILIC	POS	4.251	248.1492				5.28E-05	0.54	1.09	5.02E-02	0.43	1.50	7.62E-04	0.76	1.06	2.12E-03	0.33	1.05	2266903	4112794	7956865	11493475	5695452	5635168	10218279	14990131
HILIC_NEG_253_79378a3_05	HILIC	NEG	3.05	253.7938				1.06E-01	0.25	0.95	5.03E-02	-0.43	1.20	8.62E-01	0.03	0.51	1.83E-02	0.46	0.97	452871	88315	490078	166319	522568	171971	457587	155435
RP_POS_188_07062a3_06	RP	POS	3.06	188.0706				4.05E-02	-0.55	1.01	5.03E-02	-0.31	1.24	9.83E-03	-0.71	1.23	1.69E-01	-0.39	0.55	2111283	1813637	1395644	1049477	1601075	1237811	1190214	779091
RP_POS_986_69482a0_5	RP	POS	0.50	986.6948				9.69E-03	0.46	0.99	5.04E-02	-0.41	1.44	1.87E-01	0.26	0.64	1.91E-03	0.66	1.33	283461	160665	377875	212627	419399	221905	336352	196423
HILIC_NEG_216_9808a0_826	HILIC	NEG	0.826	216.9808				1.12E-05	0.58	1.25	5.04E-02	0.43	1.40	2.09E-04	0.80	1.15	3.10E-03	0.37	0.95	226989	61863	325747	186342	289229	121610	362266	229444
RP_NEG_897_62317a9_312	RP	NEG	9.31	897.6232				2.16E-02	0.27	0.91	5.05E-02	0.45	1.61	3.07E-02	0.50	0.95	2.82E-01	0.05	1.31	1077585	1570065	4580179	14760036	1668946	3320133	7491412	20293931
RP_NEG_704_3385a10_824	RP	NEG	10.82	704.3385				1.06E-02	-0.62	1.32	5.08E-02	-0.34	1.76	2.34E-03	-0.79	1.36	7.63E-02	-0.44	1.03	1135528	340896	961147	249598	1009796	244933	912497	247078
RP_POS_558_29565a10_198	RP	POS	10.20	558.2957				6.52E-02	-0.49	1.19	5.08E-02	-0.32	1.55	2.06E-02	-0.65	1.10	2.29E-01	-0.32	0.97	522956	320175	409446	192915	447041	184122	371851	195975
HILIC_POS_371_24026a1_353	HILIC	POS	1.353	371.2403				3.24E-03	-0.54	0.92	5.11E-02	0.40	1.14	1.22E-01	-0.35	0.62	1.51E-04	-0.74	1.53	1808928	280352	1623895	346767	1556297	272214	1691492	399403
HILIC_POS_160_09683a0_769	HILIC	POS	0.769	160.0968				2.57E-02	0.37	0.71	5.12E-02	0.41	1.12	5.94E-03	0.58	0.99	3.63E-01	0.17	0.33	1253999	1025805	1794718	1539028	1495067	1351848	2094370	1665777
RP_POS_785_50189a11_143	RP	POS	11.14	785.5019				8.71E-06	0.53	1.19	5.13E-02	-0.44	1.46	3.05E-03	0.31	1.26	4.40E-04	0.75	1.32	79395	44669	567382	1037796	770086	1294605	364679	645106
HILIC_NEG_134_89474a4_522	HILIC	NEG	4.522	134.8947				4.43E-01	-0.16	0.38	5.16E-02	0.38	1.13	9.01E-01	0.03	0.25	1.21E-01	-0.35	0.97	24930269	16895409	22311997	15926559	19217443	14639066	25406551	16692561
RP_POS_619_33777a14_261	RP	POS	14.26	619.3378				5.98E-01	-0.12	0.36	5.16E-02	0.37	1.42	8.03E-01	0.06	0.36	2.15E-01	-0.30	0.80	3330284	1363498	3189682	1096611	2976696	1033453	3402668	1126522
RP_POS_518_37616a11_485	RP	POS	11.49	518.3762				1.96E-02	-0.48	0.77	5.17E-02	0.38	1.41	2.13E-01	-0.29	0.69	2.23E-03	-0.67	1.19	1461657	219739	1354463	217374	1312229	183038	1396697	241503
RP_NEG_251_78772a15_552	RP	NEG	15.55	251.7877				4.13E-02	-0.49	0.91	5.18E-02	-0.35	1.22	9.63E-03	-0.66	1.06	2.14E-01	-0.31	0.62	1902535	102200	1861289	75890	1876019	76561	1846559	73019
HILIC_POS_260_00885a0_541	HILIC	POS	0.541	260.0089				7.58E-03	0.69	1.89	5.18E-02	0.32	1.18	2.94E-03	0.85	1.84	3.48E-02	0.53	1.47	23451136	4586599	25876205	2910089	25308764	1745286	26443645	3661546
RP_POS_617_47375a11_16	RP	POS	11.16	617.4738				1.43E-01	-0.28	0.56	5.20E-02	-0.40	1.21	1.19E-02	-0.48	1.05	7.23E-01	-0.09	0.63	1602950	1330143	1191054	1473878	1478104	1846388	904004	900920
RP_POS_241_15385a0_71	RP	POS	0.71	241.1539				5.03E-04	0.54	0.91	5.21E-02	0.42	1.29	4.25E-04	0.74	1.25	4.26E-02	0.33	0.84	781772	124474	895852	228131	851561	182117	940143	260728
RP_POS_423_7695a13_208	RP	POS	13.21	423.7695				8.87E-04	0.72	1.25	5.22E-02	0.36	1.40	2.31E-04	0.90	1.38	1.47E-02	0.54	1.02	787853	321410	1014648	295707	957312	255133	1071983	323833
RP_NEG_568_36279a10_822	RP	NEG	10.82	568.3628				2.37E-02	-0.55	1.23	5.23E-02	-0.34	1.68	5.93E-03	-0.72	1.24	1.31E-01	-0.38	0.97	34231813	11701699	28998895	8304197	30607399	8016792	27390392	8353298
RP_NEG_299_25983a10_358	RP	NEG	10.36	299.2598				2.53E-02	0.44	1.05	5.24E-02	0.39	1.24	6.32E-03	0.63	1.10	2.36E-01	0.24	0.76	2362333	867710	2777197	954258	2592341	818013	2962054	1049246
RP_POS_524_37048a11_249	RP	POS	11.25	524.3705				1.65E-01	-0.30	1.07	5.26E-02	-0.38	1.38	4.12E-02	-0.49	0.94	6.38E-01	-0.11	0.98	2737035	1122670	2421221	1037825	2621960	996118	2220482	1049597
RP_POS_179_10696a6_861	RP	POS	6.86	179.1070				4.43E-01	0.09	0.57	5.27E-02	0.44	1.17	1.46E-01	0.32	0.67	1.60E-01	-0.13	0.80	1326507	53753	1348722	272445	1295694	137739	1401750	353916
RP_POS_537_39233a15_125	RP	POS	15.13	537.3923				8.24E-01	0.05	0.44	5.33E-02	0.37	1.33	3.62E-01	0.23	0.58	5.62E-01	-0.13	0.31	4851852	3085912	4986367	2561444	4491538	2036993	5481196	2933742
HILIC_POS_544_33899a1_204	HILIC	POS	1.204	544.3390				9.01E-02	0.36	0.83	5.35E-02	-0.38	1.11	4.69E-01	0.17	0.33	1.68E-02	0.55	1.04	45722724	22141836	53391417	20888975	57417848	19072510	49364987	22017197
RP_POS_872_62769a11_156	RP	POS	11.16	872.6277				1.32E-06	0.58	1.26	5.37E-02	-0.43	1.47	2.13E-03	0.36	1.23	1.27E-04	0.79	1.41	62127	18859	281056	424005	362921	510600	199192	298063
RP_POS_151_00517a11_211	RP	POS	11.21	151.0052				6.13E-02	-0.36	0.96	5.39E-02	-0.39	1.22	1.24E-02	-0.56	0.93	4.26E-01	-0.17	1.04	2376564	358144	2233883	397200	2310294	377585	2157471	405302
RP_NEG_199_8047a4_571	RP	NEG	4.57	199.8047				5.00E-03	-0.60	0.97	5.40E-02	-0.37	1.18	1.03E-03	-0.78	1.22	6.41E-02	-0.42	0.76	7683948	2748856	6068352	2572582	6563105	2419658	5573599	2648984
RP_POS_899_62939a11_151	RP	POS	11.15	899.6294				5.77E-07	0.59	1.28	5.42E-02	-0.43	1.48	1.25E-03	0.38	1.28	8.69E-05	0.81	1.42	29761	11847	257141	424917	339026	510946	175256	300074
HILIC_POS_264_19574a0_714	HILIC	POS	0.714	264.1957				2.62E-02	0.26	0.86	5.42E-02	-0.44	1.45	1.52E-01	0.04	0.65	3.71E-02	0.48	0.89	10237	5284	14911428	66027855	27742602	91494960	2080255	10050005
RP_POS_397_3107a11_609	RP	POS	11.61	397.3107				3.18E-02	-0.41	0.95	5.43E-02	0.39	1.16	2.81E-01	-0.22	0.49	7.71E-03	-0.61	1.23	4730507	775484	4372798	874913	4204661	951161	4540935	764307
HILIC_NEG_112_98573a0_927	HILIC	NEG	0.927	112.9857				3.87E-02	-0.45	1.05	5.45E-02	-0.37	1.16	7.79E-03	-0.63	1.13	2.54E-01	-0.27	0.49	5336710	1004404	4913978	894320	5085624	896930	4742333	866791
RP_POS_726_82373a0_493	RP	POS	0.49	726.8237				2.42E-08	-0.78	1.33	5.47E-02	0.40	1.39	9.78E-04	-0.58	1.15	8.13E-08	-0.98	1.63	2440629	368837	1781009	892328	1609886	868100	1952132	891846
RP_POS_293_09735a0_753	RP	POS	0.75	293.0974				4.86E-02	-0.38	0.71	5.48E-02	-0.39	1.39	2.82E-03	-0.57	1.22	4.46E-01	-0.18	0.70	49024943	34473671	34424276	39282819	41983813	48585924	26864740	25309184
RP_POS_327_33542a10_849	RP	POS	10.85	327.3354				3.20E-04	-0.77	1.29	5.49E-02	-0.36	1.27	1.90E-05	-0.95	1.64	1.43E-02	-0.59	1.14	3143446	619571	2663865	580924	2775446	689157	2552285	426013
RP_POS_716_52216a13_151	RP	POS	13.15	716.5222				3.42E-01	0.18	0.50	5.50E-02	0.40	1.26	1.02E-01	0.38	0.61	9.00E-01	-0.02	0.42	672354	801247	837223	977276	649738	771626	1024707	1123604
RP_POS_257_14709a0_55	RP	POS	0.55	257.1471				4.75E-04	0.44	0.90	5.50E-02	0.43	1.26	2.78E-03	0.66	1.10	2.65E-02	0.23	0.71	2310479	1285827	4274252	4979586	3315025	2696096	5233480	6399365
RP_POS_241_10295a0_553	RP	POS	0.55	241.1030				2.74E-01	-0.18	0.88	5.51E-02	-0.41	1.30	7.46E-02	-0.39	0.75	8.82E-01	0.03	0.90	1963475	402458	1859800	617422	1978198	488983	1741402	708862
RP_NEG_221_94638a15_474	RP	NEG	15.47	221.9464				2.93E-01	0.21	1.06	5.52E-02	-0.38	1.38	9.28E-01	0.02	0.54	7.08E-02	0.41	0.91	21968071	4622053	22970414	4734053	23876349	4539639	22064478	4795480
RP_POS_275_62604a10_124	RP	POS	10.12	275.6260				2.36E-20	1.30	2.14	5.53E-02	0.36	1.23	1.73E-12	1.48	2.22	1.05E-14	1.12	2.25	2532616	822626	5235509	1926556	4866038	1403643	5604979	2291328
RP_POS_696_52594a11_183	RP	POS	11.18	696.5259				3.39E-05	0.49	1.15	5.58E-02	-0.43	1.44	5.91E-03	0.28	1.21	9.23E-04	0.71	1.29	63953	34640	243055	408548	321428	514792	164682	244299
RP_POS_620_69714a10_841	RP	POS	10.84	620.6971				7.73E-01	-0.04	1.32	5.58E-02	-0.43	1.26	6.89E-02	-0.25	1.06	4.22E-01	0.17	1.10	751655	174631	737442	383323	810881	469586	664002	255646
RP_POS_379_28134a10_874	RP	POS	10.87	379.2813				4.41E-04	0.45	0.83	5.58E-02	0.43	1.18	2.64E-03	0.67	0.95	1.85E-02	0.24	0.87	258207	328753	705894	1096742	495193	562732	916595	1422309
RP_POS_276_62238a10_123	RP	POS	10.12	276.6224				8.12E-21	1.32	2.17	5.59E-02	0.35	1.22	1.03E-12	1.50	2.25	2.90E-15	1.14	2.29	859651	296687	1846709	688474	1714957	496157	1978460	822234
RP_POS_767_55023a11_168	RP	POS	11.17	767.5502				8.51E-07	0.59	1.27	5.59E-02	-0.43	1.47	1.04E-03	0.37	1.29	1.28E-04	0.80	1.40	37443	17183	333290	562367	440959	685687	225620	380975
RP_POS_333_14444a6_868	RP	POS	6.87	333.1444				6.70E-01	0.06	0.64	5.61E-02	0.43	1.45	2.33E-01	0.27	0.59	1.25E-01	-0.16	0.82	486003	328105	528051	794636	375183	292627	680920	1068859
RP_NEG_624_26141a10_123	RP	NEG	10.12	624.2614				1.82E-20	1.27	2.10	5.61E-02	0.36	1.21	2.92E-12	1.45	2.20	4.71E-14	1.09	2.17	404636	160544	961173	410675	882683	307758	1039662	483179
RP_POS_273_121a0_55	RP	POS	0.55	273.1210				1.15E-01	0.21	0.88	5.62E-02	0.43	1.23	4.38E-02	0.43	1.03	9.89E-01	0.00	0.85	296276	157877	377186	426603	295597	285405	458775	522162
HILIC_NEG_343_72137a1_364	HILIC	NEG	1.364	343.7214				2.56E-08	0.97	1.67	5.64E-02	-0.37	1.02	1.09E-04	0.78	1.39	2.58E-09	1.15	2.18	159708	42398	219556	60064	231003	52553	208110	65268
HILIC_NEG_88_0399a5_548	HILIC	NEG	5.548	88.0399				1.02E-01	0.31	0.54	5.64E-02	-0.39	1.40	5.94E-01	0.12	0.41	1.51E-02	0.51	1.00	183672	128015	228328	145209	255999	128013	200657	157009
RP_POS_608_47235a11_194	RP	POS	11.19	608.4724				1.12E-05	0.52	1.17	5.65E-02	-0.43	1.44	1.95E-03	0.31	1.29	6.10E-04	0.74	1.29	44031	25819	240675	422840	321569	534947	159781	248421
HILIC_NEG_160_93544a0_926	HILIC	NEG	0.926	160.9354				3.17E-02	-0.33	0.72	5.69E-02	-0.42	1.07	3.01E-04	-0.54	1.38	5.82E-01	-0.12	0.30	763336	174947	666150	321434	727516	402226	604784	198185
RP_POS_637_49054a10_376	RP	POS	10.38	637.4905				2.24E-02	-0.48	1.07	5.71E-02	0.37	1.30	2.04E-01	-0.29	0.65	3.80E-03	-0.66	1.21	1161860	98343	1115126	95808	1096926	90575	1133325	98315
RP_NEG_465_24997a8_447	RP	NEG	8.45	465.2500				2.83E-01	-0.22	0.51	5.72E-02	-0.38	1.13	6.23E-02	-0.41	0.85	8.94E-01	-0.03	0.56	1043844	724592	884359	720595	1021256	783776	747463	629731
RP_POS_634_53656a10_861	RP	POS	10.86	634.5366				8.47E-01	-0.03	0.58	5.73E-02	0.43	1.13	3.77E-01	0.19	0.54	9.17E-02	-0.24	0.90	455497	116318	448920	269712	397597	190705	500243	324392
RP_NEG_231_93193a14_001	RP	NEG	14.00	231.9319				4.03E-01	0.18	0.58	5.74E-02	-0.37	1.31	1.00E+00	0.00	0.59	1.41E-01	0.37	0.69	6234570	3421522	6804060	2999727	7373581	3298685	6234539	2576256
HILIC_POS_171_18553a5_413	HILIC	POS	5.413	171.1855				3.86E-01	0.16	0.97	5.77E-02	-0.39	1.15	8.68E-01	-0.04	0.35	9.24E-02	0.36	0.78	66984485	17648892	70274956	21163711	74286151	20741394	66263761	21021529
HILIC_NEG_215_07324a0_699	HILIC	NEG	0.699	215.0732				4.15E-07	0.62	1.11	5.77E-02	0.42	1.40	1.62E-04	0.83	1.27	3.23E-05	0.41	1.31	274919	514135	2149472	3364401	1508342	1831548	2790602	4321568
RP_POS_579_26361a10_123	RP	POS	10.12	579.2636				2.73E-21	1.34	2.21	5.77E-02	0.35	1.24	6.98E-13	1.51	2.27	4.49E-16	1.17	2.38	283675	106431	641349	243414	595102	170787	687595	293559
RP_POS_828_55084a12_796	RP	POS	12.80	828.5508				2.04E-04	-0.86	1.40	5.79E-02	-0.33	1.14	2.34E-05	-1.03	1.84	4.91E-03	-0.70	1.10	16989497	7477301	11121571	5939678	12247261	6674083	9995881	4914274

Supplementary table 1: Metabolomics results (in asceding order according to p-value from progressive ALD vs non-progressive ALD comparison, with molecular features with ID_level of 1-2 first)

								all_ALD_vs_control			Prog_ALD_vs_non-prog_ALD			Prog_ALD_vs_control_ALD			Non-prog_ALD_vs_control			Healthy_control		all_ALD		Non-prog_ALD		Progressive_ALD	
								t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA								
Feature_ID	RP_HILIC	POS_NEG	Average.Rt	Average.Mz	Metabolite.name	curated_MSMS	ID_level	p	d	VIP	p	d	VIP	p	d	VIP	p	d	VIP	Mean	SD	Mean	SD	Mean	SD	Mean	SD
RP_POS_380_33856a10_535	RP	POS	10.54	380.3386				1.00E-01	-0.33	0.91	5.81E-02	0.38	1.13	5.23E-01	-0.14	0.53	2.14E-02	-0.52	1.02	652608	167884	595118	173814	562239	172008	627997	171015
RP_POS_789_53241a11_168	RP	POS	11.17	789.5324				2.29E-06	0.56	1.24	5.82E-02	-0.42	1.48	2.46E-03	0.35	1.28	1.87E-04	0.77	1.39	127732	73654	982438	1698910	1304689	2058161	660188	1176239
RP_POS_347_22156a7_611	RP	POS	7.61	347.2216				1.23E-01	-0.40	1.43	5.84E-02	0.32	1.12	3.77E-01	-0.24	0.70	3.99E-02	-0.56	1.17	576093	555890	411448	349906	345328	334610	477568	355641
RP_POS_242_92522a15_413	RP	POS	15.41	242.9252				9.88E-01	0.00	0.38	5.85E-02	0.39	1.23	4.01E-01	0.19	0.51	3.49E-01	-0.20	0.55	2965113	1150078	2961459	1273785	2720718	1136976	3202199	1366447
RP_POS_593_47668a11_153	RP	POS	11.15	593.4767				1.91E-01	-0.36	0.65	5.85E-02	-0.30	1.16	6.27E-02	-0.51	0.89	4.87E-01	-0.21	0.52	1429434	2270937	869713	1251108	1107151	1584112	632276	733500
HILIC_POS_87_09225a0_898	HILIC	POS	0.898	87.0923				4.94E-01	-0.15	0.61	5.85E-02	-0.36	1.08	1.84E-01	-0.33	0.51	8.93E-01	0.03	0.18	6138735	1069744	5993781	923280	6168290	789556	5819271	1018205
RP_POS_771_96576a10_502	RP	POS	10.50	771.9658				2.54E-01	-0.22	1.14	5.89E-02	-0.39	1.44	5.31E-02	-0.41	0.97	9.23E-01	-0.02	1.24	4268334	511295	4143393	598054	4256201	612273	4030585	567263
RP_POS_248_99841a0_523	RP	POS	0.52	248.9984				1.21E-03	0.40	1.06	5.91E-02	-0.43	1.41	1.87E-01	0.18	0.85	1.64E-03	0.61	1.26	426648	58635	530759	296268	586656	333246	474862	244768
RP_POS_1004_71155a0_496	RP	POS	0.50	1004.7116				9.10E-01	-0.02	0.91	5.94E-02	-0.40	1.52	2.66E-01	-0.22	0.78	4.07E-01	0.18	1.10	298608	139349	295139	182517	329510	195792	260768	162971
RP_POS_482_32413a10_167	RP	POS	10.17	482.3241				8.03E-02	-0.35	0.96	5.95E-02	-0.38	1.26	1.13E-02	-0.54	1.06	4.97E-01	-0.16	0.53	2394071	1051536	2006880	1126259	2218987	1251193	1794773	951580
RP_POS_796_54486a12_342	RP	POS	12.34	796.5449				3.47E-02	0.36	0.75	5.95E-02	0.40	1.17	8.95E-03	0.56	1.03	3.90E-01	0.16	0.59	682197	177595	769739	259368	720906	225389	818572	283283
RP_POS_1015_67017a10_371	RP	POS	10.37	1015.6702				8.13E-01	0.05	0.98	5.97E-02	-0.37	1.41	5.90E-01	-0.13	0.65	3.06E-01	0.23	0.96	2504489	1952488	2596652	1748512	2925567	1532536	2267737	1899349
HILIC_POS_175_10789a3_134	HILIC	POS	3.134	175.1079				3.90E-01	-0.14	0.69	5.99E-02	0.40	1.19	7.72E-01	0.06	0.10	8.02E-02	-0.35	0.61	2140820	402394	2060402	599230	1947801	583087	2173003	599679
RP_POS_621_89874a11_09	RP	POS	11.09	621.8987				2.08E-05	0.57	1.27	6.00E-02	-0.41	1.32	3.71E-03	0.37	1.15	2.96E-04	0.78	1.30	404739	111734	566807	308956	625035	381053	508579	201828
RP_NEG_874_77637a0_496	RP	NEG	0.50	874.7764				7.24E-01	-0.07	0.80	6.02E-02	-0.38	1.41	2.28E-01	-0.26	0.67	6.00E-01	0.12	0.89	1287192	180456	1274008	190220	1309721	201667	1238296	172723
RP_POS_768_54993a13_308	RP	POS	13.31	768.5499				1.83E-01	0.24	0.84	6.02E-02	0.39	1.10	5.15E-02	0.44	0.94	8.17E-01	0.04	0.51	2716296	1067286	3029342	1361675	2773502	1119846	3285182	1535749
RP_POS_266_6391a10_121	RP	POS	10.12	266.6391				2.09E-20	1.32	2.16	6.04E-02	0.35	1.18	1.02E-12	1.49	2.24	5.53E-15	1.15	2.27	333956	117824	713647	264313	663965	192882	763330	314496
RP_POS_387_25375a10_659	RP	POS	10.66	387.2538				9.10E-01	0.02	0.47	6.07E-02	0.37	1.13	3.95E-01	0.21	0.67	4.87E-01	-0.16	0.75	1961926	881891	1981802	797228	1832381	704625	2131222	861427
RP_POS_333_14429a6_705	RP	POS	6.71	333.1443	Unknown	333.1439(100), 315.134(45)	4	9.82E-01	0.00	0.65	6.07E-02	0.42	1.45	3.64E-01	0.21	0.57	1.14E-01	-0.20	0.82	757982	510586	760984	941279	583417	428536	938550	1241815
RP_POS_308_65976a10_932	RP	POS	10.93	308.6598				4.11E-04	-0.83	1.59	6.07E-02	-0.33	1.46	8.01E-05	-0.99	1.65	6.18E-03	-0.66	1.32	1265296	337546	1015702	264375	1065224	261892	966179	260042
RP_NEG_291_16168a9_607	RP	NEG	9.61	291.1617				1.14E-01	-0.39	0.86	6.08E-02	-0.33	1.13	3.85E-02	-0.56	0.83	3.75E-01	-0.22	0.68	2932690	129843	2892881	90050	2909748	80586	2876014	96482
HILIC_NEG_246_07503a1_544	HILIC	NEG	1.544	246.0750				1.81E-05	0.56	1.03	6.09E-02	0.41	1.20	5.03E-04	0.77	1.14	1.34E-03	0.35	1.28	288046	292114	760051	925970	585844	517019	934259	1184523
RP_POS_796_07617a13_294	RP	POS	13.29	796.0762				7.62E-02	-0.42	0.79	6.12E-02	0.34	1.13	3.16E-01	-0.25	0.71	2.10E-02	-0.59	1.01	3302706	1514969	2773633	1143081	2559928	1136224	2987339	1120591
RP_NEG_401_1474a10_827	RP	NEG	10.83	401.1474				1.74E-10	1.19	2.05	6.15E-02	0.34	1.36	2.10E-10	1.35	2.16	1.28E-07	1.02	1.90	753530	416005	1435167	519019	1338211	477514	1532123	545028
RP_POS_367_19345a11_38	RP	POS	11.38	367.1935				3.38E-10	0.90	1.79	6.16E-02	0.38	1.29	1.65E-07	1.10	1.81	1.98E-06	0.71	1.73	237632	140267	510584	310138	452595	238683	568573	361250
HILIC_NEG_247_96234a0_699	HILIC	NEG	0.699	247.9623				5.45E-08	0.69	1.22	6.17E-02	0.41	1.41	3.14E-05	0.89	1.43	3.28E-05	0.49	1.33	28917	32988	109921	127422	86051	81133	133791	158300
HILIC_POS_304_10083a4_448	HILIC	POS	4.448	304.1008				9.17E-06	0.66	0.99	6.18E-02	0.40	1.23	6.35E-06	0.85	1.44	1.03E-02	0.46	0.97	684790	80275	785754	163940	755175	160397	816332	163296
RP_POS_568_42688a11_441	RP	POS	11.44	568.4269				2.55E-07	-1.32	2.21	6.19E-02	-0.26	1.14	5.63E-08	-1.45	2.10	2.53E-06	-1.19	2.07	6517965	2644632	3433754	1654024	3742276	1508151	3125232	1748899
RP_POS_384_20297a10_855	RP	POS	10.86	384.2030				4.03E-01	0.16	0.73	6.20E-02	-0.39	1.16	8.58E-01	-0.04	0.71	8.96E-02	0.35	0.83	6568608	1807594	6895082	2190417	7303456	2002430	6486707	2311644
RP_POS_191_03995a0_523	RP	POS	0.52	191.0400				6.25E-03	0.35	0.98	6.20E-02	-0.42	1.36	3.60E-01	0.14	0.74	3.08E-03	0.56	1.19	3008910	460252	3519155	1645068	3825905	1780730	3212405	1450756
HILIC_NEG_429_58261a1_365	HILIC	NEG	1.365	429.5826				1.76E-10	-0.96	1.59	6.21E-02	-0.37	1.16	1.62E-09	-1.15	1.96	1.36E-05	-0.78	1.57	218056	36103	150977	69974	164013	68762	137941	69409
HILIC_POS_315_08023a7_326	HILIC	POS	7.326	315.0802				2.15E-02	0.38	0.79	6.22E-02	-0.40	1.22	3.39E-01	0.19	0.61	3.54E-03	0.58	1.01	1238545	164479	1328137	247507	1374226	244208	1282047	244533
HILIC_POS_562_32739a1_203	HILIC	POS	1.203	562.3274				1.45E-01	-0.33	0.56	6.23E-02	-0.35	1.27	3.86E-02	-0.50	0.92	5.37E-01	-0.15	0.24	565077	250696	492201	212621	531792	212801	452610	207014
HILIC_POS_255_09749a4_568	HILIC	POS	4.568	255.0975				6.63E-08	0.68	1.15	6.27E-02	0.41	1.11	4.20E-05	0.88	1.33	2.68E-05	0.48	1.37	363100	436712	1490574	1804726	1153722	1115836	1827426	2259177
RP_NEG_782_82819a0_493	RP	NEG	0.49	782.8282				5.87E-08	-0.73	1.25	6.28E-02	0.40	1.36	3.10E-03	-0.53	1.08	7.71E-08	-0.93	1.62	2389300	259022	1898984	717329	1765655	658176	2032312	755083
HILIC_NEG_345_71869a1_363	HILIC	NEG	1.363	345.7187				1.81E-08	0.96	1.64	6.29E-02	-0.36	0.99	1.29E-04	0.77	1.35	1.82E-09	1.14	2.19	354705	88411	482964	131821	507466	113374	458462	145015
RP_POS_419_31543a11_966	RP	POS	11.97	419.3154				7.73E-01	0.05	0.74	6.30E-02	0.40	1.34	2.05E-01	0.25	0.73	4.78E-01	-0.15	0.81	68494194	3776336	68740134	5260673	67762927	5513907	69717340	4854086
HILIC_NEG_132_92355a4_983	HILIC	NEG	4.983	132.9236				5.06E-01	0.13	0.47	6.30E-02	0.38	1.02	1.67E-01	0.32	0.50	7.57E-01	-0.06	0.24	5066364	3350846	5536757	3773199	4835419	3181574	6238094	4199807
RP_POS_333_14444a6_414	RP	POS	6.41	333.1444				9.75E-01	0.00	0.74	6.31E-02	0.41	1.47	3.83E-01	0.20	0.58	1.20E-01	-0.21	0.89	826388	502492	822445	913832	651831	468238	993060	1186831
RP_POS_411_77005a13_402	RP	POS	13.40	411.7701				5.42E-02	0.45	0.89	6.32E-02	-0.34	1.13	2.78E-01	0.28	0.51	1.04E-02	0.62	1.22	3793066	1237132	4265686	959989	4444105	757357	4087268	1106078
RP_POS_855_60291a11_156	RP	POS	11.16	855.6029				3.39E-07	0.61	1.28	6.32E-02	-0.41	1.46	6.20E-04	0.40	1.31	8.45E-05	0.81	1.42	39569	15323	349284	565774	454565	684289	244003	394792
RP_POS_829_52753a11_138	RP	POS	11.14	829.5275				2.62E-06	0.56	1.22	6.32E-02	-0.42	1.42	1.72E-03	0.35	1.28	2.51E-04	0.77	1.35	58270	36613	757252	1400493	1017990	1718321	496513	933498
HILIC_POS_202_1185a4_014	HILIC	POS	4.014	202.1185				1.58E-01	0.21	0.76	6.32E-02	0.41	1.09	4.58E-02	0.41	0.83	9.82E-01	0.00	0.25	1257320	662376	1510033	1336905	1261645	1063211	1758422	1534528
HILIC_POS_117_52146a3_723	HILIC	POS	3.723	117.5215				1.19E-03	0.54	1.12	6.32E-02	0.39	1.14	1.37E-03	0.74	1.26	2.64E-02	0.35	1.31	732024	697947	1276472	1047484	1081325	646916	1471620	1311723
RP_POS_276_11893a0_604	RP	POS	0.60	276.1189				2.25E-03	0.39	0.92	6.32E-02	-0.42	1.23	2.14E-01	0.18	0.72	1.96E-03	0.60	1.04	443827	129872	603680	458602	688828	508976	518532	388679
RP_POS_316_66666a10_932	RP	POS	10.93	316.6667				4.67E-04	-0.79	1.61	6.33E-02	-0.34	1.58	9.31E-05	-0.95	1.67	8.27E-03	-0.62	1.27	1150347	280615	943017	238696	987287	233651	898747	237743
RP_POS_833_55853a11_162	RP	POS	11.16	833.5585				7.32E-07	0.59	1.27	6.35E-02	-0.41	1.47	1.27E-03	0.38	1.30	1.10E-04	0.80	1.42	62701	46091	951111	1677753	1262885	2017441	639337	1191096
HILIC_POS_247_144a1_433	HILIC	POS	1.433	247.1440				1.50E-01	-0.40	0.71	6.41E-02	-0.28	1.04	5.41E-02	-0.55	0.97	3.79E-01	-0.26	0.37	39290360	50029043	25735571	25757970	30511711	31056829	20959430	18149532
RP_NEG_132_86658a15_51	RP	NEG	15.51	132.8666				9.90E-01	0.00	0.54	6.42E-02	-0.38	1.12	3.71E-01	-0.19	0.52	4.23E-01	0.19	0.56	2237273	85580	2237058	90766	2253847	98584	2220269	79694
RP_NEG_610_24341a10_124	RP	NEG	10.12	610.2434				6.13E-21	1.33	2.17	6.44E-02	0.34	1.19	4.97E-13	1.50	2.26	8.19E-15	1.16	2.23	827862	287582	1785537	662667	1662905	503322	1908169	776655
HILIC_POS_421_37119a0_89	HILIC	POS	0.89	421.3712				9.10E-03	0.44	0.79	6.45E-02	0.39	1.09	3.84E-03	0.64	1.10	1.56E-01	0.25	0.54	727625	138575	812614	202059	775244	158884	849983	233227
RP_POS_805_57501a13_995	RP	POS	14.00	805.5750				2.84E-01	-0.24	0.49	6.47E-02	0.36	1.37	8.16E-01	-0.06	0.52	7.22E-02	-0.41	0.79	626393	372608	546833	324656	486856	268344	606811	365520
RP_POS_196_00293a3_79	RP	POS	3.79	196.0029				5.57E-01	0.12	0.99	6.47E-02	-0.36	1.11	8.08E-01	-0.06	0.70	1.86E-01	0.31	0.78	11040837	4848104	11614200	4530564	12450377	4322910	10778022	4621302
RP_POS_257_17468a9_576	RP	POS	9.58	257.1747				3.28E-04	0.43	0.85	6.47E-02	-0.42	1.29	1.80E-02	0.22	0.96	3.37E-03	0.64	1.00	456572	267921	1414397	2535437	1884745	3263452	944048	1373490
RP_POS_1040_75098a0_49	RP	POS	0.49	1040.7510				2.65E-03	-0.52	1.07	6.49E-02	0.39	1.32	1.20E-01	-0.33	0.77	2.17E-04	-0.71	1.31	535439	160107	422409	227897	380367	198964	464451	248476
RP_POS_921_61121a11_148	RP	POS	11.15	921.6112				8.61E-07	0.59	1.26	6.49E-02	-0.41	1.46	1.01E-03	0.38	1.30	1.38E-04	0.79	1.40	90946	56769	812220	1370514	1065626	1665150	558814	944023
RP_POS_277_21378a10_823	RP	POS	10.82	277.2138				4.94E-10	0.85	1.67	6.50E-02	0.39	1.36	5.62E-08	1.05	1.87	5.19E-05	0.66	1.57	437605	304645	1083328	791206	937483	726797	1229172	832554
RP_POS_332_26157a8_999	RP	POS	9.00	332.2616				1.20E-01	0.25	0.62	6.51E-02	0.40	1.23	4.04E-02	0.45	0.90	7.37E-01	0.06	0.34	805494	341608	932760	538991	833221	396225	1032298	640106
RP_POS_343_33771a11_161	RP	POS	11.16	343.3377				1.43E-02	-0.51	0.97	6.52E-02	0.36	1.28	1.43E-01	-0.34	0.64	2.67E-03	-0.69	1.24	19221840	5502939	16410671	5309801	15432748	5104689	17388593	5380876
RP_NEG_588_3324a10_306	RP	NEG	10.31	588.3324				1.40E-02	0.51	0.98	6.53E-02	-0.36	1.45	1.63E-01	0.33	0.61	1.74E-03	0.69	1.21	48299798	13257064	55132319	13147158	57554772	11051833	52709866	14666422
HILIC_NEG_171_02744a0_7	HILIC	NEG	0.7	171.0274				9.31E-08	0.68	1.21	6.56E-02	0.40	1.37	4.25E-05	0.88	1.41	5.55E-05	0.47	1.29	54853	56394	195161	226541	153341	145845	236980	280801
RP_POS_385_15353a10_283	RP	POS	10.28	385.1535				1.38E-01	-0.32	0.83	6.56E-02	0.36	1.19	5.64E-01	-0.14	0.51	2.59E-02	-0.50	1.00	948169	81212	923879	73001	910432	56522	937327	84871
RP_NEG_199_80472a2_464	RP	NEG	2.46	199.8047				6.92E-01	0.08	0.98	6.56E-02	0.36	1.18	2.64E-01	0.27	0.44	6.68E-01	-0.10	0.82	4617424	2461103	4814041	2314670	4388331	2157365	5239750	2408454
HILIC_POS_123_0555a4_568	HILIC	POS	4.568	123.0555				2.00E-08	0.68	1.18	6.60E-02	0.41	1.13	4.88E-05	0.88	1.35	4.56E-06	0.47	1.48	219282	58190	607402	629904	491164	369171	723639	798621
HILIC_POS_246_18526a0_741	HILIC	POS	0.741	246.1853				1.10E-02	0.30	0.86	6.64E-02	-0.42	1.41	1.78E-02	0.09	1.07	2.68E-02	0.51	0.92	185497	100460	438834	962413	617158	1332012	260510	179524
RP_NEG_391_20853a11_162	RP	NEG	11.16	391.2085				1.35E-01	-0.30	0.64	6.65E-02	-0.37	1.35	3.67E-02	-0.48	0.77	5.91E-01	-0.12	0.41	1367701	150895	1320609	158142	1349609	143191	1291610	168251
RP_POS_223_09242a0_553	RP	POS	0.55	223.0924				2.88E-01	-0.18	0.88	6.65E-02	-0.40	1.25	8.58E-02	-0.37	0.74	8.98E-01	0.02	0.89	1987297	400517	1886897	616646	2000084	489084	1773711	709167
RP_POS_582_86255a0_496	RP	POS	0.50	582.8626				1.63E-08	-0.73	1.28	6.68E-02	0.39	1.34	1.41E-03	-0.54	1.11	2.52E-07	-0.93	1.59	15110061	983619	12881136	3265426	12283114	3227675	13479158	3224264
HILIC_NEG_130_05096a1_536	HILIC	NEG	1.536	130.0510				6.98E-02	0.31	0.81	6.69E-02	0.39	1.22	2.19E-02	0.51	0.86	5.13E-01	0.12	0.46	545576	132043	600637	187247	566312	150154	634963	214214
HILIC_POS_637_42957a1_23	HILIC	POS	1.23	637.4296				5.77E-01	-0.13	0.49	6.69E-02	-0.35	1.20	2.25E-01	-0.30	0.64	8.40E-01	0.05	0.15	2493702	1003738	2383535	834735	2536334	798251	2230736	850254
HILIC_POS_154_15907a4_852	HILIC	POS	4.852	154.1591				5.91E-02	-0.45	0.83	6.69E-02	-0.33	1.11	1.45E-02	-0.62	1.03	2.62E-01	-0.29	0.44	7754925	2025713	7002690	1486179	7274834	1604868	6730546	1317491
RP_POS_154_05864a0_574	RP	POS	0.57	154.0586				1.13E-02	0.41	0.77	6.71E-02	-0.39	1.32	2.49E-01	0.22	0.65	2.19E-03	0.61	1.04	336581	208952	465090	330673	525572	331753	404608	321551
RP_POS_888_5127a13_068	RP	POS	13.07	888.5127				9.29E-01	0.02	0.35	6.72E-02	-0.36	1.14	5.22E-01	-0.16	0.49	3.77E-01	0.20	0.58	1638045	588214	1648476	528694	1745275	429669	1551677	600833
RP_POS_899_63373a9_302	RP	POS	9.30	899.6337				5.15E-02	0.23	0.87	6.72E-02	0.42	1.54	5.53E-02	0.44	0.91	5.88E-01	0.02	1.25	1101460	1802203	3550648	12024919	1328775	1911318	5772520	16685931
RP_POS_362_11719a6_373	RP	POS	6.37	362.1172				7.91E-06	0.64	1.15	6.72E-02	0.39	1.18	1.79E-04	0.84	1.22	5.48E-04	0.44	1.12	31454926	9721488	44462279	21871509	40444684	12770887	48479874	27757014
RP_NEG_219_9514a15_478	RP	NEG	15.48	219.9514				5.99E-01	0.11	0.40	6.78E-02	-0.37	1.15	7.34E-01	-0.08	0.56	2.01E-01	0.29	0.67	1042429	548039	1101503	556178	1202972	549826	1000033	549236
RP_NEG_427_16379a10_973	RP	NEG	10.97	427.1638				7.65E-01	0.05	0.90	6.79E-02	-0.39	1.18	4.88E-01	-0.15	0.82	1.86E-01	0.25	0.86	1654872	273028	1673737	404536	1747565	352907	1599909	441556
RP_POS_877_58472a11_155	RP	POS	11.16	877.5847				5.79E-07	0.59	1.28	6.80E-02	-0.41	1.46	1.16E-03	0.39	1.30	9.86E-05	0.80	1.42	54643	44190	919476	1616512	1214963	1934561	623990	1165692
RP_POS_777_9873a10_372	RP	POS	10.37	777.9873				8.54E-01	-0.04	0.97	6.80E-02	-0.35	1.48	3.70E-01	-0.22	0.72	5.64E-01	0.14	0.87	492728	272663	482745	239360	526389	227814	439101	244886
RP_POS_265_17737a9_75	RP	POS	9.75	265.1774				4.95E-03	0.37	0.84	6.81E-02	0.41	1.19	1.09E-02	0.57	0.89	9.60E-02	0.16	0.63	1356770	512405	1875736	1573087	1587061	723791	2164411	2075034
RP_POS_770_56854a12_95	RP	POS	12.95	770.5685				4.72E-03	-0.64	1.04	6.81E-02	0.33	1.24	4.21E-02	-0.48	0.86	1.25E-03	-0.81	1.20	2560170	978750	1993060	803734	1846525	848628	2139596	735641
RP_POS_400_07724a6_323	RP	POS	6.32	400.0772				9.88E-01	0.00	0.69	6.81E-02	0.38	1.44	4.04E-01	0.19	0.64	2.98E-01	-0.19	0.64	18856227	11492230	18894985	14509263	16243418	10147375	21546552	17550383
RP_NEG_478_29346a10_124	RP	NEG	10.12	478.2935				1.79E-19	1.18	2.01	6.82E-02	0.36	1.16	1.03E-10	1.36	2.07	3.22E-13	1.00	2.10	537717	206588	1360716	679316	1236642	490316	1484790	812731
RP_POS_617_47461a11_361	RP	POS	11.36	617.4746				4.27E-02	-0.36	0.72	6.84E-02	-0.38	1.15	2.85E-03	-0.55	1.13	4.44E-01	-0.17	0.75	4006667	2334138	2949523	3028869	3502143	3601674	2396904	2222616
RP_POS_193_15468a0_542	RP	POS	0.54	193.1547				1.26E-02	0.38	1.00	6.87E-02	0.40	1.08	8.52E-03	0.58	1.14	2.26E-01	0.18	0.82	5542981	2581613	7250441	4934873	6350255	3390308	8150627	6004582
RP_POS_303_07074a7_589	RP	POS	7.59	303.0707				2.60E-02	0.26	0.74	6.88E-02	0.42	1.33	4.13E-02	0.47	1.00	1.29E-01	0.05	0.56	75539	128502	549128	2083106	166553	386480	931702	2884295
RP_NEG_816_8219a0_49	RP	NEG	0.49	816.8219				1.03E-07	-0.72	1.29	6.88E-02	0.39	1.38	2.03E-03	-0.52	1.13	7.15E-07	-0.91	1.56	2033513	290689	1495216	804093	1349035	805802	1641396	783198
RP_POS_153_06593a1_744	RP	POS	1.74	153.0659				1.24E-01	-0.28	0.50	6.89E-02	-0.38	1.14	2.92E-02	-0.47	0.77	6.47E-01	-0.09	0.70	1671775	772828	1411086	961058	1585753	904619	1236419	992732

Supplementary table 1: Metabolomics results (in asceding order according to p-value from progressive ALD vs non-progressive ALD comparison, with molecular features with ID_level of 1-2 first)

							all_ALD_vs_control			Prog_ALD_vs_non-prog_ALD			Prog_ALD_vs_control_ALD			Non-prog_ALD_vs_control			Healthy_control		all_ALD		Non-prog_ALD		Progressive_ALD	
							t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA								
Feature_ID	RP_HILIC	POS_NEG	Average.Rt	Average.Mz	Metabolite.name	curated_MSMS	ID_level	p	d	VIP	p	d	VIP	p	d	VIP	p	d	VIP	Mean	SD	Mean	SD	Mean	SD	Mean	SD
HILIC_POS_151_09929a0_512	HILIC	POS	0.512	151.0993				5.54E-02	0.22	0.69	6.94E-02	0.42	1.05	6.03E-02	0.43	0.69	6.21E-01	0.01	0.18	434041	231395	1067541	3243123	473130	475488	1661952	4505905
RP_POS_714_74377a0_501	RP	POS	0.50	714.7438				2.76E-02	0.40	0.87	6.95E-02	-0.38	1.31	2.84E-01	0.21	0.53	7.12E-03	0.59	1.13	285058	174296	370757	222957	411201	238126	330314	200977
HILIC_POS_104_07101a0_683	HILIC	POS	0.683	104.0710				2.24E-07	0.72	1.34	6.99E-02	0.39	1.13	1.59E-05	0.92	1.38	1.48E-04	0.53	1.39	234087	162928	502132	394401	430522	282727	573742	473159
RP_POS_873_55383a11_134	RP	POS	11.13	873.5538				1.78E-06	0.57	1.24	6.99E-02	-0.41	1.42	1.53E-03	0.36	1.29	2.08E-04	0.77	1.37	53607	31677	898974	1663473	1201127	2023832	596820	1143915
RP_POS_419_75659a13_296	RP	POS	13.30	419.7566				1.74E-01	-0.31	0.77	6.99E-02	0.34	1.11	5.72E-01	-0.13	0.55	5.52E-02	-0.48	1.00	6731631	1832634	6236600	1534011	5958769	1600380	6514430	1426765
RP_POS_597_44849a11_609	RP	POS	11.61	597.4485				1.12E-01	-0.47	0.81	7.00E-02	-0.26	1.11	4.50E-02	-0.59	0.95	2.70E-01	-0.34	0.61	3808511	5631000	2133268	2550529	2596174	3054486	1670363	1837380
RP_POS_510_35541a10_666	RP	POS	10.67	510.3554				4.76E-05	-0.86	1.54	7.00E-02	-0.33	1.37	7.24E-06	-1.03	1.73	2.09E-03	-0.70	1.21	21200865	7365824	14619029	7003516	15887131	7263367	13350928	6562102
RP_POS_577_48181a11_152	RP	POS	11.15	577.4818				1.29E-01	-0.29	0.57	7.00E-02	-0.37	1.13	1.01E-02	-0.48	1.09	6.63E-01	-0.11	0.60	1366979	1203665	978200	1352542	1224361	1743613	732038	729536
HILIC_NEG_200_99734a6_093	HILIC	NEG	6.093	200.9973				8.76E-01	0.03	0.80	7.00E-02	-0.39	1.16	3.69E-01	-0.17	0.53	2.75E-01	0.22	1.06	351188	140490	356347	217711	395763	226782	316931	202885
RP_POS_814_57062a13_247	RP	POS	13.25	814.5706				4.22E-01	-0.20	0.72	7.01E-02	-0.32	1.10	1.58E-01	-0.36	0.61	8.92E-01	-0.04	0.68	1127082	1036025	967630	717590	1097617	808938	837643	592887
RP_POS_774_5036a12_16	RP	POS	12.16	774.5036				1.49E-01	0.22	0.92	7.01E-02	-0.40	1.10	9.19E-01	0.02	0.66	4.02E-02	0.42	0.70	361717	237106	452385	461172	535894	509784	368876	394447
RP_POS_1061_65186a10_197	RP	POS	10.20	1061.6519				3.39E-02	-0.55	1.21	7.07E-02	-0.30	1.23	8.83E-03	-0.70	1.23	1.47E-01	-0.40	0.99	380362	376747	224938	236959	267774	266400	182102	196803
RP_NEG_269_05478a8_651	RP	NEG	8.65	269.0548				8.13E-01	-0.03	0.29	7.13E-02	0.41	1.18	4.62E-01	0.17	0.64	1.98E-02	-0.24	1.14	26366034	20412521	24934952	48475435	16123875	16128824	33746029	65796004
HILIC_POS_235_16545a3_699	HILIC	POS	3.699	235.1655				1.00E-02	0.30	0.73	7.14E-02	0.41	1.24	2.59E-02	0.51	0.74	3.90E-02	0.10	0.67	7767394	5751322	25415164	66476325	13328002	17219053	37502326	91289272
HILIC_POS_166_05316a6_092	HILIC	POS	6.092	166.0532				9.78E-01	0.00	0.56	7.17E-02	0.39	1.05	4.00E-01	0.19	0.31	1.85E-01	-0.20	0.85	683295	302053	681288	492054	592366	295795	770209	620922
RP_POS_779_55688a13_72	RP	POS	13.72	779.5569				9.37E-09	0.97	1.66	7.18E-02	0.35	1.09	4.14E-08	1.15	1.76	9.84E-06	0.80	1.57	579419	350619	1101334	525801	1006700	464603	1195968	569598
RP_POS_221_07846a5_517	RP	POS	5.52	221.0785				5.81E-03	0.39	0.80	7.19E-02	0.40	1.09	1.06E-02	0.59	0.91	8.72E-02	0.19	0.80	241884	291864	485013	695190	359147	308662	610880	921324
RP_POS_917_57996a11_13	RP	POS	11.13	917.5800				9.89E-07	0.58	1.26	7.21E-02	-0.40	1.41	9.41E-04	0.38	1.32	1.66E-04	0.78	1.38	43484	45979	950251	1735806	1263099	2113637	637403	1191775
RP_POS_624_84137a0_497	RP	POS	0.50	624.8414				4.14E-07	-0.70	1.30	7.22E-02	0.38	1.24	5.44E-03	-0.51	1.03	2.40E-07	-0.90	1.57	2571626	248628	2167554	614306	2057163	557700	2277945	653104
RP_POS_808_03345a10_932	RP	POS	10.93	808.0335				5.79E-02	-0.45	1.23	7.24E-02	-0.33	1.65	1.64E-02	-0.61	1.17	2.51E-01	-0.29	1.00	3699869	1436419	3161782	1085531	3356718	1074188	2966846	1072088
RP_NEG_475_32828a9_718	RP	NEG	9.72	475.3283				8.51E-01	-0.04	0.31	7.24E-02	0.34	1.69	6.40E-01	0.13	0.38	3.18E-01	-0.21	0.71	1140149	2573658	1045184	2097824	665583	782394	1424784	2825832
RP_POS_377_26608a10_69	RP	POS	10.69	377.2661				3.98E-03	0.37	0.87	7.24E-02	0.40	1.19	6.35E-03	0.57	0.95	1.87E-01	0.16	0.78	2192337	1685562	4198932	6160144	3089881	4266345	5307984	7480460
RP_POS_368_21887a10_382	RP	POS	10.38	368.2189				1.08E-01	-0.33	0.92	7.27E-02	0.36	1.27	5.31E-01	-0.15	0.61	1.80E-02	-0.51	1.07	850444	191320	786757	193371	752029	156216	821484	220643
RP_NEG_369_17465a8_165	RP	NEG	8.17	369.1747				2.55E-12	0.88	1.48	7.28E-02	0.38	1.18	5.70E-08	1.07	1.69	2.84E-06	0.69	1.71	697945	416140	2276833	1890633	1937631	1610316	2616035	2096189
RP_POS_524_37067a11_154	RP	POS	11.15	524.3707				1.58E-01	-0.33	1.03	7.28E-02	-0.33	1.42	5.07E-02	-0.49	0.97	5.08E-01	-0.16	0.87	5812881	2008095	5254372	1575476	5536821	1513499	4971924	1600442
RP_NEG_323_22241a11_162	RP	NEG	11.16	323.2224				3.87E-01	-0.18	0.53	7.33E-02	-0.35	1.27	1.21E-01	-0.36	0.67	9.69E-01	-0.01	0.26	1518442	244751	1475814	226449	1516355	231726	1435273	215763
RP_NEG_243_06261a0_708	RP	NEG	0.71	243.0626				1.80E-01	0.20	0.79	7.36E-02	0.40	1.23	4.09E-02	0.39	0.76	9.95E-01	0.00	0.87	3244670	420429	3398698	865787	3243840	799687	3553556	908864
RP_POS_188_12802a10_38	RP	POS	10.38	188.1280				4.39E-01	-0.14	0.78	7.36E-02	0.38	1.15	8.23E-01	0.05	0.58	7.70E-02	-0.33	0.88	2914948	224925	2876442	293969	2823786	222896	2929098	345337
RP_POS_203_05922a15_342	RP	POS	15.34	203.0592				5.45E-01	0.13	0.42	7.37E-02	0.35	1.05	1.82E-01	0.30	0.55	8.40E-01	-0.05	0.61	9071097	2420367	9366089	2269142	8960419	2395817	9771758	2080216
HILIC_POS_583_255a1_293	HILIC	POS	1.293	583.2550				3.53E-02	0.32	0.73	7.37E-02	0.39	1.23	1.96E-02	0.52	0.78	3.90E-01	0.13	0.42	571129	455421	820288	845547	668680	559293	971897	1041525
RP_POS_766_57104a14_127	RP	POS	14.13	766.5710				2.10E-01	-0.23	0.50	7.38E-02	0.37	1.10	8.56E-01	-0.04	0.31	3.73E-02	-0.41	0.80	1618618	581686	1458414	739907	1326157	648467	1590671	806158
RP_NEG_310_86508a15_501	RP	NEG	15.50	310.8651				1.35E-01	-0.32	0.70	7.42E-02	-0.35	1.05	3.28E-02	-0.49	0.88	5.48E-01	-0.14	0.44	840550	174884	787383	164831	816804	171769	757963	153694
RP_POS_784_77875a0_497	RP	POS	0.50	784.7788				7.90E-01	0.05	0.83	7.43E-02	-0.37	1.38	5.40E-01	-0.13	0.57	3.00E-01	0.23	0.96	1552251	194225	1563069	212942	1601058	224430	1525081	195704
RP_POS_511_83414a11_118	RP	POS	11.12	511.8341				3.48E-07	0.61	1.29	7.43E-02	-0.40	1.40	6.31E-04	0.41	1.31	8.81E-05	0.81	1.40	101588	40301	414576	569645	516421	685013	312730	406450
RP_POS_569_40137a11_2	RP	POS	11.20	569.4014				1.56E-05	0.51	1.15	7.44E-02	-0.40	1.38	1.14E-03	0.31	1.35	9.96E-04	0.71	1.25	263157	106160	2124265	4092685	2857634	5237669	1390896	2304601
RP_POS_1018_12756a10_5	RP	POS	10.50	1018.1276				7.93E-01	-0.05	0.59	7.45E-02	-0.37	1.12	2.96E-01	-0.23	0.56	5.34E-01	0.13	0.73	1724825	347487	1705633	388102	1774819	362454	1636447	403955
RP_POS_1074_74927a0_492	RP	POS	0.49	1074.7493				4.11E-07	-0.69	1.27	7.48E-02	0.38	1.37	5.39E-03	-0.50	1.11	5.10E-07	-0.88	1.55	1218529	169062	930860	447839	851086	419213	1010633	465280
RP_POS_184_09444a0_539	RP	POS	0.54	184.0944				8.57E-02	0.26	0.73	7.48E-02	-0.39	1.30	7.29E-01	0.07	0.68	1.14E-02	0.46	1.12	426939	103502	473030	192484	507313	177294	438748	202546
RP_NEG_494_95419a10_967	RP	NEG	10.97	494.9542				6.84E-01	-0.10	0.75	7.49E-02	0.33	1.05	8.16E-01	0.06	0.40	2.69E-01	-0.26	1.12	308371	443841	273639	322250	215977	176634	331300	414518
HILIC_NEG_271_99979a0_699	HILIC	NEG	0.699	271.9998				1.07E-09	0.79	1.38	7.49E-02	0.38	1.32	1.38E-06	0.98	1.70	1.90E-05	0.60	1.37	193404	290469	909793	960563	738583	755876	1081004	1110414
RP_NEG_188_89304a15_406	RP	NEG	15.41	188.8930				1.52E-01	0.31	1.03	7.52E-02	-0.34	1.09	5.67E-01	0.14	0.48	3.86E-02	0.48	1.06	859625	263270	935649	238101	977999	218986	893298	250849
RP_POS_1014_74402a0_493	RP	POS	0.49	1014.7440				4.30E-02	-0.36	0.84	7.53E-02	0.37	1.28	3.99E-01	-0.17	0.48	8.12E-03	-0.54	1.11	824083	111210	773303	148421	746916	144913	799690	148615
RP_NEG_445_33279a11_155	RP	NEG	11.16	445.3328				1.49E-01	-0.34	1.01	7.53E-02	-0.33	1.72	4.67E-02	-0.50	1.35	4.83E-01	-0.18	0.79	1381978	850694	1141405	651651	1257239	655588	1025572	633077
HILIC_POS_205_41711a2_972	HILIC	POS	2.972	205.4171				6.78E-05	0.62	1.21	7.55E-02	0.38	1.11	1.31E-04	0.80	1.27	8.95E-03	0.43	0.98	267928	347371	634486	630870	522294	511830	746678	718650
RP_POS_166_98495a11_552	RP	POS	11.55	166.9850				2.23E-01	-0.22	0.52	7.56E-02	0.37	1.26	8.68E-01	-0.04	0.35	3.61E-02	-0.41	0.91	13190882	2689657	12475568	3349355	11880028	2733593	13071107	3803809
RP_NEG_394_97168a8_709	RP	NEG	8.71	394.9717				4.08E-01	-0.19	0.36	7.59E-02	-0.34	1.35	1.60E-01	-0.36	0.65	9.40E-01	-0.02	0.36	1882916	323664	1830095	269364	1877917	234706	1782273	294688
HILIC_NEG_144_06659a0_747	HILIC	NEG	0.747	144.0666				3.47E-03	0.35	0.68	7.59E-02	0.41	1.25	1.59E-02	0.56	0.75	4.80E-03	0.15	1.08	89592	34614	149069	189731	115089	44499	183049	261522
HILIC_POS_104_07106a4_678	HILIC	POS	4.678	104.0711				1.11E-01	0.26	0.56	7.60E-02	0.38	1.06	4.86E-02	0.45	0.69	6.51E-01	0.07	0.44	5133754	2460024	6071361	3860353	5384026	2391313	6758696	4840068
RP_POS_381_20718a10_864	RP	POS	10.86	381.2072				8.31E-02	-0.36	0.68	7.61E-02	-0.35	1.25	1.52E-02	-0.53	0.98	4.45E-01	-0.18	0.44	740044	248877	650728	249103	694916	275053	606540	213850
RP_POS_200_20068a9_286	RP	POS	9.29	200.2007				5.88E-01	-0.11	0.86	7.62E-02	0.36	1.10	7.56E-01	0.07	0.86	1.76E-01	-0.29	0.93	1259499	44389	1254513	46921	1246191	40635	1262834	51532
RP_NEG_154_9733a15_453	RP	NEG	15.45	154.9733				8.42E-01	0.04	0.62	7.62E-02	-0.34	1.07	5.94E-01	-0.12	0.32	4.01E-01	0.21	0.58	2888700	110100	2893013	91703	2909281	103046	2876744	76368
RP_NEG_331_17712a8_142	RP	NEG	8.14	331.1771				1.80E-01	-0.39	0.72	7.63E-02	0.25	1.13	3.93E-01	-0.27	0.39	7.39E-02	-0.52	1.04	1956520	3881425	988065	1747795	676153	698192	1299976	2342198
RP_NEG_271_22839a10_135	RP	NEG	10.14	271.2284				6.77E-01	0.07	0.43	7.63E-02	-0.37	1.18	5.95E-01	-0.11	0.48	1.90E-01	0.26	0.81	3109776	315433	3138853	415331	3212447	381869	3065258	437770
RP_POS_1082_73108a0_493	RP	POS	0.49	1082.7311				1.35E-03	-0.53	0.92	7.63E-02	0.37	1.22	1.01E-01	-0.34	0.78	8.97E-05	-0.71	1.27	531181	113552	442039	178597	410373	150254	473704	199556
RP_POS_385_1983a7_048	RP	POS	7.05	385.1983				7.25E-02	-0.46	2.02	7.64E-02	0.30	1.05	2.50E-01	-0.30	1.22	2.42E-02	-0.61	1.52	2494138	1227796	2067108	803740	1924727	797038	2209488	792805
RP_POS_340_19611a0_707	RP	POS	0.71	340.1961				2.44E-14	0.95	1.64	7.64E-02	0.37	1.09	7.64E-08	1.13	1.72	2.59E-09	0.76	1.74	103349	107706	741116	703310	616226	494573	866005	850265
RP_POS_489_82062a11_124	RP	POS	11.12	489.8206				7.38E-07	0.59	1.28	7.65E-02	-0.39	1.39	6.14E-04	0.39	1.32	1.54E-04	0.79	1.38	62814	30260	263298	376272	330113	459742	196483	256080
RP_NEG_748_83472a0_492	RP	NEG	0.49	748.8347				2.06E-09	-0.78	1.38	7.65E-02	0.38	1.38	4.21E-04	-0.59	1.28	9.22E-08	-0.97	1.64	2482221	297678	1771182	969435	1599534	963694	1942831	953915
RP_POS_548_5036a13_933	RP	POS	13.93	548.5036				4.67E-01	0.16	0.59	7.66E-02	-0.34	1.10	9.89E-01	0.00	0.42	1.87E-01	0.33	0.61	3147266	1018252	3293091	840484	3441922	902634	3144259	753186
RP_POS_409_75241a12_694	RP	POS	12.69	409.7524				4.00E-03	0.60	1.22	7.66E-02	-0.34	1.08	5.97E-02	0.43	0.85	7.51E-04	0.77	1.33	1556869	627980	1940164	621431	2050159	594918	1830170	633731
RP_POS_497_39594a13_803	RP	POS	13.80	497.3959				3.69E-04	-0.75	1.25	7.68E-02	-0.33	1.07	6.60E-05	-0.92	1.49	9.80E-03	-0.59	1.00	6363907	971711	5617965	931404	5782717	953943	5453214	887316
RP_POS_961_6059a11_125	RP	POS	11.13	961.6059				9.36E-07	0.58	1.26	7.69E-02	-0.39	1.41	1.18E-03	0.39	1.31	1.48E-04	0.78	1.39	53672	51956	832038	1485415	1095343	1789643	568733	1055290
RP_POS_502_3266a10_7	RP	POS	10.70	502.3266				7.64E-02	-0.40	0.99	7.71E-02	-0.33	1.62	2.18E-02	-0.57	1.02	3.27E-01	-0.24	0.86	5158175	1845957	4505505	1519401	4774009	1487238	4237002	1518310
RP_POS_594_16241a9_667	RP	POS	9.67	594.1624				6.46E-01	-0.09	0.63	7.73E-02	0.37	1.07	6.42E-01	0.10	0.54	2.02E-01	-0.27	0.73	1356488	65705	1349998	79608	1335939	77546	1364057	79922
RP_POS_745_50641a11_176	RP	POS	11.18	745.5064				1.85E-05	0.51	1.19	7.74E-02	-0.40	1.42	5.80E-03	0.31	1.25	6.90E-04	0.71	1.34	274842	116791	1011960	1627328	1300105	1996944	723816	1092342
RP_POS_393_29688a11_173	RP	POS	11.17	393.2969				2.46E-05	0.53	1.11	7.75E-02	-0.39	1.29	1.97E-03	0.34	1.21	7.83E-04	0.73	1.18	1771621	251853	2240775	974408	2413461	1237150	2068088	571769
RP_POS_546_35242a11_158	RP	POS	11.16	546.3524				1.29E-01	-0.36	1.02	7.76E-02	-0.32	1.49	4.10E-02	-0.52	0.92	4.33E-01	-0.20	0.89	1675107	599231	1496281	459583	1577361	452101	1415202	457090
HILIC_NEG_161_04555a4_993	HILIC	NEG	4.993	161.0456				8.01E-01	-0.04	0.91	7.78E-02	0.37	1.01	5.19E-01	0.14	0.23	2.15E-01	-0.23	0.94	1870955	965005	1816641	1299992	1587167	1055206	2046115	1481054
RP_POS_690_78375a0_499	RP	POS	0.50	690.7838				4.22E-01	0.14	0.82	7.78E-02	-0.37	1.46	8.35E-01	-0.04	0.56	1.19E-01	0.33	1.04	730643	210802	768024	274313	816392	280704	719655	261651
RP_POS_1037_65222a10_37	RP	POS	10.37	1037.6522				5.96E-01	-0.12	0.98	7.80E-02	-0.34	1.44	2.43E-01	-0.29	0.76	8.22E-01	0.05	0.87	507376	358330	469695	310034	524333	285470	415057	326525
RP_POS_539_31317a10_325	RP	POS	10.33	539.3132				3.23E-03	-0.74	1.36	7.81E-02	-0.29	1.05	9.01E-04	-0.89	1.51	2.14E-02	-0.59	1.14	700776	310247	517079	207949	553699	201983	480459	209366
RP_POS_441_29688a10_579	RP	POS	10.58	441.2969				6.84E-01	0.09	0.84	7.83E-02	0.35	1.08	2.59E-01	0.26	0.64	7.14E-01	-0.09	0.78	1807379	408965	1840857	380929	1773813	394571	1907902	358212
RP_POS_353_26578a10_863	RP	POS	10.86	353.2658				5.90E-01	0.10	0.43	7.84E-02	0.37	1.05	2.20E-01	0.28	0.62	6.31E-01	-0.09	0.43	5804738	4206849	6301571	5369217	5354988	3980055	7248155	6369920
RP_POS_934_81274a0_487	RP	POS	0.49	934.8127				1.16E-04	0.49	0.91	7.85E-02	-0.39	1.17	8.46E-02	0.30	0.58	6.56E-05	0.69	1.33	382465	31773	433328	114932	453543	110301	413113	116997
HILIC_NEG_211_97729a1_213	HILIC	NEG	1.213	211.9773				9.55E-04	-0.62	1.27	7.87E-02	-0.35	0.97	4.13E-04	-0.80	1.37	2.40E-02	-0.44	1.27	416779	93744	347156	113319	367087	97063	327225	125349
HILIC_POS_188_17578a6_233	HILIC	POS	6.233	188.1758				1.59E-05	0.57	0.97	7.89E-02	0.39	1.45	1.22E-04	0.76	1.19	1.13E-02	0.38	1.06	1028036	534047	1873932	1633152	1586786	1363092	2161077	1833716
HILIC_POS_227_17538a1_111	HILIC	POS	1.111	227.1754				6.57E-02	0.23	0.79	7.89E-02	0.40	1.43	6.04E-02	0.43	0.61	6.35E-01	0.03	0.26	662032	467339	1011206	1689633	711764	450347	1310648	2319952
RP_NEG_197_08168a5_516	RP	NEG	5.52	197.0817				6.85E-03	0.38	0.81	7.92E-02	0.39	1.06	1.21E-02	0.58	0.91	9.02E-02	0.19	0.82	378535	494352	774153	1141270	572542	504816	975765	1514524
RP_POS_253_21368a10_464	RP	POS	10.46	253.2137				6.30E-02	-0.34	0.73	7.94E-02	0.37	1.06	4.63E-01	-0.16	0.53	1.11E-02	-0.52	0.91	716152	46447	697056	58736	686752	54819	707359	61224
HILIC_POS_188_07068a1_433	HILIC	POS	1.433	188.0707				1.21E-01	-0.43	0.86	7.96E-02	-0.27	1.04	4.47E-02	-0.57	1.06	3.15E-01	-0.30	0.44	3684979	4586897	2341858	2408648	2764854	2848096	1918863	1801323
HILIC_POS_171_18535a6_125	HILIC	POS	6.125	171.1854				9.78E-01	-0.01	0.87	7.96E-02	-0.35	1.05	4.36E-01	-0.18	0.76	4.58E-01	0.17	0.73	18762610	5969663	18728678	5823113	19749352	5633550	17708003	5886114
HILIC_NEG_202_96533a0_7	HILIC	NEG	0.7	202.9653				3.04E-09	0.83	1.43	7.98E-02	0.37	1.38	1.01E-06	1.02	1.69	1.21E-05	0.65	1.45	2541706	2447602	7210167	5871936	6180198	4574351	8240135	6824462
RP_POS_525_37543a11_202	RP	POS	11.20	525.3754				9.34E-05	0.47	1.15	7.99E-02	-0.39	1.40	1.88E-02	0.28	1.20	1.21E-03	0.67	1.28	1144151	862475	3321345	5154243	4226239	6271432	2416452	3559869
RP_NEG_528_2868a10_124	RP	NEG	10.12	528.2868				4.96E-21	1.30	2.14	8.02E-02	0.33	1.11	1.49E-12	1.47	2.22	9.58E-15	1.14	2.22	1039824	371518	2326576	915975	2166090	693400	2487061	1077858
RP_POS_265_0835a7_928	RP	POS	7.93	265.0835				9.31E-01	-0.02	0.43	8.03E-02	0.35	1.21	5.72E-01	0.15	0.23	3.24E-01	-0.19	0.77	1942467	10247731	1765838	9286729	125212	42746	3406465	12990448
RP_POS_657_45441a11_188	RP	POS	11.19	657.4544				2.27E-04	0.44	1.11	8.04E-02	-0.40	1.38	1.32E-02	0.24	1.24	3.21E-03	0.63	1.23	580729	158004	1418666	2173745	1800309	2776456	1037024	1241295
RP_POS_470_28525a11_129	RP	POS	11.13	470.2853				4.59E-07	0.60	1.28	8.06E-02	-0.39	1.41	6.52E-04	0.41	1.33	1.16E-04	0.79	1.40	21906	12754	452492	797201	592110	961911	312873	564777
RP_POS_200_20108a9_477	RP	POS	9.48	200.2011				1.37E-02	0.37	0.92	8.06E-02	0.38	1.41	1.50E-02	0.56	0.92	1.58E-01	0.18	0.59	10800726	703654	11263016	1360422	11024025	669107	11502008	1781852

Supplementary table 1: Metabolomics results (in asceding order according to p-value from progressive ALD vs non-progressive ALD comparison, with molecular features with ID_level of 1-2 first)

							all_ALD_vs_control			Prog_ALD_vs_non-prog_ALD			Prog_ALD_vs_control_ALD			Non-prog_ALD_vs_control			Healthy_control		all_ALD		Non-prog_ALD		Progressive_ALD	
							t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA								
Feature_ID	RP_HILIC	POS_NEG	Average.Rt	Average.Mz	Metabolite.name	curated_MSMS	ID_level	p	d	VIP	p	d	VIP	p	d	VIP	p	d	VIP	Mean	SD	Mean	SD	Mean	SD	Mean	SD
RP_NEG_529_46448a15_056	RP	NEG	15.06	529.4645				5.08E-01	-0.11	0.57	8.07E-02	0.38	1.34	5.27E-01	0.08	0.34	2.14E-01	-0.30	0.68	15922791	2111703	15585269	3441701	14978939	4615663	16190699	1371115
RP_POS_172_9769a0_837	RP	POS	0.84	172.9769				5.22E-02	-0.44	0.82	8.07E-02	-0.33	1.12	1.30E-02	-0.60	1.00	2.59E-01	-0.28	0.55	32021417	14721781	26294979	12141811	28415873	12701466	24174085	11284882
RP_POS_874_55469a13_296	RP	POS	13.30	874.5547				7.42E-01	0.07	0.30	8.07E-02	0.33	1.07	3.32E-01	0.24	0.66	7.09E-01	-0.09	0.25	2992721	1097026	3063520	898780	2906566	864899	3220474	913112
RP_POS_310_87701a15_419	RP	POS	15.42	310.8770				4.17E-01	-0.17	0.40	8.12E-02	-0.34	1.08	1.61E-01	-0.34	0.57	9.92E-01	0.00	0.51	1681058	401613	1615418	371411	1680229	312862	1550607	415033
RP_POS_570_79486a10_303	RP	POS	10.30	570.7949				3.77E-01	0.18	0.56	8.15E-02	-0.35	1.35	9.97E-01	0.00	0.32	9.26E-02	0.35	0.74	320093	112492	340638	117191	361077	94574	320200	133982
HILIC_POS_118_08655a0_627	HILIC	POS	0.627	118.0866				3.42E-07	0.62	1.20	8.15E-02	0.39	0.99	1.28E-07	0.81	1.70	2.07E-02	0.42	0.73	765584	156339	1417318	1167673	1213737	1312974	1620900	972761
RP_POS_481_81656a14_965	RP	POS	14.97	481.8166				5.48E-01	-0.11	0.42	8.15E-02	-0.36	1.21	8.17E-02	-0.30	0.77	7.94E-01	0.07	0.43	122924	150593	103720	173184	134135	236146	73306	54266
RP_POS_701_48053a11_182	RP	POS	11.18	701.4805				1.70E-04	0.44	1.13	8.18E-02	-0.39	1.39	1.57E-02	0.25	1.23	2.49E-03	0.64	1.26	434478	133864	1118914	1737521	1422416	2185810	815411	1064808
RP_POS_785_52875a13_157	RP	POS	13.16	785.5288				5.12E-01	-0.15	0.36	8.20E-02	0.33	1.14	9.52E-01	0.02	0.21	1.99E-01	-0.31	0.65	5388122	1177010	5236912	956984	5070483	907129	5403341	985350
HILIC_POS_112_03961a1_809	HILIC	POS	1.809	112.0396				2.32E-02	0.36	0.64	8.24E-02	-0.38	1.30	3.31E-01	0.17	0.36	7.61E-03	0.55	0.87	379487	391457	601420	666622	717230	721316	485610	591753
RP_POS_797_5899a13_998	RP	POS	14.00	797.5899				6.52E-02	-0.46	0.90	8.26E-02	0.30	1.12	2.33E-01	-0.31	0.74	2.12E-02	-0.61	0.95	11950780	4856658	10210969	3239191	9648714	3132394	10773223	3277467
RP_POS_957_47552a0_488	RP	POS	0.49	957.4755				4.50E-07	0.61	1.20	8.30E-02	-0.38	1.34	4.67E-03	0.42	1.09	2.03E-05	0.80	1.45	218229	30449	339987	220400	378200	237989	301773	196278
RP_POS_613_42731a11_194	RP	POS	11.19	613.4273				4.78E-05	0.48	1.13	8.33E-02	-0.39	1.36	3.01E-03	0.28	1.30	1.70E-03	0.68	1.24	482047	159156	1803892	3097140	2342728	3959021	1265056	1764633
RP_POS_583_2547a9_295	RP	POS	9.30	583.2547				2.25E-01	-0.21	0.74	8.35E-02	0.37	1.38	8.99E-01	-0.03	0.36	1.32E-02	-0.40	1.23	779207	463757	653560	617177	546032	267775	761088	821151
RP_POS_308_88013a15_42	RP	POS	15.42	308.8801				3.68E-01	-0.19	1.13	8.35E-02	-0.34	1.17	1.31E-01	-0.36	0.68	9.46E-01	-0.01	1.17	2124089	533804	2026206	520188	2116264	466647	1936149	558929
RP_POS_279_15674a9_575	RP	POS	9.58	279.1567				3.46E-04	0.47	0.86	8.38E-02	-0.38	1.21	1.58E-02	0.28	0.87	2.27E-03	0.67	1.00	3784654	1888277	6160164	5533610	7120765	7007941	5199562	3297301
HILIC_POS_104_07104a5_179	HILIC	POS	5.179	104.0710				6.86E-03	0.44	0.98	8.41E-02	0.37	1.07	3.06E-03	0.63	0.98	1.42E-01	0.26	0.74	580257	201771	712612	317184	657779	270352	767445	352192
RP_POS_167_08563a7_928	RP	POS	7.93	167.0856				9.37E-01	-0.02	0.43	8.41E-02	0.34	1.19	5.70E-01	0.15	0.23	3.25E-01	-0.19	0.76	3685948	20693138	3358873	19075025	30340	20179	6687405	26693219
RP_POS_501_3754a10_937	RP	POS	10.94	501.3754				7.99E-01	0.05	0.57	8.43E-02	-0.34	1.38	6.02E-01	-0.12	0.27	3.57E-01	0.22	0.60	28134054	4703438	28375274	4391611	29133747	4861145	27616801	3763153
HILIC_POS_224_12804a6_135	HILIC	POS	6.135	224.1280				1.18E-01	0.31	1.06	8.44E-02	-0.35	0.96	5.45E-01	0.13	0.54	3.08E-02	0.48	1.26	5845766	2295491	6604717	2518585	7039373	2535909	6170061	2449408
RP_POS_309_05768a8_02	RP	POS	8.02	309.0577				2.49E-02	0.33	1.10	8.46E-02	0.38	1.32	8.82E-03	0.52	1.41	4.06E-01	0.14	0.59	369221	466603	657823	963930	491531	855901	824114	1043208
RP_POS_550_82623a10_932	RP	POS	10.93	550.8262				3.41E-02	-0.50	1.26	8.50E-02	-0.31	1.60	9.89E-03	-0.66	1.22	1.64E-01	-0.35	1.07	1877941	605390	1623143	457626	1701961	454179	1544325	451842
HILIC_POS_104_07104a5_353	HILIC	POS	5.353	104.0710				8.91E-02	0.26	0.53	8.51E-02	-0.38	1.39	7.03E-01	0.07	0.23	1.63E-02	0.45	0.79	1635393	562905	1881997	1035357	2060300	1001527	1703693	1047792
RP_POS_838_63074a14_677	RP	POS	14.68	838.6307				1.42E-04	0.73	1.26	8.51E-02	0.34	1.10	7.27E-05	0.90	1.39	4.84E-03	0.56	1.10	2148271	1410804	3359854	1629417	3079123	1409613	3640586	1793415
RP_POS_304_21173a4_828	RP	POS	4.83	304.2117				3.83E-02	0.35	0.67	8.51E-02	-0.37	1.47	3.71E-01	0.17	0.47	1.09E-02	0.53	1.00	1057668	524818	1311042	764050	1442617	812576	1179467	695592
RP_POS_646_75616a0_501	RP	POS	0.50	646.7562				7.20E-04	0.60	1.16	8.57E-02	-0.35	1.26	2.67E-02	0.42	0.97	3.39E-04	0.77	1.35	195842	154151	317307	208991	353234	226165	281381	185636
RP_POS_805_01013a10_618	RP	POS	10.62	805.0101				4.79E-03	0.66	1.45	8.58E-02	-0.31	1.15	4.69E-02	0.50	1.06	8.56E-04	0.81	1.60	3458593	1113995	4099265	878600	4250357	735111	3948172	986231
HILIC_NEG_144_92345a1_342	HILIC	NEG	1.342	144.9235				4.60E-02	-0.43	0.97	8.61E-02	-0.33	1.16	7.88E-03	-0.60	1.11	2.78E-01	-0.27	0.44	7505589	4061152	5857205	3635120	6482148	4236943	5232262	2819420
RP_POS_153_06555a0_711	RP	POS	0.71	153.0656				4.47E-02	-0.37	0.66	8.64E-02	-0.35	1.13	1.19E-02	-0.55	0.87	3.40E-01	-0.19	0.82	3004804	1336225	2416569	1634567	2696921	1532988	2136217	1699322
RP_POS_120_97954a11_209	RP	POS	11.21	120.9795				6.71E-01	-0.10	0.87	8.64E-02	-0.33	1.20	2.90E-01	-0.26	0.47	7.87E-01	0.07	1.20	2596196	529228	2552146	434242	2626614	437835	2477677	421857
RP_POS_870_52057a12_693	RP	POS	12.69	870.5206				1.29E-04	0.73	1.38	8.66E-02	-0.34	1.05	8.54E-03	0.56	1.08	2.26E-05	0.90	1.52	3639968	1118158	4610607	1311907	4835494	1231142	4385721	1363232
HILIC_NEG_347_71643a1_363	HILIC	NEG	1.363	347.7164				1.89E-08	0.95	1.65	8.66E-02	-0.34	0.91	1.04E-04	0.78	1.37	3.26E-09	1.12	2.19	252489	61938	342325	92850	358247	80810	326404	101835
RP_POS_292_04221a6_862	RP	POS	6.86	292.0422				2.32E-02	-0.38	0.90	8.69E-02	0.36	1.22	3.19E-01	-0.20	0.71	4.64E-03	-0.56	1.14	1761529	129528	1691592	197044	1657857	192604	1725327	197550
HILIC_POS_544_33893a1_088	HILIC	POS	1.088	544.3389				9.72E-02	0.36	0.76	8.74E-02	-0.33	0.97	4.31E-01	0.19	0.39	2.12E-02	0.52	1.13	5440593	2488724	6277111	2259214	6663689	1895118	5890532	2532943
RP_POS_560_30206a10_312	RP	POS	10.31	560.3021				1.74E-01	0.27	0.93	8.75E-02	-0.35	1.63	6.64E-01	0.10	0.66	4.48E-02	0.44	0.91	1904195	432249	2027100	460530	2105805	440715	1948394	470778
RP_POS_1005_63196a11_119	RP	POS	11.12	1005.6320				7.68E-07	0.59	1.25	8.76E-02	-0.38	1.38	1.92E-03	0.40	1.26	9.85E-05	0.78	1.41	122355	73634	708585	1104741	897605	1290666	519565	852690
RP_POS_809_48456a10_881	RP	POS	10.88	809.4846				1.20E-02	0.30	0.93	8.77E-02	-0.39	1.28	4.34E-01	0.10	0.72	1.08E-02	0.49	1.09	2158745	167898	2491021	1266071	2707512	1452093	2274529	1017036
RP_POS_538_34021a11_127	RP	POS	11.13	538.3402				2.52E-07	0.61	1.31	8.79E-02	-0.38	1.40	5.71E-04	0.42	1.33	8.10E-05	0.80	1.43	39745	27115	810379	1390966	1048291	1658174	572467	1021764
RP_POS_1071_724a10_932	RP	POS	10.93	1071.7240				1.47E-02	-0.58	1.25	8.80E-02	-0.31	1.55	3.51E-03	-0.73	1.29	9.40E-02	-0.42	1.02	875852	456926	652149	349288	711760	371215	592538	318499
RP_NEG_701_1557a9_766	RP	NEG	9.77	701.1557				5.86E-01	-0.12	0.39	8.81E-02	-0.33	1.05	2.31E-01	-0.29	0.53	8.63E-01	0.04	0.26	4683758	311079	4650269	264808	4695450	278717	4605089	244599
RP_POS_353_26627a10_768	RP	POS	10.77	353.2663				5.22E-02	0.32	0.56	8.81E-02	0.37	1.02	2.20E-02	0.50	0.83	4.33E-01	0.13	0.44	913161	505500	1150628	809442	1012345	625331	1288912	945357
HILIC_POS_202_1548a3_509	HILIC	POS	3.509	202.1548				3.68E-01	0.16	0.47	8.82E-02	0.36	1.16	1.30E-01	0.34	0.54	9.23E-01	-0.02	0.04	1500770	1471027	1792969	1902777	1468073	1526989	2117864	2183550
RP_NEG_275_82349a15_561	RP	NEG	15.56	275.8235				3.81E-02	-0.44	0.89	8.82E-02	-0.33	1.46	9.29E-03	-0.60	1.03	2.40E-01	-0.27	0.71	1056667	45225	1037297	43363	1044693	43712	1029902	42151
RP_NEG_407_20792a7_044	RP	NEG	7.04	407.2079				9.81E-02	-0.42	2.02	8.84E-02	0.29	1.05	3.00E-01	-0.27	1.20	3.63E-02	-0.57	1.55	5616556	2989103	4661924	1960347	4327875	1986742	4995973	1894589
HILIC_POS_156_10188a0_49	HILIC	POS	0.49	156.1019				1.19E-01	0.29	0.48	8.85E-02	0.35	1.17	4.71E-02	0.46	0.72	5.52E-01	0.11	0.28	528619	127857	572140	157355	545274	114774	599005	188097
RP_POS_768_58582a14_362	RP	POS	14.36	768.5858				2.12E-02	-0.49	0.83	8.86E-02	0.33	1.01	1.76E-01	-0.33	0.61	3.39E-03	-0.66	1.12	1741433	1035422	1249133	963785	1084804	785731	1413461	1097377
RP_NEG_606_30365a10_124	RP	NEG	10.12	606.3037				4.60E-22	1.37	2.22	8.86E-02	0.31	1.10	1.23E-13	1.52	2.30	1.47E-15	1.21	2.28	3398824	1076448	7120045	2464790	6699708	1924161	7540383	2865552
RP_POS_163_97665a10_741	RP	POS	10.74	163.9767				9.70E-01	0.01	0.33	8.90E-02	0.33	1.03	4.82E-01	0.17	0.41	5.26E-01	-0.15	0.46	2190533	1028818	2198259	863505	2051385	851686	2345133	858547
RP_POS_494_31418a11_136	RP	POS	11.14	494.3142				3.85E-07	0.60	1.29	8.91E-02	-0.38	1.38	7.98E-04	0.42	1.31	9.57E-05	0.79	1.41	44114	32642	636059	1086994	821233	1292782	450885	803717
RP_POS_478_38855a13_932	RP	POS	13.93	478.3886				8.09E-02	0.42	0.75	8.93E-02	-0.30	1.15	2.91E-01	0.27	0.51	2.62E-02	0.57	0.95	6393135	1722790	6982007	1250840	7194603	1217934	6769412	1259178
RP_POS_535_35516a10_932	RP	POS	10.93	535.3552				8.57E-02	-0.41	1.05	8.95E-02	-0.31	1.53	2.90E-02	-0.56	1.02	3.04E-01	-0.26	0.86	795582	273871	703196	203134	737695	195542	668698	206648
RP_POS_593_26196a8_418	RP	POS	8.42	593.2620				5.37E-01	0.14	0.33	8.98E-02	0.33	1.09	2.49E-01	0.30	0.45	8.99E-01	-0.03	0.43	1153136	2777754	1493022	2404738	1083845	1614486	1902199	2955553
HILIC_POS_208_1333a1_357	HILIC	POS	1.357	208.1333				2.67E-01	0.17	0.43	9.03E-02	0.37	0.92	1.32E-01	0.36	0.77	9.05E-01	-0.01	0.15	721565	1160473	1046506	2067064	693714	756217	1399298	2794073
RP_NEG_254_99406a4_57	RP	NEG	4.57	254.9941				3.13E-03	-0.64	0.99	9.03E-02	-0.32	1.11	8.23E-04	-0.80	1.27	3.69E-02	-0.47	0.81	2173386	1163525	1452037	1075006	1634176	1037930	1269898	1090806
RP_POS_514_31171a11_118	RP	POS	11.12	514.3117				5.46E-07	0.60	1.29	9.03E-02	-0.38	1.39	7.20E-04	0.41	1.34	1.32E-04	0.78	1.40	76144	41159	1177066	2053308	1525699	2469809	828434	1473154
RP_POS_357_19315a11_043	RP	POS	11.04	357.1932				1.35E-04	0.72	1.65	9.04E-02	0.34	1.30	1.20E-04	0.89	1.59	3.43E-03	0.56	1.50	465293	320048	742677	378687	678432	291868	806922	442859
RP_POS_500_27686a9_93	RP	POS	9.93	500.2769				1.23E-04	0.62	1.23	9.04E-02	-0.36	1.00	9.96E-03	0.44	1.09	1.62E-04	0.80	1.34	578426	422589	987119	689081	1103917	774557	870322	575826
RP_POS_522_25916a10_049	RP	POS	10.05	522.2592				2.17E-05	0.68	1.29	9.06E-02	-0.35	1.00	3.51E-03	0.50	1.18	4.26E-05	0.86	1.42	608248	479693	1132464	804916	1268791	894338	996136	686464
RP_POS_499_82727a4_156	RP	POS	4.16	499.8273				1.55E-02	0.38	0.89	9.07E-02	-0.37	1.01	2.65E-01	0.20	0.56	5.74E-03	0.56	0.93	1609409	1786082	2702113	3111956	3228836	3356299	2175390	2781230
RP_NEG_278_88992a15_47	RP	NEG	15.47	278.8899				3.30E-01	0.15	0.72	9.09E-02	-0.37	1.09	8.75E-01	-0.04	0.24	1.62E-02	0.34	1.37	898552	38100	907949	68464	919584	36916	896314	88494
RP_POS_778_53662a12_381	RP	POS	12.38	778.5366				5.65E-02	-0.36	1.12	9.10E-02	-0.35	1.03	1.02E-02	-0.54	1.32	3.88E-01	-0.19	0.48	5878083	2472188	4864485	2837148	5344350	3061605	4384620	2533718
HILIC_NEG_217_0298a4_977	HILIC	NEG	4.977	217.0298				6.87E-01	-0.08	0.37	9.12E-02	0.34	1.00	7.07E-01	0.09	0.23	2.09E-01	-0.25	0.92	3758067	2719373	3531511	2865342	3046303	2022840	4016718	3466349
HILIC_POS_203_05269a5_167	HILIC	POS	5.167	203.0527				1.45E-01	0.27	0.83	9.13E-02	0.35	0.97	4.06E-02	0.45	0.86	6.46E-01	0.09	0.48	16771643	6077637	18695681	7402200	17445069	7004303	19946293	7645338
RP_NEG_212_00209a3_784	RP	NEG	3.78	212.0021				2.64E-02	-0.52	1.00	9.13E-02	-0.31	1.03	9.53E-03	-0.68	1.11	1.24E-01	-0.37	0.67	1669298	1101716	1180972	846786	1324090	727370	1037855	936941
RP_POS_553_43188a10_709	RP	POS	10.71	553.4319				4.35E-01	-0.16	0.80	9.14E-02	-0.34	1.60	1.39E-01	-0.33	1.47	9.48E-01	0.01	0.33	3465177	256672	3423693	268870	3469103	276161	3378282	256095
HILIC_NEG_312_83633a6_125	HILIC	NEG	6.125	312.8363				3.15E-01	0.18	0.74	9.16E-02	0.36	1.26	7.72E-02	0.36	0.99	9.93E-01	0.00	0.03	789119	151785	823265	204355	788770	211020	857759	193433
RP_POS_404_73193a12_458	RP	POS	12.46	404.7319				4.47E-01	0.16	0.60	9.17E-02	-0.34	1.02	9.58E-01	-0.01	0.80	1.45E-01	0.33	0.66	474715	295751	520642	293613	570184	269720	471100	310514
RP_POS_264_95346a15_333	RP	POS	15.33	264.9535				2.02E-01	-0.22	0.67	9.17E-02	-0.36	1.00	4.43E-02	-0.40	0.93	8.53E-01	-0.04	0.30	2817908	91116	2791161	131106	2813280	134670	2769042	124876
RP_NEG_808_83472a0_487	RP	NEG	0.49	808.8347				2.49E-01	0.16	0.88	9.17E-02	0.38	1.42	7.02E-02	0.35	0.89	8.79E-01	-0.03	1.01	5174334	735365	5421386	1690450	5136113	1503522	5706658	1829454
HILIC_POS_371_23959a1_133	HILIC	POS	1.133	371.2396				1.40E-02	-0.52	0.94	9.18E-02	-0.33	1.01	4.08E-03	-0.68	1.10	1.12E-01	-0.35	0.77	3218811	1145571	2632368	1095582	2817195	1023292	2447541	1143788
RP_POS_463_3028a11_147	RP	POS	11.15	463.3028				1.75E-05	0.57	1.04	9.18E-02	0.37	1.34	1.53E-04	0.76	1.31	8.52E-03	0.39	1.10	441138	196963	736541	563063	641489	462154	831593	639159
RP_POS_264_87231a15_465	RP	POS	15.47	264.8723				1.29E-01	0.31	1.00	9.19E-02	-0.34	0.99	5.32E-01	0.14	0.85	3.74E-02	0.48	1.04	1749643	539673	1919931	555517	2013597	563781	1826264	536417
RP_POS_615_45837a11_158	RP	POS	11.16	615.4584				2.00E-01	-0.34	0.60	9.22E-02	-0.28	1.04	7.19E-02	-0.48	0.83	4.87E-01	-0.20	0.55	3629636	5269124	2349028	3105455	2873820	3852973	1824236	2019174
RP_POS_275_63217a10_497	RP	POS	10.50	275.6322				3.80E-01	-0.19	0.60	9.22E-02	0.33	1.00	9.10E-01	-0.03	0.41	1.11E-01	-0.36	0.73	469562	173592	439198	153022	413372	113870	465024	181610
HILIC_NEG_182_98662a6_093	HILIC	NEG	6.093	182.9866				8.95E-01	0.02	0.84	9.22E-02	-0.37	1.10	3.86E-01	-0.16	0.65	3.16E-01	0.20	1.10	325639	154604	330531	246477	372058	261466	289003	225517
HILIC_POS_141_0659a5_265	HILIC	POS	5.265	141.0659				7.30E-01	0.06	0.69	9.32E-02	-0.36	0.96	4.82E-01	-0.12	0.26	2.78E-01	0.24	0.38	1278183	1125699	1368240	1675323	1650002	1950270	1086478	1305805
HILIC_POS_139_05026a1_057	HILIC	POS	1.057	139.0503				5.28E-01	-0.11	0.40	9.32E-02	-0.35	1.12	8.79E-02	-0.29	0.75	7.96E-01	0.06	0.16	816983	453331	754426	573435	851169	739962	657683	312604
RP_POS_290_1601a1_51	HILIC	POS	1.51	290.1601				2.28E-04	0.43	1.04	9.38E-02	0.38	1.00	2.67E-03	0.62	0.92	2.78E-02	0.24	0.69	240239	398839	9040791	22991172	5175244	15385807	12906338	28297663
HILIC_NEG_278_98141a5_102	HILIC	NEG	5.102	278.9814				1.76E-01	0.19	0.44	9.39E-02	0.37	1.10	8.40E-02	0.38	0.66	9.70E-01	0.00	0.60	4394235	1465995	4967619	3321013	4408998	2045595	5526240	4178759
RP_POS_1023_64001a10_625	RP	POS	10.63	1023.6400				7.93E-03	0.51	1.24	9.39E-02	0.34	1.46	3.59E-03	0.68	1.23	8.21E-02	0.34	1.10	859719	487880	1141817	556319	1048474	445327	1235161	639686
RP_POS_194_15164a7_794	RP	POS	7.79	194.1516				3.09E-04	0.42	0.87	9.42E-02	-0.38	1.16	1.08E-02	0.23	0.92	4.51E-03	0.61	0.97	21552	58563	537741	1377015	769334	1774883	306148	755891
RP_POS_308_97095a15_44	RP	POS	15.44	308.9710				3.29E-01	0.18	0.41	9.43E-02	-0.35	1.03	9.57E-01	0.01	0.36	1.09E-01	0.36	0.70	2681649	360381	2756854	421947	2827505	449907	2686203	383547
RP_NEG_473_40143a13_181	RP	NEG	13.18	473.4014				2.45E-02	-0.48	0.84	9.49E-02	-0.32	1.00	5.65E-03	-0.65	1.11	1.70E-01	-0.32	0.56	14546471	1083618	14046054	990511	14211570	1037258	13880538	922189
RP_POS_379_2608a11_202	RP	POS	11.20	379.2608				6.30E-07	0.63	1.47	9.50E-02	0.37	1.01	1.43E-04	0.82	1.34	1.31E-04	0.45	1.50	503374	393236	1379515	1518400	1125073	968371	1633957	1894271
RP_POS_516_32715a11_131	RP	POS	11.13	516.3272				2.80E-07	0.61	1.30	9.51E-02	-0.37	1.38	6.45E-04	0.43	1.31	8.56E-05	0.80	1.42	42846	23626	825909	1419682	1063441	1684591	588377	1057892
HILIC_NEG_201_95786a1_374	HILIC	NEG	1.374	201.9579				4.28E-02	-0.37	0.67	9.52E-02	-0.35	0.96	6.27E-03	-0.54	1.00	3.68E-01	-0.20	0.31	3169332	1119011	2668963	1395602	2902065	1548198	2435862	1194718
RP_POS_308_66025a10_502	RP	POS	10.50	308.6603				3.01E-01	-0.21	0.61	9.53E-02	0.33	0.99	8.48E-01	-0.04	0.32	8.73E-02	-0.38	0.79	1947756	677855	1803778	680880	1690124	617475	1917433	727336
RP_POS_1070_7865a0_488	RP	POS	0.49	1070.7865				3.28E-05	0.50	0.95	9.56E-02	-0.37	1.13	5.51E-02	0.31	0.70	6.73E-05	0.69	1.32	442418	25141	517518	167685	545475	165323	489562	166983

Supplementary table 1: Metabolomics results (in asceding order according to p-value from progressive ALD vs non-progressive ALD comparison, with molecular features with ID_level of 1-2 first)

								all_ALD_vs_control			Prog_ALD_vs_non-prog_ALD			Prog_ALD_vs_control_ALD			Non-prog_ALD_vs_control			Healthy_control		all_ALD		Non-prog_ALD		Progressive_ALD	
								t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA								
Feature_ID	RP_HILIC	POS_NEG	Average.Rt	Average.Mz	Metabolite.name	curated_MSMS	ID_level	p	d	VIP	p	d	VIP	p	d	VIP	p	d	VIP	Mean	SD	Mean	SD	Mean	SD	Mean	SD
HILIC_NEG_568_36401a1_057	HILIC	NEG	1.057	568.3640				6.28E-01	-0.10	0.43	9.57E-02	-0.33	1.13	2.63E-01	-0.27	0.62	7.93E-01	0.06	0.10	352257	118385	340739	109532	359000	103481	322477	113361
RP_POS_481_34918a11_205	RP	POS	11.21	481.3492				2.92E-06	0.55	1.22	9.57E-02	-0.37	1.38	9.88E-04	0.37	1.36	3.99E-04	0.74	1.32	247656	107301	2743263	5028205	3583895	6204967	1902632	3337348
RP_POS_492_29816a11_123	RP	POS	11.12	492.2982				5.09E-07	0.60	1.29	9.60E-02	-0.37	1.38	7.94E-04	0.41	1.33	1.23E-04	0.78	1.41	39874	28148	815364	1441947	1055964	1722077	574763	1056961
RP_POS_233_0696a15_34	RP	POS	15.34	233.0696				4.52E-01	-0.15	0.76	9.63E-02	-0.34	1.10	1.66E-01	-0.32	0.56	9.37E-01	0.02	0.88	1645799	444469	1576661	462648	1653650	427520	1499672	487426
HILIC_NEG_200_9707a0_701	HILIC	NEG	0.701	200.9707				1.27E-12	1.04	1.78	9.65E-02	0.33	1.37	2.70E-09	1.21	2.10	5.68E-08	0.88	1.80	196515	144410	513589	302727	463211	257337	563967	337277
HILIC_POS_199_1806a5_648	HILIC	POS	5.648	199.1806				5.10E-01	0.12	0.61	9.65E-02	-0.35	1.38	8.23E-01	-0.05	0.29	1.59E-01	0.30	0.51	3979574	775841	4089019	916384	4241424	866562	3936614	947800
RP_NEG_828_57788a13_385	RP	NEG	13.39	828.5779				3.36E-01	-0.20	0.50	9.67E-02	-0.33	1.05	1.08E-01	-0.36	0.71	8.95E-01	-0.03	0.40	53582748	17347193	50157983	17452304	53058440	17709062	47257526	16870160
RP_POS_172_16959a7_794	RP	POS	7.79	172.1696				3.06E-04	0.42	0.87	9.68E-02	-0.38	1.15	1.08E-02	0.24	0.92	4.52E-03	0.61	0.97	136260	304853	2490731	6272121	3537570	8073657	1443891	3472958
RP_POS_732_76514a0_499	RP	POS	0.50	732.7651				5.41E-02	0.35	0.97	9.71E-02	-0.34	1.26	3.71E-01	0.18	0.69	1.50E-02	0.53	1.14	285490	184634	363592	227798	401412	234886	325772	216223
RP_POS_752_82928a0_493	RP	POS	0.49	752.8293				6.78E-02	0.25	0.89	9.71E-02	0.37	1.42	2.84E-02	0.44	0.96	6.68E-01	0.07	0.99	1307664	311631	1484595	786466	1353940	651311	1615250	889177
HILIC_POS_184_0925a5_028	HILIC	POS	5.028	184.0943				2.26E-03	0.46	0.83	9.76E-02	0.36	1.08	1.06E-03	0.64	1.13	1.10E-01	0.28	0.53	2908893	1327422	3990248	2531814	3570471	2372103	4410025	2639033
RP_POS_1021_62463a10_324	RP	POS	10.32	1021.6246				1.25E-02	0.47	1.16	9.76E-02	-0.34	1.34	1.92E-01	0.30	0.78	1.22E-03	0.64	1.37	4509958	1992144	5608661	2415725	6009627	1899975	5207696	2802238
RP_POS_389_17798a11_048	RP	POS	11.05	389.1780				2.50E-09	0.84	1.74	9.78E-02	0.35	1.10	2.46E-07	1.01	1.77	5.15E-05	0.66	1.61	409647	224317	840766	539402	751385	487084	930146	578180
RP_POS_536_40613a11_244	RP	POS	11.24	536.4061				1.62E-05	-1.02	1.62	9.78E-02	-0.28	1.03	2.12E-06	-1.16	1.90	4.49E-04	-0.88	1.39	959518	449392	539461	343305	596417	404109	482505	261146
RP_POS_352_24509a11_253	RP	POS	11.25	352.2451				1.38E-03	0.65	1.29	9.79E-02	0.32	1.17	3.43E-04	0.81	1.50	2.58E-02	0.49	0.98	3244651	777386	3781073	798438	3648837	791965	3913310	790646
RP_POS_1067_62854a10_324	RP	POS	10.32	1067.6285				2.55E-05	-1.10	1.83	9.79E-02	-0.25	1.09	4.92E-06	-1.22	1.94	2.96E-04	-0.97	1.49	766080	483137	334317	293887	383075	349138	285559	218523
RP_POS_338_34259a11_063	RP	POS	11.06	338.3426				1.02E-02	-0.50	0.91	9.80E-02	0.33	1.06	1.18E-01	-0.33	0.74	2.85E-03	-0.66	1.11	1897569	112849	1834689	127662	1813549	130812	1855829	122082
RP_POS_1048_12097a0_487	RP	POS	0.49	1048.1210				3.18E-07	0.62	1.17	9.82E-02	-0.37	1.26	6.57E-03	0.44	1.02	7.18E-06	0.80	1.48	282265	25916	395840	203266	429476	205892	362204	196918
RP_POS_537_16754a0_709	RP	POS	0.71	537.1675				4.65E-07	0.65	1.03	9.83E-02	0.36	1.16	7.70E-05	0.83	1.22	2.76E-04	0.47	1.11	575782	267972	1136044	942763	979749	666298	1292339	1141024
RP_POS_447_3461a11_152	RP	POS	11.15	447.3461				5.51E-02	-0.43	1.13	9.84E-02	-0.31	1.66	1.70E-02	-0.59	1.41	2.51E-01	-0.27	0.82	1381057	682575	1117776	578036	1213355	562668	1022197	582949
RP_POS_355_17245a8_141	RP	POS	8.14	355.1725				9.49E-02	-0.49	0.92	9.86E-02	0.23	1.14	2.30E-01	-0.38	0.52	3.76E-02	-0.61	1.21	681293	1252834	289267	558340	196361	219139	382173	751141
RP_POS_499_32358a9_702	RP	POS	9.70	499.3236				8.80E-01	-0.03	0.28	9.90E-02	0.32	1.69	6.41E-01	0.13	0.45	3.50E-01	-0.19	0.61	489040	1187984	453632	1021112	283896	378288	623368	1380116
RP_NEG_470_34955a9_367	RP	NEG	9.37	470.3496				4.66E-11	1.10	1.76	9.91E-02	0.31	1.00	4.66E-10	1.26	1.94	2.31E-07	0.95	1.75	652950	279096	1148765	426475	1078367	400780	1219164	443548
RP_POS_499_8269a6_196	RP	POS	6.20	499.8269				9.29E-01	0.02	0.41	9.96E-02	-0.32	1.07	5.19E-01	-0.14	0.41	4.99E-01	0.18	0.51	1262497	1725025	1292962	1476404	1537188	1879232	1048735	866476
RP_POS_562_32642a10_933	RP	POS	10.93	562.3264				1.21E-01	-0.37	0.99	9.97E-02	-0.30	1.32	4.16E-02	-0.52	0.93	3.91E-01	-0.21	0.84	4349838	1554838	3876040	1186819	4071575	1187185	3680505	1165499
RP_POS_219_02661a0_547	RP	POS	0.55	219.0266				2.20E-03	-0.37	1.05	9.99E-02	0.37	1.31	3.22E-01	-0.18	0.94	1.41E-04	-0.56	1.43	12925509	1030841	11018993	5807784	10061834	4783539	11976153	6587650
HILIC_NEG_144_92345a1_485	HILIC	NEG	1.485	144.9235				8.59E-01	-0.03	0.25	9.99E-02	0.36	1.07	4.74E-01	0.15	0.31	2.47E-01	-0.21	0.46	18145647	3487551	17997640	5575120	17079232	4772640	18916049	6188601
RP_POS_211_09677a6_516	RP	POS	6.52	211.0968				9.24E-03	0.34	0.78	1.00E-01	-0.37	0.99	2.11E-01	0.16	0.54	1.31E-02	0.53	0.87	4199930	13881679	17284017	43008226	24383751	52993873	10184283	28739237
RP_POS_533_84686a11_113	RP	POS	11.11	533.8469				4.48E-07	0.60	1.29	1.00E-01	-0.37	1.36	5.90E-04	0.42	1.33	1.28E-04	0.78	1.40	50847	33133	468637	771327	595857	926067	341416	558035
RP_POS_257_16812a6_67	RP	POS	6.67	257.1681	Unknown	257.1661(100)	4	2.19E-01	0.21	0.50	1.00E-01	-0.35	1.14	8.30E-01	0.04	0.26	9.33E-02	0.39	0.71	2686221	2460023	3374861	3460234	3945589	4245737	2804134	2345155
RP_POS_560_35254a11_121	RP	POS	11.12	560.3525				2.23E-07	0.62	1.29	1.00E-01	-0.37	1.37	5.09E-04	0.44	1.32	7.99E-05	0.80	1.42	111353	61839	710734	1072891	887531	1273531	533937	800006
RP_NEG_440_88892a15_335	RP	NEG	15.34	440.8889				7.47E-01	-0.06	0.61	1.01E-01	-0.33	0.99	2.96E-01	-0.23	0.62	6.55E-01	0.10	0.42	1878810	68277	1874271	71042	1885947	73324	1862595	67397
RP_POS_595_2561a10_375	RP	POS	10.38	595.2561				7.03E-01	0.07	0.97	1.01E-01	-0.34	1.49	6.41E-01	-0.10	0.91	2.47E-01	0.24	0.78	576681	85164	583681	103155	600617	98531	566744	105855
RP_POS_309_17834a0_607	RP	POS	0.61	309.1783				6.75E-03	0.39	0.99	1.01E-01	0.36	1.29	4.11E-03	0.57	1.34	2.02E-01	0.21	0.48	210545	207686	372321	457298	297220	399386	447422	501488
RP_POS_277_07236a15_433	RP	POS	15.43	277.0724				8.30E-01	-0.04	0.55	1.01E-01	-0.33	1.10	3.61E-01	-0.21	0.41	5.64E-01	0.12	0.52	5943725	244425	5932812	260434	5975535	238306	5890088	276625
RP_POS_553_45911a10_577	RP	POS	10.58	553.4591				1.02E-01	-0.32	0.87	1.01E-01	0.33	1.11	4.97E-01	-0.16	0.47	1.92E-02	-0.49	1.10	1560804	279158	1465059	297033	1416295	241660	1513823	339125
RP_POS_884_4939a13_062	RP	POS	13.06	884.4939				9.25E-02	-0.45	0.71	1.01E-01	-0.27	1.03	3.81E-02	-0.58	0.89	2.50E-01	-0.32	0.51	740787	358023	625907	205954	659677	204726	592136	203616
HILIC_POS_149_01862a0_708	HILIC	POS	0.708	149.0186				1.12E-09	0.88	1.52	1.01E-01	0.34	1.29	1.97E-07	1.05	1.85	1.01E-05	0.71	1.48	168077	175923	496660	385436	433449	330940	559872	427175
HILIC_NEG_312_83636a4_84	HILIC	NEG	4.84	312.8364				5.23E-01	-0.14	0.42	1.02E-01	-0.32	1.20	2.11E-01	-0.30	0.52	9.13E-01	0.03	0.45	1373003	442584	1316145	411078	1383473	392695	1248818	421852
HILIC_NEG_295_73611a3_059	HILIC	NEG	3.059	295.7361				2.57E-02	-0.27	0.86	1.02E-01	0.37	1.09	7.03E-01	-0.08	0.58	5.54E-05	-0.45	1.42	1763429	112411	1577792	796445	1446971	493583	1708613	1001521
HILIC_POS_358_29495a0_629	HILIC	POS	0.629	358.2950				5.97E-02	-0.42	0.84	1.02E-01	-0.31	0.98	1.88E-02	-0.57	0.95	2.68E-01	-0.26	0.49	1315297	848306	992911	736227	1113381	712388	872441	746998
HILIC_NEG_223_00764a1_3	HILIC	NEG	1.3	223.0076				2.86E-10	1.04	1.73	1.02E-01	0.32	1.00	3.42E-09	1.20	1.89	1.02E-06	0.88	1.68	339253	135993	570088	214630	534966	198391	605210	226264
RP_NEG_204_98103a2_206	RP	NEG	2.21	204.9810				8.05E-01	-0.04	0.46	1.02E-01	0.35	1.46	5.73E-01	0.14	0.49	1.29E-01	-0.22	0.76	966479	1811524	862437	2716994	415346	1109660	1309527	3643553
RP_POS_193_08624a6_516	RP	POS	6.52	193.0862				8.85E-03	0.34	0.77	1.03E-01	-0.37	0.98	2.05E-01	0.16	0.54	1.31E-02	0.52	0.87	568833	1943520	2441623	6152363	3449604	7577355	1433641	4121382
HILIC_NEG_119_03493a4_985	HILIC	NEG	4.985	119.0349				4.58E-01	0.11	0.33	1.03E-01	0.36	1.01	1.98E-01	0.29	0.60	6.00E-01	-0.07	0.60	1931805	1064591	2139580	2058928	1801700	1129053	2477461	2656527
RP_NEG_842_82892a0_49	RP	NEG	0.49	842.8289				1.14E-01	0.21	0.89	1.03E-01	0.37	1.40	4.62E-02	0.40	0.96	8.37E-01	0.03	0.97	1075969	256577	1205917	680062	1094717	555294	1317116	775126
RP_POS_1039_67114a10_197	RP	POS	10.20	1039.6711				9.42E-02	-0.48	1.14	1.03E-01	-0.24	1.28	4.37E-02	-0.60	1.00	2.18E-01	-0.36	0.97	1717962	2297462	994950	1089207	1172793	1112752	817107	1046036
RP_POS_338_23251a9_524	RP	POS	9.52	338.2325				3.16E-01	-0.16	0.49	1.03E-01	0.35	1.23	9.43E-01	0.02	0.51	4.98E-02	-0.34	0.77	2543030	156953	2505154	253568	2463709	201711	2546600	292767
RP_POS_288_87952a15_428	RP	POS	15.43	288.8795				5.50E-01	-0.08	0.39	1.04E-01	-0.36	1.08	1.98E-01	-0.27	0.41	5.04E-01	0.10	0.35	2587882	121208	2566648	282442	2612739	213424	2520557	333602
RP_POS_286_23605a10_142	RP	POS	10.14	286.2361				2.55E-02	0.42	0.88	1.04E-01	0.33	1.18	8.24E-03	0.59	1.02	2.17E-01	0.25	0.83	643619	192449	737686	230734	700092	211536	775280	244808
RP_POS_333_14423a6_19	RP	POS	6.19	333.1442				7.41E-01	0.05	0.70	1.04E-01	0.36	1.39	3.13E-01	0.23	0.59	3.17E-01	-0.13	0.74	945333	552303	993381	1071448	818031	567310	1168732	1390984
RP_POS_694_49353a13_57	RP	POS	13.57	694.4935				5.17E-01	0.14	1.17	1.04E-01	0.32	0.99	2.05E-01	0.30	0.72	9.40E-01	-0.02	0.71	1387736	211445	1415073	189212	1384258	193195	1445888	181853
RP_POS_1050_65881a10_324	RP	POS	10.32	1050.6588				2.39E-03	-0.78	1.35	1.04E-01	-0.27	1.12	5.12E-04	-0.91	1.52	1.79E-02	-0.65	1.02	482603	348899	269753	222895	306113	265845	233393	164336
RP_NEG_994_7774a0_491	RP	NEG	0.49	994.7774				7.86E-09	-0.83	1.38	1.04E-01	0.34	1.28	4.09E-04	-0.66	1.24	1.83E-08	-1.00	1.67	1021842	167425	723632	376874	662271	345345	784993	400024
RP_POS_300_28967a8_869	RP	POS	8.87	300.2897				1.64E-12	0.88	1.53	1.04E-01	0.35	1.10	4.77E-07	1.05	1.63	5.16E-08	0.71	1.81	243135	55802	495961	304128	446396	219232	545525	365786
RP_POS_169_05809a0_524	RP	POS	0.52	169.0581				3.40E-02	0.28	0.91	1.04E-01	-0.37	1.20	5.71E-01	0.09	0.65	1.14E-02	0.46	1.10	4346235	651454	4854378	2072598	5191406	2142727	4517350	1963644
RP_NEG_195_81113a2_201	RP	NEG	2.20	195.8111				6.20E-02	0.38	1.07	1.04E-01	-0.32	1.12	2.80E-01	0.22	0.97	2.83E-02	0.54	0.74	10121673	1868255	10848404	1904649	11158620	2302944	10538188	1352577
RP_POS_288_64056a10_619	RP	POS	10.62	288.6406				3.11E-01	0.23	0.90	1.04E-01	-0.31	0.96	7.60E-01	0.08	0.60	1.05E-01	0.38	1.03	2326242	494742	2424778	401313	2490051	331927	2359504	454446
RP_POS_813_98932a10_313	RP	POS	10.31	813.9893				4.74E-01	-0.13	0.77	1.05E-01	-0.34	1.18	1.47E-01	-0.30	0.73	8.33E-01	0.04	0.37	602634	138878	580614	182083	610168	183042	551060	178039
RP_POS_770_60406a14_273	RP	POS	14.27	770.6041				1.88E-01	0.22	0.43	1.05E-01	0.35	0.99	7.46E-02	0.40	0.64	7.87E-01	0.05	0.28	1197112	1237844	1576147	1836566	1277649	1412594	1874646	2153491
HILIC_NEG_197_80779a0_882	HILIC	NEG	0.882	197.8078				3.01E-01	0.20	0.82	1.05E-01	0.33	1.11	1.03E-01	0.37	0.89	8.59E-01	0.04	0.09	969561	178726	1008257	193836	976823	183195	1039692	200835
HILIC_NEG_200_85893a7_101	HILIC	NEG	7.101	200.8589				5.04E-02	-0.33	0.75	1.05E-01	0.35	1.42	4.54E-01	-0.15	0.54	8.40E-03	-0.50	0.90	1819826	207535	1724135	312052	1673521	281201	1774749	335317
RP_POS_544_33746a10_501	RP	POS	10.50	544.3375				4.79E-03	0.54	1.04	1.05E-01	0.33	1.05	1.57E-03	0.71	1.21	6.66E-02	0.38	0.85	5894190	1936410	7086906	2196091	6730846	2052775	7442966	2295962
RP_POS_1001_65619a10_623	RP	POS	10.62	1001.6562				2.67E-03	0.56	1.39	1.05E-01	0.33	1.45	2.39E-03	0.72	1.27	2.91E-02	0.39	1.21	2806705	2110853	4229091	2605290	3805581	1730869	4652601	3217397
HILIC_NEG_188_94977a1_307	HILIC	NEG	1.307	188.9498				5.47E-04	0.59	1.18	1.05E-01	0.34	1.11	3.71E-04	0.76	1.21	2.18E-02	0.42	0.82	15857381	4316428	19414131	6230295	18404043	5479503	20424219	6805746
RP_POS_450_16068a0_708	RP	POS	0.71	450.1607				1.73E-01	0.18	0.49	1.05E-01	0.37	1.06	7.13E-02	0.36	0.68	9.84E-01	0.00	0.52	987667	263061	1111617	775887	985734	604909	1237500	904452
HILIC_NEG_153_86874a7_679	HILIC	NEG	7.679	153.8687				7.13E-01	0.07	0.18	1.06E-01	0.33	0.91	3.08E-01	0.24	0.43	6.89E-01	-0.09	0.15	1666598	445767	1700152	450375	1627169	414733	1773135	476383
RP_POS_233_07869a6_516	RP	POS	6.52	233.0787	Sinapyl alcohol [M+Na]+	233.0768(100)	3	1.01E-02	0.34	0.78	1.06E-01	-0.36	0.97	2.17E-01	0.16	0.54	1.33E-02	0.52	0.88	1156812	3953516	4709821	11671789	6604771	14265482	2814870	8025542
RP_POS_448_88812a0_496	RP	POS	0.50	448.8881				4.52E-09	-0.74	1.33	1.06E-01	0.35	1.31	4.60E-04	-0.56	1.25	7.49E-07	-0.91	1.58	2127059	113853	1797298	482494	1719158	498606	1875439	457475
RP_POS_280_06039a1_587	RP	POS	1.59	280.0604				7.20E-02	0.22	0.77	1.06E-01	0.37	1.06	5.99E-02	0.40	0.72	7.35E-01	0.03	0.44	1448099	511614	1943140	2573050	1525229	1469067	2361050	3295710
RP_POS_221_0247a0_547	RP	POS	0.55	221.0247				1.56E-03	-0.38	1.07	1.06E-01	0.37	1.31	2.76E-01	-0.20	0.96	1.51E-04	-0.57	1.43	1028607	88103	860930	493541	781053	415955	940806	553261
RP_POS_658_83557a0_494	RP	POS	0.49	658.8356				2.42E-09	-0.77	1.36	1.06E-01	0.35	1.32	3.55E-04	-0.60	1.26	2.40E-07	-0.94	1.60	2734629	288329	2000374	1024258	1834729	1031718	2166018	999590
RP_NEG_539_25092a7_183	RP	NEG	7.18	539.2509				4.76E-01	-0.14	0.59	1.06E-01	-0.33	1.09	1.94E-01	-0.30	0.63	8.70E-01	0.03	0.43	1569761	641549	1472518	743839	1592938	590813	1352098	859785
HILIC_NEG_186_04558a1_298	HILIC	NEG	1.298	186.0456				1.71E-13	1.01	1.63	1.06E-01	0.33	0.96	4.70E-09	1.17	1.79	6.92E-08	0.84	1.71	2383530	984801	4979137	2618933	4555534	2241558	5402739	2909778
RP_POS_385_29352a10_537	RP	POS	10.54	385.2935				8.98E-01	-0.03	0.55	1.07E-01	0.32	0.99	5.60E-01	0.13	0.54	4.44E-01	-0.19	0.61	8370610	1555655	8330589	1437563	8098235	1569547	8562943	1265579
RP_POS_555_85974a11_107	RP	POS	11.11	555.8597				6.78E-08	0.65	1.33	1.07E-01	-0.36	1.35	1.90E-04	0.47	1.39	5.36E-05	0.82	1.43	51670	32160	518235	798103	647338	951124	389133	590157
RP_POS_295_22424a10_136	RP	POS	10.14	295.2242				7.68E-02	-0.28	0.68	1.07E-01	-0.35	1.29	2.56E-02	-0.46	0.98	5.57E-01	-0.10	0.71	3852876	341199	3703042	580264	3796762	521240	3609323	625035
RP_POS_536_32458a11_113	RP	POS	11.11	536.3246				3.44E-07	0.61	1.30	1.07E-01	-0.36	1.36	5.68E-04	0.43	1.35	1.12E-04	0.79	1.41	72393	46211	1392837	2414639	1783024	2878926	1002650	1783544
RP_POS_338_198a10_867	RP	POS	10.87	338.1980				4.87E-02	0.32	1.26	1.07E-01	-0.35	0.99	4.65E-01	0.14	0.87	9.79E-03	0.49	1.29	1785414	370137	1963391	603515	2060715	571791	1866066	624194
RP_POS_517_37042a10_461	RP	POS	10.46	517.3704				9.09E-01	0.02	0.49	1.07E-01	0.34	0.96	3.78E-01	0.19	0.49	4.88E-01	-0.15	0.50	19450963	1038683	19476328	1245877	19275538	1218762	19677118	1252373
HILIC_POS_171_18547a5_647	HILIC	POS	5.647	171.1855				4.26E-02	-0.37	1.07	1.08E-01	0.33	1.52	3.56E-01	-0.21	0.70	5.86E-03	-0.54	1.60	224184131	17263737	216488245	21250822	213061843	17229178	219914647	24322971
RP_POS_496_33978a10_646	RP	POS	10.65	496.3398				4.50E-05	0.65	1.31	1.08E-01	-0.34	1.00	7.30E-03	0.48	1.08	5.21E-05	0.82	1.50	10234301	11289764	22075214	19074233	25147330	20196079	19003097	17548081
RP_POS_582_36597a11_116	RP	POS	11.12	582.3660				5.11E-07	0.60	1.28	1.08E-01	-0.36	1.35	1.15E-03	0.42	1.30	1.01E-04	0.78	1.41	127691	58370	554534	789218	681787	923794	427281	609917
RP_POS_472_30124a11_141	RP	POS	11.14	472.3012				1.76E-06	0.57	1.21	1.08E-01	-0.36	1.31	4.28E-03	0.39	1.16	1.28E-04	0.75	1.39	43624	20328	405614	711619	520262	809964	290966	583329
HILIC_POS_305_19666a1_431	HILIC	POS	1.431	305.1967				8.32E-02	-0.42	0.82	1.08E-01	-0.29	0.92	2.60E-02	-0.57	1.05	2.88E-01	-0.28	0.44	510884	391506	378473	277795	423191	308009	333754	238671
RP_POS_1069_71533a10_932	RP	POS	10.93	1069.7153				2.82E-02	-0.52	1.25	1.08E-01	-0.29	1.60	8.89E-03	-0.67	1.22	1.34E-01	-0.38	1.03	5500305	2642197	4345828	2001128	4667661	2007644	4023995	1961819
RP_POS_168_00821a15_616	RP	POS	15.62	168.0082				2.38E-01	0.27	0.64	1.08E-01	0.30	1.05	9.51E-02	0.42	0.66	6.15E-01	0.12	0.70	13702671	2494703	14281008	1979330	13962829	1865326	14599188	2056549
RP_POS_677_90826a10_921	RP	POS	10.92	677.9083				1.43E-01	0.19	0.89	1.08E-01	-0.37	1.22	9.74E-01	0.00	0.73	8.40E-02	0.37	0.98	814160	133662	892479	476036	969238	600522	815721	291880

Supplementary table 1: Metabolomics results (in asceding order according to p-value from progressive ALD vs non-progressive ALD comparison, with molecular features with ID_level of 1-2 first)

								all_ALD_vs_control			Prog_ALD_vs_non-prog_ALD			Prog_ALD_vs_control_ALD			Non-prog_ALD_vs_control			Healthy_control		all_ALD		Non-prog_ALD		Progressive_ALD	
								t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA								
Feature_ID	RP_HILIC	POS_NEG	Average.Rt	Average.Mz	Metabolite.name	curated_MSMS	ID_level	p	d	VIP	p	d	VIP	p	d	VIP	p	d	VIP	Mean	SD	Mean	SD	Mean	SD	Mean	SD
RP_NEG_524_33661a10_699	RP	NEG	10.70	524.3366				3.91E-02	-0.47	1.06	1.08E-01	-0.30	1.71	1.31E-02	-0.62	1.14	1.82E-01	-0.32	0.86	9585661	3132750	8287877	2573437	8701429	2455992	7874325	2645634
HILIC_POS_207_14926a0_708	HILIC	POS	0.708	207.1493				1.58E-02	-0.84	1.77	1.08E-01	0.08	1.24	2.19E-02	-0.80	1.21	1.17E-02	-0.88	1.50	2872705	5587394	345738	772785	221118	466862	470358	978226
RP_POS_375_22675a11_049	RP	POS	11.05	375.2268				3.13E-09	0.85	1.81	1.08E-01	0.33	1.11	4.00E-07	1.02	1.78	2.24E-05	0.68	1.70	625611	347128	1259876	774749	1135323	670245	1384429	855473
HILIC_POS_118_65576a3_718	HILIC	POS	3.718	118.6558				8.36E-02	0.29	0.62	1.09E-01	0.34	1.00	4.80E-02	0.46	0.81	4.48E-01	0.12	0.57	911593	833449	1249259	1241385	1049098	730900	1449419	1580362
HILIC_POS_675_54272a0_912	HILIC	POS	0.912	675.5427				7.31E-01	-0.06	0.28	1.09E-01	0.34	0.97	6.14E-01	0.11	0.27	2.76E-01	-0.23	0.47	891096	318800	867345	395587	803806	397662	930884	387037
RP_POS_360_08688a6_516	RP	POS	6.52	360.0869				8.56E-03	0.35	0.80	1.09E-01	-0.36	0.97	1.94E-01	0.17	0.56	1.18E-02	0.53	0.90	119387	404535	483633	1161703	670561	1412623	296704	812302
RP_POS_545_40076a10_878	RP	POS	10.88	545.4008				4.82E-01	-0.16	0.70	1.09E-01	0.30	1.45	9.74E-01	-0.01	0.67	2.23E-01	-0.31	0.73	23173273	1449003	22972852	1188787	22781908	1331003	23163795	1004636
HILIC_POS_147_14906a5_856	HILIC	POS	5.856	147.1491				6.37E-01	0.10	0.39	1.09E-01	0.32	1.05	2.92E-01	0.26	0.57	7.48E-01	-0.07	0.35	55612486	53867460	60828521	54875956	52007982	41437779	69649061	64871633
HILIC_NEG_197_80795a4_003	HILIC	NEG	4.003	197.8080				2.24E-01	0.21	0.77	1.09E-01	-0.34	1.16	8.54E-01	0.04	0.27	5.39E-02	0.38	1.05	726060	660353	909259	933375	1059040	875229	759478	973832
RP_NEG_251_092a7_386	RP	NEG	7.39	251.0920				8.74E-01	-0.03	0.39	1.09E-01	-0.33	0.98	3.77E-01	-0.19	0.38	5.58E-01	0.13	0.41	607271	30059	606280	31971	611408	32480	601152	30929
RP_POS_346_00806a0_743	RP	POS	0.74	346.0081				2.90E-02	-0.38	1.00	1.10E-01	0.34	1.39	3.01E-01	-0.21	0.94	6.29E-03	-0.55	1.09	23739514	10575179	18458768	14572699	16124518	13885693	20793018	15004291
HILIC_NEG_134_89471a4_07	HILIC	NEG	4.07	134.8947				1.54E-01	-0.32	0.97	1.10E-01	0.30	1.31	4.78E-01	-0.17	0.35	5.27E-02	-0.48	1.13	21863024	10881315	18788428	8897383	17364497	8551892	20212358	9092285
RP_POS_919_54797a10_838	RP	POS	10.84	919.5480				3.47E-06	0.56	1.18	1.10E-01	-0.36	1.31	1.44E-03	0.38	1.25	3.76E-04	0.74	1.33	529451	110023	1000509	942061	1151586	1145566	849432	658914
RP_POS_594_41913a10_832	RP	POS	10.83	594.4191				1.20E-10	1.18	2.02	1.10E-01	0.29	1.51	5.71E-10	1.33	2.10	4.38E-08	1.04	1.94	189834	151912	442709	194335	411607	171903	473810	211608
RP_POS_633_40338a15_1	RP	POS	15.10	633.4034				1.73E-01	0.28	0.65	1.10E-01	-0.32	0.96	6.19E-01	0.12	0.26	4.40E-02	0.44	0.82	4350292	1305794	4718589	1332497	4931861	1153766	4505316	1470827
HILIC_NEG_199_80501a4_007	HILIC	NEG	4.007	199.8050				1.81E-01	0.23	0.91	1.10E-01	-0.34	1.10	7.68E-01	0.06	0.27	4.81E-02	0.40	1.16	329270	319805	427261	454481	499937	448955	354585	452750
RP_POS_1076_79224a0_49	RP	POS	0.49	1076.7922				2.66E-06	0.57	1.11	1.10E-01	-0.35	1.19	1.66E-02	0.40	0.92	1.63E-05	0.75	1.47	2214488	120126	2572487	692726	2683240	683352	2461734	691035
RP_NEG_481_28101a9_356	RP	NEG	9.36	481.2810				8.06E-03	0.31	0.52	1.11E-01	0.37	0.96	2.87E-02	0.49	0.74	3.70E-02	0.13	0.66	1174364	1128661	5484751	15823248	2941011	5671407	8028491	21459028
RP_POS_281_24756a9_997	RP	POS	10.00	281.2476				3.62E-07	0.77	1.46	1.11E-01	0.33	1.45	1.72E-05	0.93	1.46	5.88E-05	0.60	1.58	991069	494184	1698590	964960	1544211	682916	1852969	1168883
RP_POS_553_45825a13_806	RP	POS	13.81	553.4583				6.89E-03	-0.60	1.09	1.11E-01	-0.30	0.94	1.95E-03	-0.75	1.20	5.60E-02	-0.45	1.05	14623239	2555892	13201447	2207487	13553771	2201177	12849123	2178747
RP_POS_577_87262a11_102	RP	POS	11.10	577.8726				7.25E-07	0.59	1.28	1.11E-01	-0.36	1.34	9.99E-04	0.41	1.32	1.50E-04	0.77	1.39	81595	39735	478161	746831	597426	886582	358895	558426
RP_POS_273_05969a7_721	RP	POS	7.72	273.0597				6.78E-01	0.06	0.65	1.11E-01	0.36	1.17	3.00E-01	0.24	0.86	1.92E-01	-0.13	0.90	23348290	20731570	26197901	57813256	16922804	22734198	35472997	77849514
RP_POS_715_5744a12_604	RP	POS	12.60	715.5744				4.99E-12	-1.56	2.66	1.12E-01	-0.22	0.94	7.31E-13	-1.67	2.62	1.05E-10	-1.44	2.32	869544	290071	344980	237896	382877	246229	307082	225353
RP_POS_468_35709a11_238	RP	POS	11.24	468.3571				3.52E-01	-0.17	0.69	1.12E-01	-0.33	1.08	1.24E-01	-0.34	0.73	9.73E-01	-0.01	0.18	2114142	801859	1952829	972405	2107725	893951	1797932	1030693
RP_NEG_929_10693a9_374	RP	NEG	9.37	929.1069				4.98E-01	-0.14	0.39	1.12E-01	-0.32	1.07	1.82E-01	-0.30	0.59	9.14E-01	0.02	0.28	1469982	124205	1452620	128641	1473105	131823	1432134	123293
RP_POS_599_46405a11_609	RP	POS	11.61	599.4641				4.88E-01	-0.11	0.48	1.12E-01	-0.35	0.98	3.57E-02	-0.28	0.84	7.75E-01	0.07	0.53	1379211	1092386	1189560	1918036	1496370	2538261	882750	893269
RP_POS_293_20859a10_29	RP	POS	10.29	293.2086				6.26E-01	-0.09	0.81	1.12E-01	0.34	1.28	6.98E-01	0.08	0.66	1.93E-01	-0.25	0.76	2670722	335517	2634167	452111	2562247	406014	2706087	487419
RP_POS_237_14825a8_618	RP	POS	8.62	237.1483				2.32E-01	0.24	1.00	1.12E-01	0.32	1.08	1.09E-01	0.40	0.77	6.97E-01	0.07	0.61	742645	648056	904376	693667	793805	443506	1014947	866325
RP_POS_609_15997a9_21	RP	POS	9.21	609.1600				1.63E-03	-0.63	1.03	1.13E-01	-0.31	1.18	2.86E-04	-0.78	1.32	3.58E-02	-0.47	1.14	2116117	125005	2030622	133281	2051805	144157	2009439	119136
RP_POS_307_06067a8_02	RP	POS	8.02	307.0607	Unknown	73.0653(100), 307.1872(30)	4	7.53E-02	-0.28	0.79	1.13E-01	0.35	1.26	6.09E-01	-0.10	0.83	1.00E-02	-0.45	1.02	3431527	1709006	2665704	3001237	2188569	2558127	3142838	3345154
RP_POS_420_7645a13_998	RP	POS	14.00	420.7645				3.13E-01	-0.22	0.71	1.13E-01	0.31	1.06	7.85E-01	-0.06	0.77	1.18E-01	-0.37	0.69	15027476	3766680	14264563	3401040	13724864	3409893	14804261	3338922
RP_POS_632_37695a14_266	RP	POS	14.27	632.3770				5.17E-01	0.13	0.63	1.13E-01	-0.32	0.96	9.15E-01	-0.02	0.24	1.92E-01	0.29	0.51	1530722	470635	1593000	465719	1666899	432133	1519100	490235
HILIC_NEG_312_83682a5_419	HILIC	NEG	5.419	312.8368				9.68E-01	-0.01	0.15	1.13E-01	-0.32	1.30	4.46E-01	-0.17	0.41	5.15E-01	0.15	0.27	3370157	1061547	3361551	1077176	3532325	1146807	3190777	984689
RP_POS_304_23038a8_476	RP	POS	8.48	304.2304				2.43E-04	0.58	1.28	1.13E-01	0.34	0.96	5.03E-04	0.75	1.31	1.12E-02	0.42	0.99	685633	313528	979596	533337	894964	413455	1064229	623810
RP_NEG_630_3031a10_042	RP	NEG	10.04	630.3031				1.88E-02	0.40	0.91	1.14E-01	-0.34	0.95	2.53E-01	0.23	0.73	4.21E-03	0.57	1.17	815795	504043	1093945	740679	1211315	709317	976576	759712
HILIC_NEG_217_87839a0_882	HILIC	NEG	0.882	217.8784				9.42E-02	0.32	1.00	1.14E-01	0.32	1.15	3.28E-02	0.49	0.93	4.34E-01	0.16	0.35	649739	147253	702153	164602	676118	148983	728188	176525
RP_POS_788_60583a14_241	RP	POS	14.24	788.6058				2.45E-01	-0.24	0.60	1.14E-01	0.31	0.97	7.06E-01	-0.09	0.44	8.13E-02	-0.40	0.76	2232088	1528152	1870725	1460991	1639691	1392513	2101759	1504835
RP_POS_245_14952a4_597	RP	POS	4.60	245.1495				4.62E-06	0.55	1.13	1.14E-01	0.35	1.00	9.90E-04	0.73	1.14	3.05E-05	0.37	1.34	233210	180532	946115	1442586	716965	721719	1175265	1891174
RP_POS_417_24396a12_686	RP	POS	12.69	417.2440				2.76E-03	0.58	1.19	1.14E-01	-0.32	0.98	4.90E-02	0.42	0.88	7.36E-04	0.74	1.26	712952	304575	912725	344069	967104	338289	858345	344540
RP_POS_125_03907a15_514	RP	POS	15.51	125.0391				4.61E-01	-0.14	0.44	1.15E-01	0.33	0.94	8.98E-01	0.03	0.34	1.89E-01	-0.30	0.54	14902573	1863810	14608517	2200533	14260788	2514291	14956245	1793066
HILIC_NEG_112_9857a2_171	HILIC	NEG	2.171	112.9857				6.12E-01	0.10	0.38	1.15E-01	0.32	1.17	2.43E-01	0.26	0.48	8.03E-01	-0.06	0.48	3930556	1198134	4055348	1228689	3861443	1248000	4249253	1189928
RP_NEG_714_84039a0_495	RP	NEG	0.50	714.8404				1.01E-07	-0.73	1.30	1.15E-01	0.34	1.30	2.15E-03	-0.57	1.14	1.77E-07	-0.90	1.58	2380546	229585	1977972	584967	1885661	532876	2070282	624506
HILIC_POS_235_18036a0_535	HILIC	POS	0.535	235.1804				1.39E-02	-0.88	1.77	1.15E-01	0.00	0.92	1.41E-02	-0.88	1.32	1.37E-02	-0.88	1.41	33006849	71409518	84725	459935	11593	35248	157857	644392
RP_NEG_240_97899a6_484	RP	NEG	6.48	240.9790				1.13E-01	0.18	0.73	1.16E-01	-0.36	0.99	1.81E-01	0.00	0.80	1.15E-01	0.37	0.72	44592	19592	2831971	17444377	5604450	24477141	59493	73861
RP_NEG_637_14557a9_481	RP	NEG	9.48	637.1456				8.37E-01	-0.04	0.50	1.16E-01	-0.31	1.02	3.71E-01	-0.20	0.45	6.25E-01	0.11	0.53	6927991	420896	6910437	412869	6975487	438645	6845386	378623
RP_NEG_371_22076a10_941	RP	NEG	10.94	371.2208				2.34E-07	0.88	1.69	1.16E-01	0.31	1.00	7.85E-07	1.04	1.74	7.65E-05	0.72	1.57	1673088	762817	2669430	1126729	2491884	1005640	2846976	1220369
HILIC_NEG_113_9261a5_424	HILIC	NEG	5.424	113.9261				1.51E-01	0.27	0.77	1.16E-01	-0.32	1.01	6.10E-01	0.11	0.18	4.31E-02	0.43	1.10	3303838	702460	3520038	817824	3648744	794744	3391332	828190
RP_POS_166_98488a10_776	RP	POS	10.78	166.9849				8.30E-01	-0.05	0.55	1.16E-01	0.30	1.00	6.98E-01	0.10	0.50	4.15E-01	-0.20	0.56	14631387	6529640	14358015	5206467	13538658	4683002	15177372	5609564
RP_POS_617_47437a11_256	RP	POS	11.26	617.4744				8.55E-01	0.03	0.46	1.16E-01	-0.34	1.05	4.27E-01	-0.14	0.51	3.80E-01	0.20	0.74	1450735	1401467	1509102	1984468	1821856	2398162	1196348	1416261
RP_POS_387_18262a11_049	RP	POS	11.05	387.1826				3.84E-09	0.83	1.77	1.16E-01	0.33	1.08	3.74E-07	1.00	1.77	4.69E-05	0.67	1.65	1161082	652114	2376282	1523692	2136606	1372079	2615959	1640372
HILIC_POS_240_10188a1_756	HILIC	POS	1.756	240.1019				4.75E-01	-0.16	0.26	1.17E-01	-0.30	0.89	1.85E-01	-0.31	0.53	9.82E-01	-0.01	0.01	1986892	1045798	1838364	910772	1981549	990753	1695179	807779
RP_NEG_199_80457a1_457	RP	NEG	1.46	199.8046				4.93E-01	0.13	0.47	1.17E-01	-0.33	0.98	8.53E-01	-0.04	0.40	1.66E-01	0.29	0.60	8816352	2741794	9225380	3415146	9762049	3325647	8688710	3452066
RP_POS_149_01227a15_342	RP	POS	15.34	149.0123				8.61E-01	-0.04	0.65	1.17E-01	-0.31	0.96	3.86E-01	-0.19	0.67	6.16E-01	0.12	0.90	190942748	71086866	188413996	68666645	199205112	74656486	177622879	60952461
RP_POS_780_58868a13_637	RP	POS	13.64	780.5887				1.15E-02	-0.52	0.86	1.17E-01	-0.31	0.96	2.45E-03	-0.67	1.20	1.14E-01	-0.36	0.58	1714592	675559	1354250	683792	1461615	733546	1246885	618928
RP_POS_121_0172a15_338	RP	POS	15.34	121.0172				2.21E-01	-0.29	1.15	1.17E-01	0.29	0.94	5.63E-01	-0.15	0.87	8.68E-02	-0.43	0.94	2907504	1260011	2606612	948462	2457805	914453	2755419	967526
RP_POS_365_23203a7_183	RP	POS	7.18	365.2320				4.86E-01	-0.13	0.51	1.17E-01	-0.33	1.06	2.04E-01	-0.29	0.58	8.65E-01	0.03	0.33	721991	285143	679410	339944	732784	271696	626037	392238
RP_POS_165_05441a0_709	RP	POS	0.71	165.0544				3.77E-01	0.15	0.91	1.18E-01	0.34	1.07	1.47E-01	0.32	1.16	9.29E-01	-0.02	0.56	12752949	2829112	13323843	4025904	12692267	3273356	13955419	4606264
RP_POS_505_27695a9_335	RP	POS	9.34	505.2770				1.36E-02	0.29	0.49	1.18E-01	0.36	0.94	3.93E-02	0.47	0.70	4.18E-02	0.11	0.65	481550	495811	2646755	8576514	1293059	2681531	4000452	11733880
RP_POS_366_06021a0_734	RP	POS	0.73	366.0602				1.44E-06	0.59	1.00	1.18E-01	0.35	0.94	1.44E-04	0.76	1.22	1.83E-03	0.41	1.02	321268	194086	929062	1144731	749488	893058	1108636	1335739
RP_POS_512_33429a10_088	RP	POS	10.09	512.3343				6.01E-01	0.10	1.43	1.18E-01	-0.32	1.07	7.77E-01	-0.06	0.85	2.32E-01	0.26	1.51	5258756	1793077	5456838	2038202	5775968	2040387	5137708	2005565
RP_POS_348_28976a11_049	RP	POS	11.05	348.2898				9.74E-10	0.84	1.75	1.18E-01	0.33	1.08	4.87E-07	1.01	1.74	1.45E-05	0.68	1.64	1151556	608729	2408167	1565802	2163000	1338185	2653335	1743589
RP_POS_122_97486a15_402	RP	POS	15.40	122.9749				3.08E-01	-0.24	0.56	1.18E-01	0.29	1.47	7.25E-01	-0.09	0.63	1.19E-01	-0.38	0.80	10217472	5164521	9184835	4114393	8541253	3786455	9828417	4361122
RP_POS_318_909a15_426	RP	POS	15.43	318.9090				7.60E-01	0.07	0.55	1.19E-01	-0.31	0.95	7.28E-01	-0.09	0.43	3.25E-01	0.22	0.44	9452675	1066990	9517832	965840	9668971	771234	9366693	1115039
RP_POS_301_07391a7_589	RP	POS	7.59	301.0739				2.69E-01	0.15	0.62	1.19E-01	0.36	1.14	1.64E-01	0.32	0.82	6.94E-01	-0.03	0.65	1632445	2180805	2470193	6494096	1447682	1872862	3492703	8919972
RP_POS_478_3884a13_641	RP	POS	13.64	478.3884				2.12E-03	-0.60	1.34	1.19E-01	0.31	1.59	2.19E-02	-0.44	1.03	1.55E-03	-0.76	1.46	7344531	996452	6675027	1106985	6501729	1322560	6848325	815710
HILIC_POS_176_12823a4_066	HILIC	POS	4.066	176.1282				6.94E-05	0.60	0.98	1.19E-01	0.33	1.08	1.65E-04	0.77	1.25	9.72E-03	0.43	0.88	1748379	682772	2490651	1322275	2283937	1146636	2697365	1459633
RP_NEG_311_16968a10_423	RP	NEG	10.42	311.1697				8.94E-01	-0.03	0.39	1.19E-01	0.30	0.94	6.22E-01	0.12	0.23	4.64E-01	-0.18	0.39	11022779	5893225	10867879	4948067	10094915	4982408	11640842	4839698
RP_NEG_1091_72742a10_933	RP	NEG	10.93	1091.7274				4.82E-02	-0.48	1.18	1.19E-01	-0.28	1.58	1.89E-02	-0.62	1.13	1.73E-01	-0.34	0.96	10212491	4328049	8532887	3087939	9014539	2866276	8051236	3252131
RP_POS_583_38617a14_266	RP	POS	14.27	583.3862				3.83E-02	-0.46	0.96	1.20E-01	-0.29	1.24	1.22E-02	-0.61	1.28	1.89E-01	-0.31	0.62	3164496	924592	2776776	798133	2901156	794995	2652396	789585
HILIC_POS_229_155a4_222	HILIC	POS	4.222	229.1550				3.78E-01	0.14	0.82	1.20E-01	0.34	1.19	1.67E-01	0.31	0.52	8.40E-01	-0.03	0.74	8512185	2388731	9031782	4063218	8397133	2690035	9666430	5029724
RP_POS_793_55914a12_82	RP	POS	12.82	793.5591				1.57E-06	-1.21	1.97	1.20E-01	-0.23	0.96	4.15E-07	-1.33	2.02	1.59E-05	-1.10	1.65	2398098	1185076	1139850	772923	1260191	790652	1019509	743187
RP_POS_534_31653a10_088	RP	POS	10.09	534.3165				4.38E-01	0.15	1.42	1.20E-01	-0.32	1.03	9.51E-01	-0.01	0.84	1.55E-01	0.31	1.52	819560	295308	868253	341197	921326	338570	815179	338863
RP_POS_322_67517a10_931	RP	POS	10.93	322.6752				3.69E-03	-0.67	1.59	1.21E-01	-0.28	1.62	1.22E-03	-0.81	1.56	2.76E-02	-0.53	1.27	1242357	335847	1042594	268755	1084355	259156	1000834	274248
HILIC_POS_162_05009a4_852	HILIC	POS	4.852	162.0501				8.17E-01	-0.04	0.91	1.21E-01	-0.33	1.05	3.25E-01	-0.21	0.79	5.73E-01	0.12	0.59	2543862	547556	2516412	676848	2621552	689320	2411272	654121
RP_POS_884_16089a0_484	RP	POS	0.48	884.1609				4.93E-05	0.49	0.95	1.21E-01	-0.35	1.10	5.78E-02	0.32	0.75	9.07E-05	0.67	1.34	278444	28901	357030	179046	384840	173883	329220	181535
HILIC_POS_480_34457a1_11	HILIC	POS	1.11	480.3446				2.47E-01	-0.26	0.72	1.21E-01	-0.29	1.12	1.01E-01	-0.41	0.64	6.28E-01	-0.12	0.19	4720347	1961947	4272079	1601963	4520890	1529435	4023268	1649070
RP_POS_172_13307a10_38	RP	POS	10.38	172.1331				3.45E-01	-0.19	0.81	1.21E-01	0.31	0.96	8.92E-01	-0.03	0.59	9.92E-02	-0.35	0.93	11801318	799621	11645030	833786	11515451	675844	11774608	955799
HILIC_NEG_244_98708a6_093	HILIC	NEG	6.093	244.9871				9.49E-01	0.01	0.77	1.22E-01	-0.33	1.03	4.21E-01	-0.16	0.48	3.80E-01	0.18	1.01	222012	80076	223201	120656	241879	123767	204523	115682
RP_POS_816_42133a7_549	RP	POS	7.55	816.4213				5.52E-01	-0.13	0.77	1.22E-01	0.30	1.04	9.35E-01	0.02	0.63	2.47E-01	-0.28	0.77	919781	71081	911377	62409	901722	63378	921033	60515
RP_POS_513_84448a14_671	RP	POS	14.67	513.8445				5.27E-01	0.10	0.81	1.23E-01	0.34	1.02	2.58E-01	0.27	0.66	6.29E-01	-0.07	0.49	223890	340002	275301	542523	190911	223492	359690	728140
RP_POS_585_27002a11_94	RP	POS	11.94	585.2700				3.33E-01	-0.18	0.71	1.23E-01	0.32	1.30	9.25E-01	-0.02	0.43	4.78E-02	-0.34	0.98	1167939	1471567	864469	1699525	600136	696101	1128801	2282227
RP_POS_352_24469a10_271	RP	POS	10.27	352.2447				7.06E-01	-0.07	1.00	1.23E-01	0.33	1.01	6.87E-01	0.09	0.85	2.10E-01	-0.23	0.76	12371775	874152	12299938	1098890	12129848	791998	12470027	1324182
RP_POS_166_98485a11_212	RP	POS	11.21	166.9849				5.17E-03	-0.52	1.10	1.23E-01	-0.31	0.99	2.29E-03	-0.68	1.20	6.90E-02	-0.36	1.29	14125127	1025448	13486813	1252658	13680293	1122159	13293332	1354508
HILIC_NEG_161_98665a0_546	HILIC	NEG	0.546	161.9867				4.37E-01	0.13	0.32	1.23E-01	0.34	1.25	2.18E-01	0.30	0.52	7.81E-01	-0.04	0.12	709323	660310	830391	1019729	672101	454179	988681	1357756
HILIC_POS_64_01662a0_709	HILIC	POS	0.709	64.0166				1.07E-06	0.74	1.30	1.23E-01	0.32	1.39	1.38E-05	0.91	1.52	3.53E-04	0.58	1.27	670463	324186	1105177	609687	1010972	501843	1199382	693589
RP_NEG_676_30573a10_537	RP	NEG	10.54	676.3057				3.16E-02	-0.40	0.82	1.23E-01	-0.32	0.95	9.02E-03	-0.55	1.04	2.57E-01	-0.24	0.53	1906713	111092	1853961	137975	1875260	136620	1832662	137374
RP_POS_206_89355a0_519	RP	POS	0.52	206.8936				8.63E-01	0.03	0.30	1.23E-01	-0.31	1.04	5.78E-01	-0.12	0.34	4.01E-01	0.19	0.48	1297026	612106	1318822	643141	1418095	662787	1219549	613435
RP_POS_547_36115a10_678	RP	POS	10.68	547.3612				4.71E-01	-0.16	0.73	1.23E-01	0.30	1.12	9.84E-01	-0.01	0.15	1.62E-01	-0.31	1.09	3689349	1482321	3475262	1340362	3268043	978255	3682481	1607853

Supplementary table 1: Metabolomics results (in asceding order according to p-value from progressive ALD vs non-progressive ALD comparison, with molecular features with ID_level of 1-2 first)

								all_ALD_vs_control			Prog_ALD_vs_non-prog_ALD			Prog_ALD_vs_control_ALD			Non-prog_ALD_vs_control			Healthy_control		all_ALD		Non-prog_ALD		Progressive_ALD	
								t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA								
Feature_ID	RP_HILIC	POS_NEG	Average.Rt	Average.Mz	Metabolite.name	curated_MSMS	ID_level	p	d	VIP	p	d	VIP	p	d	VIP	p	d	VIP	Mean	SD	Mean	SD	Mean	SD	Mean	SD
HILIC_POS_229_15433a4_787	HILIC	POS	4.787	229.1543				7.88E-01	0.05	0.81	1.24E-01	0.33	1.18	3.67E-01	0.21	0.32	4.47E-01	-0.12	1.05	5307916	1541436	5403112	2247739	5055329	1316525	5750894	2868395
RP_POS_558_33771a11_107	RP	POS	11.11	558.3377				2.83E-07	0.61	1.31	1.24E-01	-0.34	1.34	4.69E-04	0.44	1.36	1.12E-04	0.78	1.41	75788	58254	1440719	2474884	1822793	2940285	1058646	1852541
HILIC_POS_258_0119a0_541	HILIC	POS	0.541	258.0119				4.15E-01	-0.11	0.77	1.24E-01	0.35	0.98	7.57E-01	0.06	0.33	5.41E-02	-0.28	1.56	98698064	12746501	95423695	33132773	90312409	25787837	100534981	38725130
RP_POS_586_30743a10_504	RP	POS	10.50	586.3074				1.58E-01	0.29	0.72	1.24E-01	-0.31	0.93	5.33E-01	0.14	0.57	5.77E-02	0.44	0.82	3867085	1008154	4159591	994886	4312863	1038330	4006319	934733
HILIC_NEG_59_01299a0_701	HILIC	NEG	0.701	59.0130				4.93E-04	0.41	0.84	1.24E-01	0.35	1.26	1.01E-02	0.59	0.84	2.58E-05	0.24	1.35	468062	246056	1316304	2318313	956685	698787	1675923	3179089
HILIC_NEG_100_93345a1_051	HILIC	NEG	1.051	100.9335				2.31E-02	0.42	1.02	1.24E-01	0.32	1.12	6.53E-03	0.58	1.32	2.16E-01	0.26	0.44	13905230	4853127	16352044	6075711	15416294	6040369	17287794	6025681
RP_POS_272_18582a7_728	RP	POS	7.73	272.1858				1.77E-05	-0.65	1.17	1.24E-01	-0.33	1.21	1.60E-04	-0.82	1.43	1.37E-03	-0.49	1.03	6052530	359574	5632824	680543	5737810	497772	5527839	815757
RP_NEG_193_81508a15_583	RP	NEG	15.58	193.8151				6.90E-02	-0.37	0.70	1.24E-01	-0.31	0.99	1.71E-02	-0.52	1.02	3.54E-01	-0.21	0.38	1702188	67110	1676708	69120	1687354	74714	1666062	61962
RP_POS_633_25494a8_499	RP	POS	8.50	633.2549				8.86E-01	-0.02	0.65	1.24E-01	0.34	1.30	5.24E-01	0.15	0.54	2.10E-01	-0.19	0.74	2576715	1411292	2527597	2321786	2168983	1439462	2886212	2925216
HILIC_POS_154_09747a1_969	HILIC	POS	1.969	154.0975				3.22E-02	0.29	0.84	1.24E-01	-0.35	0.88	2.34E-01	0.12	0.65	4.44E-02	0.46	0.94	361051	665532	828810	1811711	1109276	2438220	548343	725347
RP_POS_728_52191a12_215	RP	POS	12.22	728.5219				6.32E-02	0.33	0.82	1.25E-01	0.32	1.10	2.80E-02	0.49	0.89	3.77E-01	0.16	0.39	1023614	830164	1373968	1136400	1199035	932801	1548902	1294834
RP_POS_421_35245a10_708	RP	POS	10.71	421.3525				8.69E-01	-0.03	0.56	1.25E-01	-0.32	0.97	3.81E-01	-0.19	0.50	5.71E-01	0.13	0.44	7300226	596824	7279543	661257	7381212	675565	7177875	637152
RP_POS_485_81409a2_762	RP	POS	2.76	485.8141				3.16E-01	-0.24	0.47	1.25E-01	-0.28	1.24	1.19E-01	-0.38	0.68	7.01E-01	-0.10	0.39	1140209	1217081	904674	873789	1039266	1056722	770082	623669
RP_POS_271_24191a9_334	RP	POS	9.33	271.2419				1.29E-02	0.29	0.49	1.25E-01	0.35	0.92	3.95E-02	0.47	0.69	3.71E-02	0.11	0.66	420791	438798	2292526	7350750	1155584	2368438	3429467	10046006
RP_POS_210_01862a15_425	RP	POS	15.43	210.0186				7.64E-01	0.06	0.51	1.25E-01	-0.30	1.08	7.08E-01	-0.09	0.37	3.61E-01	0.22	0.82	1956754	523354	1988230	485504	2062811	486076	1913650	478139
HILIC_NEG_219_8756a0_881	HILIC	NEG	0.881	219.8756				1.15E-01	0.31	0.99	1.26E-01	0.31	1.14	4.10E-02	0.47	0.90	4.61E-01	0.16	0.34	205690	50564	222415	53870	214147	50099	230682	56690
HILIC_POS_146_11757a4_67	HILIC	POS	4.67	146.1176				5.67E-03	0.37	0.78	1.26E-01	0.34	1.19	9.84E-03	0.54	0.90	1.38E-01	0.20	0.56	700690	812802	1466362	2311427	1110999	1649394	1821725	2795748
HILIC_POS_178_05862a6_779	HILIC	POS	6.779	178.0586				4.96E-02	0.28	1.03	1.26E-01	-0.34	1.11	4.71E-01	0.11	1.02	2.80E-02	0.45	1.19	1085864	263719	1233826	582137	1323215	670997	1144438	467055
HILIC_POS_230_0956a5_436	HILIC	POS	5.436	230.0956				2.40E-02	0.40	0.91	1.26E-01	0.32	0.94	8.47E-03	0.56	1.12	2.27E-01	0.24	0.49	316289	439415	541762	592735	450834	555147	632691	620306
HILIC_POS_140_06812a5_459	HILIC	POS	5.459	140.0681				3.57E-01	0.17	0.38	1.26E-01	0.32	0.92	1.30E-01	0.33	0.72	9.41E-01	0.02	0.32	988014	94228	1006566	110211	989672	105024	1023461	113702
RP_POS_1074_69202a10_931	RP	POS	10.93	1074.6920				5.22E-03	-0.65	1.28	1.26E-01	-0.28	1.46	1.51E-03	-0.79	1.35	3.87E-02	-0.51	1.09	585895	321719	402635	255884	441859	264305	363411	243501
RP_POS_295_11246a7_093	RP	POS	7.09	295.1125				4.14E-01	0.16	0.64	1.26E-01	0.32	1.03	1.57E-01	0.31	0.65	9.89E-01	0.00	0.96	770225	57144	780147	65938	770045	62404	790248	68425
RP_POS_167_02266a15_338	RP	POS	15.34	167.0227				1.53E-01	-0.32	1.15	1.26E-01	0.29	1.01	4.69E-01	-0.18	0.89	5.55E-02	-0.47	0.99	23081470	9369949	20420012	7837976	19219431	7609152	21620592	7954915
HILIC_NEG_187_04176a1_299	HILIC	NEG	1.299	187.0418				4.30E-12	0.95	1.60	1.27E-01	0.31	0.96	2.28E-08	1.11	1.72	5.22E-07	0.80	1.60	9651460	4503715	20458260	11641575	18676425	10131887	22240095	12832918
RP_POS_353_24484a11_049	RP	POS	11.05	353.2448				7.29E-10	0.85	1.79	1.27E-01	0.32	1.08	4.38E-07	1.01	1.75	1.16E-05	0.69	1.70	6349153	3285919	13196411	8461521	11902115	7264203	14490708	9405765
RP_POS_614_33923a10_934	RP	POS	10.93	614.3392				3.18E-02	-0.48	1.19	1.27E-01	-0.29	1.49	1.05E-02	-0.62	1.16	1.60E-01	-0.33	0.99	2891669	728104	2575052	623451	2670335	617151	2479768	621217
HILIC_NEG_165_04167a0_799	HILIC	NEG	0.799	165.0417				1.59E-01	0.23	0.53	1.27E-01	-0.33	1.11	7.29E-01	0.07	0.12	5.07E-02	0.40	0.67	145353	149570	195685	235721	231697	244513	159673	223226
RP_NEG_355_26492a11_203	RP	NEG	11.20	355.2649	FA 24:6 (Tetracosahexaenoic acid)	355.2663(100), 116.9271(28), 99.9246(16)	3	8.63E-07	0.63	1.46	1.27E-01	0.34	0.94	1.95E-04	0.79	1.32	1.57E-04	0.46	1.45	538187	459315	1539125	1755425	1270313	1160426	1807936	2175285
RP_NEG_217_86539a15_575	RP	NEG	15.58	217.8654				3.47E-01	-0.20	0.47	1.27E-01	-0.30	1.27	1.36E-01	-0.35	0.68	8.38E-01	-0.05	0.35	1066200	269724	1014761	256532	1053938	252602	975584	256944
RP_POS_279_07339a15_387	RP	POS	15.39	279.0734				6.37E-01	0.09	0.36	1.27E-01	-0.31	1.02	7.41E-01	-0.07	0.16	2.86E-01	0.25	0.59	1930372	1035806	2033341	1170381	2212200	1326526	1854482	970866
RP_POS_1075_69495a10_932	RP	POS	10.93	1075.6950				1.50E-02	-0.61	1.27	1.28E-01	-0.26	1.47	5.29E-03	-0.74	1.27	6.57E-02	-0.48	1.03	660578	434923	451824	289571	496023	294199	407625	280844
HILIC_POS_203_1212a0_524	HILIC	POS	0.524	203.1212				2.85E-01	0.21	0.55	1.28E-01	-0.31	0.92	7.65E-01	0.06	0.14	1.39E-01	0.37	0.68	255082	222763	304542	234889	340481	292600	268602	152386
RP_POS_1017_68555a10_616	RP	POS	10.62	1017.6856				6.57E-03	0.53	1.29	1.28E-01	-0.30	1.25	8.98E-02	0.38	0.94	1.30E-03	0.69	1.39	1455219	883875	1974126	969663	2122096	864493	1826156	1052450
RP_POS_1045_62329a10_315	RP	POS	10.32	1045.6233				4.73E-02	0.36	0.99	1.28E-01	-0.32	1.14	3.51E-01	0.20	0.58	1.14E-02	0.51	1.07	3075367	1295286	3650171	1689215	3907572	1590415	3392770	1760822
RP_POS_499_43591a13_618	RP	POS	13.62	499.4359				3.39E-01	0.14	0.40	1.28E-01	0.34	1.01	1.60E-01	0.31	0.53	8.01E-01	-0.03	0.35	855914	117600	888125	263017	847939	168256	928311	328879
RP_POS_1046_84192a14_258	RP	POS	14.26	1046.8419				4.70E-01	0.14	0.35	1.28E-01	0.31	0.96	1.92E-01	0.30	0.75	9.59E-01	-0.01	0.33	496434	409593	557803	434292	491640	407617	623965	453854
HILIC_POS_394_31644a0_891	HILIC	POS	0.891	394.3164				8.42E-01	-0.04	0.62	1.29E-01	0.31	1.23	6.28E-01	0.12	0.19	3.53E-01	-0.19	0.38	2933879	679093	2905943	714667	2797041	588117	3014844	813534
RP_POS_329_24478a11_128	RP	POS	11.13	329.2448				1.66E-07	0.81	1.82	1.29E-01	0.31	1.16	1.83E-06	0.96	1.76	1.62E-04	0.65	1.69	1591385	849142	2812502	1561865	2574684	1398571	3050320	1690328
RP_NEG_426_96826a11_162	RP	NEG	11.16	426.9683				1.18E-01	0.26	0.92	1.29E-01	-0.32	0.93	5.97E-01	0.10	0.30	3.90E-02	0.43	1.21	21321867	6944365	23839041	10161224	25385449	10591367	22292633	9568211
RP_NEG_339_21582a10_713	RP	NEG	10.71	339.2158				2.23E-02	0.37	1.17	1.29E-01	0.33	1.15	1.40E-02	0.53	1.15	2.29E-01	0.20	1.09	1237623	165399	1331079	275503	1289114	217579	1373045	320028
RP_POS_416_26096a10_543	RP	POS	10.54	416.2610				1.09E-05	0.75	1.27	1.29E-01	-0.31	1.05	4.49E-03	0.59	1.02	1.41E-06	0.90	1.68	418321	210159	646114	310637	693407	262621	598822	348463
RP_NEG_177_95622a13_287	RP	NEG	13.29	177.9562				2.94E-01	-0.25	0.66	1.29E-01	0.27	1.04	6.61E-01	-0.12	0.37	1.19E-01	-0.39	0.90	926450	202821	885340	146140	863092	122741	907589	164543
RP_POS_1048_74414a0_493	RP	POS	0.49	1048.7441				4.24E-09	-0.78	1.33	1.29E-01	0.32	1.19	6.89E-04	-0.61	1.24	4.24E-08	-0.94	1.64	710637	87349	516158	267266	475501	245290	556816	284218
RP_NEG_556_32709a10_087	RP	NEG	10.09	556.3271				9.93E-01	0.00	1.31	1.29E-01	-0.31	1.07	4.71E-01	-0.16	0.87	4.91E-01	0.15	1.33	2768476	938137	2766769	1020949	2921972	1042704	2611567	984659
RP_POS_970_72034a0_498	RP	POS	0.50	970.7203				4.65E-01	0.14	0.92	1.29E-01	-0.31	1.34	9.28E-01	-0.02	0.67	1.86E-01	0.30	1.06	1325167	288488	1370043	335171	1420988	357800	1319099	306029
RP_POS_246_17001a2_848	RP	POS	2.85	246.1700				8.95E-02	0.31	0.62	1.29E-01	-0.32	1.16	4.60E-01	0.15	0.34	3.09E-02	0.47	0.84	1447610	760609	1733680	973682	1881614	1022371	1585747	908601
RP_POS_262_01337a1_462	RP	POS	1.46	262.0134				5.39E-04	0.41	0.75	1.30E-01	0.35	0.95	1.10E-02	0.58	0.85	3.87E-05	0.23	1.23	229287	418272	3313392	8593492	2000071	2736697	4626713	11755585
RP_POS_800_74994a0_499	RP	POS	0.50	800.7499				7.50E-01	0.06	0.57	1.30E-01	-0.31	1.16	7.04E-01	-0.09	0.28	3.26E-01	0.22	0.66	414499	212785	428399	216145	461185	201197	395613	227413
RP_NEG_613_40125a11_163	RP	NEG	11.16	613.4013				9.22E-03	0.43	1.07	1.30E-01	-0.32	1.40	1.63E-01	0.27	0.85	3.33E-03	0.59	1.30	1093480	84131	1146526	132166	1166566	134518	1126485	127975
RP_POS_388_71155a0_522	RP	POS	0.52	388.7116				9.56E-03	-0.43	0.89	1.30E-01	0.32	1.05	1.78E-01	-0.27	0.68	2.41E-03	-0.59	1.10	407463	78962	358259	122001	339760	116534	376758	125673
RP_POS_559_1311a10_529	RP	POS	10.53	559.1311				2.40E-01	-0.28	1.05	1.30E-01	0.28	0.90	5.82E-01	-0.14	0.64	9.30E-02	-0.42	0.99	375142	266829	314194	196330	284416	169550	343973	217534
HILIC_NEG_200_85863a4_682	HILIC	NEG	4.682	200.8586				5.67E-01	0.11	0.25	1.30E-01	0.32	1.09	2.47E-01	0.26	0.42	7.81E-01	-0.05	0.22	5627065	2575602	5946341	3179350	5464066	2596578	6428616	3633998
RP_POS_246_98045a15_564	RP	POS	15.56	246.9805				1.93E-01	-0.28	0.55	1.30E-01	0.30	1.10	5.90E-01	-0.13	0.30	5.99E-02	-0.43	0.92	2676959	105980	2649067	97698	2634254	84658	2663880	108026
RP_NEG_372_67331a15_575	RP	NEG	15.58	372.6733				2.24E-01	-0.26	0.70	1.30E-01	-0.30	1.08	8.32E-02	-0.41	0.84	6.44E-01	-0.11	0.40	620723	39988	610831	38186	616617	37525	605045	38336
RP_NEG_562_31647a10_041	RP	NEG	10.04	562.3165				2.25E-02	0.42	0.94	1.31E-01	-0.31	0.95	2.23E-01	0.26	0.71	4.67E-03	0.58	1.16	8359068	5906177	11336904	7294916	12442143	6573188	10231665	7862435
RP_NEG_631_24188a8_496	RP	NEG	8.50	631.2419				7.74E-01	-0.05	0.62	1.31E-01	0.33	1.30	6.14E-01	0.12	0.50	1.74E-01	-0.21	0.71	1332881	756377	1281655	1166249	1104450	694581	1458860	1483746
RP_POS_164_9845a11_213	RP	POS	11.21	164.9845				2.46E-04	-0.67	1.20	1.31E-01	-0.31	0.92	1.14E-04	-0.82	1.53	1.08E-02	-0.51	1.10	3476190	282111	3237044	363527	3292086	351473	3182002	370520
RP_POS_347_18799a11_159	RP	POS	11.16	347.1880				1.50E-01	-0.26	0.82	1.31E-01	0.32	1.16	6.29E-01	-0.10	0.61	4.98E-02	-0.42	0.87	1745887	118612	1707746	156683	1684031	161885	1731461	149149
HILIC_NEG_112_98563a1_307	HILIC	NEG	1.307	112.9856				1.11E-01	0.32	0.56	1.31E-01	-0.30	1.08	4.41E-01	0.17	0.39	3.98E-02	0.47	0.76	3189332	1177491	3581605	1234355	3768267	1286048	3394944	1163328
RP_NEG_284_22363a10_16	RP	NEG	10.16	284.2236				1.31E-02	0.47	0.94	1.31E-01	0.31	1.17	3.60E-03	0.62	1.13	1.40E-01	0.32	1.00	515587	144190	593840	169712	568179	172374	619501	164729
HILIC_POS_143_11786a2_425	HILIC	POS	2.425	143.1179				5.77E-04	0.50	1.05	1.31E-01	0.33	0.95	1.17E-03	0.67	1.25	3.33E-02	0.34	1.03	462650	353885	807816	746433	694890	615799	920743	848799
RP_NEG_293_87778a15_515	RP	NEG	15.52	293.8778				7.64E-01	-0.07	0.28	1.32E-01	0.28	1.07	7.79E-01	0.07	0.36	4.56E-01	-0.21	0.46	1227832	145831	1219416	105114	1203459	139818	1235374	47482
RP_NEG_896_565a13_427	RP	NEG	13.43	896.5650				7.53E-02	0.38	0.63	1.32E-01	-0.29	0.96	3.45E-01	0.23	0.59	1.75E-02	0.53	1.03	6074136	1379227	6574957	1286197	6769363	1020097	6380551	1491522
RP_NEG_378_77911a15_629	RP	NEG	15.63	378.7791				1.11E-01	-0.32	0.58	1.32E-01	-0.30	1.14	3.80E-02	-0.47	0.80	4.48E-01	-0.17	0.65	1734099	66606	1711889	70199	1722488	68025	1701290	71413
RP_NEG_251_09369a7_77	RP	NEG	7.77	251.0937				1.93E-02	-0.52	0.99	1.32E-01	0.28	1.14	1.09E-01	-0.38	0.71	6.44E-03	-0.66	1.07	2467366	126274	2407242	107946	2390945	107999	2423538	106474
RP_POS_183_0993a6_567	RP	POS	6.57	183.0993				4.52E-02	0.30	0.93	1.32E-01	0.33	1.13	4.39E-02	0.46	0.85	2.99E-01	0.13	1.14	580356	272102	727918	546662	645042	274943	810795	717053
RP_POS_387_25259a8_497	RP	POS	8.50	387.2526				9.28E-02	0.28	0.75	1.32E-01	0.32	1.02	4.45E-02	0.44	0.76	4.92E-01	0.12	0.60	512211	461159	694418	694307	589575	543678	799262	809903
RP_POS_547_38403a14_946	RP	POS	14.95	547.3840				8.98E-02	0.25	0.66	1.32E-01	0.33	0.95	3.74E-02	0.42	0.79	6.05E-01	0.09	0.30	2227926	355957	2389061	699869	2283458	610832	2494663	770556
HILIC_NEG_100_93343a6_101	HILIC	NEG	6.101	100.9334				6.37E-02	-0.29	0.94	1.32E-01	-0.33	1.08	2.70E-02	-0.45	0.72	4.75E-01	-0.12	0.42	34205396	3443073	32589458	6093402	33508651	5349414	31670264	6684032
RP_NEG_926_79022a0_491	RP	NEG	0.49	926.7902				6.24E-08	-0.71	1.33	1.32E-01	0.33	1.31	2.34E-03	-0.55	1.22	2.96E-07	-0.87	1.61	1483913	187898	1096807	586446	1008363	539978	1185251	622348
HILIC_POS_542_32349a1_137	HILIC	POS	1.137	542.3235				3.54E-01	-0.21	0.68	1.32E-01	-0.29	0.93	1.56E-01	-0.35	0.55	7.83E-01	-0.07	0.49	1840377	1228056	1616030	1015934	1769201	975625	1462860	1041913
RP_NEG_536_88458a0_496	RP	NEG	0.50	536.8846				3.13E-09	-0.77	1.34	1.33E-01	0.32	1.27	3.36E-04	-0.61	1.24	2.82E-07	-0.93	1.60	21619709	1266417	18530635	4307574	17881622	4301141	19179648	4257889
RP_NEG_321_20529a10_826	RP	NEG	10.83	321.2053				2.30E-11	1.13	1.98	1.33E-01	0.28	1.22	2.91E-10	1.27	2.11	9.85E-08	0.99	1.83	304365	270663	793639	408583	732157	389295	855122	421926
RP_POS_850_55292a13_727	RP	POS	13.73	850.5529				3.36E-01	0.18	0.36	1.33E-01	-0.31	1.18	9.06E-01	0.03	0.50	1.17E-01	0.34	0.61	7557736	2507809	8073505	2946860	8516877	2907967	7630132	2947497
HILIC_NEG_343_99533a6_273	HILIC	NEG	6.273	343.9953				5.42E-01	0.13	0.51	1.33E-01	-0.30	0.82	9.35E-01	-0.02	0.19	2.47E-01	0.28	0.47	19527385	6795514	20361220	6344628	21315235	6704218	19407205	5875896
HILIC_NEG_201_03835a1_301	HILIC	NEG	1.301	201.0384				9.51E-12	0.99	1.59	1.33E-01	0.30	0.93	7.15E-09	1.14	1.78	6.01E-07	0.83	1.61	714978	225516	1194583	490317	1120860	445328	1268306	525659
RP_POS_566_31891a10_305	RP	POS	10.31	566.3189				8.32E-03	0.57	1.04	1.34E-01	-0.29	1.24	7.76E-02	0.42	0.72	1.84E-03	0.71	1.21	22560481	6169032	25947312	5726917	26808114	4990243	25086510	6312666
RP_POS_409_26532a10_659	RP	POS	10.66	409.2653				5.94E-01	0.10	0.75	1.34E-01	-0.31	1.38	8.13E-01	-0.05	0.81	2.45E-01	0.26	0.67	1922537	752266	2006833	840175	2132950	853187	1880717	815969
RP_POS_451_3627a10_453	RP	POS	10.45	451.3627				1.81E-02	-0.48	0.85	1.34E-01	0.30	0.89	1.32E-01	-0.33	0.71	6.00E-03	-0.63	1.09	3482802	256641	3355091	261928	3315778	265313	3394403	255083
RP_POS_353_24472a11_129	RP	POS	11.13	353.2447				6.68E-05	0.63	1.68	1.34E-01	0.32	1.27	1.75E-04	0.79	1.58	5.58E-03	0.47	1.50	2862381	1472413	4387517	2561343	4002890	2150770	4772144	2885674
RP_POS_606_02289a10_867	RP	POS	10.87	606.0229				1.41E-03	0.40	1.05	1.34E-01	-0.34	1.12	5.80E-02	0.23	1.01	6.77E-03	0.56	1.08	425893	92838	570911	412374	632933	506737	508889	280966
RP_NEG_247_96269a1_462	RP	NEG	1.46	247.9627				3.89E-08	0.68	1.15	1.34E-01	0.33	0.95	1.14E-04	0.84	1.24	1.16E-06	0.51	1.46	567604	545511	2373037	2913451	1934370	1664869	2811705	3739669
HILIC_POS_132_10213a3_04	HILIC	POS	3.04	132.1021		132.1017(100)	4	6.03E-07	0.66	1.09	1.34E-01	0.32	1.03	1.41E-05	0.83	1.50	1.93E-03	0.50	0.97	620558	195059	973589	577148	887026	530466	1060152	613442
RP_POS_382_2478a12_208	RP	POS	12.21	382.2478				1.92E-02	-0.51	0.97	1.35E-01	0.29	1.08	1.19E-01	-0.36	0.77	6.27E-03	-0.65	1.16	602340	220714	495938	201714	465708	201033	526167	199821
RP_NEG_682_33496a10_446	RP	NEG	10.45	682.3350				3.00E-04	0.68	1.34	1.35E-01	-0.30	1.08	1.41E-02	0.53	1.03	5.97E-05	0.83	1.53	675173	335881	949931	402117	1010203	361922	889659	433930
HILIC_POS_139_12309a2_936	HILIC	POS	2.936	139.1231				4.61E-01	0.14	0.79	1.35E-01	0.31	0.94	1.69E-01	0.29	0.89	9.32E-01	-0.02	0.46	12184668	3108604	12677019	3719418	12119794	3717552	13234244	3673771
RP_POS_256_10986a4_551	RP	POS	4.55	256.1099				5.82E-01	0.08	0.48	1.35E-01	-0.33	0.89	4.81E-01	-0.09	0.51	2.78E-01	0.25	0.58	21059053	5461982	21886641	11490614	23615607	15041024	20157675	5867700

Supplementary table 1: Metabolomics results (in asceding order according to p-value from progressive ALD vs non-progressive ALD comparison, with molecular features with ID_level of 1-2 first)

								all_ALD_vs_control			Prog_ALD_vs_non-prog_ALD			Prog_ALD_vs_control_ALD			Non-prog_ALD_vs_control			Healthy_control		all_ALD		Non-prog_ALD		Progressive_ALD	
								t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA								
Feature_ID	RP_HILIC	POS_NEG	Average.Rt	Average.Mz	Metabolite.name	curated_MSMS	ID_level	p	d	VIP	p	d	VIP	p	d	VIP	p	d	VIP	Mean	SD	Mean	SD	Mean	SD	Mean	SD
RP_POS_199_13042a13_013	RP	POS	13.01	199.1304				8.07E-01	-0.05	0.67	1.35E-01	-0.29	0.96	4.35E-01	-0.20	0.48	6.78E-01	0.09	0.58	23766970	4179545	23564568	3687359	24117475	2800387	23011660	4359433
RP_POS_205_98676a0_254	RP	POS	0.25	205.9868				8.59E-01	-0.04	0.31	1.36E-01	-0.29	0.99	4.38E-01	-0.18	0.40	6.47E-01	0.11	0.56	3732910	588080	3712065	531987	3791622	520707	3632508	536417
RP_NEG_851_11426a9_304	RP	NEG	9.30	851.1143				2.13E-01	-0.22	0.57	1.36E-01	-0.32	0.96	6.32E-02	-0.38	0.72	7.63E-01	-0.06	0.32	4250577	267621	4176267	355324	4229360	364491	4123174	341293
RP_NEG_307_85608a15_525	RP	NEG	15.53	307.8561				2.29E-01	-0.24	0.64	1.36E-01	-0.30	0.88	7.74E-02	-0.39	0.70	6.91E-01	-0.09	0.29	11001180	302033	10925684	316718	10972976	326205	10878393	302809
RP_NEG_519_40668a13_181	RP	NEG	13.18	519.4067				1.83E-02	-0.52	0.89	1.36E-01	-0.28	0.88	5.88E-03	-0.67	1.09	1.07E-01	-0.38	0.64	17417368	1181192	16849735	1015589	17001332	1027745	16698138	990319
RP_POS_140_06827a0_694	RP	POS	0.69	140.0683				4.94E-02	0.27	1.24	1.37E-01	-0.33	1.38	5.43E-01	0.10	1.31	1.96E-02	0.44	1.22	298939	53319	332060	137731	352607	144023	311513	129317
RP_POS_289_64111a10_617	RP	POS	10.62	289.6411				3.35E-01	0.22	1.04	1.37E-01	-0.28	1.27	7.50E-01	0.08	0.74	1.31E-01	0.36	1.07	10846992	1972883	11220567	1583926	11456848	1350458	10984287	1769512
HILIC_NEG_217_02998a4_805	HILIC	NEG	4.805	217.0300				1.27E-01	0.23	0.50	1.37E-01	0.33	1.02	7.56E-02	0.39	0.66	6.52E-01	0.06	0.51	768804	199952	849296	386426	791542	251790	907050	481136
RP_POS_392_20059a11_125	RP	POS	11.13	392.2006				1.20E-06	0.81	1.72	1.37E-01	0.30	1.06	3.70E-06	0.96	1.70	3.12E-04	0.66	1.54	251602	130431	412344	201812	382258	182814	442429	216839
RP_POS_416_20053a11_048	RP	POS	11.05	416.2005				4.79E-09	0.83	1.77	1.37E-01	0.31	1.01	4.80E-07	0.99	1.75	4.29E-05	0.68	1.64	301938	172012	617145	395371	558230	357344	676060	425497
RP_POS_326_18066a0_702	RP	POS	0.70	326.1807				7.35E-15	0.97	1.67	1.37E-01	0.31	0.92	5.27E-08	1.12	1.75	3.67E-09	0.81	1.73	59256	59112	476643	450763	409419	343635	543867	532179
RP_NEG_271_22806a10_509	RP	NEG	10.51	271.2281				1.24E-01	-0.26	0.94	1.37E-01	0.32	1.21	6.02E-01	-0.10	0.79	3.73E-02	-0.42	0.94	8471504	1064542	8094778	1526367	7867476	1515622	8322080	1518087
RP_POS_592_46838a12_111	RP	POS	12.11	592.4684				9.10E-02	-0.35	0.67	1.37E-01	0.29	1.18	3.75E-01	-0.20	0.47	3.01E-02	-0.50	0.83	951905	461109	791107	455124	723331	445696	858882	458784
RP_POS_265_14349a7_276	RP	POS	7.28	265.1435				1.61E-06	-1.09	1.71	1.37E-01	-0.25	0.94	3.02E-07	-1.22	1.98	5.34E-05	-0.97	1.42	778225	358811	392188	297234	436453	330056	347924	256053
RP_POS_465_28467a9_334	RP	POS	9.33	465.2847				2.24E-02	0.27	0.45	1.37E-01	0.34	0.89	5.51E-02	0.44	0.65	4.96E-02	0.10	0.62	247279	258809	1347392	4720964	639985	1344716	2054799	6496177
RP_POS_136_04803a0_55	RP	POS	0.55	136.0480				5.13E-01	-0.10	1.18	1.37E-01	-0.33	1.20	1.51E-01	-0.26	1.29	7.50E-01	0.06	1.09	2395584	430825	2324370	771942	2439252	800872	2209488	731861
RP_POS_176_07059a5_864	RP	POS	5.86	176.0706				5.96E-02	-0.25	0.64	1.38E-01	-0.34	0.96	5.35E-06	-0.42	1.76	7.14E-01	-0.08	0.61	648779	388471	406626	1073451	567450	1481882	245801	281691
HILIC_NEG_98_93893a3_015	HILIC	NEG	3.015	98.9389				3.16E-01	-0.21	0.70	1.38E-01	0.29	0.96	7.70E-01	-0.07	0.43	1.26E-01	-0.36	0.74	689535	106541	668023	98355	653395	96951	682651	98532
RP_POS_473_32288a10_897	RP	POS	10.90	473.3229				1.68E-02	0.43	0.80	1.38E-01	0.31	0.98	5.06E-03	0.58	1.14	1.81E-01	0.28	0.61	1386160	504699	1657719	656392	1560163	656671	1755274	647962
RP_POS_170_09219a0_514	RP	POS	0.51	170.0922				1.91E-01	0.24	0.68	1.39E-01	-0.31	0.94	6.69E-01	0.08	0.43	8.13E-02	0.39	0.74	644020	481786	782269	608879	872695	690039	691844	506154
RP_POS_619_49023a11_61	RP	POS	11.61	619.4902				1.20E-01	-0.28	0.50	1.39E-01	-0.31	0.94	2.50E-02	-0.44	0.84	5.74E-01	-0.12	0.29	6285422	4056826	4886926	5239927	5665002	5897654	4108851	4410915
RP_POS_535_32355a10_857	RP	POS	10.86	535.3236				8.19E-06	0.58	1.10	1.39E-01	0.33	1.26	2.12E-04	0.74	1.27	4.00E-03	0.41	1.18	533735	207668	899764	697012	796274	566082	1003255	799538
RP_POS_266_84134a0_515	RP	POS	0.52	266.8413				1.00E-01	-0.29	0.63	1.39E-01	-0.31	0.90	2.67E-02	-0.45	0.94	5.18E-01	-0.14	0.41	346766	89098	313878	118775	331496	123698	296259	112107
RP_POS_367_22693a10_884	RP	POS	10.88	367.2269				1.02E-02	-0.34	0.86	1.39E-01	0.33	1.09	3.91E-01	-0.18	0.66	2.35E-04	-0.51	1.19	1405832	167326	1258237	482480	1186622	342460	1329852	585303
HILIC_POS_518_32294a1_32	HILIC	POS	1.32	518.3229				6.76E-09	0.99	1.56	1.39E-01	-0.29	1.00	4.57E-05	0.84	1.33	1.10E-09	1.13	2.16	20107604	3233652	24963221	4798116	25674511	3958334	24251931	5460105
HILIC_POS_263_14612a5_591	HILIC	POS	5.591	263.1461				1.34E-01	0.27	0.64	1.40E-01	-0.31	1.35	6.03E-01	0.11	0.56	3.13E-02	0.42	0.84	797885	863261	1084893	1121586	1251002	981462	918783	1233696
RP_POS_873_69244a10_839	RP	POS	10.84	873.6924				1.98E-08	0.84	1.51	1.40E-01	0.31	0.90	5.38E-07	1.00	1.61	5.56E-05	0.69	1.47	164813	121319	359787	238449	324484	217186	395090	255271
RP_POS_191_97209a15_548	RP	POS	15.55	191.9721				1.98E-01	-0.25	0.55	1.40E-01	0.30	0.89	6.33E-01	-0.10	0.37	8.53E-02	-0.40	0.70	4432994	949783	4173737	1069283	4015398	1208045	4332076	894162
HILIC_POS_229_15492a5_011	HILIC	POS	5.011	229.1549				4.93E-01	0.11	0.79	1.40E-01	0.32	1.10	2.39E-01	0.27	0.39	7.47E-01	-0.05	1.03	4995610	1255181	5200959	1989530	4905647	1177657	5496271	2536215
RP_POS_808_07574a13_841	RP	POS	13.84	808.0757				2.54E-02	0.42	0.98	1.40E-01	-0.30	0.90	2.16E-01	0.26	0.62	6.96E-03	0.57	1.21	1508360	623195	1814318	755320	1926055	724143	1702581	776400
RP_POS_514_87274a0_497	RP	POS	0.50	514.8727				1.97E-09	-0.75	1.34	1.40E-01	0.32	1.27	2.71E-04	-0.59	1.27	7.61E-07	-0.91	1.57	18460071	856095	15602162	4132746	14991179	4264123	16213146	3945017
RP_NEG_205_83949a1_319	RP	NEG	1.32	205.8395				1.20E-03	0.53	0.93	1.40E-01	-0.31	1.02	2.51E-02	0.37	1.00	1.81E-03	0.69	1.10	3008105	1452580	4166524	2312134	4508808	2736663	3824240	1752884
RP_NEG_160_84106a15_582	RP	NEG	15.58	160.8411				8.13E-03	-0.54	0.96	1.40E-01	-0.29	1.11	2.09E-03	-0.68	1.23	8.45E-02	-0.39	0.65	3221376	106326	3161539	109859	3177777	115605	3145301	102380
RP_POS_144_10176a0_705	RP	POS	0.71	144.1018				1.34E-01	0.17	0.73	1.40E-01	0.34	0.99	1.36E-01	0.35	0.91	8.58E-01	0.00	0.36	1524045	992700	3451390	12650490	1567434	1176766	5335346	17740000
RP_POS_203_05185a0_547	RP	POS	0.55	203.0519	Unknown	203.05185(100)	4	4.85E-06	0.58	1.13	1.40E-01	0.33	1.37	9.98E-05	0.74	1.29	6.79E-03	0.41	1.28	83353072	8064914	100303264	32488511	95502642	28937323	105103886	35329114
RP_NEG_316_9491a14_258	RP	NEG	14.26	316.9491				5.08E-01	-0.13	0.60	1.41E-01	0.31	1.09	8.98E-01	0.03	0.29	2.01E-01	-0.28	0.69	5636413	2100743	5340151	2443425	4979301	2469077	5701000	2387554
HILIC_NEG_142_92892a7_352	HILIC	NEG	7.352	142.9289				2.66E-01	-0.16	0.27	1.41E-01	-0.33	0.84	8.61E-02	-0.32	0.63	9.86E-01	0.00	0.32	3048480	222365	2979507	475937	3049794	452227	2909220	493013
RP_POS_809_58551a13_021	RP	POS	13.02	809.5855				4.39E-04	-0.78	1.33	1.41E-01	-0.27	0.89	1.11E-04	-0.92	1.54	6.66E-03	-0.65	1.11	7134577	3430902	4578288	2981452	5018595	3164687	4137981	2747477
RP_POS_285_12387a11_804	RP	POS	11.80	285.1239				1.41E-02	-0.49	1.21	1.41E-01	0.29	1.33	1.58E-01	-0.35	0.69	1.40E-03	-0.64	1.46	1316415	698209	952841	730095	844750	453307	1060932	920665
RP_POS_335_25513a10_902	RP	POS	10.90	335.2551				5.20E-02	-0.32	0.92	1.41E-01	0.32	1.15	4.66E-01	-0.16	0.79	6.18E-03	-0.47	1.08	748850	127432	688816	205126	658520	161473	719112	238884
HILIC_NEG_199_80507a0_882	HILIC	NEG	0.882	199.8051				1.80E-01	0.27	0.93	1.41E-01	0.30	1.06	6.71E-02	0.42	0.92	5.76E-01	0.12	0.21	449829	84304	473205	86058	460512	83341	485898	87684
RP_NEG_197_80789a2_201	RP	NEG	2.20	197.8079				5.64E-01	0.11	0.66	1.41E-01	-0.30	1.14	8.46E-01	-0.04	0.42	2.61E-01	0.26	0.45	12722088	2243615	12993666	2491815	13361459	2836382	12625872	2055206
HILIC_POS_171_18575a7_097	HILIC	POS	7.097	171.1858				7.03E-01	0.08	0.99	1.41E-01	-0.30	1.02	7.30E-01	-0.08	0.94	3.18E-01	0.23	0.85	6763088	1682337	6896385	1808724	7163084	1863968	6629686	1729217
RP_POS_580_35052a11_101	RP	POS	11.10	580.3505				1.94E-07	0.62	1.30	1.41E-01	-0.33	1.32	4.59E-04	0.46	1.36	8.99E-05	0.78	1.41	41953	33462	1273144	2198700	1597707	2576949	948582	1706333
HILIC_NEG_568_36389a1_173	HILIC	NEG	1.173	568.3639				3.02E-01	-0.24	0.61	1.41E-01	-0.28	1.12	1.33E-01	-0.38	0.81	6.84E-01	-0.10	0.24	2439190	786250	2280189	623861	2372156	615135	2188223	625056
RP_POS_298_69098a10_932	RP	POS	10.93	298.6910				2.73E-04	-0.84	1.63	1.41E-01	-0.26	1.45	8.87E-05	-0.97	1.66	3.20E-03	-0.71	1.39	993262	267308	787846	217040	819825	216685	755866	214789
RP_POS_232_05246a8_574	RP	POS	8.57	232.0525				6.07E-01	0.07	0.63	1.42E-01	0.33	1.02	3.05E-01	0.24	0.87	2.67E-01	-0.10	0.77	1688458	1472943	1949898	4350538	1305633	1570231	2594162	5909983
RP_NEG_197_80798a4_573	RP	NEG	4.57	197.8080				1.61E-03	-0.69	1.08	1.42E-01	-0.27	0.95	4.86E-04	-0.83	1.30	1.76E-02	-0.56	0.95	17501279	6400276	13268280	5654156	14100365	5762865	12436195	5474285
RP_POS_321_12079a11_804	RP	POS	11.80	321.1208				2.98E-02	-0.43	1.11	1.42E-01	0.30	1.32	2.56E-01	-0.28	0.66	2.83E-03	-0.58	1.37	595043	339380	438276	367080	384095	208978	492458	471786
RP_POS_441_297a13_095	RP	POS	13.10	441.2970				1.01E-01	0.24	0.46	1.43E-01	0.33	0.98	4.92E-02	0.40	0.76	6.35E-01	0.08	0.51	8745438	1352792	9363468	2868695	8941687	2372839	9785249	3260882
RP_NEG_894_54907a12_821	RP	NEG	12.82	894.5491				8.47E-06	-1.03	1.68	1.43E-01	-0.25	0.98	3.22E-06	-1.16	1.80	1.20E-04	-0.91	1.47	4296869	1294610	3032425	1036427	3184703	986719	2880146	1072076
RP_NEG_211_91728a13_292	RP	NEG	13.29	211.9173				1.80E-01	0.25	0.42	1.43E-01	-0.30	1.09	6.42E-01	0.10	0.62	5.49E-02	0.40	0.79	2096482	650828	2283789	763237	2395909	717657	2171670	797660
HILIC_NEG_253_0929a1_279	HILIC	NEG	1.279	253.0929				1.69E-12	0.86	1.44	1.43E-01	0.31	1.03	2.01E-07	1.02	1.62	1.39E-06	0.71	1.73	20850	18297	219596	245262	183556	208812	255636	274374
RP_NEG_235_92616a13_287	RP	NEG	13.29	235.9262				5.49E-02	-0.43	0.79	1.43E-01	0.28	0.87	2.20E-01	-0.29	0.50	2.12E-02	-0.57	1.00	947363	218991	862785	185990	835487	191645	890083	177882
RP_POS_331_26315a11_049	RP	POS	11.05	331.2632				4.66E-10	0.83	1.74	1.43E-01	0.31	1.02	5.99E-07	0.98	1.71	1.53E-05	0.67	1.67	1456373	767708	3263301	2311536	2924267	2011848	3602334	2552123
RP_POS_305_09622a7_093	RP	POS	7.09	305.0962				3.26E-01	-0.19	0.74	1.44E-01	0.30	1.01	8.46E-01	-0.04	0.35	1.21E-01	-0.34	0.76	988168	68366	974079	74751	963122	73624	985037	74994
HILIC_NEG_113_92623a4_793	HILIC	NEG	4.793	113.9262				9.86E-01	0.00	0.48	1.44E-01	0.29	1.70	5.51E-01	0.14	0.48	5.43E-01	-0.15	0.27	3293876	1066123	3290115	958221	3149703	999087	3430527	903716
RP_POS_421_32828a11_341	RP	POS	11.34	421.3283				2.58E-01	-0.21	0.70	1.44E-01	0.30	1.20	7.83E-01	-0.06	0.75	8.91E-02	-0.36	0.69	1931086	256976	1868275	310090	1822894	306547	1913655	310000
RP_POS_229_15436a0_709	RP	POS	0.71	229.1544				2.79E-02	0.32	0.55	1.45E-01	0.32	0.93	2.46E-02	0.48	0.79	2.69E-01	0.16	0.71	6107647	1167572	6813615	2403024	6461705	1713566	7165525	2911675
HILIC_POS_130_08643a4_986	HILIC	POS	4.986	130.0864				2.77E-01	0.28	0.68	1.45E-01	0.25	1.25	1.57E-01	0.40	0.58	5.51E-01	0.15	0.33	5941064	11697005	8373014	7652726	7252323	4817322	9493706	9620492
RP_POS_194_11528a10_386	RP	POS	10.39	194.1153				9.00E-01	0.02	0.88	1.45E-01	0.30	1.30	4.59E-01	0.17	0.66	5.44E-01	-0.12	0.72	1314057	269408	1321091	294017	1278159	243783	1364023	333862
RP_POS_261_98135a15_59	RP	POS	15.59	261.9814				5.81E-02	-0.36	0.74	1.46E-01	0.30	1.02	3.31E-01	-0.22	0.39	1.55E-02	-0.51	1.20	7407599	249288	7306366	282989	7265098	260318	7347635	300930
RP_POS_165_09105a11_237	RP	POS	11.24	165.0911				1.71E-01	-0.25	0.72	1.46E-01	-0.30	1.04	8.63E-02	-0.41	0.77	5.81E-01	-0.10	0.40	704942	243568	632503	296740	675841	211207	589165	359812
RP_NEG_317_11475a5_92	RP	NEG	5.92	317.1148				7.35E-01	-0.05	0.67	1.46E-01	0.32	1.34	6.27E-01	0.11	0.46	7.71E-02	-0.21	0.90	1703300	959012	1615473	1956667	1328850	854588	1902096	2614812
HILIC_POS_421_37061a1_388	HILIC	POS	1.388	421.3706				3.44E-01	-0.15	0.66	1.46E-01	-0.32	0.93	1.35E-01	-0.31	0.50	9.66E-01	0.01	0.46	1141351	238735	1086236	397023	1144114	346581	1028359	437626
HILIC_NEG_148_04633a0_927	HILIC	NEG	0.927	148.0463				1.66E-04	0.54	0.89	1.46E-01	-0.32	1.34	4.75E-02	0.39	0.65	3.36E-05	0.70	1.41	103308	50140	158094	109256	174015	94679	142172	120979
RP_POS_319_12875a5_922	RP	POS	5.92	319.1288				7.91E-01	-0.04	0.68	1.46E-01	0.32	1.33	5.94E-01	0.12	0.49	1.17E-01	-0.20	0.86	1506157	834487	1447434	1639213	1207640	822438	1687227	2152933
RP_POS_820_81677a0_493	RP	POS	0.49	820.8168				7.80E-03	0.35	1.00	1.46E-01	0.33	1.36	8.71E-03	0.51	1.08	2.08E-01	0.19	1.08	851327	230827	1065796	680656	966678	573897	1164914	765920
RP_POS_1066_12915a10_324	RP	POS	10.32	1066.1292				1.00E-02	-0.71	1.27	1.47E-01	-0.22	1.03	4.33E-03	-0.82	1.29	3.32E-02	-0.60	1.00	653758	461258	422243	249673	458562	246260	385925	250219
RP_POS_421_35123a10_657	RP	POS	10.66	421.3512				7.20E-01	0.07	0.31	1.47E-01	0.30	0.86	3.00E-01	0.22	0.45	7.10E-01	-0.08	0.60	5195327	382090	5224382	441453	5160167	463927	5288596	412425
RP_POS_801_98761a10_197	RP	POS	10.20	801.9876				3.00E-02	-0.54	1.19	1.47E-01	-0.25	1.17	9.75E-03	-0.67	1.21	1.20E-01	-0.42	0.96	311599	275639	194286	186371	221403	211237	167169	155097
RP_POS_187_13335a10_271	RP	POS	10.27	187.1334				9.17E-01	-0.02	0.62	1.47E-01	0.29	1.00	6.26E-01	0.12	0.58	4.65E-01	-0.17	0.90	1916090	149095	1912975	135799	1893220	116309	1932729	151443
RP_POS_164_98398a15_442	RP	POS	15.44	164.9840				5.01E-02	-0.45	0.85	1.47E-01	-0.27	0.98	1.39E-02	-0.59	1.18	2.15E-01	-0.32	0.55	586869991	164880262	522519956	130726028	541535137	151769786	503504774	103708096
HILIC_NEG_136_89165a4_071	HILIC	NEG	4.071	136.8917				5.37E-01	-0.14	0.86	1.47E-01	0.28	1.09	9.93E-01	0.00	0.20	2.52E-01	-0.28	0.86	6380996	3283410	5979664	2805151	5572304	2762547	6387024	2815673
HILIC_NEG_312_83673a4_757	HILIC	NEG	4.757	312.8367				1.01E-02	-0.42	0.70	1.47E-01	-0.31	1.01	1.12E-03	-0.58	1.16	2.10E-01	-0.27	0.53	1139969	151097	1045632	238680	1080318	275121	1010946	192229
RP_POS_173_07838a0_722	RP	POS	0.77	173.0784				9.99E-03	0.32	1.10	1.48E-01	-0.33	1.28	3.27E-01	0.15	1.09	8.23E-03	0.48	1.20	2943178	362064	3427187	1734824	3679057	1842780	3175316	1598544
HILIC_NEG_179_05621a4_984	HILIC	NEG	4.984	179.0562				3.04E-02	0.33	0.85	1.48E-01	0.32	0.87	3.40E-02	0.49	0.84	2.07E-01	0.17	0.50	18710063	7997907	23292364	15365282	21053375	8319931	25531352	19938655
RP_POS_252_15695a7_139	RP	POS	7.14	252.1570				7.45E-01	0.08	0.59	1.48E-01	-0.27	0.90	8.29E-01	-0.06	0.53	4.06E-01	0.21	0.51	761027	600346	798708	445539	863333	425495	734082	459883
RP_NEG_134_8934a11_209	RP	NEG	11.21	134.8934				1.11E-01	0.29	0.54	1.48E-01	-0.30	1.05	5.28E-01	0.14	0.85	2.76E-02	0.44	0.92	449949	109170	488287	138448	508372	123058	468203	150866
RP_NEG_334_78738a15_4	RP	NEG	15.40	334.7874				9.41E-01	-0.02	0.76	1.48E-01	-0.25	0.87	5.85E-01	-0.14	0.33	7.02E-01	0.11	0.62	1316043	103016	1314607	65410	1324098	73123	1305116	55798
RP_NEG_960_78442a0_491	RP	NEG	0.49	960.7844				7.45E-09	-0.75	1.35	1.48E-01	0.31	1.27	3.75E-04	-0.59	1.28	8.08E-07	-0.90	1.57	3134606	348975	2301916	1195968	2128568	1218292	2475264	1159444
HILIC_POS_524_37189a1_096	HILIC	POS	1.096	524.3719				3.32E-01	-0.22	0.57	1.48E-01	-0.28	1.08	1.48E-01	-0.36	0.63	7.36E-01	-0.08	0.15	12475540	4810459	11553990	3990076	12132252	3908844	10975729	4025523
RP_POS_777_69281a7_775	RP	POS	7.78	777.6928				9.45E-08	-1.38	2.61	1.49E-01	0.20	0.99	7.49E-07	-1.28	2.11	2.47E-08	-1.48	2.35	1537510	420323	1023164	252565	986604	219727	1059724	279056
RP_POS_810_98871a10_618	RP	POS	10.62	810.9887				4.68E-03	0.63	1.36	1.49E-01	-0.27	1.08	4.59E-02	0.49	1.02	1.01E-03	0.76	1.48	1862684	790621	2325495	689636	2425322	570551	2225668	784243
HILIC_POS_285_09973a1_437	HILIC	POS	1.437	285.0997				8.50E-02	-0.46	0.98	1.49E-01	-0.24	0.86	3.58E-02	-0.58	1.09	2.26E-01	-0.34	0.55	405963	412128	270175	242307	305196	267586	235153	210993
RP_POS_223_09402a10_796	RP	POS	10.80	223.0940				6.26E-02	-0.44	0.74	1.50E-01	0.26	0.86	2.26E-01	-0.31	0.56	2.26E-02	-0.57	1.00	9049853	4180533	7509819	3213530	7045578	3009992	7974059	3371115
RP_POS_419_35126a12_236	RP	POS	12.24	419.3513				4.34E-01	-0.14	0.42	1.50E-01	0.31	0.91	9.36E-01	0.02	0.30	1.54E-01	-0.29	0.72	1956914	280295	1907605	382892	1852390	374459	1962819	386993
RP_POS_319_12878a6_048	RP	POS	6.05	319.1288				8.33E-01	-0.03	0.69	1.50E-01	0.32	1.33	5.76E-01	0.13	0.51	1.42E-01	-0.19	0.81	925065	528735	895883	1019480	748342	520936	1043425	1335698

Supplementary table 1: Metabolomics results (in asceding order according to p-value from progressive ALD vs non-progressive ALD comparison, with molecular features with ID_level of 1-2 first)

							all_ALD_vs_control			Prog_ALD_vs_non-prog_ALD			Prog_ALD_vs_control_ALD			Non-prog_ALD_vs_control			Healthy_control		all_ALD		Non-prog_ALD		Progressive_ALD	
							t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA								
Feature_ID	RP_HILIC	POS_NEG	Average.Rt	Average.Mz	Metabolite.name	curated_MSMS	ID_level	p	d	VIP	p	d	VIP	p	d	VIP	p	d	VIP	Mean	SD	Mean	SD	Mean	SD	Mean	SD
RP_POS_997_47577a0_483	RP	POS	0.48	997.4758				1.16E-07	0.68	1.16	1.51E-01	-0.31	1.10	2.09E-03	0.52	1.02	2.72E-06	0.84	1.49	233262	58196	365484	211799	395995	209911	334972	211354
RP_POS_425_33893a12_021	RP	POS	12.02	425.3389				8.91E-02	-0.46	0.73	1.51E-01	-0.23	1.06	3.75E-02	-0.57	0.95	2.30E-01	-0.34	0.52	477230	521633	308196	296669	350959	339158	265432	243025
HILIC_NEG_200_85873a5_355	HILIC	NEG	5.355	200.8587				7.79E-01	0.06	0.41	1.51E-01	-0.29	0.92	6.96E-01	-0.09	0.18	3.73E-01	0.20	0.55	4842801	2460778	4984123	2506535	5345061	2497694	4623185	2487832
RP_NEG_204_79147a15_58	RP	NEG	15.58	204.7915				2.59E-01	-0.23	0.50	1.51E-01	-0.29	0.92	1.05E-01	-0.38	0.69	6.91E-01	-0.09	0.36	676245	31641	668934	31257	673434	30211	664434	31935
RP_POS_685_43463a11_915	RP	POS	11.92	685.4346				1.28E-01	-0.22	0.43	1.51E-01	0.32	1.24	6.88E-01	-0.06	0.71	6.39E-02	-0.38	0.70	4994679	491873	4788360	1024411	4640769	1178785	4935951	828410
HILIC_POS_558_29517a1_275	HILIC	POS	1.275	558.2952				4.79E-02	-0.43	1.00	1.51E-01	-0.28	0.97	1.98E-02	-0.57	0.95	2.02E-01	-0.29	0.62	1862508	547242	1642199	491605	1712925	451645	1571472	523537
RP_POS_872_54028a13_071	RP	POS	13.07	872.5403				6.36E-01	0.11	0.44	1.51E-01	-0.27	1.10	9.07E-01	-0.03	0.27	3.00E-01	-0.24	0.69	6994618	2118469	7191503	1747907	7443072	1470788	6939934	1969856
RP_NEG_317_11478a6_043	RP	NEG	6.04	317.1148				8.59E-01	-0.03	0.68	1.51E-01	0.32	1.35	5.63E-01	0.13	0.47	1.09E-01	-0.19	0.89	940175	553187	913328	1146756	747524	469793	1079132	1542767
RP_POS_812_034a13_195	RP	POS	13.20	812.0340				3.51E-03	0.61	0.98	1.52E-01	0.28	1.08	1.17E-03	0.75	1.31	3.78E-02	0.47	0.79	697797	379979	933031	374321	879222	375133	986839	369403
RP_POS_323_25537a10_556	RP	POS	10.56	323.2554				4.37E-03	-0.53	1.06	1.52E-01	0.29	1.09	6.96E-02	-0.39	0.88	1.28E-03	-0.68	1.17	5143254	574885	4778883	696453	4678773	667331	4878992	717084
RP_NEG_231_93213a15_412	RP	NEG	15.41	231.9321				1.25E-01	0.32	0.63	1.52E-01	0.28	1.05	3.52E-02	0.46	0.94	4.56E-01	0.18	0.40	14971957	1914211	15572846	1836751	15309196	2094463	15836496	1512457
RP_POS_293_9454a15_349	RP	POS	15.35	293.9454				7.93E-01	-0.05	0.43	1.53E-01	0.31	1.29	5.83E-01	0.11	0.33	3.37E-01	-0.20	0.92	2580541	516600	2549660	731713	2444729	756507	2654590	697826
HILIC_POS_130_08646a4_124	HILIC	POS	4.124	130.0865				1.82E-02	-0.47	1.44	1.53E-01	0.29	0.94	1.34E-01	-0.33	0.69	6.10E-03	-0.62	1.46	2300848	671882	1964142	708225	1862589	702534	2065694	706258
RP_NEG_291_00827a7_31	RP	NEG	7.31	291.0083				5.96E-01	-0.10	0.55	1.53E-01	-0.30	0.90	2.34E-01	-0.25	0.70	8.25E-01	0.05	0.48	2621281	537758	2560488	630535	2650905	666665	2470070	584924
RP_POS_331_26279a11_132	RP	POS	11.13	331.2628				1.84E-05	0.67	1.73	1.53E-01	0.30	1.21	7.69E-05	0.82	1.62	2.46E-03	0.51	1.58	530274	345943	923591	621948	834437	534948	1012745	692200
HILIC_POS_242_07883a3_016	HILIC	POS	3.016	242.0788				4.25E-10	0.81	1.48	1.53E-01	0.31	1.24	9.52E-07	0.96	1.56	1.95E-05	0.65	1.51	5401856	4725854	18058296	16746692	15657985	14559132	20458607	18517571
RP_POS_351_22708a11_132	RP	POS	11.13	351.2271				3.06E-06	0.70	1.65	1.53E-01	0.30	1.09	3.21E-05	0.85	1.57	8.24E-04	0.55	1.51	777081	330242	1205805	643382	1113631	545991	1297978	721723
HILIC_POS_167_09274a1_16	HILIC	POS	1.16	167.0927				4.86E-02	0.23	0.66	1.53E-01	0.33	0.86	8.42E-02	0.40	0.76	1.28E-01	0.07	0.87	606439	342722	1303517	3440045	807602	818952	1799433	4768306
RP_POS_385_23456a11_095	RP	POS	11.10	385.2346				1.92E-03	-0.60	1.01	1.53E-01	0.29	0.89	3.75E-02	-0.45	0.81	5.21E-04	-0.74	1.21	2123090	209835	1979507	240848	1945036	225620	2013977	252724
HILIC_POS_130_09758a1_559	HILIC	POS	1.559	130.0976				4.64E-02	-0.47	1.06	1.53E-01	-0.26	0.92	1.66E-02	-0.60	1.26	1.78E-01	-0.34	0.76	795743	663206	534145	502378	606039	529223	462250	468287
RP_NEG_351_25143a11_611	RP	NEG	11.61	351.2514				1.62E-01	-0.25	0.63	1.54E-01	-0.30	1.09	4.41E-02	-0.40	0.77	6.51E-01	-0.10	0.58	2249002	368970	2133644	491512	2203974	528673	2063314	445543
RP_NEG_188_93326a15_487	RP	NEG	15.49	188.9333				4.84E-01	-0.12	0.51	1.54E-01	0.31	1.13	8.16E-01	0.04	0.40	2.47E-01	-0.27	0.59	2188902	166109	2161962	245687	2126696	315207	2197228	141643
RP_NEG_285_16486a8_337	RP	POS	8.34	285.1649				8.49E-01	0.04	0.36	1.54E-01	-0.29	0.85	6.45E-01	-0.10	0.31	4.34E-01	0.18	0.40	647741	431084	664468	425565	725309	442500	603627	403170
RP_POS_328_06067a6_515	RP	POS	6.52	328.0607				1.44E-03	0.42	0.86	1.54E-01	-0.32	0.87	4.46E-02	0.26	0.73	5.61E-03	0.58	0.96	176630	648482	892125	1874218	1160560	2282676	623690	1318866
RP_POS_615_4585a11_255	RP	POS	11.26	615.4585				8.11E-01	0.04	0.41	1.54E-01	-0.32	0.98	3.26E-01	-0.12	0.53	4.13E-01	0.19	0.63	1941857	2276345	2079963	4130193	2673570	5596257	1486356	1558173
RP_POS_516_3078a9_748	RP	POS	9.75	516.3078				5.02E-07	0.70	1.28	1.54E-01	-0.31	0.85	1.45E-03	0.55	1.19	5.40E-06	0.85	1.51	123353	159421	379108	390904	434940	400157	323277	377152
RP_NEG_185_11795a8_007	RP	NEG	8.01	185.1180				9.78E-02	-0.39	0.65	1.54E-01	-0.26	0.87	2.95E-02	-0.52	0.92	3.24E-01	-0.26	0.47	1569160	1341635	1133109	1005129	1276916	1224283	989302	707187
RP_NEG_253_78329a15_551	RP	NEG	15.55	253.7833				2.23E-01	-0.25	0.65	1.54E-01	-0.28	1.15	8.83E-02	-0.40	0.68	6.22E-01	-0.11	0.59	842458	54025	829040	52231	836497	51796	821582	52110
HILIC_POS_72_08159a4_858	HILIC	POS	4.858	72.0816				8.15E-01	-0.04	1.02	1.54E-01	-0.30	1.13	3.70E-01	-0.19	0.66	5.93E-01	0.11	0.70	22557803	5485903	22275804	7021675	23278430	6557301	21273179	7386764
RP_POS_569_4342a11_165	RP	POS	11.17	569.4342				9.22E-01	0.02	0.76	1.55E-01	0.29	0.99	4.92E-01	0.16	0.70	5.80E-01	-0.12	0.66	2199058	516368	2209338	507927	2136833	455645	2281843	550367
RP_POS_277_2139a10_463	RP	POS	10.46	277.2139				3.56E-10	0.80	1.44	1.55E-01	-0.31	1.21	4.12E-06	0.65	1.56	2.84E-06	0.95	1.65	918918	206041	1516995	799637	1631164	932808	1402826	628616
RP_POS_212_16457a7_139	RP	POS	7.14	212.1646				8.30E-01	0.05	0.61	1.55E-01	-0.26	0.88	7.67E-01	-0.08	0.54	4.76E-01	0.18	0.48	1105347	858327	1140710	619009	1228948	572420	1052473	656209
RP_POS_338_01166a4_555	RP	POS	4.56	338.0117				5.78E-03	-0.60	0.94	1.55E-01	-0.27	0.97	2.48E-03	-0.73	1.14	4.17E-02	-0.46	0.79	2630212	1630410	1693252	1492169	1905918	1376289	1480586	1584962
RP_NEG_317_11484a5_729	RP	NEG	5.73	317.1148				6.61E-01	-0.06	0.65	1.55E-01	0.32	1.31	6.84E-01	0.09	0.44	6.55E-02	-0.22	0.90	956558	544325	892014	1109203	733249	496156	1050779	1479243
RP_NEG_367_24704a10_224	RP	NEG	10.22	367.2470				2.09E-01	0.22	0.92	1.55E-01	0.30	1.00	7.85E-02	0.37	0.93	7.25E-01	0.07	0.69	1485892	201898	1542855	273163	1503954	258340	1581756	284485
RP_POS_208_13345a0_714	RP	POS	0.71	208.1335				1.74E-01	0.24	0.74	1.56E-01	0.30	0.91	6.58E-02	0.39	0.81	6.51E-01	0.09	0.56	789328	70300	810773	94351	797344	88682	824201	98758
HILIC_POS_306_08121a0_555	HILIC	POS	0.555	306.0812				9.46E-01	-0.01	0.93	1.56E-01	0.31	0.93	5.05E-01	0.14	0.76	3.11E-01	-0.17	1.31	7817801	1263947	7796754	2132966	7492852	1604626	8100656	2535473
RP_POS_446_88773a0_497	RP	POS	0.50	446.8877				2.51E-09	-0.74	1.34	1.56E-01	0.31	1.26	3.00E-04	-0.58	1.28	1.17E-06	-0.89	1.57	32393030	1247569	27649770	6999660	26653847	7236824	28645692	6677917
RP_POS_596_60864a14_01	RP	POS	14.01	596.6086				4.75E-01	0.17	0.69	1.56E-01	-0.27	1.21	8.96E-01	0.03	0.66	2.36E-01	0.30	0.84	5295419	2519773	5646662	1987503	5929168	2022223	5364156	1930982
RP_NEG_289_93567a15_678	RP	NEG	15.68	289.9357				3.86E-02	-0.42	0.77	1.56E-01	0.28	0.87	2.20E-01	-0.27	0.50	1.26E-02	-0.56	0.96	1022668	301946	891337	314251	846684	304585	935989	320439
RP_POS_401_76367a12_691	RP	POS	12.69	401.7637				1.71E-03	0.60	1.17	1.56E-01	-0.29	0.87	3.61E-02	0.45	0.89	4.69E-04	0.74	1.28	1186786	443789	1495660	519769	1569508	486037	1421812	546325
RP_POS_305_9855a4_554	RP	POS	4.55	305.9855				4.94E-03	-0.61	0.95	1.56E-01	-0.27	0.97	2.14E-03	-0.74	1.17	3.69E-02	-0.47	0.81	2978357	1809835	1916808	1662254	2152981	1532957	1680636	1766006
HILIC_NEG_100_93342a7_429	HILIC	NEG	7.429	100.9334				8.62E-01	0.03	0.41	1.57E-01	0.31	0.95	3.64E-01	0.18	0.56	5.32E-01	-0.12	0.34	27008617	2529352	27110833	3762373	26576616	3699651	27645051	3785491
RP_POS_363_18268a11_126	RP	POS	11.13	363.1827				2.82E-07	0.84	1.75	1.57E-01	0.29	1.07	2.12E-06	0.98	1.73	9.29E-05	0.70	1.59	910211	456214	1518638	734753	1414312	651089	1622963	802878
RP_POS_904_77698a0_493	RP	POS	0.49	904.7770				3.68E-08	-0.76	1.34	1.57E-01	0.30	1.24	6.89E-04	-0.61	1.25	4.02E-07	-0.91	1.60	1254036	184552	916208	474210	848899	457198	983517	485863
RP_POS_780_55298a12_693	RP	POS	12.69	780.5530				2.24E-03	0.57	1.18	1.57E-01	-0.29	0.89	4.26E-02	0.43	0.89	7.58E-04	0.71	1.22	146960222	62414057	189621998	75740793	200363481	73908700	178880514	76762269
RP_POS_258_01196a4_299	RP	POS	4.30	258.0120				9.56E-01	0.01	0.30	1.57E-01	0.30	0.90	5.38E-01	0.16	0.41	3.76E-01	-0.14	0.47	5837503	27150359	6161778	32596141	1507919	2923851	10815637	45759709
HILIC_NEG_200_94971a0_857	HILIC	NEG	0.857	200.9497				2.24E-01	0.15	0.61	1.58E-01	0.32	1.12	1.73E-01	0.31	0.46	8.78E-01	-0.01	0.18	386869	496077	653757	2001877	368366	575687	939149	2756660
RP_POS_499_82721a3_138	RP	POS	3.14	499.8272				1.83E-01	0.17	0.76	1.58E-01	-0.32	0.97	9.00E-01	0.01	0.42	1.53E-01	0.33	1.10	1589941	1420189	2326586	4894634	3024106	6763376	1629067	1291371
RP_POS_136_98967a15_5	RP	POS	15.50	136.9897				8.36E-01	0.05	0.37	1.58E-01	-0.28	0.84	7.03E-01	-0.09	0.28	4.33E-01	0.18	0.65	62337503	24167987	63334769	21539968	66383246	19971647	60286291	22794228
RP_NEG_215_03256a0_549	RP	NEG	0.55	215.0326				1.07E-01	0.22	0.54	1.58E-01	0.32	0.95	8.40E-02	0.38	0.63	6.01E-01	0.06	0.81	205851707	21216687	216327629	52543077	208870957	30841764	223784301	67180388
RP_POS_465_37885a10_709	RP	POS	10.71	465.3789				7.89E-01	-0.06	0.94	1.58E-01	-0.28	1.19	3.77E-01	-0.20	1.23	7.30E-01	0.08	0.60	6726027	511213	6698395	485292	6767048	539260	6629743	418812
RP_POS_750_54266a13_523	RP	POS	13.52	750.5427				9.03E-01	-0.02	0.69	1.59E-01	-0.29	0.84	4.31E-01	-0.17	0.43	5.91E-01	0.12	0.75	12456323	3578688	12364587	3949827	12922488	4163701	11806687	3680904
HILIC_POS_162_1125a5_026	HILIC	POS	5.026	162.1125				4.88E-02	0.34	0.61	1.59E-01	0.30	0.90	1.97E-02	0.49	0.85	3.34E-01	0.19	0.34	14643392	11133116	19729614	16052760	17462427	15036473	21996802	16853949
HILIC_POS_585_27039a1_29	HILIC	POS	1.29	585.2704				1.44E-01	0.24	0.65	1.59E-01	0.30	1.11	8.41E-02	0.39	0.57	5.74E-01	0.09	0.24	1589284	1087586	1962531	1648114	1729352	1103770	2195709	2039294
RP_POS_972_76611a0_491	RP	POS	0.49	972.7661				3.42E-07	-0.75	1.25	1.59E-01	0.30	1.16	1.76E-03	-0.60	1.11	2.57E-07	-0.90	1.57	899220	140451	691952	289879	651033	256830	732871	316853
HILIC_NEG_117_05573a0_603	HILIC	NEG	0.603	117.0557				1.02E-04	0.50	0.98	1.60E-01	0.31	1.20	2.81E-03	0.66	0.92	1.39E-03	0.35	1.07	497864	159215	739007	531299	663853	292900	814162	687750
RP_POS_156_0416a0_549	RP	POS	0.55	156.0416				1.47E-03	-0.45	1.09	1.60E-01	0.31	1.22	1.16E-01	-0.30	1.01	4.03E-04	-0.61	1.31	2455138	477376	2009846	1074879	1858350	971161	2161342	1159446
HILIC_NEG_215_03285a4_804	HILIC	NEG	4.804	215.0329				7.90E-02	0.27	0.54	1.60E-01	0.31	0.98	5.75E-02	0.42	0.71	4.44E-01	0.11	0.53	2307616	589745	2578347	1114134	2421042	736324	2735651	1383926
RP_POS_345_25681a10_65	RP	POS	10.65	345.2568				1.97E-01	-0.19	0.64	1.60E-01	0.31	0.86	8.92E-01	-0.03	0.45	4.88E-03	-0.34	1.09	2235273	322682	2119992	680406	2023737	317588	2216246	903096
RP_POS_441_29816a15_229	RP	POS	15.23	441.2982				8.86E-01	0.03	0.31	1.60E-01	0.29	1.28	4.45E-01	0.17	0.41	5.95E-01	-0.12	0.62	13246780	6222905	13432950	6745482	12483793	6431850	14382107	6980286
RP_POS_293_04486a7_72	RP	POS	7.72	293.0449				5.85E-01	-0.07	0.56	1.61E-01	0.32	0.99	6.81E-01	0.09	0.65	2.27E-04	-0.23	1.55	1742638	807313	1528381	3641284	1012699	861662	2044063	5050081
RP_POS_787_47137a10_886	RP	POS	10.89	787.4714				9.15E-02	0.20	0.79	1.61E-01	-0.32	1.03	7.51E-01	0.04	0.62	5.94E-02	0.36	0.97	2550097	213983	2763019	1192542	2930751	1370945	2595286	967693
HILIC_POS_325_17117a0_523	HILIC	POS	0.523	325.1712				3.94E-02	0.35	0.89	1.61E-01	0.30	0.97	2.24E-02	0.50	0.85	2.61E-01	0.20	0.45	5436278	3400020	7060765	4889523	6373313	4014410	7748218	5587739
RP_POS_610_30902a10_325	RP	POS	10.33	610.3090				2.17E-01	-0.29	0.82	1.61E-01	-0.26	1.01	9.52E-02	-0.42	0.83	5.20E-01	-0.16	0.63	1580294	546406	1448787	410911	1506516	425888	1391057	391100
RP_POS_260_00888a4_299	RP	POS	4.30	260.0089				9.65E-01	-0.01	0.25	1.61E-01	0.29	0.89	5.92E-01	0.14	0.35	3.22E-01	-0.16	0.52	840129	4435938	798020	5279948	50806	22666	1545234	7428638
HILIC_POS_176_12799a5_341	HILIC	POS	5.341	176.1280				5.82E-01	0.11	0.27	1.61E-01	0.29	0.98	2.72E-01	0.25	0.44	8.62E-01	-0.04	0.48	454864	481643	510399	530374	435894	479513	584904	571903
HILIC_POS_288_28952a0_524	HILIC	POS	0.524	288.2895				3.64E-01	-0.19	0.47	1.61E-01	0.28	0.90	8.18E-01	-0.06	0.33	1.45E-01	-0.33	0.57	644365	122486	621923	114067	605899	102281	637947	123704
RP_POS_386_19916a10_857	RP	POS	10.86	386.1992				1.37E-01	-0.31	0.94	1.61E-01	-0.28	0.91	5.79E-02	-0.45	0.92	4.37E-01	-0.17	0.65	2253674	672614	2049122	643407	2139492	598620	1958752	679249
RP_POS_334_30774a11_603	RP	POS	11.60	334.3077				5.08E-08	0.77	1.32	1.62E-01	0.30	1.32	2.21E-05	0.92	1.43	6.92E-06	0.62	1.44	2851277	1036079	4626927	2442451	4283473	1658611	4970381	3010176
RP_POS_165_05449a1_268	RP	POS	1.27	165.0545				2.42E-01	0.20	0.95	1.62E-01	0.30	1.07	1.12E-01	0.35	1.13	7.76E-01	0.05	0.60	3227659	788060	3437923	1112138	3281778	905553	3594067	1276385
RP_NEG_403_16251a11_163	RP	NEG	11.16	403.1625				9.55E-01	-0.01	0.59	1.62E-01	-0.30	1.00	4.49E-01	-0.16	0.39	4.71E-01	0.14	0.64	2357467	113791	2356012	159738	2378418	147195	2333606	169889
RP_POS_301_1181a5_921	RP	POS	5.92	301.1181				7.61E-01	-0.05	0.68	1.62E-01	0.31	1.34	6.34E-01	0.11	0.48	1.24E-01	-0.20	0.85	650769	372918	621110	713319	520670	361932	721550	936189
RP_POS_301_87332a15_557	RP	POS	15.56	301.8733				5.89E-01	0.12	0.57	1.62E-01	-0.27	0.88	9.33E-01	-0.02	0.13	2.96E-01	0.25	0.47	1494936	77663	1503314	69714	1513085	73514	1493544	64963
HILIC_POS_256_01511a0_541	HILIC	POS	0.541	256.0151				9.02E-01	0.02	0.67	1.62E-01	0.31	0.93	3.55E-01	0.17	0.33	4.20E-01	-0.14	0.93	187422625	20814794	188168218	47559358	181504710	44545529	194831726	49950225
HILIC_POS_583_25488a0_525	HILIC	POS	0.525	583.2549				2.87E-03	0.43	0.93	1.62E-01	0.31	1.22	7.40E-03	0.59	0.97	4.48E-02	0.28	1.04	644068	429832	1008329	922186	878856	611726	1137803	1144460
RP_POS_619_61267a11_246	RP	POS	11.25	619.6127				4.65E-06	0.57	1.03	1.63E-01	0.31	1.32	1.14E-03	0.73	1.13	8.98E-06	0.42	1.33	2987950	4282327	12561046	18490219	9960349	8855381	15161742	24464926
RP_POS_150_96902a15_487	RP	POS	15.49	150.9690				3.28E-01	0.19	0.93	1.63E-01	0.29	0.95	1.61E-01	0.33	0.86	8.17E-01	0.05	0.67	50466974	7916390	52099992	8829065	50862219	6790187	53337765	10404917
HILIC_POS_266_16507a0_637	HILIC	POS	0.637	266.1651				1.19E-01	0.18	0.42	1.63E-01	0.32	0.85	1.40E-01	0.34	0.64	1.50E-02	0.02	0.82	4639	3167	1057505	6696614	113057	304182	2001952	9417620
RP_POS_223_09453a10_282	RP	POS	10.28	223.0945				7.32E-01	0.07	0.25	1.63E-01	-0.27	0.83	7.82E-01	-0.06	0.20	3.84E-01	0.21	0.41	6497565	2221869	6649841	2029878	6933769	2160278	6365913	1869112
RP_POS_721_43457a10_915	RP	POS	10.92	721.4346				1.87E-05	0.58	1.25	1.63E-01	-0.31	1.06	6.96E-04	0.43	1.29	7.14E-04	0.74	1.19	1200400	393360	1754359	1032941	1899137	1297067	1609580	656162
RP_NEG_199_80464a15_584	RP	NEG	15.58	199.8046				1.21E-01	-0.32	0.64	1.63E-01	-0.28	1.00	4.05E-02	-0.46	0.82	4.31E-01	-0.18	0.39	16560734	491215	16404346	478404	16471231	511206	16337461	438121
RP_NEG_243_75459a15_587	RP	NEG	15.59	243.7546				1.47E-01	-0.28	0.59	1.63E-01	-0.29	0.98	4.40E-02	-0.42	0.80	5.55E-01	-0.13	0.26	10131479	318933	10032416	369832	10084119	399962	9980713	333042
RP_POS_184_0732a10_501	RP	POS	10.50	184.0732				6.23E-02	0.37	1.11	1.64E-01	-0.28	1.23	3.11E-01	0.23	0.80	1.74E-02	0.51	1.16	2283940	470429	2467879	492154	2536654	434881	2399105	539074
RP_POS_941_55951a10_836	RP	POS	10.84	941.5595				6.65E-07	0.61	1.19	1.64E-01	-0.31	1.13	1.72E-04	0.45	1.39	2.66E-04	0.76	1.37	381955	116904	765330	698205	863062	856828	667599	480920
HILIC_POS_188_13931a0_727	HILIC	POS	0.727	188.1393				1.68E-01	0.16	0.46	1.64E-01	-0.32	0.83	5.64E-01	0.00	0.21	1.66E-01	0.32	0.42	16143	9892	118373	736245	221949	1035936	14798	10798
RP_POS_133_03468a10_571	RP	POS	10.57	133.0347				4.15E-02	0.38	0.69	1.64E-01	-0.29	0.84	2.90E-01	0.24	0.55	8.68E-03	0.53	1.16	1707188	632514	1987960	753313	2093222	626853	1882698	854976
RP_POS_230_17509a7_139	RP	POS	7.14	230.1751				7.77E-01	0.07	0.59	1.64E-01	-0.26	0.87	8.18E-01	-0.06	0.53	4.39E-01	0.20	0.48	1018731	798320	1062227	586667	1144130	544827	980324	620366

Supplementary table 1: Metabolomics results (in asceding order according to p-value from progressive ALD vs non-progressive ALD comparison, with molecular features with ID_level of 1-2 first)

							all_ALD_vs_control			Prog_ALD_vs_non-prog_ALD			Prog_ALD_vs_control_ALD			Non-prog_ALD_vs_control			Healthy_control		all_ALD		Non-prog_ALD		Progressive_ALD	
							t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA								
Feature_ID	RP_HILIC	POS_NEG	Average.Rt	Average.Mz	Metabolite.name	curated_MSMS	ID_level	p	d	VIP	p	d	VIP	p	d	VIP	p	d	VIP	Mean	SD	Mean	SD	Mean	SD	Mean	SD
RP_POS_225_11047a6_819	RP	POS	6.82	225.1105				2.55E-01	0.25	0.61	1.64E-01	0.27	0.84	1.18E-01	0.38	0.67	6.24E-01	0.11	0.48	1574800	307718	1644996	273618	1606798	250629	1683195	292350
RP_POS_323_99603a4_552	RP	POS	4.55	323.9960				2.21E-03	-0.65	1.01	1.64E-01	-0.27	0.96	1.04E-03	-0.78	1.23	2.06E-02	-0.51	0.87	853143	496689	530872	476704	597337	439412	464407	506984
HILIC_POS_375_32153a4_054	HILIC	POS	4.054	375.3215				9.18E-01	0.02	0.43	1.65E-01	-0.28	0.81	5.97E-01	-0.12	0.30	4.51E-01	0.16	0.42	4427326	1226150	4453644	1306040	4635644	1196885	4271643	1395047
RP_POS_799_39441a7_549	RP	POS	7.55	799.3944				8.42E-01	-0.04	0.85	1.65E-01	0.28	0.98	6.79E-01	0.10	0.74	4.46E-01	-0.18	0.88	645409	47669	643491	44797	637250	45897	649733	43225
RP_POS_575_49164a14_002	RP	POS	14.00	575.4916				9.53E-01	0.01	0.28	1.65E-01	-0.28	0.93	5.94E-01	-0.13	0.38	4.90E-01	0.15	0.48	2447747	822727	2457674	810601	2570634	712737	2344714	890799
RP_POS_600_46643a10_463	RP	POS	10.46	600.4664				5.87E-02	-0.36	0.95	1.65E-01	0.28	0.91	3.40E-01	-0.22	0.68	1.21E-02	-0.51	1.13	4037282	398280	3875942	452356	3812896	357894	3938987	526525
RP_POS_805_55402a12_82	RP	POS	12.82	805.5540				2.16E-06	-1.16	1.87	1.65E-01	-0.22	0.93	7.51E-07	-1.27	1.94	2.12E-05	-1.06	1.62	27415116	9954002	16997826	6961583	17966118	6915136	16029533	6941453
RP_POS_685_4342a11_61	RP	POS	11.61	685.4342				8.81E-01	-0.02	0.61	1.65E-01	0.30	0.92	4.55E-01	0.13	0.57	4.07E-01	-0.18	0.71	2785540	283920	2775134	476404	2708821	545671	2841447	389643
HILIC_NEG_247_95482a0_833	HILIC	NEG	0.833	247.9548				8.30E-01	-0.04	0.79	1.65E-01	-0.29	1.15	3.88E-01	-0.19	0.56	5.83E-01	0.11	0.57	407610	104615	402643	137825	421813	126818	383472	146787
RP_POS_474_25967a10_139	RP	POS	10.14	474.2597				2.89E-04	0.55	1.10	1.66E-01	0.30	0.91	3.51E-04	0.70	1.32	2.29E-02	0.41	0.82	1217650	962887	2145328	1788023	1896753	1684468	2393902	1869696
HILIC_POS_269_12582a1_435	HILIC	POS	1.435	269.1258				9.67E-02	-0.46	0.94	1.66E-01	-0.22	0.83	4.47E-02	-0.57	1.06	2.27E-01	-0.35	0.55	747879	861230	476905	457195	540485	523318	413325	374446
RP_NEG_217_02945a0_549	RP	NEG	0.55	217.0295				1.23E-01	0.21	0.53	1.66E-01	0.31	0.93	9.48E-02	0.37	0.62	6.46E-01	0.06	0.82	69921387	7077748	73311269	17888681	70818459	10520143	75804078	22873245
HILIC_POS_400_34122a0_615	HILIC	POS	0.615	400.3412				1.40E-04	0.73	1.52	1.66E-01	-0.27	0.87	3.37E-03	0.60	1.33	1.08E-04	0.87	1.61	1330227	534583	1789514	615992	1875101	664877	1703926	556439
RP_NEG_493_24509a9_147	RP	NEG	9.15	493.2451				4.62E-02	0.25	0.80	1.66E-01	0.31	1.37	6.35E-02	0.41	0.95	3.27E-01	0.10	0.96	1836321	1358599	2915871	4794336	2247510	2406866	3584232	6303631
HILIC_NEG_230_0128a0_626	HILIC	NEG	0.626	230.0128				8.23E-02	0.20	0.46	1.66E-01	-0.32	0.82	2.24E-01	0.04	0.44	1.15E-01	0.36	0.47	22437	50786	191569	959462	325680	1336630	57459	191409
HILIC_NEG_200_85867a7_017	HILIC	NEG	7.017	200.8587				2.27E-01	-0.26	0.47	1.66E-01	-0.27	0.97	8.70E-02	-0.39	0.84	6.05E-01	-0.12	0.20	2892691	1271902	2582429	1167419	2744413	1244461	2420444	1072993
RP_NEG_870_54944a13_159	RP	NEG	13.16	870.5494				4.29E-01	0.16	0.34	1.67E-01	0.28	0.88	1.77E-01	0.30	0.63	9.39E-01	0.02	0.42	7658154	2653201	8093184	2795157	7705533	2876391	8480835	2684202
RP_NEG_385_04672a8_81	RP	NEG	8.81	385.0467				4.05E-03	0.38	0.94	1.67E-01	0.31	0.87	1.29E-02	0.54	0.92	5.96E-02	0.23	0.91	988374	407958	1384525	1145546	1225234	712839	1543817	1446170
RP_POS_194_00798a15_625	RP	POS	15.63	194.0080				5.13E-01	-0.13	0.46	1.67E-01	-0.28	1.02	2.24E-01	-0.27	0.47	9.59E-01	0.01	0.52	5846218	2034819	5569586	2171051	5870617	2171676	5268554	2149884
RP_POS_1058_77356a0_491	RP	POS	0.49	1058.7736				6.53E-03	0.35	0.99	1.67E-01	0.31	1.33	8.68E-03	0.51	1.09	1.87E-01	0.20	1.05	747080	175229	924404	561695	846518	480154	1002289	628103
HILIC_POS_126_05524a0_723	HILIC	POS	0.723	126.0552				1.66E-01	0.16	0.46	1.67E-01	-0.32	0.82	3.91E-01	0.00	0.35	1.67E-01	0.32	0.41	24219	15198	4185100	29837579	8348766	41992276	21434	12572
RP_NEG_230_01279a2_224	RP	NEG	2.22	230.0128				1.50E-02	0.30	0.48	1.67E-01	-0.32	0.88	2.65E-02	0.14	0.86	4.80E-02	0.45	0.58	1266175	1635806	3451643	8370366	4617755	11523825	2285530	2445860
RP_POS_429_37219a11_237	RP	POS	11.24	429.3722				1.66E-01	-0.25	0.72	1.67E-01	-0.29	0.98	8.52E-02	-0.40	0.77	5.64E-01	-0.11	0.30	890416	353876	782776	446011	844582	342446	720969	526161
HILIC_POS_98_06068a0_723	HILIC	POS	0.723	98.0607				1.65E-01	0.16	0.46	1.68E-01	-0.32	0.82	1.42E-01	0.00	0.53	1.67E-01	0.32	0.41	15897	16307	1420764	10031711	2819357	14118491	22171	21882
RP_POS_182_02361a11_209	RP	POS	11.21	182.0236				4.93E-03	-0.59	1.33	1.68E-01	-0.27	0.94	2.09E-03	-0.73	1.24	3.97E-02	-0.46	1.26	1420880	147070	1333986	140353	1353411	133238	1314561	145869
RP_NEG_243_96844a1_3	HILIC	NEG	1.3	243.9684				2.11E-07	0.87	1.42	1.68E-01	0.28	1.25	5.65E-06	1.01	1.46	1.08E-05	0.73	1.71	40971977	7133853	50428955	10888877	48919651	7819885	51938260	13181633
RP_POS_665_47351a10_851	RP	POS	10.85	665.4735				8.25E-01	0.04	0.87	1.68E-01	-0.28	1.12	6.87E-01	-0.10	0.77	3.83E-01	0.18	0.92	1478982	733259	1512267	759171	1617375	634040	1407159	860169
RP_NEG_297_15439a12_418	RP	NEG	12.42	297.1544				7.79E-01	-0.06	0.63	1.68E-01	0.28	0.90	7.14E-01	0.09	0.54	3.40E-01	-0.20	0.62	1554214	967022	1497569	1048175	1352443	861813	1642694	1197521
RP_POS_425_78445a14_328	RP	POS	14.33	425.7845				8.43E-01	-0.04	0.44	1.68E-01	0.26	0.88	7.29E-01	0.09	0.52	4.50E-01	-0.18	0.42	1072578	728450	1044123	610391	959642	520251	1128603	683763
RP_POS_850_71875a0_5	RP	POS	0.50	850.7188				1.98E-01	0.25	0.78	1.68E-01	-0.28	1.28	6.32E-01	0.10	0.46	7.51E-02	0.39	0.92	511732	249373	580186	287131	619904	286767	540467	284809
RP_POS_428_80298a10_653	RP	POS	10.65	428.8030				9.65E-01	-0.01	0.25	1.68E-01	0.27	0.90	5.86E-01	0.13	0.71	5.22E-01	-0.15	0.40	775652	295648	773000	282311	733953	270768	812046	290858
RP_NEG_195_81117a15_584	RP	NEG	15.58	195.8112				1.66E-01	-0.29	0.66	1.68E-01	-0.28	0.98	5.71E-02	-0.42	0.78	5.29E-01	-0.15	0.45	28277556	844486	28037297	837922	28153186	904741	27921407	756697
RP_POS_287_19672a0_612	RP	POS	0.61	287.1967				2.28E-01	0.19	1.07	1.68E-01	0.30	1.18	1.05E-01	0.34	1.34	8.35E-01	0.04	0.55	2991040	4044770	4226401	7244475	3224740	6052174	5228062	8207284
HILIC_POS_62_06092a3_773	HILIC	POS	3.773	62.0609				1.62E-05	0.59	1.11	1.68E-01	0.30	1.00	2.97E-04	0.74	1.25	2.65E-03	0.44	1.12	2316430	616615	3173685	1568935	2956800	1236462	3390570	1829894
HILIC_POS_177_07468a1_233	HILIC	POS	1.233	177.0747				1.71E-06	-1.07	1.94	1.69E-01	-0.24	0.88	2.02E-06	-1.18	1.84	1.49E-05	-0.95	2.16	721217	154255	555096	133862	573609	97407	536583	161296
RP_NEG_262_99371a8_012	RP	NEG	8.01	262.9937				1.00E-01	-0.32	0.54	1.69E-01	-0.28	0.94	3.14E-02	-0.46	0.86	4.31E-01	-0.17	0.48	4592413	224835	4513442	255473	4548721	270385	4478164	237100
RP_POS_133_03165a0_71	RP	POS	0.71	133.0317				4.20E-01	-0.10	0.46	1.69E-01	0.32	0.94	8.09E-01	0.05	0.28	1.95E-03	-0.26	1.41	4671177	616754	4475827	2156950	4176397	770357	4775256	2936561
RP_POS_172_13304a10_271	RP	POS	10.27	172.1330				7.53E-01	-0.06	0.81	1.69E-01	0.28	0.83	7.53E-01	0.08	0.78	3.25E-01	-0.20	0.62	8178793	461579	8148923	476707	8083054	363830	8214791	563835
RP_POS_341_26624a10_536	RP	POS	10.54	341.2662				6.38E-01	-0.09	0.53	1.69E-01	0.28	0.88	8.16E-01	0.05	0.44	2.90E-01	-0.23	0.53	3010690	694676	2941921	774595	2835034	777868	3048807	764098
RP_POS_185_03024a0_713	RP	POS	0.71	185.0302				9.42E-05	0.62	1.05	1.69E-01	0.29	0.85	3.66E-04	0.76	1.25	4.32E-03	0.47	0.98	968251	171541	1141404	296262	1100506	235021	1182301	344507
RP_POS_1047_7334a10_932	RP	POS	10.93	1047.7334				1.02E-01	-0.41	1.04	1.69E-01	-0.24	1.43	4.98E-02	-0.53	0.93	2.65E-01	-0.29	0.85	32602795	19053242	26571692	12936956	28356065	11914605	24787319	13772782
RP_POS_199_13045a12_888	RP	POS	12.89	199.1305				7.10E-01	-0.08	0.51	1.69E-01	-0.27	0.93	3.81E-01	-0.22	0.63	8.03E-01	0.06	0.18	20966252	9335289	20269680	8595685	21455345	7422830	19084015	9555736
RP_POS_577_00537a10_874	RP	POS	10.87	577.0054				2.74E-01	0.14	0.75	1.69E-01	-0.31	0.90	8.76E-01	-0.02	0.45	1.50E-01	0.29	0.82	548038	87192	589035	339662	635930	411262	542140	243865
RP_POS_319_12885a5_731	RP	POS	5.73	319.1289				7.07E-01	-0.06	0.66	1.69E-01	0.31	1.30	6.69E-01	0.10	0.47	1.02E-01	-0.21	0.86	885988	499525	835619	1004256	696657	510625	974582	1318141
RP_POS_604_37885a11_108	RP	POS	11.11	604.3789				2.07E-07	0.62	1.29	1.69E-01	-0.31	1.29	6.29E-04	0.47	1.33	8.34E-05	0.77	1.41	22774	21988	328199	546039	403510	626940	252888	444718
RP_POS_126_05495a0_71	RP	POS	0.71	126.0550				1.68E-01	0.16	0.58	1.69E-01	-0.32	0.85	5.22E-01	0.00	0.77	1.69E-01	0.32	0.58	3907	2878	717946	5141090	1431444	7236164	4448	4731
RP_POS_511_29587a11_476	RP	POS	11.48	511.2959				2.41E-01	-0.22	0.57	1.70E-01	0.29	1.01	7.30E-01	-0.07	0.50	8.43E-02	-0.36	0.74	2038793	110965	2010653	134297	1992151	127595	2029154	139501
HILIC_NEG_234_82022a6_157	HILIC	NEG	6.157	234.8202				6.02E-02	0.35	1.55	1.70E-01	0.28	1.56	2.86E-02	0.50	1.57	2.91E-01	0.21	1.15	872943	145001	932034	171916	908345	150261	955723	189710
RP_POS_429_31924a10_451	RP	POS	10.45	429.3192				9.59E-02	-0.32	0.75	1.70E-01	0.28	1.11	4.34E-01	-0.17	0.51	2.80E-02	-0.46	0.93	31599547	1934915	30906368	2257176	30595517	2036160	31217220	2439367
HILIC_POS_64_01661a2_223	HILIC	POS	2.223	64.0166				9.33E-01	-0.02	0.61	1.70E-01	-0.28	0.93	4.80E-01	-0.16	0.34	5.67E-01	0.12	0.35	3125229	765039	3111858	841014	3227605	816131	2996112	857690
RP_POS_818_60266a14_573	RP	POS	14.57	818.6027				4.68E-05	-0.87	1.49	1.70E-01	-0.25	0.81	8.66E-06	-1.00	1.71	1.58E-03	-0.75	1.35	2538753	1052624	1599666	982327	1734938	1119460	1464394	811844
RP_POS_408_16104a4_275	RP	POS	4.28	408.1610				5.67E-02	0.27	0.70	1.70E-01	0.31	0.97	5.12E-02	0.42	0.91	3.91E-01	0.12	0.49	1679095	628857	2030786	1450562	1830812	963486	2230760	1800357
HILIC_NEG_161_02644a1_297	HILIC	NEG	1.297	161.0264				4.02E-06	0.76	1.32	1.70E-01	0.28	0.93	5.30E-06	0.90	1.56	1.28E-03	0.61	1.06	341130	113651	474558	181160	449650	180580	499466	180090
RP_POS_230_96573a15_325	RP	POS	15.33	230.9657				1.84E-01	-0.20	0.44	1.70E-01	-0.30	0.98	6.55E-02	-0.35	0.74	7.80E-01	-0.05	0.37	1020679	51485	1002938	96320	1016181	93698	989695	98017
RP_POS_599_88562a11_096	RP	POS	11.10	599.8856				4.81E-07	0.60	1.29	1.71E-01	-0.31	1.26	4.76E-04	0.45	1.34	1.88E-04	0.75	1.38	82135	32927	414734	615228	499384	729422	330085	466965
RP_NEG_159_10199a6_563	RP	NEG	6.56	159.1020				2.32E-02	0.34	0.94	1.71E-01	0.30	1.06	3.37E-02	0.49	0.87	1.42E-01	0.19	1.13	1059093	548626	1396149	1096229	1244937	559413	1547362	1438177
RP_POS_1058_72009a10_931	RP	POS	10.93	1058.7201				2.28E-02	-0.52	1.14	1.71E-01	-0.25	1.42	7.61E-03	-0.65	1.21	1.11E-01	-0.40	0.93	427719	257719	309689	207142	338154	222903	281224	188021
HILIC_NEG_202_92886a4_213	HILIC	NEG	4.213	202.9289				1.16E-01	-0.32	0.69	1.71E-01	0.28	0.99	4.28E-01	-0.18	0.49	4.20E-02	-0.45	0.86	3453653	1015203	3121565	1050764	2977207	1014806	3265923	1076282
HILIC_NEG_500_27789a1_711	HILIC	NEG	1.711	500.2779				2.15E-06	0.86	1.45	1.71E-01	-0.27	0.77	8.43E-04	0.72	1.17	2.86E-07	0.99	2.05	468475	165350	656859	216217	686574	175548	627144	248665
HILIC_POS_144_10185a3_51	HILIC	POS	3.51	144.1019				1.98E-01	0.22	0.51	1.71E-01	0.29	0.95	8.10E-02	0.36	0.66	7.14E-01	0.07	0.28	493483418	565301033	662929831	837530419	547907021	770563639	777952640	892446655
RP_POS_782_73035a0_501	RP	POS	0.50	782.7304				9.30E-01	0.02	0.83	1.71E-01	-0.29	1.25	4.87E-01	-0.13	0.58	4.43E-01	0.16	0.96	479628	227993	484244	328700	529389	355872	439099	295785
HILIC_NEG_262_98703a2_172	HILIC	NEG	2.172	262.9870				4.58E-01	0.14	0.53	1.71E-01	-0.28	1.00	9.95E-01	0.00	0.24	2.19E-01	0.28	0.50	838920	385688	899352	436410	959291	488334	839413	372817
RP_NEG_462_17764a6_604	RP	NEG	6.60	462.1776				3.67E-03	0.46	1.55	1.71E-01	-0.29	0.83	7.74E-02	0.31	1.33	3.21E-03	0.61	1.12	1031435	1219816	1929704	2103558	2218471	2299887	1640937	1865627
RP_POS_549_30853a10_522	RP	POS	10.52	549.3085				4.71E-01	-0.21	0.57	1.71E-01	-0.21	0.84	2.92E-01	-0.31	0.54	7.30E-01	-0.10	0.57	552513	600949	472310	292985	512505	313169	432115	268440
RP_POS_537_39258a13_626	RP	POS	13.63	537.3926				4.86E-01	-0.16	0.50	1.71E-01	0.26	0.80	9.20E-01	-0.02	0.27	2.28E-01	-0.29	0.68	798377	340526	751481	287480	712049	262975	790913	307648
HILIC_POS_156_07684a7_096	HILIC	POS	7.096	156.0768				7.70E-01	-0.05	1.04	1.72E-01	-0.29	1.04	3.12E-01	-0.20	1.08	6.54E-01	0.10	0.90	1374039	508316	1340516	702216	1436796	752535	1244236	641132
HILIC_NEG_149_04254a0_928	HILIC	NEG	0.928	149.0425				5.71E-05	0.57	0.94	1.72E-01	-0.30	1.27	3.00E-02	0.42	0.70	1.37E-05	0.72	1.47	426044	208065	677206	475846	742439	405240	611974	533457
RP_POS_365_17801a11_125	RP	POS	11.13	365.1780				5.18E-07	0.81	1.70	1.72E-01	0.28	1.03	3.94E-06	0.95	1.67	1.59E-04	0.67	1.55	316404	157031	522450	259909	486868	232168	558033	282840
RP_POS_321_23993a10_005	RP	POS	10.01	321.2399				7.30E-11	0.86	1.50	1.73E-01	0.29	1.45	3.03E-06	1.01	1.52	2.24E-08	0.72	1.78	1092323	552069	2481547	1695925	2249082	1113593	2714012	2112024
RP_POS_161_13258a8_589	RP	POS	8.59	161.1326				8.33E-01	0.05	0.32	1.73E-01	0.26	0.83	4.68E-01	0.18	0.60	7.22E-01	-0.08	0.40	13132306	1646167	13200655	1408601	13008017	1340423	13393292	1461622
RP_POS_267_19308a9_919	RP	POS	9.92	267.1931				1.85E-04	0.58	1.55	1.73E-01	0.29	1.25	2.21E-04	0.73	1.49	1.62E-02	0.44	1.29	916257	222758	1133556	395983	1079427	378065	1187686	409747
HILIC_POS_249_06113a4_123	HILIC	POS	4.123	249.0611				5.15E-03	-0.46	1.20	1.73E-01	-0.29	1.43	5.00E-03	-0.61	1.29	7.06E-02	-0.31	1.18	1328035	195408	1195388	306152	1237263	250732	1153513	350607
RP_POS_602_36322a11_096	RP	POS	11.10	602.3632				3.40E-07	0.61	1.30	1.73E-01	-0.30	1.29	5.39E-04	0.46	1.36	1.37E-04	0.76	1.40	76902	90868	1040894	1757408	1281053	2054795	800735	1378442
RP_POS_266_15903a4_569	RP	POS	4.57	266.1590				1.96E-01	0.19	0.37	1.73E-01	0.30	0.95	1.45E-01	0.34	0.57	7.67E-01	0.03	0.33	1086787	72923	1113445	159480	1091569	67635	1135322	214093
HILIC_POS_133_98238a5_19	HILIC	POS	5.19	133.9824				5.30E-02	0.30	0.59	1.74E-01	0.30	0.82	4.44E-02	0.44	0.67	3.25E-01	0.15	0.38	23585	31114	39209	57809	31302	39044	47117	71414
RP_POS_816_55237a13_022	RP	POS	13.02	816.5524				3.73E-05	-0.84	1.65	1.74E-01	-0.26	0.87	1.34E-05	-0.97	1.74	1.28E-03	-0.71	1.43	1997026	680718	1370638	702063	1466420	723971	1274856	673043
RP_POS_774_54211a13_381	RP	POS	13.38	774.5421				4.16E-03	-0.53	1.21	1.74E-01	0.28	0.87	9.68E-02	-0.39	0.79	3.32E-04	-0.67	1.37	3030068	991309	2391841	1242230	2222112	841726	2561569	1533123
RP_POS_187_1321a10_38	RP	POS	10.38	187.1321				7.66E-01	0.07	0.69	1.74E-01	0.26	1.09	4.38E-01	0.20	0.55	7.88E-01	-0.06	0.57	2531039	297325	2548445	247326	2514717	210801	2582173	277182
HILIC_POS_283_17523a0_615	HILIC	POS	0.615	283.1752				9.01E-01	0.03	1.05	1.74E-01	-0.24	1.04	7.41E-01	-0.09	0.85	5.98E-01	0.15	1.05	589173	1539473	625452	972776	758197	1172356	492706	708180
RP_NEG_380_92154a15_428	RP	NEG	15.43	380.9215				6.43E-01	-0.09	0.29	1.74E-01	-0.27	0.96	2.88E-01	-0.23	0.66	8.57E-01	0.04	0.44	1092494	54410	1087336	54918	1094818	60336	1079854	48360
RP_POS_548_38831a11_476	RP	POS	11.48	548.3883				5.84E-01	-0.09	0.47	1.75E-01	0.29	0.96	8.01E-01	0.05	0.42	2.45E-01	-0.24	0.54	2990458	175914	2968705	244873	2935368	249208	3002042	238278
RP_POS_553_45856a12_423	RP	POS	12.42	553.4586				6.19E-01	0.10	0.51	1.75E-01	0.27	0.84	3.00E-01	0.24	0.58	8.73E-01	-0.04	0.42	10727554	4710575	11207343	4776066	10557218	4611831	11857468	4894445
HILIC_POS_118_08667a4_858	HILIC	POS	4.858	118.0867				7.91E-01	-0.05	1.02	1.75E-01	-0.29	1.11	3.75E-01	-0.19	0.67	6.51E-01	0.09	0.75	83253906	22891366	81943148	28227241	85784576	27013463	78101721	29154286
RP_POS_1063_67004a10_198	RP	POS	10.20	1063.6700				3.35E-01	-0.25	0.91	1.75E-01	-0.23	1.26	1.88E-01	-0.37	0.75	6.06E-01	-0.14	0.84	512716	656901	393088	390809	446269	376412	339907	401399
RP_POS_552_33136a10_932	RP	POS	10.93	552.3314				4.02E-02	-0.48	1.21	1.75E-01	-0.25	1.63	1.72E-02	-0.61	1.16	1.47E-01	-0.36	0.99	6301263	1888046	5531327	1452587	5728977	1412790	5333677	1478980
RP_POS_798_06024a13_378	RP	POS	13.38	798.0602				8.68E-01	-0.03	0.55	1.75E-01	-0.28	0.80	4.32E-01	-0.17	0.45	6.32E-01	0.11	0.36	991194	441380	975862	481730	1041388	491585	910336	467381
RP_NEG_508_34042a10_934	RP	NEG	10.93	508.3404				1.53E-01	-0.34	1.06	1.75E-01	-0.25	1.60	7.49E-02	-0.46	0.98	3.88E-01	-0.21	0.87	2268941	625659	2093781	477997	2158795	434316	2028768	514169
RP_POS_749_3819a4_792	RP	POS	4.79	749.3819				8.44E-08	0.66	1.17	1.75E-01	0.30	1.25	8.45E-06	0.81	1.46	1.48E-03	0.51	1.14	365258	156029	869007	837005	755246	800190	982767	865295

Supplementary table 1: Metabolomics results (in asceding order according to p-value from progressive ALD vs non-progressive ALD comparison, with molecular features with ID_level of 1-2 first)

							all_ALD_vs_control			Prog_ALD_vs_non-prog_ALD			Prog_ALD_vs_control_ALD			Non-prog_ALD_vs_control			Healthy_control		all_ALD		Non-prog_ALD		Progressive_ALD	
							t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA								
Feature_ID	RP_HILIC	POS_NEG	Average.Rt	Average.Mz	Metabolite.name	curated_MSMS	ID_level	p	d	VIP	p	d	VIP	p	d	VIP	p	d	VIP	Mean	SD	Mean	SD	Mean	SD	Mean	SD
RP_POS_379_25018a12_766	RP	POS	12.77	379.2502				6.77E-02	-0.35	0.76	1.76E-01	0.28	0.89	3.43E-01	-0.21	0.50	2.20E-02	-0.49	0.90	2423625	633437	2173852	740459	2073372	701357	2274333	771520
RP_POS_591_68073a10_88	RP	POS	10.88	591.6807				9.09E-01	-0.01	0.87	1.76E-01	-0.31	0.87	2.55E-01	-0.17	0.65	4.43E-01	0.14	0.83	774488	70567	770186	354229	818248	390844	722124	309910
RP_POS_317_05591a0_587	RP	POS	0.59	317.0559				8.12E-01	-0.05	0.60	1.77E-01	-0.27	1.13	3.80E-01	-0.19	0.48	7.06E-01	0.09	0.75	697280	662408	664808	689351	758292	782290	571324	574713
RP_POS_441_29712a11_645	RP	POS	11.65	441.2971				6.04E-01	-0.11	0.38	1.77E-01	-0.27	1.09	1.97E-01	-0.24	0.76	9.22E-01	0.03	0.32	28012144	22101145	25698701	21049259	28570373	29476974	22827030	3076249
HILIC_POS_371_2406a7_098	HILIC	POS	7.098	371.2406				9.81E-01	0.00	1.03	1.77E-01	-0.28	1.06	5.32E-01	-0.13	0.97	5.18E-01	0.14	0.91	2053342	529347	2055996	590585	2136021	609764	1975971	565524
RP_POS_424_36362a10_539	RP	POS	10.54	424.3636				1.19E-01	-0.29	0.72	1.77E-01	0.28	0.83	4.94E-01	-0.15	0.46	3.24E-02	-0.43	0.92	1067382	192972	1002734	226051	972101	191915	1033367	253957
RP_POS_824_55511a13_999	RP	POS	14.00	824.5551				2.85E-02	-0.51	0.98	1.77E-01	0.25	0.89	1.33E-01	-0.38	0.82	9.04E-03	-0.63	1.11	7734896	2730693	6534776	2186904	6238461	1874140	6831091	2443585
RP_POS_319_2244a9_925	RP	POS	9.93	319.2244				1.39E-11	0.97	1.61	1.77E-01	-0.27	1.37	2.02E-06	0.83	1.57	4.06E-09	1.11	1.87	1349306	304650	1997967	676367	2089536	684754	1906397	662028
RP_POS_807_51276a12_688	RP	POS	12.69	807.5128				1.11E-03	0.57	1.22	1.77E-01	-0.28	0.87	3.56E-02	0.43	0.93	4.01E-04	0.71	1.23	615885	472835	976477	653956	1064980	622312	887974	678813
HILIC_NEG_238_07747a0_929	HILIC	NEG	0.929	238.0775				1.45E-05	0.57	1.04	1.78E-01	0.30	1.02	1.13E-03	0.72	1.10	1.58E-04	0.43	1.55	3182108	2710066	7408821	8062619	6314836	4438364	8502806	10449726
HILIC_POS_174_11252a4_87	HILIC	POS	4.87	174.1125				4.59E-01	-0.18	0.75	1.78E-01	0.25	0.98	8.35E-01	-0.05	0.13	2.35E-01	-0.30	0.78	561191	675352	464399	498743	396968	468488	531831	523264
HILIC_POS_179_00494a3_757	HILIC	POS	3.757	179.0049				2.66E-01	0.13	0.47	1.78E-01	0.31	1.38	2.13E-01	0.29	0.58	5.27E-01	-0.02	0.35	1220806	1234515	2294202	9354636	1021257	1599416	3567148	13074375
RP_POS_792_5882a13_244	RP	POS	13.24	792.5882				6.18E-02	-0.46	0.95	1.78E-01	-0.24	0.84	2.53E-02	-0.58	0.98	1.92E-01	-0.34	0.69	4831882	2507183	3918516	1724637	4151623	1847866	3685408	1576053
RP_POS_418_74777a12_821	RP	POS	12.82	418.7478				8.87E-06	-1.03	1.67	1.78E-01	-0.23	0.89	3.10E-06	-1.15	1.81	1.30E-04	-0.92	1.44	6350818	2159410	4248887	1716772	4480778	1752264	4016995	1665710
RP_POS_582_59283a14_006	RP	POS	14.01	582.5928				9.09E-01	0.03	0.61	1.78E-01	-0.25	1.16	7.07E-01	-0.10	0.58	5.65E-01	0.15	0.67	1121603	905105	1141390	656209	1230026	688698	1052754	616175
RP_POS_465_29639a11_153	RP	POS	11.15	465.2964				2.29E-03	-0.47	0.99	1.78E-01	0.29	1.00	5.28E-02	-0.32	0.97	3.36E-03	-0.61	1.11	1314838	49010	1275375	91541	1263003	104285	1287746	75782
RP_NEG_915_12708a9_653	RP	NEG	9.65	915.1271				2.80E-01	-0.21	0.47	1.78E-01	-0.28	0.82	1.01E-01	-0.34	0.62	7.65E-01	-0.07	0.36	5384238	323321	5309877	372870	5360232	396890	5259522	343811
HILIC_POS_310_14163a0_518	HILIC	POS	0.518	310.1416				2.77E-01	0.14	0.88	1.78E-01	-0.31	0.81	7.94E-01	-0.02	0.29	2.10E-01	0.29	0.82	905592	1431079	1546998	5298530	2266798	7374933	827198	1129064
RP_POS_300_28876a10_691	RP	POS	10.69	300.2888				1.27E-13	1.11	1.88	1.79E-01	-0.26	0.97	1.24E-08	0.97	1.80	3.21E-10	1.24	2.07	726690	160296	1090410	320735	1133681	342501	1047139	294470
RP_POS_433_7717a14_327	RP	POS	14.33	433.7717				4.27E-01	0.18	0.43	1.79E-01	0.25	0.82	2.27E-01	0.31	0.60	8.12E-01	0.06	0.25	1667200	981162	1819784	778798	1714832	695878	1924736	847765
RP_NEG_339_23337a10_658	RP	NEG	10.66	339.2334				6.72E-05	0.63	1.00	1.79E-01	-0.28	0.87	2.97E-03	0.49	1.04	3.13E-04	0.77	1.13	5258817	4343421	9724865	7436043	10727053	8681017	8722676	5857313
RP_POS_420_24786a12_822	RP	POS	12.82	420.2479				2.68E-05	-1.01	1.67	1.80E-01	-0.22	1.03	1.04E-05	-1.12	1.74	2.66E-04	-0.89	1.46	1980344	845086	1217416	628454	1301948	623241	1132884	628456
HILIC_NEG_234_82027a3_049	HILIC	NEG	3.049	234.8203				2.64E-01	0.20	0.90	1.80E-01	-0.29	0.97	7.81E-01	0.05	0.26	1.21E-01	0.34	0.59	604284	89294	626725	121591	643084	134573	610367	105899
RP_POS_390_7088a0_519	RP	POS	0.52	390.7088				9.84E-03	-0.40	1.00	1.80E-01	0.29	0.99	1.73E-01	-0.26	0.74	4.20E-03	-0.55	1.15	342713	61366	302337	108226	287783	107103	316891	108451
HILIC_POS_153_06589a0_74	HILIC	POS	0.74	153.0659				2.56E-01	-0.20	0.47	1.80E-01	-0.28	0.82	1.11E-01	-0.34	0.55	7.59E-01	-0.06	0.25	8817576	4410032	7705061	5795001	8484445	5290885	6925678	6214200
RP_POS_246_86243a15_458	RP	POS	15.46	246.8624				2.75E-01	-0.26	0.43	1.80E-01	-0.25	1.10	1.39E-01	-0.38	0.61	5.92E-01	-0.13	0.41	2571960	798882	2401495	615175	2484182	573324	2318808	649578
RP_NEG_307_85663a1_013	RP	NEG	1.01	307.8566				3.25E-01	0.19	0.57	1.80E-01	-0.28	0.82	8.28E-01	0.05	0.27	1.11E-01	0.33	0.64	31847	12854	34537	14744	36519	12658	32555	16462
HILIC_NEG_134_89482a4_126	HILIC	NEG	4.126	134.8948				8.98E-01	-0.03	0.39	1.81E-01	0.26	1.12	6.76E-01	0.10	0.25	5.03E-01	-0.16	0.35	19144809	9893394	18894370	8639757	17734205	8143183	20054535	9041894
RP_POS_315_66678a10_932	RP	POS	10.93	315.6668				4.56E-04	-0.82	1.66	1.81E-01	-0.24	1.58	1.81E-04	-0.93	1.64	3.98E-03	-0.70	1.42	3465003	878006	2820778	694671	2914041	688806	2727515	694823
RP_NEG_135_02882a0_569	RP	NEG	0.57	135.0288				8.86E-01	0.02	0.45	1.81E-01	-0.29	0.86	5.38E-01	-0.12	0.52	4.05E-01	0.17	0.53	1561395	505114	1578263	754207	1679515	772328	1477011	729281
RP_POS_384_34857a11_063	RP	POS	11.06	384.3486				2.30E-05	-0.67	1.05	1.81E-01	0.28	0.86	3.68E-03	-0.53	1.02	4.60E-05	-0.81	1.25	2474809	63424	2405056	108907	2390435	113309	2419677	103384
RP_POS_406_7872a10_655	RP	POS	10.66	406.7872				1.06E-01	-0.34	1.21	1.81E-01	0.27	0.83	3.85E-01	-0.20	0.63	3.82E-02	-0.47	1.13	792145	307490	690060	300964	649680	280310	730439	317972
RP_POS_166_98486a10_888	RP	POS	10.89	166.9849				3.25E-05	-0.78	1.29	1.82E-01	0.26	0.91	3.37E-03	-0.64	1.05	5.62E-06	-0.91	1.55	13990508	3627641	10501106	4432818	9906749	3703388	11095464	5026404
HILIC_POS_375_32175a0_528	HILIC	POS	0.528	375.3218				3.30E-03	-0.59	1.42	1.82E-01	-0.26	0.79	2.48E-03	-0.72	1.29	2.42E-02	-0.46	1.14	3150912	765528	2668069	796764	2774873	635088	2561265	925205
RP_POS_583_25421a11_668	RP	POS	11.67	583.2542				4.05E-01	-0.17	0.57	1.82E-01	0.27	1.10	8.87E-01	-0.04	0.30	1.09E-01	-0.31	0.88	1041983	2038570	695473	2012338	424573	756545	966373	2731212
RP_NEG_388_87476a15_403	RP	NEG	15.40	388.8748				3.44E-01	-0.19	0.65	1.82E-01	0.27	0.84	7.82E-01	-0.06	0.65	1.75E-01	-0.33	0.53	1417133	221765	1374047	223872	1344052	255806	1404042	184357
HILIC_NEG_431_58038a1_366	HILIC	NEG	1.366	431.5804				2.99E-10	-0.93	1.53	1.82E-01	-0.27	0.89	3.14E-08	-1.07	1.79	5.03E-06	-0.80	1.61	244530	39509	170633	80318	181384	76428	159882	83407
HILIC_NEG_136_89172a3_131	HILIC	NEG	3.131	136.8917				1.51E-04	-0.64	1.10	1.82E-01	0.28	0.95	9.20E-03	-0.50	1.02	1.20E-04	-0.78	1.30	34391022	7579479	27436035	11177159	25940334	11337452	28931736	10922636
RP_POS_343_29544a8_988	RP	POS	8.99	343.2954				9.91E-02	-0.39	0.84	1.82E-01	-0.25	0.89	2.49E-02	-0.51	1.11	3.38E-01	-0.26	0.67	1124509	271590	1036194	210070	1064426	280872	1007962	92972
RP_POS_199_13034a13_497	RP	POS	13.50	199.1303				5.61E-01	0.10	0.60	1.82E-01	-0.29	1.04	8.27E-01	-0.04	0.58	2.56E-01	0.24	0.43	20255200	7215005	21204602	10054230	22549718	10941085	19859486	8991008
RP_NEG_207_83698a1_323	RP	NEG	1.32	207.8370				2.89E-02	0.39	0.67	1.83E-01	-0.28	0.91	2.08E-01	0.25	0.74	1.40E-02	0.53	0.96	2902755	1191524	3492762	1598703	3706460	1701039	3279063	1475511
RP_POS_776_57794a11_889	RP	POS	11.89	776.5779				1.88E-09	0.73	1.52	1.83E-01	0.29	0.92	2.31E-05	0.88	1.52	3.04E-06	0.59	1.45	161069	114815	736247	853416	622003	609394	850491	1036101
HILIC_POS_256_16983a0_517	HILIC	POS	0.517	256.1698				2.10E-01	0.14	0.38	1.83E-01	0.31	0.77	1.96E-01	0.30	0.53	1.24E-01	-0.01	0.92	143389	129162	713324	4513211	105902	48241	1320747	6355984
RP_POS_203_99384a15_42	RP	POS	15.42	203.9938				3.67E-01	0.19	0.65	1.83E-01	-0.26	0.84	7.92E-01	0.06	0.46	1.58E-01	0.32	0.77	3298769	811592	3445781	738799	3544530	669370	3347033	796763
HILIC_NEG_183_93427a2_945	HILIC	NEG	2.945	183.9343				2.49E-03	-0.54	0.86	1.83E-01	0.28	0.93	5.60E-02	-0.40	0.73	8.16E-04	-0.67	1.17	483736	82192	426416	110728	411619	104129	441212	116111
RP_NEG_892_79675a0_492	RP	NEG	0.49	892.7968				6.62E-10	-0.77	1.39	1.84E-01	0.29	1.28	1.63E-04	-0.63	1.36	3.72E-07	-0.92	1.60	4830368	380114	3537066	1806210	3296090	1820198	3778041	1777565
RP_POS_343_19147a11_16	RP	POS	11.16	343.1915				4.11E-01	-0.14	0.68	1.84E-01	0.28	0.99	9.88E-01	0.00	0.55	1.63E-01	-0.29	0.80	1349606	101492	1330907	137220	1312615	135445	1349200	137894
RP_POS_391_3399a10_88	RP	POS	10.88	391.3399				5.36E-01	0.10	0.66	1.84E-01	-0.29	0.98	8.46E-01	-0.04	0.41	1.99E-01	0.25	0.99	4594302	278277	4634387	416075	4689846	388897	4578928	438466
RP_POS_1020_1355a0_483	RP	POS	0.48	1020.1355				5.11E-05	0.48	1.07	1.84E-01	-0.30	1.11	3.66E-02	0.33	0.95	3.41E-04	0.63	1.35	238091	19870	329438	213277	357854	218883	301023	205779
RP_NEG_197_80806a7_099	RP	NEG	7.10	197.8081				7.64E-01	0.06	0.45	1.84E-01	-0.26	0.80	7.68E-01	-0.07	0.29	3.97E-01	0.20	0.53	4495348	470017	4523833	448082	4583522	436094	4464144	456293
HILIC_POS_300_2016a0_616	HILIC	POS	0.616	300.2016				8.54E-01	0.05	1.07	1.84E-01	-0.23	1.03	7.83E-01	-0.07	0.88	5.60E-01	0.16	1.07	1949142	4890717	2119878	3213353	2548423	3850447	1691333	2379340
RP_POS_315_19296a9_988	RP	POS	9.99	315.1930				8.21E-04	0.49	1.21	1.84E-01	0.29	0.96	3.25E-03	0.64	1.15	1.72E-02	0.35	1.24	1361033	403873	1738030	830776	1627199	586230	1848862	1012783
RP_POS_183_98911a6_427	RP	POS	6.43	183.9891				3.42E-02	0.35	0.89	1.84E-01	-0.29	0.92	2.29E-01	0.20	0.61	2.54E-02	0.49	1.02	692578	729348	1064659	1150193	1217997	1351961	911320	892805
HILIC_POS_176_06577a4_248	HILIC	POS	4.248	176.0658				4.55E-01	-0.13	1.18	1.85E-01	0.28	1.10	9.55E-01	0.01	0.28	1.51E-01	-0.27	0.82	943392	272524	897383	378093	847040	323120	947725	423376
RP_POS_199_13052a11_58	RP	POS	11.58	199.1305				5.75E-01	-0.12	0.43	1.85E-01	0.26	0.87	9.70E-01	0.01	0.14	2.76E-01	-0.25	0.64	5395134	1854680	5187356	1680905	4963723	1526050	5410989	1810430
HILIC_NEG_117_9191a1_049	HILIC	NEG	1.049	117.9191				4.27E-03	0.49	0.98	1.85E-01	0.28	0.92	2.24E-03	0.63	1.19	7.29E-02	0.35	0.70	683418	148553	783157	213429	754786	206413	811528	218596
RP_NEG_276_99142a6_926	RP	NEG	6.93	276.9914				5.10E-01	0.12	0.50	1.85E-01	-0.28	0.79	9.00E-01	-0.03	0.34	2.13E-01	0.26	0.55	5286050	1483837	5505183	2014798	5772986	2021606	5237381	1992087
RP_POS_173_02892a15_735	RP	POS	15.74	173.0289				4.76E-01	-0.16	0.58	1.85E-01	-0.25	0.90	2.24E-01	-0.29	0.54	8.88E-01	-0.04	0.36	65846146	44711629	59578402	36688716	64457298	41188359	54699506	31217538
RP_POS_569_43103a14_513	RP	POS	14.51	569.4310				4.84E-01	-0.15	0.59	1.85E-01	-0.26	0.96	2.23E-01	-0.28	0.48	9.39E-01	-0.02	0.59	4481785	2342799	4152086	2175304	4441131	2308157	3863041	2015533
RP_POS_276_89249a15_46	RP	POS	15.46	276.8925				5.20E-01	0.15	0.54	1.86E-01	-0.25	0.78	9.09E-01	0.03	0.24	2.73E-01	0.27	0.56	2717069	906847	2830168	687187	2921440	646690	2738897	720333
RP_POS_807_57269a13_859	RP	POS	13.86	807.5727				2.76E-03	0.61	1.47	1.86E-01	-0.26	0.82	2.69E-02	0.48	1.12	1.41E-03	0.74	1.40	2103397	1032908	2766486	1063722	2907678	1121193	2625295	994155
RP_POS_307_16873a4_555	RP	POS	4.56	307.1687				4.42E-03	-0.60	0.95	1.86E-01	-0.26	0.94	2.13E-03	-0.72	1.18	3.48E-02	-0.47	0.84	3631682	2209911	2303992	2145746	2588800	2009328	2019184	2258201
RP_POS_605_23621a11_803	RP	POS	11.80	605.2362				4.35E-02	-0.40	1.02	1.86E-01	0.27	1.29	2.85E-01	-0.27	0.59	5.46E-03	-0.53	1.31	1677146	1030946	1237417	1099659	1091033	592540	1383801	1431204
RP_NEG_130_94281a15_605	RP	NEG	15.61	130.9428				1.73E-01	-0.24	0.59	1.86E-01	0.28	0.91	6.14E-01	-0.10	0.59	7.02E-02	-0.38	0.85	2923561	67105	2903082	89484	2891215	92141	2914948	86027
RP_POS_182_08177a1_268	RP	POS	1.27	182.0818				2.57E-01	0.19	0.94	1.87E-01	0.28	1.03	1.27E-01	0.34	1.13	7.73E-01	0.05	0.60	19995370	4852856	21257029	6946531	20335867	5712090	22178192	7945671
HILIC_NEG_100_93342a1_331	HILIC	NEG	1.331	100.9334				1.34E-02	-0.43	1.06	1.87E-01	-0.28	1.05	6.66E-03	-0.57	0.93	1.38E-01	-0.29	0.52	15134894	2390874	13770681	3334026	14212486	3160712	13328877	3474169
RP_POS_189_07846a6_096	RP	POS	6.10	189.0785				3.08E-05	-1.00	1.74	1.87E-01	-0.22	0.78	1.06E-05	-1.11	1.73	3.21E-04	-0.90	1.47	2685762	1377318	1455329	1009567	1589026	1049557	1321633	959794
RP_NEG_636_26288a10_331	RP	NEG	10.33	636.2629				4.83E-02	-0.49	1.13	1.87E-01	-0.23	1.13	2.44E-02	-0.61	1.15	1.39E-01	-0.38	0.88	2606534	434645	2439049	293042	2477838	263867	2400260	317496
RP_POS_366_06067a1_463	RP	POS	1.46	366.0607				4.61E-01	0.09	0.37	1.87E-01	0.30	0.85	2.99E-01	0.24	0.43	1.26E-01	-0.06	0.66	830256	797491	1186989	4613878	572423	620054	1801555	6469538
RP_POS_606_35541a10_868	RP	POS	10.87	606.3554				2.56E-01	0.15	0.62	1.88E-01	-0.30	0.90	9.74E-01	0.00	0.50	1.36E-01	0.30	0.78	644561	114681	695258	395347	747552	459818	642965	314285
HILIC_POS_388_30545a0_917	HILIC	POS	0.917	388.3055				2.71E-06	0.81	1.43	1.88E-01	0.27	1.15	5.09E-06	0.94	1.68	4.33E-04	0.67	1.26	596979	281914	923497	407298	869722	388954	977272	421879
RP_POS_553_45923a13_288	RP	POS	13.29	553.4592				1.27E-01	0.32	0.67	1.88E-01	-0.26	0.98	4.30E-01	0.18	0.65	4.55E-02	0.45	0.86	13139959	4637484	14598556	4583620	15203720	4180956	13993392	4921394
HILIC_POS_161_01843a1_017	HILIC	POS	1.017	161.0184				1.64E-01	0.21	0.46	1.88E-01	-0.29	1.11	7.23E-01	0.07	0.19	6.15E-02	0.36	0.72	370873	113145	412152	215642	440611	218039	383692	211560
RP_POS_573_14655a11_014	RP	POS	11.01	573.1466				3.18E-01	0.21	0.60	1.89E-01	-0.26	0.86	7.29E-01	0.08	0.38	1.41E-01	0.34	0.77	979404	300797	1040108	283137	1077454	274044	1002761	289867
RP_NEG_269_21237a10_292	RP	NEG	10.29	269.2124				5.50E-01	-0.12	0.77	1.89E-01	0.27	1.02	9.41E-01	0.02	0.70	2.58E-01	-0.25	0.61	1370361	201720	1345298	216339	1316783	216246	1373812	214798
HILIC_NEG_195_81093a4_011	HILIC	NEG	4.011	195.8109				8.31E-02	0.30	0.98	1.89E-01	-0.28	0.78	4.28E-01	0.16	0.28	2.82E-02	0.44	1.15	515470	489793	707847	669781	796100	641877	619595	691713
RP_NEG_162_83859a15_582	RP	NEG	15.58	162.8386				1.38E-01	-0.30	0.59	1.89E-01	-0.26	0.89	5.14E-02	-0.43	0.81	4.59E-01	-0.17	0.29	3173231	110840	3139180	112603	3154014	118499	3124346	105482
HILIC_POS_132_10204a2_639	HILIC	POS	2.639	132.1020				1.31E-01	-0.54	1.00	1.89E-01	0.03	0.87	1.44E-01	-0.53	0.76	1.20E-01	-0.56	0.85	874391	2627822	154184	170723	131669	124231	176698	205960
RP_POS_345_66989a5_958	RP	POS	5.96	345.6699				1.16E-01	-0.29	1.02	1.89E-01	-0.27	0.85	5.08E-02	-0.43	0.97	4.57E-01	-0.15	0.77	729401	149522	677837	186308	702365	174028	653308	196509
RP_POS_301_03546a15_445	RP	POS	15.45	301.0355				2.33E-01	-0.28	0.67	1.89E-01	0.24	0.81	5.43E-01	-0.16	0.46	1.02E-01	-0.40	0.69	3835286	1059637	3587383	829657	3478134	739629	3696632	905152
RP_POS_583_25513a7_159	RP	POS	7.16	583.2551				9.38E-01	-0.01	0.67	1.90E-01	0.28	1.18	5.80E-01	0.13	0.40	3.55E-01	-0.15	0.86	894156	526468	884786	753201	785431	498539	984142	936756
RP_POS_287_23691a9_749	RP	POS	9.75	287.2369				5.70E-04	0.47	0.86	1.90E-01	0.29	0.84	1.54E-03	0.62	1.02	3.96E-02	0.33	0.76	277615	158760	451353	403230	398265	355483	504440	443157
RP_NEG_228_16061a7_134	RP	NEG	7.13	228.1606				7.91E-01	0.06	0.60	1.90E-01	-0.24	0.82	8.16E-01	-0.06	0.55	4.54E-01	0.18	0.49	1211570	835948	1254451	641087	1338809	575572	1170094	696109
RP_NEG_308_9993a7_742	RP	NEG	7.74	308.9993				2.11E-01	0.21	0.54	1.90E-01	-0.28	0.80	7.13E-01	0.07	0.54	7.79E-02	0.36	0.71	6974315	774595	7195462	1095967	7339626	1074103	7051298	1109364
HILIC_POS_218_1385a2_109	HILIC	POS	2.109	218.1385				7.37E-01	-0.06	0.45	1.90E-01	-0.28	0.84	3.48E-01	-0.20	0.40	6.97E-01	0.08	0.18	42944640	17843589	41623717	23344796	44692443	22362543	38554991	24120099
RP_NEG_198_93556a15_778	RP	NEG	15.78	198.9356				9.35E-01	-0.02	0.65	1.90E-01	-0.27	0.78	5.02E-01	-0.15	0.58	6.06E-01	0.12	0.43	12023156	5599422	11929652	5839713	12696646	5961138	11162657	5671395
RP_POS_929_48486a0_484	RP	POS	0.48	929.4849				7.67E-07	0.59	1.19	1.91E-01	-0.29	1.18	3.87E-03	0.44	1.11	5.94E-05	0.73	1.42	120408	13129	286597	314144	327817	333477	245377	291054
RP_NEG_595_49506a11_477	RP	NEG	11.48	595.4951				2.15E-01	-0.22	0.36	1.91E-01	-0.28	0.82	5.78E-02	-0.35	0.70	7.29E-01	-0.08	0.25	1751151	1150870	1427990	1593155	1637057	1815377	1218923	1320337

Supplementary table 1: Metabolomics results (in asceding order according to p-value from progressive ALD vs non-progressive ALD comparison, with molecular features with ID_level of 1-2 first)

								all_ALD_vs_control			Prog_ALD_vs_non-prog_ALD			Prog_ALD_vs_control_ALD			Non-prog_ALD_vs_control			Healthy_control		all_ALD		Non-prog_ALD		Progressive_ALD	
								t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA								
Feature_ID	RP_HILIC	POS_NEG	Average.Rt	Average.Mz	Metabolite.name	curated_MSMS	ID_level	p	d	VIP	p	d	VIP	p	d	VIP	p	d	VIP	Mean	SD	Mean	SD	Mean	SD	Mean	SD
RP_POS_419_31485a13_932	RP	POS	13.93	419.3149				2.67E-01	0.24	0.48	1.91E-01	0.25	0.84	1.25E-01	0.37	0.92	6.19E-01	0.12	0.38	4803716	2353785	5325363	2053119	5056147	2026823	5594579	2064144
RP_POS_327_22635a11_254	RP	POS	11.25	327.2264				3.01E-05	0.74	1.71	1.91E-01	0.26	1.06	6.89E-05	0.87	1.62	1.10E-03	0.61	1.62	7223335	2794452	10000543	3787071	9503860	3207620	10497225	4264297
RP_POS_368_27933a8_328	RP	POS	8.33	368.2793				7.15E-07	0.67	1.08	1.91E-01	0.28	0.77	1.03E-04	0.81	1.30	1.66E-04	0.53	1.37	430421	184638	745507	508284	678806	378252	812208	508131
RP_NEG_239_75981a15_587	RP	NEG	15.59	239.7598				4.94E-02	-0.38	0.73	1.92E-01	-0.27	0.84	1.62E-02	-0.51	0.92	2.64E-01	-0.25	0.45	8507052	286248	8387034	318536	8428772	338005	8345295	295295
RP_POS_190_98807a0_843	RP	POS	0.84	190.9881				6.33E-01	-0.09	0.42	1.92E-01	-0.27	0.77	2.85E-01	-0.23	0.43	8.35E-01	0.05	0.44	7058826	2985078	6755180	3498005	7213083	3634198	6297277	3329637
RP_POS_166_98491a11_09	RP	POS	11.09	166.9849				2.41E-02	0.44	0.95	1.93E-01	0.26	0.79	9.99E-03	0.57	1.03	1.51E-01	0.31	0.60	10184800	4764597	12480918	5222671	11798132	5130133	13163704	5276320
RP_POS_414_3002a8_564	RP	POS	8.56	414.3002				1.24E-01	0.18	0.87	1.93E-01	0.30	0.94	1.56E-01	0.33	0.90	5.40E-02	0.03	0.85	295758	624499	3546133	20916760	797616	1633361	6294650	29425595
RP_POS_1006_75824a0_493	RP	POS	0.49	1006.7582				2.17E-09	-0.76	1.38	1.93E-01	0.28	1.26	2.57E-04	-0.62	1.34	5.42E-07	-0.90	1.59	2314230	223222	1671254	914941	1551858	914728	1790651	908569
RP_POS_607_25189a11_805	RP	POS	11.81	607.2519				1.66E-02	-0.49	1.24	1.93E-01	0.26	1.33	1.42E-01	-0.36	0.83	2.74E-03	-0.62	1.31	4483035	1781114	3584450	1810563	3347741	1236484	3821159	2231577
RP_POS_279_22971a11_161	RP	POS	11.16	279.2297				2.70E-01	-0.25	0.46	1.93E-01	-0.24	0.92	1.09E-01	-0.38	0.82	6.14E-01	-0.13	0.45	1708748	803635	1534754	640691	1618448	761767	1451060	484524
RP_POS_401_19681a10_143	RP	POS	10.14	401.1968		401.1967(100)	4	4.30E-01	-0.22	0.73	1.94E-01	-0.20	0.90	2.68E-01	-0.22	0.59	6.71E-01	-0.13	0.70	5149212	9458242	3763698	4665015	4372157	5062013	3155239	4193964
RP_POS_371_25653a10_854	RP	POS	10.85	371.2565				5.39E-06	-0.75	1.25	1.94E-01	-0.27	1.02	2.25E-05	-0.89	1.41	5.85E-04	-0.62	1.12	1772475	445181	1261422	695550	1352124	614934	1170720	763229
RP_POS_647_45807a13_32	RP	POS	13.32	647.4581				2.37E-01	-0.26	0.52	1.94E-01	-0.25	0.90	9.83E-02	-0.38	0.85	5.91E-01	-0.13	0.34	7571027	8297615	5606422	7384736	6568452	8021352	4644391	6629535
RP_POS_299_1387a11_805	RP	POS	11.81	299.1387				2.90E-02	-0.44	1.11	1.94E-01	0.26	1.32	2.15E-01	-0.31	0.67	3.93E-03	-0.57	1.34	4409086	2356395	3323738	2460892	3002299	1429581	3645177	3159273
RP_NEG_723_08887a9_357	RP	NEG	9.36	723.0889				3.13E-03	-0.60	1.06	1.95E-01	-0.26	0.91	1.17E-03	-0.72	1.24	3.57E-02	-0.47	0.84	3197036	192044	3075017	201014	3101181	206149	3048852	194276
RP_POS_524_27441a10_216	RP	POS	10.22	524.2744				3.29E-06	0.82	1.53	1.95E-01	-0.26	0.94	1.54E-03	0.69	1.20	3.39E-07	0.95	1.84	1103681	341027	1489493	470688	1550779	363633	1428206	554727
RP_POS_290_91843a15_37	RP	POS	15.37	290.9184				1.01E-02	-0.52	0.87	1.95E-01	-0.26	0.97	3.21E-03	-0.64	1.26	8.74E-02	-0.39	0.61	2187754	464441	1932877	489679	1996534	521230	1869220	452232
RP_NEG_394_97629a10_261	RP	NEG	10.26	394.9763				9.08E-01	0.02	0.38	1.96E-01	0.26	1.09	5.21E-01	0.16	0.62	5.92E-01	-0.11	0.46	1124642	803367	1143753	848876	1033425	651971	1254080	1002985
HILIC_NEG_234_82019a7_019	HILIC	NEG	7.019	234.8202				7.84E-01	-0.06	0.17	1.96E-01	-0.25	1.55	4.24E-01	-0.19	0.36	7.79E-01	0.07	0.20	1143872	467273	1118342	422079	1173123	444229	1063562	395567
RP_POS_700_52673a13_495	RP	POS	13.50	700.5267				2.74E-02	-0.54	1.03	1.96E-01	-0.23	0.76	1.29E-02	-0.66	1.09	9.34E-02	-0.43	0.75	1296561	796251	950125	559396	1022715	538810	877536	575469
RP_POS_587_54944a15_22	RP	POS	15.22	587.5494				1.15E-01	0.37	0.72	1.96E-01	-0.24	0.83	2.98E-01	0.26	0.49	5.88E-02	0.49	0.88	15278841	2423546	16027798	1817804	16263672	1963255	15791923	1645706
RP_POS_872_5401a12_82	RP	POS	12.82	872.5401				2.18E-05	-0.97	1.61	1.96E-01	-0.22	0.92	1.10E-05	-1.09	1.71	2.43E-04	-0.86	1.42	4580873	1419892	3270339	1160089	3420778	1099395	3119900	1210051
HILIC_POS_166_08385a3_509	HILIC	POS	3.509	166.0839				2.42E-01	0.20	0.54	1.96E-01	0.28	0.90	1.08E-01	0.34	0.67	7.65E-01	0.06	0.36	3138139	3846289	4189360	5761799	3442125	5293075	4936595	6157761
RP_POS_185_11484a13_809	RP	POS	13.81	185.1148				1.74E-01	-0.31	0.72	1.96E-01	0.25	0.88	4.64E-01	-0.18	0.51	7.14E-02	-0.43	1.11	8111944	4197718	6976507	3526365	6519320	3150764	7433694	3843228
RP_POS_195_12225a10_652	RP	POS	10.65	195.1223				5.17E-01	0.13	0.73	1.97E-01	-0.26	0.98	9.85E-01	0.00	0.35	2.44E-01	0.26	0.70	1629694	468267	1692939	504453	1758275	505720	1627603	499674
RP_POS_417_73984a12_693	RP	POS	12.69	417.7398				1.62E-03	0.59	1.21	1.97E-01	-0.26	0.82	3.22E-02	0.46	0.94	5.61E-04	0.72	1.27	5865386	2195446	7413794	2647386	7756580	2487690	7071007	2780637
RP_POS_624_3764a11_089	RP	POS	11.09	624.3764				1.27E-07	0.63	1.31	1.97E-01	-0.29	1.27	3.36E-04	0.49	1.37	8.68E-05	0.77	1.41	46841	35060	775709	1279003	941322	1477673	610097	1032273
RP_POS_548_80963a10_618	RP	POS	10.62	548.8096				6.29E-03	0.62	1.37	1.97E-01	-0.24	1.03	4.56E-02	0.50	1.04	1.73E-03	0.74	1.47	3023515	875438	3512934	722115	3606429	589740	3419439	829402
RP_NEG_335_04788a0_62	RP	NEG	0.62	335.0479				1.64E-05	0.51	1.09	1.97E-01	-0.29	1.16	6.52E-03	0.36	1.08	8.23E-04	0.65	1.27	4309636	755772	16029926	25836481	19375305	29870716	12684548	20822364
RP_NEG_412_62927a15_583	RP	NEG	15.58	412.6293				2.69E-01	-0.24	0.60	1.98E-01	-0.25	0.86	1.16E-01	-0.37	0.66	6.38E-01	-0.11	0.42	1669239	72635	1653109	65450	1661573	69876	1644645	60216
RP_NEG_269_24805a11_381	RP	NEG	11.38	269.2481				1.32E-03	-0.67	1.11	1.98E-01	-0.25	1.05	2.79E-04	-0.79	1.36	2.14E-02	-0.55	0.85	943868	218470	793793	214296	821523	246529	766064	174460
RP_POS_677_47821a10_868	RP	POS	10.87	677.4782				2.29E-01	-0.22	0.49	1.98E-01	0.27	0.93	6.86E-01	-0.08	0.32	9.35E-02	-0.35	0.69	8111819	549114	7967094	689373	7877973	690569	8056216	683427
RP_POS_376_31848a10_829	RP	POS	10.83	376.3185				6.49E-01	0.12	0.87	1.98E-01	0.22	0.94	4.08E-01	0.23	0.71	9.84E-01	0.01	0.61	646739	584322	697155	371956	649074	334628	745235	403524
HILIC_POS_426_35788a0_608	HILIC	POS	0.608	426.3579				2.94E-07	0.95	1.76	1.98E-01	0.25	0.76	1.48E-07	1.08	1.99	7.19E-05	0.83	1.69	1159881	519060	1801439	642286	1718438	682203	1884440	594997
HILIC_NEG_134_89473a4_009	HILIC	NEG	4.009	134.8947				1.20E-01	-0.32	0.59	1.98E-01	-0.26	0.88	5.34E-02	-0.45	0.72	3.88E-01	-0.19	0.80	18077081	8213843	15447430	8086014	16491356	7797773	14403504	8310975
HILIC_POS_478_32684a1_309	HILIC	POS	1.309	478.3268				5.31E-03	0.56	0.88	1.98E-01	-0.25	0.71	4.76E-02	0.44	0.74	2.28E-03	0.69	1.18	448805	193842	564238	201144	590198	201783	538278	199128
RP_NEG_237_93413a1_459	RP	NEG	1.46	237.9341				5.20E-12	0.91	1.48	1.98E-01	0.27	0.78	1.18E-07	1.04	1.69	6.15E-07	0.77	1.50	303919	279482	1067423	874770	954483	758425	1180363	972019
RP_NEG_187_86122a15_536	RP	NEG	15.54	187.8612				1.09E-01	-0.36	0.85	1.98E-01	-0.24	0.99	4.77E-02	-0.48	0.81	3.26E-01	-0.24	0.69	579426	36455	567751	30650	571706	30957	563796	30130
HILIC_POS_570_35577a1_192	HILIC	POS	1.192	570.3558				2.70E-04	0.67	1.17	1.98E-01	-0.26	0.79	1.16E-02	0.54	0.97	7.76E-05	0.80	1.54	3012022	1612105	4353905	1998646	4611860	1792536	4095949	2172950
RP_POS_814_01208a10_932	RP	POS	10.93	814.0121				4.42E-02	-0.48	1.18	1.99E-01	-0.23	1.61	1.97E-02	-0.60	1.14	1.49E-01	-0.36	0.96	1406903	655902	1145720	491771	1209148	491861	1082292	488338
HILIC_NEG_221_01254a1_297	HILIC	NEG	1.297	221.0125				1.09E-12	0.99	1.64	1.99E-01	0.26	0.89	1.80E-08	1.12	1.73	7.15E-08	0.86	1.73	332142	190297	789804	468250	729437	405133	850171	520980
RP_NEG_215_86778a3_128	RP	NEG	3.13	215.8678				1.61E-01	-0.25	0.89	1.99E-01	-0.27	0.78	4.67E-02	-0.39	0.85	6.01E-01	-0.11	0.53	1504842	784568	1260339	1027199	1392752	1150261	1127925	879162
HILIC_NEG_124_04037a0_692	HILIC	NEG	0.692	124.0404				1.18E-01	-0.39	0.74	1.99E-01	-0.22	1.08	5.46E-02	-0.50	0.82	2.96E-01	-0.28	0.48	140060	110292	106779	74037	116316	79591	97242	67487
RP_POS_1070_66125a10_617	RP	POS	10.62	1070.6613				1.47E-03	0.66	1.39	2.00E-01	-0.25	0.84	2.24E-02	0.53	1.09	3.66E-04	0.78	1.50	866367	524017	1223689	523182	1291020	448487	1156358	585348
RP_NEG_235_92589a0_104	RP	NEG	0.10	235.9259				7.84E-01	0.06	0.52	2.00E-01	0.25	0.89	4.35E-01	0.18	0.54	7.65E-01	-0.07	0.52	5256595	2234785	5379715	2092169	5110859	2006330	5648571	2161202
RP_NEG_314_84808a15_494	RP	NEG	15.49	314.8481				5.41E-01	0.17	0.53	2.00E-01	-0.21	0.78	8.26E-01	0.06	0.28	3.34E-01	0.27	0.68	967483	108689	979906	59870	987602	51773	972210	66638
RP_POS_590_85297a0_494	RP	POS	0.49	590.8530				2.85E-09	-0.76	1.38	2.01E-01	0.28	1.26	1.78E-04	-0.62	1.35	1.08E-06	-0.89	1.56	1548707	157838	1119599	610669	1041208	628738	1197991	587871
RP_NEG_458_57303a15_583	RP	NEG	15.58	458.5730				6.57E-02	-0.33	0.55	2.01E-01	-0.27	0.80	2.58E-02	-0.47	0.81	3.40E-01	-0.20	0.34	678781	28609	667062	36932	671802	36975	662321	36643
RP_POS_365_26575a10_744	RP	POS	10.74	365.2658				1.79E-02	-0.52	1.37	2.01E-01	0.24	0.79	1.08E-01	-0.39	0.94	5.16E-03	-0.64	1.20	1055046	295988	911285	264298	877340	220252	945231	300450
RP_POS_409_24481a11_17	RP	POS	11.17	409.2448				1.70E-02	0.43	1.00	2.01E-01	-0.27	0.91	1.43E-01	0.29	0.71	8.64E-03	0.56	1.11	2054514	155676	2138587	205781	2165001	215092	2112173	194595
RP_POS_450_35699a11_394	RP	POS	11.39	450.3570				3.32E-02	-0.42	0.75	2.01E-01	0.26	1.03	2.11E-01	-0.29	0.59	8.35E-03	-0.55	0.97	7235630	705232	6916694	760527	6819029	624068	7014358	871596
RP_NEG_266_01834a6_762	RP	NEG	6.76	266.0183				1.77E-02	-0.75	1.48	2.01E-01	-0.14	1.21	1.03E-02	-0.82	1.25	3.41E-02	-0.68	1.07	7365956	12068540	1946572	3998438	2459959	4548044	1433186	3328466
RP_POS_518_32135a11_255	RP	POS	11.26	518.3214				4.01E-04	0.56	1.35	2.01E-01	-0.27	0.97	2.42E-02	0.42	1.07	3.68E-04	0.69	1.58	582718	272065	830087	471363	890523	475669	769651	463881
RP_NEG_297_15375a15_468	RP	NEG	15.47	297.1538				7.98E-01	0.05	1.06	2.01E-01	-0.26	0.93	7.05E-01	-0.08	0.32	4.10E-01	0.18	1.17	1651117	534763	1679809	597762	1756438	599935	1603179	591629
RP_NEG_437_29184a9_858	RP	NEG	9.86	437.2918				4.64E-01	0.13	0.32	2.02E-01	0.27	0.77	2.30E-01	0.27	0.47	9.95E-01	0.00	0.64	2460987	3727894	3057626	4693723	2455985	4058881	3659267	5224791
HILIC_POS_64_01665a4_007	HILIC	POS	4.007	64.0167				8.51E-02	0.30	0.74	2.02E-01	-0.27	1.00	4.29E-01	0.16	0.53	2.90E-02	0.44	0.77	3112343	792386	3422617	1093384	3562711	1033621	3282524	1143219
RP_POS_1067_77185a14_271	RP	POS	14.27	1067.7719				2.90E-01	0.17	0.51	2.02E-01	0.28	0.81	1.75E-01	0.31	0.64	8.37E-01	0.03	0.35	4222147	1295339	4552987	2100062	4283392	1330302	4822582	2644332
RP_POS_677_47968a10_921	RP	POS	10.92	677.4797				2.58E-01	-0.27	0.50	2.02E-01	-0.23	1.09	1.34E-01	-0.39	0.67	5.36E-01	-0.16	0.46	7128840	1217687	6862186	876571	6974420	864191	6749953	883121
RP_POS_393_19058a8_034	RP	POS	8.03	393.1906				2.11E-07	0.62	1.08	2.02E-01	0.28	1.16	3.65E-04	0.76	1.24	9.79E-06	0.48	1.33	36498	64104	1106609	1915709	860718	1180374	1352501	2428602
RP_POS_774_60046a14_012	RP	POS	14.01	774.6005				5.12E-01	0.12	0.59	2.02E-01	0.27	0.77	2.53E-01	0.26	0.59	9.61E-01	-0.01	0.43	1683912	934412	1815255	1108646	1673286	995638	1957223	1204511
HILIC_POS_386_28961a0_925	HILIC	POS	0.925	386.2896				1.92E-03	0.50	1.04	2.03E-01	0.27	1.29	2.14E-03	0.64	1.12	3.97E-02	0.37	0.70	1205244	533675	1613547	857582	1503840	758094	1723253	941612
RP_POS_1065_68384a10_618	RP	POS	10.62	1065.6838				1.96E-03	0.67	1.46	2.03E-01	-0.24	1.00	2.34E-02	0.55	1.14	4.90E-04	0.79	1.58	6267823	2682101	8016845	2468955	8332776	2059172	7700913	2805708
RP_POS_315_13321a11_803	RP	POS	11.80	315.1332				5.49E-02	-0.37	0.98	2.03E-01	0.26	1.30	3.28E-01	-0.24	0.54	7.05E-03	-0.50	1.31	992820	705125	704225	783930	603679	415356	804770	1023954
RP_POS_772_5274a13_52	RP	POS	13.52	772.5274				9.64E-01	0.01	0.61	2.03E-01	-0.26	0.76	5.68E-01	-0.12	0.34	5.33E-01	0.14	0.65	2880242	1054490	2890130	1170949	3039760	1224661	2740500	1106680
RP_POS_136_07588a1_268	RP	POS	1.27	136.0759				3.87E-01	0.15	0.99	2.03E-01	0.27	1.05	1.99E-01	0.28	1.15	9.49E-01	0.01	0.63	2521372	566912	2633386	808449	2530096	648304	2736676	937254
RP_POS_229_95404a15_592	RP	POS	15.59	229.9540				3.34E-01	-0.22	0.70	2.03E-01	0.24	0.94	6.91E-01	-0.10	0.46	1.66E-01	-0.34	0.58	3685775	113564	3664136	94065	3652130	92849	3676142	94667
HILIC_NEG_452_2778a1_867	HILIC	NEG	1.867	452.2778				8.44E-02	0.28	0.73	2.03E-01	-0.27	0.84	4.86E-01	0.15	0.26	2.18E-02	0.42	0.80	259847	82123	293810	129337	310322	112748	277298	143279
RP_POS_667_27289a11_802	RP	POS	11.80	667.2729				6.15E-02	-0.34	0.92	2.03E-01	0.27	1.28	3.99E-01	-0.21	0.52	5.01E-03	-0.47	1.32	968194	729198	666822	920681	548837	420634	784806	1227707
RP_POS_693_47516a10_468	RP	POS	10.47	693.4752				9.23E-01	0.01	0.35	2.04E-01	-0.28	1.13	5.12E-01	-0.13	0.48	3.93E-01	0.16	0.35	5365747	430610	5376548	816676	5480756	780098	5272339	846649
RP_POS_784_57642a11_168	RP	POS	11.17	784.5764				2.45E-04	0.44	1.15	2.04E-01	-0.29	1.25	2.22E-02	0.30	1.14	3.35E-03	0.58	1.30	238755	77048	440128	513627	505721	605882	374534	396404
HILIC_POS_143_99702a7_961	HILIC	POS	7.961	143.9970				5.51E-05	-0.63	1.27	2.04E-01	0.27	0.99	9.23E-03	-0.50	1.24	4.94E-05	-0.77	1.39	1794943	466107	1304187	818146	1199825	788523	1408550	841660
RP_NEG_396_97314a7_568	RP	NEG	7.57	396.9731				8.91E-01	0.03	0.21	2.04E-01	0.26	1.03	4.79E-01	0.16	0.79	6.38E-01	-0.10	0.34	2671788	668376	2690825	726972	2598119	719698	2783531	729559
RP_POS_568_29468a7_093	RP	POS	7.09	568.2947				3.65E-01	-0.17	0.56	2.04E-01	0.27	0.86	8.74E-01	-0.03	0.41	1.55E-01	-0.30	0.73	51251006	2342517	50790666	2881645	50423266	2836754	51158067	2907675
HILIC_NEG_89_02402a4_985	HILIC	NEG	4.985	89.0240				9.59E-01	0.01	0.32	2.04E-01	0.27	0.76	5.21E-01	0.14	0.56	5.11E-01	-0.13	0.82	7298098	4248728	7345981	5503611	6644136	4550474	8047827	6283752
RP_NEG_274_97604a7_752	RP	NEG	7.75	274.9760				5.43E-02	-0.30	0.53	2.04E-01	0.28	0.88	2.78E-01	-0.17	0.47	4.89E-02	-0.44	0.69	8712257	394854	8522960	674701	8436804	838186	8609115	449476
RP_POS_768_55292a13_859	RP	POS	13.86	768.5529				3.19E-01	0.21	0.53	2.05E-01	0.25	0.83	1.71E-01	0.34	0.65	6.94E-01	0.09	0.45	3102310	1880280	3480409	1751519	3257297	1472156	3703521	1982275
HILIC_POS_168_10193a1_104	HILIC	POS	1.104	168.1019				2.15E-02	0.27	0.45	2.05E-01	0.29	0.87	6.37E-02	0.41	0.56	7.35E-02	0.12	0.56	729431	1200314	6261183	23585316	3245327	9620090	9277039	31824182
RP_NEG_322_80655a15_382	RP	NEG	15.38	322.8066				6.53E-01	0.10	0.48	2.05E-01	-0.24	0.81	9.46E-01	-0.02	0.24	3.84E-01	0.22	0.46	781568	61810	787003	49371	793288	54477	780717	43317
RP_POS_1019_60614a10_335	RP	POS	10.34	1019.6061				5.87E-01	0.11	0.96	2.05E-01	-0.25	1.02	9.61E-01	-0.01	0.74	2.73E-01	0.24	0.91	1138207	591857	1203270	565173	1275224	468422	1131316	644495
RP_POS_625_38861a13_501	RP	POS	13.50	625.3886				6.06E-01	0.07	0.56	2.05E-01	0.29	0.78	3.56E-01	0.21	0.50	4.42E-01	-0.07	0.30	1828044	301973	1877161	787205	1776535	282008	1977787	1073237
RP_NEG_348_00574a2_476	RP	NEG	2.48	348.0057				3.28E-03	-0.50	1.15	2.05E-01	-0.27	1.17	3.86E-03	-0.63	1.23	4.18E-02	-0.36	1.03	1121284	178949	995920	265961	1029770	218076	962070	304989
RP_POS_263_12778a7_279	RP	POS	7.28	263.1278				3.31E-06	-1.05	1.65	2.05E-01	-0.22	0.84	1.04E-06	-1.16	1.88	7.06E-05	-0.95	1.40	810980	367774	430219	307982	469378	330794	391061	281226
RP_NEG_245_75206a15_587	RP	NEG	15.59	245.7521				3.61E-01	-0.18	0.59	2.05E-01	-0.26	0.95	1.58E-01	-0.31	0.64	8.18E-01	-0.05	0.32	2634893	98121	2616201	104946	2629539	108487	2602863	100596
RP_POS_537_53571a14_003	RP	POS	14.00	537.5357				5.81E-01	0.13	0.46	2.05E-01	-0.23	0.82	9.46E-01	0.02	0.51	3.47E-01	0.25	0.60	13748150	2191223	13981002	1596945	14183974	1750937	13778030	1415153
RP_POS_553_45807a10_888	RP	POS	10.89	553.4581				8.03E-03	-0.48	0.92	2.06E-01	0.26	1.02	8.14E-02	-0.35	0.87	4.32E-03	-0.61	1.04	3460905	1011900	2859159	1282277	2696239	1334855	3022078	1219025
RP_POS_771_57568a13_718	RP	POS	13.72	771.5757				7.85E-13	1.19	1.89	2.06E-01	0.24	1.00	8.24E-11	1.31	2.01	3.46E-09	1.07	1.88	11681897	3500093	18672309	5461878	17978542	5074868	19366077	5791069
RP_POS_788_55487a13_372	RP	POS	13.37	788.5549	PC compound	184.0733(75), 788.5593(30), 605.4916(22), 146.9818(100), 86.0969(55), 729.4908(45),	3	7.95E-01	-0.05	0.53	2.06E-01	-0.27	0.80	3.81E-01	-0.18	0.34	6.99E-01	0.08	0.45	10523805	2674579	10373959	3257620	10787500	3445280	9960419	3036738

Supplementary table 1: Metabolomics results (in asceding order according to p-value from progressive ALD vs non-progressive ALD comparison, with molecular features with ID_level of 1-2 first)

								all_ALD_vs_control			Prog_ALD_vs_non-prog_ALD			Prog_ALD_vs_control_ALD			Non-prog_ALD_vs_control			Healthy_control		all_ALD		Non-prog_ALD		Progressive_ALD	
								t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA								
Feature_ID	RP_HILIC	POS_NEG	Average.Rt	Average.Mz	Metabolite.name	curated_MSMS	ID_level	p	d	VIP	p	d	VIP	p	d	VIP	p	d	VIP	Mean	SD	Mean	SD	Mean	SD	Mean	SD
RP_NEG_367_15927a9_588	RP	NEG	9.59	367.1593				5.72E-05	0.55	0.96	2.06E-01	0.28	1.06	1.76E-03	0.69	1.01	9.74E-04	0.41	1.28	1861874	1338817	3646030	3571083	3192098	2177704	4099962	4539010
HILIC_POS_157_07605a4_124	HILIC	POS	4.124	157.0761				5.91E-03	-0.45	1.08	2.07E-01	-0.27	1.44	7.24E-03	-0.59	1.18	6.42E-02	-0.32	1.07	715220	116638	636956	185063	660438	145888	613475	216302
RP_POS_497_0578a7_643	RP	POS	7.643	497.0578				8.45E-01	0.03	0.85	2.07E-01	-0.27	0.76	6.18E-01	-0.10	0.47	4.19E-01	0.17	0.37	434665	16888	435401	22864	438297	23559	432506	22001
RP_POS_205_01593a15_441	RP	POS	15.44	205.0159				1.93E-01	-0.28	0.62	2.07E-01	0.24	1.03	5.18E-01	-0.16	0.55	7.15E-02	-0.41	0.69	4203962	1625051	3780073	1435149	3598170	1133628	3961976	1675917
HILIC_POS_267_17044a1_387	HILIC	POS	1.387	267.1704				3.96E-02	0.24	0.89	2.07E-01	0.29	0.87	9.46E-02	0.38	0.83	8.86E-03	0.09	0.96	322880	910412	5346614	24042220	2283848	4977266	8409379	33525155
RP_POS_176_10295a0_548	RP	POS	0.55	176.1030				3.69E-07	0.82	1.57	2.07E-01	0.26	1.44	1.63E-06	0.95	1.76	2.09E-04	0.69	1.41	1036077	253198	1373903	421190	1320575	409528	1427231	430007
RP_POS_699_41901a10_918	RP	POS	10.92	699.4190				3.92E-01	0.10	0.79	2.07E-01	-0.29	0.82	7.31E-01	-0.04	0.52	2.13E-01	0.25	0.82	2117834	122655	2189416	804513	2291381	961112	2087451	602277
RP_POS_585_27063a7_157	RP	POS	7.16	585.2706				9.13E-01	-0.02	0.68	2.07E-01	0.27	1.17	6.13E-01	0.12	0.39	3.65E-01	-0.15	0.86	8774942	4906381	8652983	6905772	7777405	4720625	9528561	8514914
RP_NEG_514_28595a12_402	RP	NEG	12.40	514.2860	Likely taurine conjugated bile acid (BA 24:1;O4;T)	514.285(100)	3	6.33E-01	0.06	0.48	2.07E-01	0.29	1.05	3.80E-01	0.21	0.39	1.71E-01	-0.08	1.10	410688	433757	495583	1598146	292114	262870	699053	2237561
HILIC_NEG_212_0023a0_554	HILIC	NEG	0.554	212.0023				7.14E-02	-0.41	0.72	2.08E-01	-0.24	0.91	3.56E-02	-0.53	0.81	2.23E-01	-0.29	0.54	2185814	1435136	1668595	1189645	1819023	1100349	1518167	1265877
RP_POS_214_0034a0_787	RP	POS	0.79	214.0034				2.97E-02	-0.46	0.86	2.08E-01	-0.25	0.88	1.27E-02	-0.58	0.99	1.42E-01	-0.34	0.68	2717961	1461342	2062101	1383254	2236963	1376280	1887238	1381767
RP_POS_946_75916a0_494	RP	POS	0.49	946.7592				1.65E-08	-0.74	1.31	2.08E-01	0.27	1.17	1.34E-03	-0.60	1.24	7.26E-08	-0.87	1.62	1111661	96026	898889	309852	859704	268529	938074	344579
RP_POS_162_9892a15_442	RP	POS	15.44	162.9892				1.10E-01	-0.37	0.61	2.08E-01	-0.24	0.87	4.04E-02	-0.49	0.93	3.33E-01	-0.25	0.47	35906220	10535426	32567472	8465441	33638263	9843038	31496680	6750149
HILIC_POS_239_14893a0_616	HILIC	POS	0.616	239.1489				1.76E-01	0.23	1.09	2.08E-01	-0.27	0.98	5.83E-01	0.09	1.11	1.06E-01	0.37	1.18	1056797	1245393	1445614	1806395	1674188	2166225	1217041	1339240
HILIC_POS_224_12801a5_328	HILIC	POS	5.328	224.1280				8.84E-04	0.57	1.05	2.08E-01	-0.26	0.83	2.25E-02	0.44	0.79	6.87E-04	0.71	1.14	5707342	1634549	6990364	2314514	7282841	2401742	6697887	2209148
RP_POS_787_54297a13_718	RP	POS	13.72	787.5430				2.54E-11	1.11	1.79	2.08E-01	0.24	0.91	8.69E-10	1.23	1.93	8.20E-08	0.99	1.74	2230309	698614	3500326	1089856	3362607	1036952	3638045	1133948
HILIC_NEG_186_95505a1_307	HILIC	NEG	1.307	186.9551				4.32E-05	0.78	1.27	2.08E-01	0.25	0.93	5.34E-05	0.91	1.39	1.01E-03	0.66	1.28	686986	177640	852734	206068	826701	182660	878766	225937
RP_NEG_225_06982a7_63	RP	NEG	7.63	225.0698				1.56E-01	0.17	0.42	2.08E-01	0.29	1.00	1.63E-01	0.32	0.53	6.85E-01	0.03	0.89	654220	509542	1043924	2577608	716730	881092	1371118	3525467
RP_POS_559_80048a10_617	RP	POS	10.62	559.8005				2.62E-02	-0.49	0.99	2.08E-01	-0.24	1.06	1.23E-02	-0.61	1.14	1.12E-01	-0.37	0.71	642944	242101	533417	210680	560021	201095	506812	218620
RP_NEG_221_94623a15_646	RP	NEG	15.65	221.9462				6.02E-01	-0.10	0.25	2.09E-01	0.26	1.15	8.71E-01	0.03	0.15	3.12E-01	-0.23	0.56	33397366	2034346	33170807	2396997	32868295	2654986	33473319	2091108
HILIC_POS_148_09686a4_858	HILIC	POS	4.858	148.0969				1.12E-01	-0.28	0.81	2.09E-01	-0.27	0.84	4.01E-02	-0.41	0.73	4.85E-01	-0.15	0.46	3407048	544927	3211542	740216	3304929	771868	3118155	702455
RP_POS_318_24008a9_299	RP	POS	9.30	318.2401				7.12E-01	-0.09	0.62	2.09E-01	-0.22	0.75	4.44E-01	-0.20	0.56	9.41E-01	0.02	0.28	6577106	5598434	6182797	3784492	6659951	3692853	5705644	3851654
HILIC_NEG_129_93636a6_272	HILIC	NEG	6.272	129.9364				7.02E-01	-0.08	0.41	2.09E-01	-0.25	0.75	3.61E-01	-0.20	0.35	8.24E-01	0.05	0.25	2702801	931145	2629584	962331	2750915	980188	2508254	938217
RP_POS_569_43268a11_256	RP	POS	11.26	569.4327				7.25E-02	0.37	1.17	2.10E-01	0.25	0.98	3.63E-02	0.49	1.12	2.68E-01	0.24	1.01	2248037	767262	2534722	779847	2436531	709447	2632912	840086
RP_POS_241_17329a8_341	RP	POS	8.34	241.1733				7.97E-01	0.05	0.37	2.10E-01	-0.25	0.75	7.52E-01	-0.07	0.28	4.44E-01	0.18	0.37	12870906	8188799	13298634	7964307	14300823	8213746	12296444	7657642
RP_NEG_880_60944a14_034	RP	NEG	14.03	880.6094	PC 40:5|PC 20:1_20:4 [M+HCOO]-	329.2493(100), 283.2648(68), 820.593(30)	3	4.10E-07	0.91	1.50	2.10E-01	0.25	0.95	3.07E-06	1.03	1.58	1.85E-05	0.79	1.52	3334482	1064243	4650659	1410005	4473231	1138265	4828087	1630002
RP_POS_245_17464a8_028	RP	POS	8.03	245.1746				1.41E-01	0.30	0.67	2.10E-01	0.25	0.79	6.59E-02	0.43	0.74	4.25E-01	0.18	0.60	587242	115046	622142	114388	607764	109274	636519	118632
RP_NEG_197_80794a15_584	RP	NEG	15.58	197.8079				4.09E-02	-0.41	0.74	2.11E-01	-0.25	0.87	1.28E-02	-0.54	0.98	2.17E-01	-0.29	0.48	34814028	964983	34400078	997849	34525508	1106393	34274648	869203
RP_POS_573_25446a7_093	RP	POS	7.09	573.2545				6.58E-01	-0.08	0.50	2.11E-01	0.26	0.83	8.36E-01	0.05	0.33	3.05E-01	-0.21	0.68	216332975	9776884	215414825	11326672	213991754	10373727	216837897	12143233
RP_POS_165_09056a13_129	RP	POS	13.13	165.0906				1.50E-01	-0.29	1.02	2.11E-01	-0.25	0.85	8.44E-02	-0.42	0.97	4.22E-01	-0.17	0.66	2849557	661368	2652638	670588	2736871	534706	2568405	779849
RP_POS_792_55261a13_7	RP	POS	13.70	792.5526				7.35E-01	0.05	0.78	2.12E-01	0.28	0.74	4.17E-01	0.19	0.61	4.73E-01	-0.09	0.47	1028108	833982	1102186	1609523	899557	706444	1304814	2156650
HILIC_POS_209_20125a0_511	HILIC	POS	0.511	209.2013				1.15E-06	0.58	1.12	2.12E-01	-0.28	0.99	3.16E-03	0.44	1.24	1.07E-04	0.72	1.34	106247	73898	521517	792913	620928	859999	422107	714484
RP_POS_227_20041a8_322	RP	POS	8.32	227.2004				8.10E-02	-0.37	0.74	2.12E-01	0.24	0.77	2.89E-01	-0.25	0.43	3.34E-02	-0.49	0.94	993413	46309	976906	43430	971463	41669	982350	44879
RP_NEG_271_22839a10_711	RP	NEG	10.71	271.2284				1.09E-01	0.27	1.00	2.12E-01	0.27	1.01	6.59E-02	0.40	0.95	4.55E-01	0.13	0.96	10965169	1480211	11525977	2265365	11242177	1836112	11809776	2613964
HILIC_NEG_115_9206a4_794	HILIC	NEG	4.794	115.9206				8.84E-01	0.03	0.88	2.12E-01	0.25	1.33	4.88E-01	0.16	0.94	6.71E-01	-0.10	0.17	71819852	17537991	72342983	17915795	70100757	18243246	74585209	17476429
RP_POS_571_28003a8_418	RP	POS	8.42	571.2800				9.06E-01	0.03	0.36	2.12E-01	0.24	0.85	5.84E-01	0.15	0.29	6.85E-01	-0.09	0.53	780471	1616986	817982	1315080	653091	881001	982873	1631722
HILIC_POS_138_05504a2_081	HILIC	POS	2.081	138.0550				1.25E-01	0.18	0.33	2.13E-01	0.29	0.80	1.57E-01	0.32	0.55	4.57E-01	0.04	0.26	2681848	4948011	11527254	56482899	4422389	15245879	18632119	78168337
RP_POS_430_04108a0_726	RP	POS	0.73	430.0411				5.10E-09	0.73	1.19	2.13E-01	0.27	0.80	1.07E-05	0.87	1.43	4.01E-05	0.60	1.27	121693	92042	394263	401916	343960	335254	444565	456957
HILIC_NEG_98_93883a2_941	HILIC	NEG	2.941	98.9388				3.75E-03	0.48	1.04	2.13E-01	-0.26	1.00	8.72E-02	0.35	0.76	1.14E-03	0.62	1.13	683323	99074	752290	150529	771117	135899	733464	163059
RP_POS_288_63388a10_328	RP	POS	10.33	288.6339				4.75E-04	-0.77	1.42	2.13E-01	-0.23	1.32	2.88E-04	-0.88	1.51	4.03E-03	-0.65	1.23	14952294	2242866	13288122	1986492	13536524	1811517	13039719	2136660
RP_NEG_459_27383a9_902	RP	NEG	9.90	459.2738				1.14E-01	0.29	1.10	2.13E-01	0.26	0.73	4.90E-02	0.42	0.84	4.38E-01	0.16	1.11	683649	726493	933794	889420	822598	875413	1044991	898163
RP_POS_791_54297a12_686	RP	POS	12.69	791.5430				1.62E-03	0.59	1.24	2.13E-01	-0.25	0.83	2.84E-02	0.46	0.95	7.15E-04	0.72	1.25	3559505	2048272	5005234	2473538	5314267	2404579	4696201	2526804
HILIC_POS_394_29507a0_626	HILIC	POS	0.626	394.2951				1.62E-01	0.25	0.54	2.14E-01	-0.26	1.02	5.48E-01	0.12	0.37	7.52E-02	0.38	0.63	436056	186796	493930	241396	524065	254193	463795	226419
RP_NEG_378_92041a15_317	RP	NEG	15.32	378.9204				9.21E-01	-0.02	0.81	2.14E-01	-0.25	0.77	4.96E-01	-0.15	0.68	6.43E-01	0.11	0.36	1320532	67487	1319142	71456	1328053	77066	1310230	64922
RP_POS_397_41544a11_669	RP	POS	11.67	397.4154				9.59E-01	-0.01	0.65	2.15E-01	-0.25	0.74	5.50E-01	-0.14	0.49	6.20E-01	0.11	0.39	4236235	1859052	4216946	1850640	4447510	1892785	3986382	1796805
RP_NEG_529_46478a14_275	RP	NEG	14.28	529.4648				3.82E-01	-0.18	0.56	2.15E-01	0.25	0.77	8.03E-01	-0.06	0.25	1.79E-01	-0.31	0.62	986456	748157	853587	724827	763352	688360	943821	755654
HILIC_NEG_254_97211a4_79	HILIC	NEG	4.79	254.9721				9.83E-01	0.00	1.07	2.15E-01	-0.26	1.10	5.67E-01	-0.13	0.82	5.22E-01	0.13	1.05	315494	97725	315947	116642	330465	110164	301429	122156
RP_POS_980_13605a0_488	RP	POS	0.49	980.1361				3.21E-08	0.67	1.28	2.15E-01	-0.27	1.21	3.61E-04	0.54	1.25	1.99E-05	0.81	1.48	194949	34825	352290	256977	384276	281462	320304	228284
RP_POS_516_87354a0_496	RP	POS	0.50	516.8735				4.45E-09	-0.74	1.33	2.15E-01	0.27	1.19	2.47E-04	-0.60	1.29	1.77E-06	-0.87	1.56	1349347	76135	1121536	334692	1079917	344211	1163156	322967
RP_NEG_209_83333a15_553	RP	NEG	15.55	209.8333				6.56E-01	-0.09	0.32	2.15E-01	-0.26	0.88	3.38E-01	-0.21	0.52	8.37E-01	0.04	0.44	1583531	112083	1572952	128436	1588922	120687	1556981	135065
RP_NEG_680_84668a0_493	RP	NEG	0.49	680.8467				1.30E-08	-0.71	1.35	2.16E-01	0.27	1.26	5.15E-04	-0.58	1.32	2.54E-06	-0.85	1.55	1610026	143250	1185542	648511	1104942	657949	1266143	635264
RP_POS_665_42072a10_463	RP	POS	10.46	665.4207				4.10E-03	0.54	0.97	2.16E-01	0.25	0.75	2.24E-03	0.67	1.10	4.49E-02	0.42	0.79	818172	292724	1003734	345271	960834	332241	1046634	355973
RP_NEG_636_35291a10_936	RP	NEG	10.94	636.3529				2.32E-02	-0.51	1.33	2.16E-01	-0.23	1.73	1.28E-02	-0.63	1.26	8.94E-02	-0.39	1.11	13616235	2356932	12532009	1986598	12778755	1740679	12285264	2195329
HILIC_POS_159_11298a4_857	HILIC	POS	4.857	159.1130				4.18E-01	-0.15	1.00	2.16E-01	-0.26	1.08	2.03E-01	-0.28	0.70	9.09E-01	-0.02	0.79	1127392	317755	1072307	374242	1118765	351288	1025849	393908
RP_NEG_317_05917a8_812	RP	NEG	8.81	317.0592				2.68E-01	-0.14	0.75	2.16E-01	0.28	0.82	9.69E-01	0.00	0.55	1.91E-01	-0.29	0.69	74721975	12657642	69711746	39057783	64850547	50365916	74572945	22298006
RP_NEG_351_90536a15_419	RP	NEG	15.42	351.9054				1.50E-01	-0.29	0.48	2.16E-01	-0.25	0.95	5.00E-02	-0.41	1.01	4.89E-01	-0.16	0.38	850474	209130	787660	219280	814880	250398	760439	181488
RP_NEG_212_00212a3_298	RP	NEG	3.30	212.0021				6.64E-02	-0.42	0.81	2.17E-01	-0.23	0.75	3.27E-02	-0.53	0.94	2.09E-01	-0.30	0.54	27436432	17667973	20960000	14479430	22756219	13786944	19163781	15063935
RP_POS_146_06013a4_314	RP	POS	4.31	146.0601				2.13E-02	-0.55	0.85	2.17E-01	-0.22	0.77	4.38E-03	-0.66	1.47	1.13E-01	-0.44	0.56	1154540	1577083	432271	1164438	577414	1600249	287128	368393
HILIC_NEG_113_92614a7_352	HILIC	NEG	7.352	113.9261				8.51E-01	-0.04	0.75	2.17E-01	-0.26	0.92	4.23E-01	-0.16	0.39	6.78E-01	0.09	0.55	3926277	476171	3907195	559809	3976589	611504	3837802	499403
RP_POS_132_95853a15_618	RP	POS	15.62	132.9585				2.17E-01	0.28	0.46	2.17E-01	0.24	0.82	1.13E-01	0.39	0.63	5.04E-01	0.16	0.65	74063130	12593235	77147414	10624334	75830925	9848394	78463903	11292858
RP_POS_267_89459a0_252	RP	POS	0.25	267.8946				2.62E-01	0.23	0.88	2.17E-01	-0.25	0.95	6.36E-01	0.10	0.40	1.30E-01	0.35	0.95	3267807	319135	3341635	324286	3381811	342691	3301458	302883
HILIC_NEG_133_05061a1_39	HILIC	NEG	1.39	133.0506				1.08E-02	0.30	0.86	2.17E-01	0.28	0.80	5.08E-02	0.44	0.67	1.51E-02	0.16	0.84	54566	80906	593062	2068252	335667	783408	850456	2809573
RP_POS_1030_72058a0_496	RP	POS	0.50	1030.7206				4.02E-01	-0.19	0.43	2.17E-01	-0.24	0.77	2.14E-01	-0.31	0.60	7.73E-01	-0.07	0.45	566679	142504	543072	120116	557951	116258	528194	123217
RP_POS_281_20792a10_403	RP	POS	10.40	281.2079				9.71E-01	0.00	0.63	2.17E-01	0.28	0.77	5.45E-01	0.14	0.55	1.83E-01	-0.14	0.59	3021615	234222	3018862	645386	2938673	323514	3099051	850743
RP_POS_146_06009a5_026	RP	POS	5.03	146.0601				9.36E-01	-0.02	0.36	2.18E-01	-0.24	0.77	5.66E-01	-0.14	0.51	6.75E-01	0.10	0.42	425825	295632	421130	255934	452804	261480	389456	248840
RP_POS_591_26056a6_357	RP	POS	6.36	591.2606				7.71E-01	0.05	0.41	2.18E-01	0.26	0.74	4.13E-01	0.18	0.41	7.10E-01	-0.08	0.59	1070362	64381	1074393	77700	1064775	68729	1084010	85356
HILIC_POS_123_05552a0_611	HILIC	POS	0.611	123.0555				6.55E-01	-0.08	0.64	2.18E-01	-0.26	0.92	2.80E-01	-0.21	0.40	8.10E-01	0.05	0.64	385485	178020	367777	237858	397206	260899	338347	210883
RP_POS_417_22815a7_549	RP	POS	7.55	417.2282				2.23E-01	-0.25	0.84	2.18E-01	0.25	0.93	5.80E-01	-0.12	0.76	1.09E-01	-0.37	0.80	613158	43412	602180	45020	596612	47507	607749	42128
RP_POS_587_43268a13_497	RP	POS	13.50	587.4327				4.22E-01	0.11	0.42	2.18E-01	0.28	0.83	2.60E-01	0.25	0.50	7.95E-01	-0.03	0.31	770424	111351	799056	296007	762345	168621	835768	381896
RP_POS_332_96414a6_184	RP	POS	6.18	332.9641				1.21E-01	0.29	1.07	2.18E-01	-0.26	0.88	4.16E-01	0.16	0.77	6.62E-02	0.42	1.01	175165	210269	245741	252406	276964	283119	214518	215806
RP_NEG_207_93074a1_582	RP	NEG	1.58	207.9307				3.57E-01	0.18	0.55	2.18E-01	0.25	1.00	1.76E-01	0.30	0.64	8.09E-01	0.05	0.71	1419562	674532	1550356	752281	1457362	705251	1643349	792701
RP_POS_140_95232a15_38	RP	POS	15.38	140.9523				6.91E-01	-0.08	0.20	2.19E-01	-0.26	0.83	3.37E-01	-0.20	0.44	8.09E-01	0.05	0.39	26402086	753830	26338350	880113	26447043	913982	26229658	839961
HILIC_NEG_200_85866a3_965	HILIC	NEG	3.965	200.8587				9.61E-01	-0.01	0.30	2.19E-01	-0.25	0.88	5.50E-01	-0.13	0.45	6.11E-01	0.11	0.23	2439508	825925	2431113	851817	2536260	852545	2325967	846520
RP_POS_321_24002a10_333	RP	POS	10.33	321.2400				1.67E-01	0.22	0.66	2.19E-01	-0.27	0.77	5.95E-01	0.09	0.48	1.03E-01	0.36	0.66	4196248	1241855	4613339	2031477	4864266	2405114	4362413	1557226
RP_POS_260_1601a0_705	RP	POS	0.71	260.1601				8.56E-01	0.02	0.58	2.19E-01	-0.28	0.78	7.07E-02	-0.12	0.73	4.79E-01	0.16	0.45	514878	472793	551188	1810720	775831	2519296	326545	417715
RP_POS_912_51154a12_958	RP	POS	12.96	912.5115				4.31E-04	-0.76	1.36	2.19E-01	-0.23	0.87	2.05E-04	-0.88	1.45	4.74E-03	-0.65	1.13	819201	433028	493932	393420	542425	390869	445439	393878
HILIC_NEG_164_83583a3_005	HILIC	NEG	3.005	164.8358				7.94E-01	0.06	0.82	2.20E-01	-0.24	0.84	7.78E-01	-0.07	0.38	4.51E-01	0.18	0.78	23271513	6819146	23628849	6354283	24411580	6332665	22846118	6342306
RP_POS_313_64136a10_446	RP	POS	10.45	313.6414				1.71E-03	0.60	1.23	2.20E-01	-0.25	1.00	2.85E-02	0.48	0.98	6.16E-04	0.73	1.37	630981	333215	861770	382519	908864	355520	814676	405841
HILIC_POS_117_52026a3_689	HILIC	POS	3.689	117.5203				9.21E-02	0.29	0.58	2.20E-01	0.26	1.03	6.16E-02	0.42	0.74	3.59E-01	0.16	0.39	1031878	725386	1309578	1000904	1186342	760389	1432813	1189485
RP_NEG_201_03471a0_611	RP	NEG	0.61	201.0347				2.48E-01	0.23	0.43	2.21E-01	-0.25	0.81	6.38E-01	0.10	0.31	1.18E-01	0.35	0.72	2100111	718454	2274309	781256	2370372	807067	2178247	750326
RP_POS_997_62421a10_332	RP	POS	10.33	997.6242				9.68E-01	0.01	0.96	2.21E-01	-0.24	1.12	6.62E-01	-0.11	0.69	5.78E-01	0.13	0.87	5830274	3911893	5860936	3391412	6278125	2855457	5443747	3837870
RP_POS_199_13046a13_638	RP	POS	13.64	199.1305				2.25E-01	0.25	0.87	2.21E-01	-0.24	0.94	5.65E-01	0.13	0.54	1.06E-01	0.38	0.76	27479560	11982813	30441508	11515577	31855906	11448164	29027111	11523029
RP_POS_366_18594a10_65	RP	POS	10.65	366.1859				8.76E-01	-0.02	0.57	2.21E-01	0.28	0.77	6.04E-01	0.12	0.51	1.36E-01	-0.16	0.63	431239	97700	426442	254415	395078	118043	457807	338871
HILIC_POS_363_03571a6_299	HILIC	POS	6.299	363.0357				3.19E-01	-0.21	0.48	2.21E-01	-0.24	0.72	1.58E-01	-0.33	0.55	6.98E-01	-0.09	0.23	1694644	653201	1562923	615778	1638507	607185	1487340	621105
RP_POS_301_21057a11_161	RP	POS	11.16	301.2106				7.06E-01	0.07	0.84	2.21E-01	0.26	0.97	3.86E-01	0.20	0.73	7.70E-01	-0.06	0.85	3205362	690468	3261338	829306	3159496	690182	3363180	944466
RP_POS_301_63004a10_303	RP	POS	10.30	301.6300				3.53E-03	0.68	1.14	2.21E-01	-0.22	0.85	2.33E-02	0.56	0.90	1.29E-03	0.79	1.22	936604	313233	1123845	249847	1154513	227350	1093177	269283
RP_POS_477_10568a7_035	RP	POS	7.04	477.1057				2.79E-01	-0.17	0.78	2.22E-01	0.27	1.21	8.72E-01	-0.04	0.81	3.00E-02	-0.31	1.07	2084716	1586723	1662318	2680531	1332388	1335092	1992248	3537302

Supplementary table 1: Metabolomics results (in asceding order according to p-value from progressive ALD vs non-progressive ALD comparison, with molecular features with ID_level of 1-2 first)

								all_ALD_vs_control			Prog_ALD_vs_non-prog_ALD			Prog_ALD_vs_control_ALD			Non-prog_ALD_vs_control			Healthy_control		all_ALD		Non-prog_ALD		Progressive_ALD	
								t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA								
Feature_ID	RP_HILIC	POS_NEG	Average.Rt	Average.Mz	Metabolite.name	curated_MSMS	ID_level	p	d	VIP	p	d	VIP	p	d	VIP	p	d	VIP	Mean	SD	Mean	SD	Mean	SD	Mean	SD
RP_POS_818_50824a12_693	RP	POS	12.69	818.5082				1.13E-03	0.57	1.20	2.22E-01	-0.25	0.83	3.00E-02	0.44	0.97	5.96E-04	0.69	1.24	3794310	1700462	5094619	2380408	5386310	2318592	4802927	2428747
RP_POS_341_17776a11_248	RP	POS	11.25	341.1778				3.21E-05	0.78	1.63	2.22E-01	0.24	1.14	4.87E-05	0.90	1.61	8.75E-04	0.66	1.45	2748401	600906	3325716	728757	3236438	648492	3414995	797624
RP_POS_312_32599a11_601	RP	POS	11.60	312.3260				3.61E-08	0.74	1.30	2.22E-01	0.26	1.28	4.92E-05	0.87	1.39	2.86E-06	0.61	1.47	1772391	631771	2992028	1754592	2776718	1164801	3207338	2183722
HILIC_NEG_203_08269a4_014	HILIC	NEG	4.014	203.0827				5.77E-03	-0.44	1.06	2.23E-01	-0.26	1.43	7.06E-03	-0.58	1.18	6.81E-02	-0.31	1.05	315254	55550	277295	91344	288484	75167	266106	104652
RP_POS_853_50909a10_868	RP	POS	10.87	853.5091				2.27E-05	0.51	1.16	2.23E-01	-0.27	1.15	6.56E-03	0.37	1.20	9.66E-04	0.65	1.25	612222	201903	1320410	1558868	1511228	1796847	1129592	1267582
HILIC_NEG_157_01199a1_302	HILIC	NEG	1.302	157.0120				9.33E-08	0.84	1.49	2.23E-01	0.25	0.94	1.29E-06	0.96	1.57	7.05E-05	0.71	1.34	1194897	328628	1669407	578424	1598655	542885	1740158	609127
RP_POS_441_29495a14_166	RP	POS	14.17	441.2950				3.88E-01	0.17	0.53	2.24E-01	-0.25	0.72	8.32E-01	0.05	0.65	1.82E-01	0.30	0.72	15441881	7287601	16747578	7719740	17690098	7496886	15805057	7898654
RP_POS_864_51117a13_159	RP	POS	13.16	864.5112				1.97E-01	-0.28	0.73	2.24E-01	-0.24	0.83	9.45E-02	-0.40	0.73	5.01E-01	-0.16	0.54	2666110	878897	2436680	812092	2535817	804109	2337544	815964
RP_NEG_674_29102a10_124	RP	NEG	10.12	674.2910				1.22E-19	1.50	2.44	2.24E-01	0.20	0.77	3.85E-15	1.60	2.42	2.47E-16	1.40	2.45	696608	233799	1353795	362938	1309472	295518	1398118	418086
RP_NEG_170_94081a15_774	RP	NEG	15.77	170.9408				8.71E-01	-0.04	0.34	2.24E-01	-0.22	0.73	5.68E-01	-0.15	0.48	7.83E-01	0.07	0.31	1135898	507780	1120036	362441	1164210	345581	1075862	376252
RP_NEG_626_2807a10_508	RP	NEG	10.51	626.2807				9.94E-02	-0.36	0.97	2.25E-01	0.23	0.89	3.07E-01	-0.25	0.69	4.44E-02	-0.48	1.05	2522830	804271	2256073	705026	2170170	679615	2341977	726176
RP_POS_259_08414a6_888	RP	POS	6.89	259.0841				9.41E-01	0.01	0.64	2.25E-01	-0.28	0.92	1.01E-01	-0.13	0.68	5.24E-01	0.15	0.72	5524597	4114941	5632336	12569046	7172072	17432948	4092600	3231082
RP_POS_807_56995a13_801	RP	POS	13.80	807.5700				1.51E-01	0.25	0.92	2.25E-01	-0.26	0.89	5.29E-01	0.12	0.71	7.58E-02	0.38	0.99	1278008	1034414	1613001	1410486	1784777	1515527	1441224	1289380
RP_POS_306_95697a0_522	RP	POS	0.52	306.9570				1.20E-04	0.47	1.10	2.25E-01	-0.27	1.14	2.64E-02	0.33	0.95	1.19E-03	0.61	1.28	200538	37492	284237	199593	308544	218091	259930	178097
RP_POS_550_38647a10_9	RP	POS	10.90	550.3865				2.82E-01	-0.23	0.74	2.25E-01	0.24	1.42	6.52E-01	-0.11	0.50	1.22E-01	-0.35	0.87	698778	351722	622349	327598	582469	284745	662228	364014
RP_POS_194_11497a10_271	RP	POS	10.27	194.1150				2.37E-01	-0.24	0.92	2.26E-01	0.24	0.85	6.22E-01	-0.12	0.77	9.14E-02	-0.36	0.81	895453	68820	878582	71158	869929	60580	887236	80047
HILIC_POS_203_15009a6_433	HILIC	POS	6.433	203.1501				6.34E-03	0.43	0.95	2.26E-01	0.26	0.96	7.01E-03	0.56	0.89	8.72E-02	0.30	1.02	3939384	1169131	4753071	2053969	4503511	1780476	5002631	2286149
RP_POS_307_22443a10_564	RP	POS	10.56	307.2244				4.18E-03	-0.55	1.15	2.26E-01	0.24	1.08	5.58E-02	-0.43	1.09	1.25E-03	-0.67	1.16	758803	83431	706378	96008	694717	84799	718039	105616
RP_NEG_411_89331a15_708	RP	NEG	15.71	411.8933				9.84E-02	-0.30	0.71	2.27E-01	-0.25	0.84	5.53E-02	-0.43	0.75	3.77E-01	-0.17	0.65	811237	94385	776685	120986	791375	104901	761996	134646
RP_POS_518_3244a10_041	RP	POS	10.04	518.3244				4.39E-02	0.38	0.93	2.27E-01	-0.25	0.86	2.41E-01	0.26	0.72	1.67E-02	0.50	1.10	18174279	13457563	24064618	15923980	25996872	15051085	22132365	16678323
RP_POS_194_00746a15_547	RP	POS	15.55	194.0075				1.59E-02	-0.38	1.08	2.27E-01	-0.26	1.14	1.75E-02	-0.51	1.06	1.36E-01	-0.25	0.97	5224113	407888	4974382	717098	5061455	567288	4887309	837654
RP_NEG_410_6319a15_584	RP	NEG	15.58	410.6319				4.60E-01	-0.15	0.48	2.27E-01	-0.24	0.72	2.08E-01	-0.27	0.53	9.09E-01	-0.03	0.25	724360	36541	718807	37508	723358	41696	714257	32583
RP_NEG_155_86446a15_588	RP	NEG	15.59	155.8645				4.16E-01	-0.15	0.33	2.27E-01	-0.25	0.76	1.99E-01	-0.28	0.65	9.02E-01	-0.03	0.31	495853	23439	491758	28000	495153	27310	488362	28541
RP_POS_378_90021a0_497	RP	POS	0.50	378.9002				3.25E-09	-0.72	1.35	2.27E-01	0.26	1.23	2.24E-04	-0.59	1.33	3.29E-06	-0.85	1.55	34962004	933651	29694375	7992550	28725180	8362671	30663570	7564001
RP_POS_585_27014a11_669	RP	POS	11.67	585.2701				6.79E-01	-0.09	0.54	2.27E-01	0.24	1.19	9.15E-01	0.03	0.36	3.07E-01	-0.21	0.73	952703	1693505	812942	1511699	628900	637327	996984	2035140
RP_POS_179_10689a7_866	RP	POS	7.87	179.1069				7.66E-02	-0.39	0.61	2.27E-01	-0.23	0.76	3.89E-02	-0.50	0.80	2.43E-01	-0.27	0.49	1932199	112461	1891954	99489	1904016	93373	1879893	104798
RP_NEG_414_62457a15_583	RP	NEG	15.58	414.6246				5.04E-01	-0.13	0.51	2.27E-01	-0.25	0.86	2.45E-01	-0.26	0.60	9.68E-01	-0.01	0.30	1586780	77393	1576022	82711	1586045	85115	1565999	79827
RP_NEG_259_85715a15_626	RP	NEG	15.63	259.8572				1.71E-01	0.28	0.80	2.27E-01	-0.24	0.84	5.08E-01	0.15	0.31	6.70E-02	0.40	0.90	795583	52070	810382	53896	816914	48071	803851	58915
RP_POS_163_97653a10_57	RP	POS	10.57	163.9765				2.83E-01	-0.22	0.57	2.28E-01	0.24	0.95	6.41E-01	-0.10	0.37	1.49E-01	-0.34	0.61	2572239	802366	2396811	776276	2302785	834455	2490837	709329
RP_POS_479_39282a10_88	RP	POS	10.88	479.3928				9.72E-01	-0.01	0.73	2.28E-01	0.25	1.33	6.06E-01	0.12	0.55	5.63E-01	-0.13	0.62	3625973	367293	3623335	383021	3576951	381545	3669719	382671
HILIC_NEG_114_02457a1_298	HILIC	NEG	1.298	114.0246				1.18E-07	0.82	1.44	2.28E-01	0.25	0.94	9.06E-07	0.95	1.58	1.46E-04	0.70	1.26	496518	149012	711755	268370	679264	264847	744247	270585
HILIC_POS_659_76855a0_575	HILIC	POS	0.575	659.7686				3.46E-06	0.60	1.28	2.29E-01	-0.27	0.96	1.13E-03	0.46	1.43	2.81E-04	0.73	1.45	56820	213423	463959	749494	554601	870058	373317	600982
RP_NEG_178_81479a15_52	RP	NEG	15.52	178.8148				7.14E-01	-0.07	0.60	2.29E-01	-0.25	0.79	3.33E-01	-0.19	0.57	7.89E-01	0.06	0.37	2617674	100360	2609715	124191	2624722	136522	2594709	109836
HILIC_NEG_134_89464a4_771	HILIC	NEG	4.771	134.8946				1.68E-01	-0.24	0.48	2.29E-01	0.26	0.82	5.51E-01	-0.11	0.63	9.01E-02	-0.37	0.58	15896576	3317467	14865077	4520044	14318884	5009648	15411270	3946283
RP_NEG_387_18552a8_139	RP	NEG	8.14	387.1855				1.27E-01	0.24	0.58	2.29E-01	0.26	0.76	9.55E-02	0.37	0.65	4.82E-01	0.11	0.59	1107788	1196572	1560863	2048384	1313107	1405662	1808620	2525119
HILIC_NEG_136_89163a0_824	HILIC	NEG	0.824	136.8916				7.46E-01	-0.06	0.75	2.29E-01	-0.25	0.93	4.04E-01	-0.19	0.30	7.77E-01	0.06	0.15	6046764	973275	5980712	1078174	6110875	1032668	5850550	1116989
HILIC_NEG_132_90002a0_93	HILIC	NEG	0.93	132.9000				4.86E-02	0.38	1.14	2.30E-01	0.25	0.94	1.52E-02	0.50	1.21	2.60E-01	0.26	0.88	1475714	368429	1631796	420282	1581091	468805	1682501	363118
RP_NEG_213_02251a6_647	RP	NEG	6.65	213.0225				1.25E-01	0.18	0.54	2.30E-01	0.28	0.81	1.60E-01	0.32	0.72	4.47E-01	0.04	0.45	7958113	14952849	26709835	118521368	12349551	36080281	41070118	163274830
RP_NEG_299_73135a15_599	RP	NEG	15.60	299.7314				1.60E-01	-0.30	0.81	2.30E-01	-0.23	0.71	8.34E-02	-0.42	0.73	4.18E-01	-0.19	0.72	1152212	60998	1134907	55559	1141600	51443	1128214	59150
RP_POS_323_25568a10_287	RP	POS	10.29	323.2557				1.48E-01	0.25	0.91	2.30E-01	0.26	1.10	9.19E-02	0.37	0.84	5.07E-01	0.12	0.75	4280610	600166	4481689	873941	4376340	685492	4587038	1024979
HILIC_NEG_199_03789a2_172	HILIC	NEG	2.172	199.0379				3.57E-01	0.18	0.51	2.30E-01	-0.24	0.95	7.72E-01	0.06	0.24	1.88E-01	0.31	0.53	411095	176967	444895	185590	467251	201199	422539	167598
RP_NEG_244_90852a8_371	RP	NEG	8.37	244.9085				6.79E-02	-0.40	1.16	2.30E-01	-0.23	0.74	2.42E-02	-0.51	1.14	2.54E-01	-0.28	0.50	1672792	949551	1321315	850126	1423752	967465	1218878	709067
RP_POS_192_13838a0_883	RP	POS	0.88	192.1384	Unknown	192.1387(100), 133.0642(40), 58.0657(10)	4	9.29E-02	0.34	0.69	2.30E-01	-0.24	0.74	3.24E-01	0.22	0.49	4.47E-02	0.46	0.86	27168929	4705524	28821319	4910252	29412523	5062664	28230115	4729621
RP_NEG_215_01816a6_646	RP	NEG	6.65	215.0182				1.30E-01	0.18	0.54	2.30E-01	0.28	0.82	1.64E-01	0.32	0.72	4.68E-01	0.04	0.44	371455	681797	1196531	5275781	558103	1597242	1834958	7269990
RP_POS_181_07205a2_679	RP	POS	2.68	181.0721				7.97E-04	-0.95	1.87	2.31E-01	0.17	0.73	2.99E-03	-0.86	1.38	3.31E-04	-1.03	1.92	21902375	20327949	8234285	10076949	7020208	7833367	9448362	11865597
RP_POS_299_25787a10_54	RP	POS	10.54	299.2579				1.15E-01	-0.30	0.86	2.31E-01	0.25	0.96	4.01E-01	-0.18	0.74	5.28E-02	-0.43	0.86	2762769	405179	2626992	456247	2572114	460666	2681871	449680
RP_NEG_261_85083a15_621	RP	NEG	15.62	261.8508				2.07E-01	-0.24	0.78	2.31E-01	0.25	0.90	5.96E-01	-0.11	0.51	9.33E-02	-0.36	1.15	8695299	452421	8572680	533501	8508517	532502	8636844	532067
RP_POS_949_6264a10_511	RP	POS	10.51	949.6264				3.51E-01	0.16	1.00	2.31E-01	-0.26	0.97	8.67E-01	0.04	0.72	1.33E-01	0.29	0.90	2619775	853824	2797934	1152925	2936621	1017898	2659246	1268948
RP_POS_143_01675a14_268	RP	POS	14.27	143.0168				6.38E-01	0.07	0.40	2.31E-01	0.26	0.76	3.51E-01	0.21	0.46	7.02E-01	-0.06	0.39	5271333	588315	5341153	1051071	5214577	744483	5467728	1282612
HILIC_NEG_99_92564a1_294	HILIC	NEG	1.294	99.9256				8.09E-01	0.05	0.63	2.32E-01	0.24	0.87	4.66E-01	0.17	0.33	7.64E-01	-0.07	0.13	5585270	1631754	5665128	1574947	5476069	1541452	5854187	1600787
RP_POS_888_80432a0_493	RP	POS	0.49	888.8043				3.30E-03	0.39	1.03	2.32E-01	0.27	1.30	6.83E-03	0.53	1.12	9.44E-02	0.26	1.09	526672	193584	718831	542915	653640	471080	784022	604102
RP_NEG_704_33734a10_94	RP	NEG	10.94	704.3373				2.00E-01	-0.29	1.33	2.32E-01	-0.23	1.14	1.08E-01	-0.40	1.07	4.64E-01	-0.17	1.05	2439655	525664	2305678	444341	2359016	405992	2252340	477777
RP_POS_514_03711a0_711	RP	POS	0.71	514.0371				3.81E-01	-0.13	0.85	2.32E-01	0.27	1.01	9.94E-01	0.00	0.77	1.26E-01	-0.26	0.94	589623	120982	561549	236534	533158	209378	589941	259913
HILIC_POS_143_11786a1_548	HILIC	POS	1.548	143.1179				4.05E-02	0.37	0.78	2.33E-01	0.25	0.88	2.59E-02	0.49	0.86	2.05E-01	0.25	0.46	2530779	1019716	2996301	1309547	2839272	1132276	3153329	1460292
RP_POS_311_1553a5_624	RP	POS	5.62	311.1553				1.91E-01	0.24	0.70	2.33E-01	0.25	0.91	1.15E-01	0.36	1.13	5.44E-01	0.11	0.63	694830	1010906	983381	1257963	832494	975250	1134268	1483125
RP_NEG_230_0128a2_409	RP	NEG	2.41	230.0128				1.17E-01	0.21	0.43	2.33E-01	-0.27	0.76	4.03E-01	0.07	0.74	1.40E-01	0.34	0.47	1685829	2311289	2935010	6786491	3752163	9321297	2117856	2191700
RP_POS_320_25604a9_979	RP	POS	9.98	320.2560				2.80E-01	-0.30	0.97	2.33E-01	-0.19	0.88	1.66E-01	-0.39	0.87	4.81E-01	-0.21	0.64	5788274	7735964	4224143	4066837	4711610	4585506	3736676	3450223
RP_NEG_256_98642a7_425	RP	NEG	7.43	256.9864				1.20E-01	-0.26	0.58	2.33E-01	-0.26	0.77	8.46E-02	-0.39	0.69	4.23E-01	-0.14	0.42	6416076	346380	6291596	502190	6351843	360944	6231350	609794
RP_NEG_855_66193a14_829	RP	NEG	14.83	855.6619				5.89E-03	-0.68	1.20	2.33E-01	-0.21	0.72	2.76E-03	-0.78	1.30	2.53E-02	-0.57	0.96	4536821	2008977	3426845	1411482	3595753	1424785	3257938	1391758
HILIC_POS_663_45471a10_694	HILIC	POS	10.694	663.4547				3.51E-02	-0.39	0.83	2.33E-01	-0.25	0.88	1.73E-02	-0.51	1.01	1.97E-01	-0.27	0.65	1769875	46512	1748393	56501	1755152	54783	1741634	57926
RP_NEG_529_46478a13_289	RP	NEG	13.29	529.4648				2.88E-01	-0.20	0.72	2.34E-01	0.25	0.76	7.58E-01	-0.07	0.58	9.59E-02	-0.32	0.66	3777434	1347366	3466350	1659272	3267714	1308958	3664987	1941304
RP_POS_208_89061a0_518	RP	POS	0.52	208.8906				1.58E-02	0.36	1.01	2.34E-01	-0.26	0.94	1.91E-01	0.23	0.85	1.24E-02	0.49	1.06	506590	101162	572446	200272	596380	213080	548511	185645
HILIC_NEG_119_90759a3_046	HILIC	NEG	3.046	119.9076				4.41E-02	-0.42	0.88	2.34E-01	-0.23	0.94	2.15E-02	-0.54	0.87	1.79E-01	-0.30	0.65	722829	213892	633876	206813	658588	200573	609164	211992
HILIC_NEG_209_0665a2_173	HILIC	NEG	2.173	209.0665				4.60E-01	0.14	0.53	2.34E-01	-0.25	0.98	9.32E-01	0.02	0.32	2.31E-01	0.26	0.50	4633117	1649047	4890716	1875834	5114819	1926498	4666613	1815333
RP_POS_235_99799a1_464	RP	POS	1.46	235.9980				4.99E-11	0.90	1.47	2.34E-01	0.25	0.73	1.96E-07	1.02	1.68	1.56E-06	0.77	1.48	964210	904133	3040685	2405948	2753297	2133914	3328073	2640675
HILIC_POS_144_10202a5_119	HILIC	POS	5.119	144.1020				3.15E-01	0.12	0.48	2.35E-01	0.28	1.28	2.71E-01	0.26	0.60	4.22E-01	-0.02	0.61	1150308	1434814	2623958	14364719	899845	1261447	4348070	20229773
RP_NEG_189_93207a15_38	RP	NEG	15.38	189.9321				1.97E-01	0.28	1.16	2.35E-01	-0.23	0.71	4.87E-01	0.16	0.84	9.88E-02	0.39	0.88	2261367	789015	2466396	715208	2551721	726706	2381071	700374
RP_POS_525_28772a5_108	RP	POS	5.11	525.2877				4.05E-02	0.36	1.20	2.35E-01	-0.25	1.28	2.05E-01	0.23	1.13	3.08E-02	0.48	1.22	620076	1790628	1461522	2499683	1759917	2904052	1163128	2002277
RP_POS_548_50372a11_253	RP	POS	11.25	548.5037				4.75E-01	0.13	0.86	2.35E-01	0.25	1.17	2.37E-01	0.25	0.73	9.98E-01	0.00	0.75	1395007	439186	1464584	580757	1395311	543396	1533857	613489
RP_POS_413_32349a10_944	RP	POS	10.94	413.3235				3.17E-01	-0.22	0.62	2.35E-01	0.23	0.76	6.74E-01	-0.10	0.30	1.51E-01	-0.33	0.82	27893608	5250725	26843323	4649969	26288774	4186462	27397872	5052883
RP_POS_336_93079a15_423	RP	POS	15.42	336.9308				1.60E-02	-0.53	1.03	2.35E-01	-0.22	0.87	5.93E-03	-0.64	1.18	8.56E-02	-0.42	0.86	4926836	1511044	4182687	1319453	4339986	1442538	4025388	1177299
RP_POS_431_38806a13_125	RP	POS	13.13	431.3881				1.55E-01	-0.28	1.05	2.36E-01	-0.24	0.84	8.86E-02	-0.40	0.98	4.39E-01	-0.16	0.68	2816481	628884	2628350	681117	2709498	569033	2547203	774643
HILIC_NEG_289_70312a1_362	HILIC	NEG	1.362	289.7031				1.66E-10	0.87	1.64	2.36E-01	-0.25	0.68	9.84E-05	0.75	1.37	1.55E-09	0.99	2.18	462031	66844	611227	179047	632549	153065	589906	201031
RP_POS_404_15005a7_727	RP	POS	7.73	404.1501				9.57E-01	0.01	0.24	2.36E-01	-0.25	0.81	6.12E-01	-0.12	0.26	4.20E-01	0.14	0.61	782288	52781	782936	73690	791722	49100	774150	91667
HILIC_POS_256_17532a0_615	HILIC	POS	0.615	256.1753				2.30E-01	0.21	1.09	2.36E-01	-0.25	0.95	6.53E-01	0.08	1.11	1.40E-01	0.33	1.17	611647	718336	809020	1021791	930748	1217919	687291	771916
HILIC_NEG_136_89168a0_709	HILIC	NEG	0.709	136.8917				2.51E-01	0.23	0.73	2.36E-01	-0.24	0.75	6.24E-01	0.11	0.62	1.16E-01	0.35	0.62	4706761	1423117	5045782	1481347	5221966	1435539	4869599	1519684
RP_NEG_787_10193a9_437	RP	NEG	9.44	787.1019				2.08E-01	-0.29	0.63	2.36E-01	-0.22	0.72	1.05E-01	-0.40	0.77	4.79E-01	-0.17	0.37	4110549	290490	4038335	237810	4066615	241560	4010056	232976
RP_NEG_199_03769a0_611	RP	NEG	0.61	199.0377				2.78E-01	0.22	0.40	2.36E-01	-0.24	0.78	6.66E-01	0.09	0.28	1.37E-01	0.34	0.68	6254940	2077733	6725464	2220463	6989471	2280126	6461456	2149491
RP_NEG_246_90561a8_372	RP	NEG	8.37	246.9056				5.31E-02	-0.42	1.18	2.37E-01	-0.23	0.74	1.90E-02	-0.54	1.18	2.12E-01	-0.31	0.52	1623331	908436	1266622	809679	1362895	917339	1170348	681259
HILIC_POS_394_31537a7_665	HILIC	POS	7.665	394.3154				9.25E-01	-0.02	0.38	2.37E-01	-0.25	0.71	4.95E-01	-0.14	0.50	5.77E-01	0.11	0.79	2484869	297311	2478600	412169	2527581	390105	2429618	431458
HILIC_NEG_1002_76892a0_493	RP	NEG	0.49	1002.7689				3.58E-10	-0.81	1.43	2.37E-01	0.25	1.23	7.85E-05	-0.68	1.41	1.70E-07	-0.93	1.63	1171355	131594	812798	473430	756555	468166	869041	476666
RP_POS_316_11783a7_526	RP	POS	7.53	316.1178				9.54E-05	0.47	0.92	2.37E-01	-0.27	0.71	1.43E-02	0.34	0.86	1.89E-03	0.61	1.02	155300	137585	507668	836374	607062	960598	408274	685863
RP_NEG_608_31793a10_528	RP	NEG	10.53	608.3179				6.34E-02	-0.46	0.80	2.37E-01	-0.21	0.85	3.62E-02	-0.56	0.89	1.62E-01	-0.35	0.76	11571255	1007433	11206309	697214	11289128	619038	11123490	764807
RP_POS_187_12619a6_499	RP	POS	6.50	187.1262				1.07E-01	0.34	0.67	2.37E-01	-0.23	0.76	3.41E-01	0.22	0.51	4.82E-02	0.45	0.84	39201571	21071918	46182603	20446164	48609359	19925511	43755847	20870508
RP_NEG_134_86436a15_504	RP	NEG	15.50	134.8644				4.59E-01	0.14	0.85	2.37E-01	-0.25	0.75	9.53E-01	0.01	0.54	2.35E-01	0.26	0.55	1504422	60991	1514211	75147	1523130	80070	1505292	69540
HILIC_NEG_343_99524a7_355	HILIC	NEG	7.355	343.9952				1.79E-01	0.20	0.43	2.37E-01	0.26	0.71	1.40E-01	0.33	0.47	6.28E-01	0.07	0.34	1084930	73824	1111948	151391	1093946	93278	1129951	192209
RP_POS_569_43201a15_102	RP	POS	15.10	569.4320				1.04E-01	-0.36	0.66	2.37E-01	0.23	0.70	3.12E-01	-0.25	0.40	4.66E-02	-0.47	0.80	109564536	40731885	96260419	35419218	92058396	33313781	100462442	37266631
RP_POS_387_16187a10_908	RP	POS	10.91	387.1619				6.10E-02	0.27	1.39	2.38E-01	0.26	0.92	4.22E-02	0.40	1.11	3.97E-01	0.14	1.20	965468	413168	1180677	871682	1077266	770691	1284087	958841

Supplementary table 1: Metabolomics results (in asceding order according to p-value from progressive ALD vs non-progressive ALD comparison, with molecular features with ID_level of 1-2 first)

								all_ALD_vs_control			Prog_ALD_vs_non-prog_ALD			Prog_ALD_vs_control_ALD			Non-prog_ALD_vs_control			Healthy_control		all_ALD		Non-prog_ALD		Progressive_ALD	
								t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA								
Feature_ID	RP_HILIC	POS_NEG	Average.Rt	Average.Mz	Metabolite.name	curated_MSMS	ID_level	p	d	VIP	p	d	VIP	p	d	VIP	p	d	VIP	Mean	SD	Mean	SD	Mean	SD	Mean	SD
RP_POS_230_8889a15_43	RP	POS	15.43	230.8889				6.31E-01	-0.07	1.05	2.38E-01	0.26	0.75	6.96E-01	0.06	0.69	3.50E-01	-0.20	0.93	3342703	229732	3313778	441751	3261308	539611	3366248	312204
RP_POS_614_48492a10_659	RP	POS	10.66	614.4849				8.18E-01	0.05	0.60	2.38E-01	0.23	1.02	4.93E-01	0.17	0.82	7.57E-01	-0.07	0.54	6627647	502882	6650919	476252	6594444	421299	6707394	523697
RP_POS_189_12163a6_499	RP	POS	6.50	189.1216				1.10E-01	0.33	0.66	2.38E-01	-0.23	0.76	3.50E-01	0.21	0.51	4.99E-02	0.45	0.83	1697232	938163	2005418	916934	2114116	894338	1896720	935275
HILIC_POS_244_12756a0_571	HILIC	POS	0.571	244.1276				7.36E-01	0.04	0.19	2.38E-01	-0.27	0.75	3.13E-01	-0.09	0.44	4.37E-01	0.18	0.31	4565576	2711789	4876457	7844702	5810524	10737576	3942391	2694159
RP_POS_497_39606a13_281	RP	POS	13.28	497.3961				9.35E-01	0.02	0.72	2.38E-01	0.23	0.75	5.84E-01	0.13	0.74	6.67E-01	-0.10	0.33	21185069	14202174	21414891	12908289	19885444	11691699	22944338	13970634
RP_POS_812_55548a13_266	RP	POS	13.27	812.5555				5.20E-02	-0.45	0.95	2.38E-01	-0.22	0.88	2.28E-02	-0.56	0.98	1.75E-01	-0.34	0.84	2101814	1203311	1636032	955679	1749205	1017735	1522859	885076
HILIC_POS_102_1282a0_828	HILIC	POS	0.828	102.1282				5.24E-01	-0.13	0.82	2.39E-01	0.24	0.67	9.73E-01	-0.01	0.32	2.54E-01	-0.25	0.43	3530965	922851	3409239	966931	3294892	879508	3523586	1043443
HILIC_POS_162_11266a1_873	HILIC	POS	1.873	162.1127				2.10E-01	0.16	0.55	2.39E-01	0.27	1.16	2.00E-01	0.29	0.72	7.76E-01	0.02	0.16	47294	127707	116276	498443	57100	182720	175451	679285
HILIC_POS_173_12842a0_629	HILIC	POS	0.629	173.1284				2.95E-04	0.50	0.99	2.39E-01	0.26	0.82	1.58E-03	0.63	1.02	1.70E-02	0.37	1.01	241498	162652	425118	400129	377826	338528	472410	452005
RP_POS_531_40851a12_461	RP	POS	12.46	531.4085	Unknown	531.3886(70), 105.0006(100), 57.0705(28), 71.0863(20)	4	1.26E-01	0.23	0.43	2.39E-01	0.26	0.82	7.83E-02	0.36	0.60	5.60E-01	0.10	0.34	2753075	281674	2869264	564292	2802575	483584	2935953	632788
HILIC_POS_106_08674a1_87	HILIC	POS	1.87	106.0867				2.67E-01	0.22	0.62	2.39E-01	0.24	0.91	1.58E-01	0.34	0.52	6.24E-01	0.10	0.19	4232850	1690255	4624173	1810383	4410142	1412517	4838205	2129124
RP_NEG_556_31799a10_621	RP	NEG	10.62	556.3180				1.82E-02	0.54	1.30	2.40E-01	-0.22	1.03	8.43E-02	0.43	0.97	6.99E-03	0.65	1.38	4679536	888650	5102748	717081	5187446	631236	5018050	791077
HILIC_POS_189_12328a5_681	HILIC	POS	5.681	189.1233				1.02E-01	0.29	0.96	2.40E-01	0.25	0.94	5.68E-02	0.41	0.66	3.96E-01	0.16	0.60	423245	115056	465673	155071	447369	138640	483976	169352
RP_POS_324_32504a11_45	RP	POS	11.45	324.3250				4.50E-02	0.33	0.93	2.40E-01	0.25	1.19	3.91E-02	0.46	0.92	2.29E-01	0.20	0.60	230173	140117	297436	218741	271609	166046	323263	260268
RP_POS_570_35498a10_341	RP	POS	10.34	570.3550				6.85E-06	0.82	1.49	2.40E-01	-0.23	0.85	8.76E-04	0.70	1.27	3.39E-06	0.93	1.66	1110526	541401	1689533	701288	1772238	639231	1606827	755692
RP_NEG_332_87173a15_437	RP	NEG	15.44	332.8717				7.20E-01	0.07	0.65	2.41E-01	-0.25	0.95	7.95E-01	-0.06	0.24	3.72E-01	0.19	0.71	2576481	263833	2596740	315661	2633941	310223	2559539	319773
RP_NEG_583_25708a7_16	RP	NEG	7.16	583.2571				3.16E-01	-0.18	0.87	2.41E-01	0.25	1.15	7.92E-01	-0.06	0.42	9.93E-02	-0.31	1.10	2211856	1146126	1962320	1408621	1796239	1014288	2128402	1709927
RP_POS_299_25781a10_663	RP	POS	10.66	299.2578				4.37E-01	-0.14	0.80	2.41E-01	0.25	0.93	9.52E-01	-0.01	0.71	1.93E-01	-0.26	0.77	3698131	494219	3612462	660709	3534684	627318	3690241	690007
HILIC_POS_226_95102a5_461	HILIC	POS	5.461	226.9510				5.08E-01	-0.12	0.35	2.41E-01	0.25	0.92	9.93E-01	0.00	0.37	1.95E-01	-0.24	0.64	1682050	228486	1649186	283753	1615759	215645	1682613	337479
RP_NEG_1060_7196a0_497	RP	NEG	0.50	1060.7196				8.50E-01	-0.04	0.85	2.42E-01	-0.24	1.16	4.79E-01	-0.16	0.49	7.23E-01	0.08	0.86	1285010	202310	1277123	209634	1301776	217141	1252471	200996
RP_POS_584_47095a10_875	RP	POS	10.88	584.4710				1.54E-02	-0.43	0.77	2.42E-01	0.24	0.76	1.06E-01	-0.31	0.77	1.14E-02	-0.56	0.83	5143547	522669	4858227	681840	4778027	754857	4938426	596962
RP_POS_255_23192a10_462	RP	POS	10.46	255.2319				7.08E-09	0.74	1.36	2.42E-01	-0.25	0.97	1.60E-05	0.61	1.47	1.82E-05	0.87	1.55	821794	153262	1216317	575345	1284017	671322	1148616	456916
RP_POS_695_50903a11_854	RP	POS	11.85	695.5090				1.68E-05	-0.95	1.71	2.42E-01	-0.21	0.70	1.03E-05	-1.06	1.71	2.20E-04	-0.85	1.46	1498814	511495	1014937	450593	1067913	435104	961960	463862
RP_POS_213_15973a5_858	RP	POS	5.86	213.1597				7.61E-01	-0.09	1.25	2.42E-01	0.18	0.88	9.82E-01	0.01	0.66	5.43E-01	-0.18	1.08	656116	717742	615702	369705	572237	357371	659166	380241
RP_POS_592_33716a10_446	RP	POS	10.45	592.3372				3.37E-03	0.56	1.22	2.42E-01	-0.24	0.93	4.64E-02	0.44	0.93	1.17E-03	0.68	1.35	2131693	1324395	2988419	1548170	3170342	1400211	2806497	1677630
HILIC_NEG_136_89163a5_138	HILIC	NEG	5.138	136.8916				2.51E-01	-0.25	0.64	2.42E-01	0.23	1.01	5.57E-01	-0.14	0.25	1.32E-01	-0.37	0.71	6820133	1905880	6382606	1674662	6185903	1719925	6579309	1621456
RP_POS_166_98492a15_486	RP	POS	15.49	166.9849				6.38E-01	-0.10	0.84	2.42E-01	0.24	0.76	9.27E-01	0.02	0.57	2.85E-01	-0.21	0.83	54805382	10565094	53787075	10729990	52524405	6945898	55049745	13457926
RP_POS_211_13052a8_135	RP	POS	8.14	211.1305				4.31E-03	0.46	1.44	2.42E-01	0.25	1.42	3.11E-03	0.58	1.33	7.79E-02	0.33	1.20	992293	576043	1399915	947328	1288680	926612	1511151	964010
HILIC_NEG_119_90741a2_939	HILIC	NEG	2.939	119.9074				1.30E-01	0.29	0.90	2.42E-01	-0.24	0.89	4.25E-01	0.16	0.38	6.85E-02	0.41	0.67	149681	33158	160477	38984	165055	41762	155900	35829
RP_POS_279_9552a15_411	RP	POS	15.41	279.9552				7.57E-01	0.07	0.83	2.43E-01	-0.22	0.78	8.79E-01	-0.04	0.79	4.48E-01	0.18	0.58	3510713	952593	3568343	760765	3657645	654153	3479040	851556
HILIC_POS_154_15903a5_179	HILIC	POS	5.179	154.1590				4.20E-01	0.17	0.69	2.43E-01	-0.23	1.02	8.35E-01	0.05	0.20	2.13E-01	0.28	0.51	14756448	3223609	15288488	3221632	15666438	3146561	14910538	3282877
RP_POS_359_17429a11_252	RP	POS	11.25	359.1743				2.59E-05	0.66	1.51	2.43E-01	0.25	0.96	1.83E-04	0.78	1.48	1.53E-03	0.54	1.51	229756	154564	400174	271329	368361	227572	431987	308038
RP_POS_548_50415a11_16	RP	POS	11.16	548.5042				9.72E-02	0.26	1.06	2.43E-01	0.26	1.06	4.94E-02	0.38	1.10	4.85E-01	0.13	0.94	1650089	260515	1760205	469251	1705221	450254	1815188	485787
HILIC_POS_520_33252a0_618	HILIC	POS	0.618	520.3325				5.08E-02	0.34	1.21	2.43E-01	-0.25	1.00	2.47E-01	0.21	1.17	3.61E-02	0.46	1.36	899830	2215870	1896573	3140808	2264755	3582004	1528390	2612138
RP_POS_568_42694a11_645	RP	POS	11.65	568.4269				8.17E-03	-0.77	1.39	2.43E-01	-0.16	0.80	4.61E-03	-0.85	1.28	1.95E-02	-0.69	1.19	619339	590944	316874	270186	348520	269916	285228	269430
RP_POS_347_17166a7_093	RP	POS	7.09	347.1717				3.90E-01	-0.16	0.64	2.44E-01	0.24	0.78	8.65E-01	-0.04	0.32	1.85E-01	-0.28	0.66	1388644	79748	1373765	98274	1362261	97565	1385268	98609
RP_NEG_180_89876a15_544	RP	NEG	15.54	180.8988				2.35E-01	-0.19	0.66	2.44E-01	0.25	0.70	6.95E-01	-0.07	0.74	1.37E-01	-0.32	0.63	5076127	540448	4923644	843958	4824789	972364	5022498	688209
RP_POS_177_95604a0_253	RP	POS	0.25	177.9560				1.51E-01	0.29	1.09	2.44E-01	0.24	0.71	7.37E-02	0.40	1.05	4.43E-01	0.17	0.61	9492543	2836482	10343347	2990250	9993419	2920593	10693275	3047279
RP_POS_335_22052a9_056	RP	POS	9.06	335.2205				1.80E-01	0.27	0.57	2.44E-01	-0.23	0.74	4.82E-01	0.16	0.53	9.01E-02	0.39	0.69	1627377	482641	1761115	488488	1818277	502594	1703952	472061
RP_POS_233_05968a0_734	RP	POS	0.73	233.0597				8.71E-11	0.83	1.37	2.44E-01	0.25	0.73	1.61E-06	0.95	1.57	1.94E-06	0.71	1.45	84382	118540	434092	447482	381713	372585	486470	510047
HILIC_POS_154_15926a5_334	HILIC	POS	5.334	154.1593				3.64E-01	0.18	0.61	2.45E-01	-0.23	0.79	7.63E-01	0.07	0.31	1.89E-01	0.30	0.56	21062936	7844474	22524826	7942996	23453106	8144960	21596546	7705259
RP_POS_323_198a10_122	RP	POS	10.12	323.1980				3.18E-01	0.14	0.45	2.45E-01	-0.26	0.90	9.23E-01	0.01	0.26	1.98E-01	0.27	0.62	319825	452656	446074	972486	559850	1175206	332299	709388
RP_POS_348_28726a10_432	RP	POS	10.43	348.2873				4.15E-01	-0.23	0.88	2.45E-01	-0.17	0.88	2.69E-01	-0.32	0.77	6.28E-01	-0.15	0.52	2135880	4157794	1507960	2005692	1742492	2343414	1273428	1588664
HILIC_NEG_261_81305a3_028	HILIC	NEG	3.028	261.8131				1.77E-02	-0.45	0.98	2.45E-01	0.24	0.82	1.19E-01	-0.34	0.68	8.21E-03	-0.57	0.97	537838	51177	511518	58772	504655	57943	518381	59375
HILIC_POS_476_30682a0_616	HILIC	POS	0.616	476.3068				5.84E-01	0.13	1.13	2.45E-01	-0.22	0.98	9.31E-01	0.02	0.93	3.69E-01	0.24	1.18	1800604	4919927	2323468	3755880	2762236	4320997	1884700	3072011
HILIC_POS_64_01666a5_049	HILIC	POS	5.049	64.0167				6.95E-01	0.07	0.56	2.45E-01	0.24	0.95	4.00E-01	0.19	0.48	8.03E-01	-0.05	0.11	9393052	5165125	9826844	6185534	9104451	4956944	10549236	7187919
HILIC_POS_680_48022a10_693	HILIC	POS	10.693	680.4802				2.51E-01	-0.16	0.36	2.46E-01	-0.26	0.69	1.88E-01	-0.29	0.52	7.93E-01	-0.03	0.18	2780146	66012	2758375	148248	2775706	85940	2741045	190801
RP_NEG_329_24902a11_13	RP	NEG	11.13	329.2490				1.08E-05	0.68	1.68	2.46E-01	0.25	1.16	8.62E-05	0.80	1.60	1.14E-03	0.56	1.54	3168587	1906996	5409258	3452716	5006567	3022042	5811949	3823887
HILIC_POS_170_09235a6_886	HILIC	POS	6.886	170.0924				9.54E-01	-0.01	0.22	2.46E-01	-0.23	0.67	5.85E-01	-0.13	0.30	6.79E-01	0.10	0.23	16668274	22091074	16415593	19778756	18722001	21379442	14109184	17956762
RP_POS_392_2576a12_908	RP	POS	12.91	392.2576				8.31E-06	-0.96	1.65	2.46E-01	-0.21	0.80	9.66E-06	-1.07	1.61	8.72E-05	-0.86	1.62	852593	278401	576063	258016	606138	219407	545987	290719
HILIC_NEG_136_89165a6_093	HILIC	NEG	6.093	136.8917				3.77E-01	-0.18	0.84	2.46E-01	-0.23	0.93	1.81E-01	-0.30	0.69	7.89E-01	-0.06	0.94	4761238	2142099	4370906	2197159	4626916	2311587	4114896	2067933
HILIC_POS_645_09351a0_569	HILIC	POS	0.569	645.0935				2.55E-06	0.60	1.29	2.46E-01	-0.26	0.95	9.13E-04	0.48	1.45	2.58E-04	0.73	1.45	54162	214163	474074	764197	563138	884338	385010	617794
RP_POS_464_31369a10_799	RP	POS	10.80	464.3137				4.14E-02	0.33	0.61	2.46E-01	0.25	0.90	1.27E-02	0.45	1.06	3.26E-01	0.20	0.44	1152578	397653	1351698	656989	1275164	723067	1428233	580774
HILIC_POS_184_07335a0_604	HILIC	POS	0.604	184.0734				1.91E-02	0.51	1.05	2.47E-01	0.22	0.83	9.04E-03	0.62	1.11	9.13E-02	0.39	1.09	759716	107450	811565	98253	800137	98646	822993	97502
RP_NEG_201_8889a14_27	RP	NEG	14.27	201.8889				4.59E-01	0.14	0.35	2.47E-01	-0.24	0.93	9.40E-01	0.02	0.42	1.31E-01	0.26	0.69	1208422	337452	1261784	395162	1307921	176120	1215647	529274
RP_POS_195_10159a7_699	RP	POS	7.70	195.1016				4.59E-01	-0.12	0.49	2.47E-01	0.26	0.74	9.56E-01	0.01	0.32	1.10E-01	-0.24	0.64	2162989	63306	2151212	111868	2138177	74066	2164248	139469
RP_POS_185_12843a2_82	RP	POS	2.82	185.1284				1.26E-02	0.43	0.74	2.47E-01	0.24	0.69	1.57E-02	0.56	0.98	7.08E-02	0.31	0.98	3388066	1530559	4269609	2136652	4020735	1507352	4518482	2612511
RP_NEG_393_80124a15_618	RP	NEG	15.62	393.8012				5.87E-02	-0.41	0.85	2.47E-01	-0.22	0.69	2.93E-02	-0.52	0.89	2.01E-01	-0.30	0.70	850727	42997	834216	38609	838706	37820	829726	39247
RP_POS_874_5542a13_404	RP	POS	13.40	874.5542				8.70E-01	0.03	0.51	2.47E-01	-0.23	0.83	7.17E-01	-0.08	0.34	4.95E-01	0.15	0.78	6250556	1203586	6290870	1230012	6433917	1140159	6147824	1309585
RP_POS_286_8829a15_427	RP	POS	15.43	286.8829				1.86E-02	-0.32	0.60	2.47E-01	0.26	1.15	6.75E-02	-0.19	0.71	5.03E-02	-0.45	0.74	5298615	140652	5188490	389470	5143043	521893	5233936	172866
RP_POS_963_57471a10_834	RP	POS	10.83	963.5747				9.37E-06	0.53	1.08	2.47E-01	-0.26	1.04	2.08E-03	0.40	1.16	9.48E-04	0.66	1.23	459776	60797	696695	497745	754597	588852	638794	383363
RP_POS_429_31921a10_54	RP	POS	10.54	429.3192				7.95E-01	-0.05	0.58	2.47E-01	0.23	0.77	7.61E-01	0.07	0.37	4.73E-01	-0.17	0.66	12876368	1614987	12790137	1662930	12596832	1856941	12983442	1436183
RP_POS_441_29739a12_619	RP	POS	12.62	441.2974				4.44E-02	0.36	0.88	2.47E-01	-0.24	0.74	2.16E-01	0.23	0.73	3.04E-02	0.48	0.82	15990137	6331633	18861339	8442679	19842454	9488101	17880224	7212752
HILIC_POS_159_09143a4_124	HILIC	POS	4.124	159.0914				2.88E-02	-0.40	1.05	2.47E-01	-0.24	1.34	2.07E-02	-0.52	0.97	1.46E-01	-0.28	0.82	2846778	679094	2519308	838310	2616718	709229	2421899	947364
RP_POS_499_82715a5_878	RP	POS	5.88	499.8272				3.22E-01	0.17	0.57	2.48E-01	0.25	0.70	2.27E-01	0.29	0.61	7.58E-01	0.05	0.42	1322169	2225985	1823072	3126841	1458698	1397114	2187446	4186993
RP_POS_259_19043a8_028	RP	POS	8.03	259.1904				1.24E-01	0.32	0.79	2.48E-01	0.23	0.77	6.16E-02	0.44	0.78	3.65E-01	0.21	0.70	1947856	320051	2048673	309877	2012715	304823	2084631	313769
RP_POS_402_77362a12_817	RP	POS	12.82	402.7736				8.81E-06	-1.10	1.80	2.48E-01	-0.18	1.08	3.39E-06	-1.19	1.86	7.66E-05	-1.00	1.56	1093558	512382	599624	356596	641005	382581	558243	327190
RP_POS_617_26111a11_803	RP	POS	11.80	617.2611				1.14E-02	-0.52	1.07	2.48E-01	0.23	1.26	9.77E-02	-0.41	0.68	2.34E-03	-0.63	1.31	416713	239823	288943	240611	260987	167677	316898	295396
RP_NEG_364_86996a0_5	RP	NEG	0.50	364.8700				7.83E-01	0.04	0.97	2.49E-01	-0.26	1.43	6.41E-01	-0.09	1.00	3.77E-01	0.17	1.00	872163	201296	886514	377874	930272	388236	842755	365865
HILIC_POS_645_42814a0_569	HILIC	POS	0.569	645.4281				1.87E-06	0.60	1.29	2.49E-01	-0.26	0.94	8.13E-04	0.47	1.46	2.63E-04	0.73	1.46	59257	191538	484809	780577	575255	904770	394364	629072
RP_NEG_191_86061a15_551	RP	NEG	15.55	191.8606				5.94E-01	-0.11	0.47	2.49E-01	-0.23	1.30	3.19E-01	-0.23	0.67	9.73E-01	0.01	0.29	972073	61126	965392	61780	972544	62759	958240	60567
RP_POS_431_27911a10_659	RP	POS	10.66	431.2791				5.54E-01	0.10	0.59	2.49E-01	0.25	0.73	2.83E-01	0.23	0.55	9.10E-01	-0.02	0.69	1729361	548141	1803216	776263	1713372	722437	1893060	824063
RP_POS_768_80524a0_494	RP	POS	0.49	768.8052				2.59E-09	-0.74	1.39	2.49E-01	0.25	1.25	2.11E-04	-0.62	1.37	1.32E-06	-0.87	1.57	2369056	208803	1690411	987988	1576128	1000310	1804694	972053
RP_POS_312_90988a0_497	RP	POS	0.50	312.9099				4.04E-08	-0.67	1.32	2.49E-01	0.25	1.25	5.77E-04	-0.54	1.31	1.62E-05	-0.79	1.50	1444182	54277	1198188	405382	1151294	429796	1245082	377903
RP_POS_613_26489a11_803	RP	POS	11.80	613.2649				4.11E-02	-0.40	1.06	2.49E-01	0.23	1.28	2.48E-01	-0.29	0.63	6.97E-03	-0.52	1.28	2157361	1335383	1579014	1443418	1411636	838306	1746393	1857283
RP_POS_358_83374a0_5	RP	POS	0.50	358.8337				7.33E-01	0.05	1.12	2.50E-01	-0.26	1.31	6.54E-01	-0.08	1.01	3.65E-01	0.18	1.23	480603	173982	496492	347364	536670	376469	456314	314265
RP_POS_163_98746a15_397	RP	POS	15.40	163.9875				7.26E-01	0.07	0.29	2.50E-01	0.23	0.74	4.17E-01	0.19	0.71	8.55E-01	-0.04	0.47	55952682	22272184	57533652	21532317	55043694	21371335	60023611	21618432
HILIC_NEG_202_92896a2_998	HILIC	NEG	2.998	202.9290				2.03E-01	-0.24	0.83	2.50E-01	0.24	0.95	5.72E-01	-0.12	0.42	9.19E-02	-0.36	0.70	4993066	1043013	4709302	1205446	4569934	1169429	4848670	1236387
RP_NEG_573_12891a9_262	RP	NEG	9.26	573.1289				2.66E-01	-0.26	0.59	2.50E-01	0.21	0.73	5.41E-01	-0.16	0.30	1.42E-01	-0.37	0.64	5069564	627036	4933655	477411	4878481	455019	4988830	497232
RP_NEG_765_16815a9_304	RP	NEG	9.30	765.1682				7.04E-01	0.06	0.38	2.50E-01	-0.25	1.05	7.53E-01	-0.07	0.19	2.97E-01	0.19	0.49	8167541	451306	8209309	750344	8296029	655470	8122589	832186
RP_POS_339_1824a11_247	RP	POS	11.25	339.1824				3.80E-05	0.76	1.61	2.50E-01	0.23	1.12	7.89E-05	0.87	1.58	9.17E-04	0.64	1.45	7870370	1655923	9459414	2085626	9218404	1816950	9700425	2317023
RP_POS_308_89911a0_252	RP	POS	0.25	308.8991				6.80E-01	-0.09	0.64	2.51E-01	-0.23	0.86	3.93E-01	-0.20	0.41	9.10E-01	0.03	0.92	1176439	233886	1157064	218460	1182268	215579	1131860	220574
RP_POS_339_25064a9_607	RP	POS	9.61	339.2506				1.18E-05	0.68	1.27	2.51E-01	0.24	1.24	1.38E-04	0.80	1.31	8.44E-04	0.55	1.29	1147313	149132	1322635	273291	1291090	226108	1354180	312640
RP_POS_818_60303a14_119	RP	POS	14.12	818.6030				5.59E-03	-0.70	1.18	2.51E-01	-0.19	0.75	2.65E-03	-0.79	1.25	2.25E-02	-0.60	0.94	1707885	969144	1171393	650790	1246414	673737	1096373	624732
RP_POS_169_03589a0_71	RP	POS	0.71	169.0359	Uric acid	169.0353(100), 141.04(15), 126.0299(10), 152.01(3)	3	6.21E-04	0.54	0.98	2.51E-01	0.25	0.68	2.23E-03	0.66	1.15	1.07E-02	0.41	0.92	69416225	13329244	81151959	23285333	78466733	17909985	83837185	27568027
RP_POS_812_54028a11_613	RP	POS	11.61	812.5403				7.08E-01	0.06	0.31	2.51E-01	-0.25	0.83	6.53E-01	-0.07	0.23	4.16E-01	0.19	0.46	5347137	9610014	6234777	16362270	8123930	20800797	4345624	10047633
HILIC_POS_327_20132a0_616	HILIC	POS	0.616	327.2013				7.29E-01	-0.11	1.02	2.52E-01	-0.16	0.96	5.49E-01	-0.18	0.76	9.32E-01	-0.03	0.94	331983	1038463	266042	425685	315085	493852	216998	342512
RP_POS_360_27438a7_568	RP	POS	7.57	360.2744				1.39E-04	0.62	1.14	2.52E-01	0.24	0.89	5.09E-04	0.74	1.22	4.01E-03	0.50	1.17	456844	201283	648879	324146	611547	269786	686210	369672

Supplementary table 1: Metabolomics results (in asceding order according to p-value from progressive ALD vs non-progressive ALD comparison, with molecular features with ID_level of 1-2 first)

								all_ALD_vs_control			Prog_ALD_vs_non-prog_ALD			Prog_ALD_vs_control_ALD			Non-prog_ALD_vs_control			Healthy_control		all_ALD		Non-prog_ALD		Progressive_ALD	
								t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA								
Feature_ID	RP_HILIC	POS_NEG	Average.Rt	Average.Mz	Metabolite.name	curated_MSMS	ID_level	p	d	VIP	p	d	VIP	p	d	VIP	p	d	VIP	Mean	SD	Mean	SD	Mean	SD	Mean	SD
RP_POS_274_7912a0_522	RP	POS	0.52	274.7912				1.66E-05	-0.60	1.20	2.52E-01	0.25	1.14	5.98E-03	-0.47	1.10	1.05E-04	-0.72	1.36	470994	59141	390955	144635	374320	148776	407591	139881
HILIC_POS_344_22815a0_617	HILIC	POS	0.617	344.2282				7.46E-01	-0.10	1.02	2.52E-01	-0.16	0.96	5.59E-01	-0.18	0.77	9.55E-01	-0.02	0.95	3783743	11415471	3105876	4825716	3661116	5586963	2550635	3899616
RP_POS_1054_69275a10_617	RP	POS	10.62	1054.6928				7.49E-03	0.57	1.33	2.52E-01	-0.22	0.99	5.60E-02	0.46	1.12	2.36E-03	0.68	1.37	669156	445794	917473	414101	965104	345798	869842	471437
RP_POS_792_58698a13_829	RP	POS	13.83	792.5870				1.17E-05	-0.99	1.57	2.52E-01	-0.20	0.72	8.90E-06	-1.09	1.63	1.09E-04	-0.89	1.48	2391807	974215	1453829	820700	1548173	745374	1359486	887184
RP_POS_273_20667a8_908	RP	POS	8.91	273.2067				1.80E-01	0.28	0.62	2.53E-01	0.23	0.69	1.07E-01	0.39	0.72	4.43E-01	0.17	0.41	595989	116969	628132	114161	615007	94411	641256	130639
RP_POS_415_28159a9_859	RP	POS	9.86	415.2816	Chenodeoxycholic acid [M+Na]+	415.278(100)		4.56E-01	0.14	0.36	2.53E-01	0.24	0.69	2.43E-01	0.26	0.46	9.32E-01	0.02	0.67	1394188	1929712	1706227	2375270	1433314	2171062	1979141	2556060
HILIC_NEG_303_68158a1_369	HILIC	NEG	1.369	303.6816				2.98E-18	-1.23	2.13	2.53E-01	-0.22	0.94	3.72E-13	-1.33	2.31	3.63E-10	-1.12	2.22	296056	35483	188198	83680	197807	84574	178588	82501
RP_POS_844_5213a12_959	RP	POS	12.96	844.5213				1.74E-03	-0.66	1.37	2.53E-01	-0.22	0.77	9.57E-04	-0.77	1.48	1.50E-02	-0.55	1.09	9100067	3040423	7075190	2937766	7412519	2889163	6737861	2976170
RP_NEG_397_23651a11_049	RP	NEG	11.05	397.2365				2.08E-09	0.82	1.77	2.53E-01	0.24	0.89	1.82E-06	0.94	1.68	1.32E-05	0.70	1.72	436757	251128	954425	667765	877730	587747	1031121	737204
RP_POS_386_28986a7_98	RP	POS	7.98	386.2899				7.30E-04	0.55	1.09	2.53E-01	0.24	0.96	1.34E-03	0.67	1.18	1.73E-02	0.43	1.09	888319	429118	1249803	699544	1169471	617559	1330134	770818
RP_POS_668_40118a11_078	RP	POS	11.08	668.4012				2.53E-07	0.62	1.28	2.53E-01	-0.25	1.21	6.17E-04	0.49	1.34	1.12E-04	0.74	1.39	43663	29141	319054	495464	375928	558675	262181	421023
RP_POS_499_8273a2_965	RP	POS	2.97	499.8273				5.09E-01	-0.16	0.52	2.54E-01	-0.21	0.77	3.00E-01	-0.26	0.56	8.43E-01	-0.05	0.50	2125252	2027399	1866057	1528716	2041350	1568879	1690764	1482413
RP_POS_321_23962a10_542	RP	POS	10.54	321.2396				1.62E-01	-0.26	0.84	2.54E-01	0.24	0.98	5.13E-01	-0.14	0.70	7.72E-02	-0.38	0.84	5622176	773837	5385431	963398	5274966	970870	5495896	952744
RP_POS_308_92014a15_458	RP	POS	15.46	308.9201				5.46E-01	0.13	0.57	2.54E-01	-0.22	0.92	9.38E-01	0.02	0.45	3.00E-01	0.24	0.88	3061337	784830	3156085	707200	3237165	670079	3075005	740303
RP_POS_192_03242a0_706	RP	POS	0.71	192.0324				5.40E-04	0.47	0.99	2.54E-01	0.25	0.71	5.55E-03	0.60	1.03	7.92E-03	0.35	1.11	538500	473705	1070813	1243220	928062	819440	1213564	1552311
HILIC_POS_564_35913a0_619	HILIC	POS	0.619	564.3591				2.27E-04	0.48	1.25	2.54E-01	-0.25	1.00	1.78E-02	0.36	1.34	1.92E-03	0.61	1.46	561275	1230574	2235970	3842112	2676491	4345243	1795449	3247729
RP_POS_292_63455a7_158	RP	POS	7.16	292.6346				5.31E-01	-0.12	0.86	2.54E-01	0.24	1.14	9.98E-01	0.00	0.42	2.31E-01	-0.24	0.94	492376	215536	463552	252842	434557	203598	492547	293249
RP_NEG_203_08163a2_484	RP	NEG	2.48	203.0816				5.91E-04	-0.72	1.38	2.54E-01	-0.22	1.10	5.56E-04	-0.83	1.39	4.44E-03	-0.61	1.25	4703550	1164379	3842879	1132140	3972552	961974	3713206	1276686
RP_POS_646_38892a11_085	RP	POS	11.09	646.3889				1.73E-07	0.62	1.30	2.54E-01	-0.25	1.22	3.91E-04	0.50	1.37	1.11E-04	0.75	1.40	54323	40274	521823	829077	616784	945278	426862	690517
RP_POS_164_98444a13_12	RP	POS	13.12	164.9844				7.22E-01	-0.08	0.30	2.54E-01	-0.23	0.81	4.24E-01	-0.19	0.62	8.72E-01	0.04	0.26	13751674	4630987	13419807	4334875	13915929	4243333	12923685	4411074
RP_POS_246_09058a0_614	RP	POS	0.61	246.0906				1.55E-02	0.45	0.97	2.54E-01	0.23	0.95	9.07E-03	0.57	1.19	1.07E-01	0.33	0.76	244721	299360	404699	365250	362898	349441	446501	379292
RP_POS_560_46979a14_267	RP	POS	14.27	560.4698				6.96E-01	-0.08	0.37	2.55E-01	0.23	1.15	8.69E-01	0.04	0.21	3.94E-01	-0.19	0.46	31619872	9456632	30860195	9749966	29744454	9976136	31975935	9486826
HILIC_POS_285_12802a5_592	HILIC	POS	5.592	285.1280				2.10E-01	0.22	0.70	2.55E-01	-0.24	1.18	6.58E-01	0.10	0.58	6.94E-02	0.34	0.71	199282	234559	265718	321758	302555	266429	228880	367989
RP_POS_293_17477a8_696	RP	POS	8.70	293.1748				2.40E-01	-0.24	0.51	2.55E-01	0.23	0.94	5.83E-01	-0.13	0.45	1.11E-01	-0.36	0.66	1078566	59784	1064179	59029	1057425	54387	1070933	63158
RP_POS_661_52698a11_968	RP	POS	11.97	661.5270				3.12E-06	-1.12	1.96	2.55E-01	-0.18	0.67	1.11E-06	-1.21	2.01	3.55E-05	-1.03	1.63	1011159	451817	546621	331119	584469	362544	508774	295221
RP_POS_463_12979a10_133	RP	POS	10.13	463.1298				6.86E-01	0.09	0.40	2.55E-01	-0.22	0.75	9.33E-01	-0.02	0.36	4.08E-01	0.20	0.49	629631	125260	639638	107441	651908	106092	627368	108444
RP_POS_743_44574a10_909	RP	POS	10.91	743.4457				1.26E-04	0.50	1.14	2.56E-01	-0.25	1.11	4.32E-03	0.38	1.12	2.64E-03	0.63	1.20	1200580	363521	1709368	1115308	1836842	1359533	1581894	794806
RP_NEG_394_01221a2_473	RP	NEG	2.47	394.0122				7.44E-03	-0.45	1.10	2.56E-01	-0.24	1.17	8.76E-03	-0.57	1.17	6.55E-02	-0.33	0.97	1043108	168181	935791	253407	964725	209132	906857	290337
HILIC_POS_694_46509a0_51	HILIC	POS	0.51	694.4651				7.98E-07	0.61	1.33	2.56E-01	-0.25	1.00	8.22E-04	0.49	1.50	1.46E-04	0.74	1.51	59347	173388	506781	803104	598467	908058	415096	679258
RP_POS_309_9057a0_253	RP	POS	0.25	309.9057				7.61E-01	0.06	0.38	2.56E-01	-0.23	0.78	7.99E-01	-0.06	0.24	4.10E-01	0.18	0.43	1088351	143497	1097499	158022	1115529	146493	1079469	168308
RP_POS_515_41296a14_267	RP	POS	14.27	515.4130				3.72E-01	0.13	0.43	2.56E-01	0.25	0.72	2.34E-01	0.26	0.54	9.53E-01	0.01	0.39	485619044	66178432	501016525	125935231	486636302	87589932	515396749	154754689
RP_POS_464_19171a6_602	RP	POS	6.60	464.1917				3.27E-03	0.46	1.58	2.56E-01	-0.24	0.72	5.83E-02	0.34	1.40	3.78E-03	0.59	1.12	1941198	2313122	3669858	4006053	4126544	4293252	3213171	3683311
RP_POS_550_31537a10_618	RP	POS	10.62	550.3154				6.32E-03	0.62	1.40	2.57E-01	-0.21	1.03	4.15E-02	0.52	1.07	1.94E-03	0.73	1.50	7689201	2111914	8868144	1731935	9065620	1348709	8670668	2040052
RP_POS_392_22147a11_167	RP	POS	11.17	392.2215				1.19E-02	0.45	0.95	2.57E-01	-0.24	0.82	1.04E-01	0.33	0.73	6.64E-03	0.57	1.07	1087954	70509	1128069	92535	1138610	93406	1117529	91372
RP_POS_764_52203a12_954	RP	POS	12.95	764.5220	PE 38:6 + PC 35:6	623.509(55), 313.2715(3), 764.547(2), 184.0735(100)	3	9.75E-01	0.01	0.68	2.57E-01	0.24	0.68	6.09E-01	0.12	0.57	5.45E-01	-0.11	0.36	5568929	3322848	5591415	3855989	5151356	2497880	6031473	4837989
RP_POS_621_30939a11_426	RP	POS	11.43	621.3094				6.64E-01	-0.09	0.22	2.57E-01	0.22	0.98	9.46E-01	0.02	0.37	3.83E-01	-0.21	0.35	505844	104455	496809	92995	486219	88872	507399	96672
RP_POS_700_48743a12_272	RP	POS	12.27	700.4874				1.48E-01	0.29	0.71	2.57E-01	0.23	0.74	8.63E-02	0.41	0.79	4.05E-01	0.18	0.36	388422	504003	539868	522368	480371	452759	599365	582316
RP_POS_318_24036a9_213	RP	POS	9.21	318.2404		318.2419(100)	4	1.97E-01	-0.34	0.96	2.57E-01	-0.19	0.83	1.05E-01	-0.44	0.87	3.87E-01	-0.25	0.58	5534517	8913967	3347573	5342771	3956180	6255843	2738966	4216808
RP_POS_583_25452a11_94	RP	POS	11.94	583.2545				5.77E-01	-0.08	0.49	2.57E-01	0.26	1.06	8.41E-01	0.05	0.30	3.52E-02	-0.21	1.04	1185935	1548260	939877	3437640	546620	746205	1333135	4796193
HILIC_POS_454_29251a1_965	HILIC	POS	1.965	454.2925				8.94E-02	0.29	0.81	2.58E-01	-0.24	0.82	4.24E-01	0.17	0.27	3.35E-02	0.41	0.75	1130621	418593	1296045	613913	1365866	562919	1226225	659276
RP_POS_294_11243a8_289	RP	POS	8.29	294.1124				1.55E-06	0.66	1.09	2.58E-01	0.24	0.90	8.89E-05	0.78	1.25	5.72E-04	0.54	1.11	680661	129808	885150	334117	847185	283924	923115	376818
RP_POS_645_29108a11_804	RP	POS	11.80	645.2911				3.25E-02	-0.42	1.07	2.58E-01	0.23	1.30	2.16E-01	-0.31	0.65	5.41E-03	-0.53	1.28	8679052	4985849	6407333	5450413	5786933	3222100	7027733	6989481
RP_NEG_171_02673a0_737	RP	NEG	0.74	171.0267				7.00E-08	0.71	1.21	2.58E-01	0.25	0.77	9.24E-05	0.83	1.29	6.22E-06	0.59	1.40	235736	235556	716265	729785	633291	497423	799238	902530
RP_NEG_172_99072a3_098	RP	NEG	3.10	172.9907				1.17E-01	0.24	0.86	2.59E-01	0.25	0.96	8.01E-02	0.36	1.20	5.04E-01	0.11	0.36	19370169	18820322	27155778	36343322	23030223	30573276	31281333	41220985
RP_POS_297_24182a9_925	RP	POS	9.93	297.2418				5.93E-09	0.89	1.49	2.59E-01	-0.23	1.19	1.75E-05	0.78	1.42	1.82E-07	1.01	1.72	1343469	234152	1726173	435555	1775591	445712	1676755	423844
HILIC_POS_59_06126a0_541	HILIC	POS	0.541	59.0613				5.18E-02	-0.30	0.45	2.59E-01	-0.25	0.72	1.47E-02	-0.42	0.83	3.88E-01	-0.18	0.29	2464994	351413	2289796	636717	2362041	713580	2217552	547032
RP_POS_350_98441a15_406	RP	POS	15.41	350.9844				2.49E-01	-0.19	0.81	2.59E-01	0.24	0.74	6.74E-01	-0.07	0.67	1.61E-01	-0.32	0.89	2921257	191458	2870004	283780	2837783	341463	2902226	209737
RP_POS_203_97173a1_459	RP	POS	1.46	203.9717				3.40E-11	0.88	1.44	2.59E-01	0.24	0.78	3.26E-07	1.00	1.65	1.73E-06	0.76	1.45	471618	474284	1686738	1452384	1521998	1286753	1851477	1597113
RP_POS_396_26321a12_768	RP	POS	12.77	396.2632				2.11E-02	-0.45	0.93	2.59E-01	0.23	0.72	1.26E-01	-0.33	0.65	1.04E-02	-0.56	1.02	1057336	318914	898761	359969	857974	357536	939548	361349
RP_POS_298_27408a9_958	RP	POS	9.96	298.2741	Unknown	298.274(45), 95.0858(100), 263.2368(65)	4	2.60E-01	-0.34	0.99	2.59E-01	-0.15	0.79	1.76E-01	-0.42	0.84	3.94E-01	-0.27	0.66	5390696	9506860	3416100	3828321	3849881	4289498	2982319	3290499
HILIC_POS_176_13916a3_702	HILIC	POS	3.702	176.1392				8.95E-01	0.02	0.73	2.59E-01	0.24	0.89	5.08E-01	0.14	0.25	6.64E-01	-0.09	0.63	4526557	1325125	4563835	1568277	4386207	1558362	4741463	1573625
HILIC_NEG_144_92352a7_948	HILIC	NEG	7.948	144.9235				8.47E-03	-0.50	0.77	2.60E-01	0.23	1.26	6.78E-02	-0.39	0.80	4.54E-03	-0.62	1.03	62038350	18012883	51693530	20714350	49348858	20778098	54038202	20590694
RP_POS_400_1817a0_71	RP	POS	0.71	400.1817				1.52E-01	0.19	0.48	2.60E-01	0.26	0.83	9.55E-02	0.31	0.56	7.05E-01	0.06	0.79	314483	71080	351073	220712	326099	197306	376048	241286
RP_POS_293_93311a15_509	RP	POS	15.51	293.9331				6.37E-01	0.10	0.34	2.60E-01	-0.22	0.70	9.87E-01	0.00	0.52	3.66E-01	0.21	0.36	3127954	441742	3169127	378416	3211937	345379	3126316	407790
RP_POS_790_55884a11_613	RP	POS	11.61	790.5588				7.31E-01	0.05	0.31	2.60E-01	-0.25	0.81	6.52E-01	-0.07	0.22	4.34E-01	0.18	0.46	3124805	5562923	3589643	9219699	4634299	11667465	2544987	5777850
RP_POS_583_25494a5_914	RP	POS	5.91	583.2549				1.67E-01	0.20	0.72	2.61E-01	0.25	1.12	1.32E-01	0.33	0.59	5.91E-01	0.08	0.91	381747	275701	486198	571660	421575	392295	550822	705578
RP_NEG_455_60333a15_584	RP	NEG	15.58	455.6033				2.07E-01	-0.26	0.59	2.61E-01	0.22	0.97	5.17E-01	-0.15	0.33	9.92E-02	-0.37	0.69	722661	39310	712516	38225	708202	36290	716831	39964
RP_POS_330_75305a0_522	RP	POS	0.52	330.7531				6.20E-05	-0.62	1.12	2.61E-01	0.24	1.01	8.22E-03	-0.50	1.01	9.87E-05	-0.74	1.31	423085	69666	348791	127810	334373	125654	363209	129580
HILIC_POS_226_04488a5_119	HILIC	POS	5.119	226.0449				7.54E-01	0.05	0.89	2.61E-01	0.24	1.00	4.03E-01	0.17	0.29	7.42E-01	-0.07	0.66	1039444	234645	1055962	323158	1019511	309372	1092414	335517
HILIC_POS_111_05559a6_789	HILIC	POS	6.789	111.0556				8.10E-01	-0.05	0.73	2.62E-01	-0.23	0.84	4.72E-01	-0.16	0.45	7.80E-01	0.06	0.40	1095740	345806	1078767	347752	1117977	355851	1039558	338472
RP_NEG_193_08643a7_695	RP	NEG	7.70	193.0864				2.28E-02	-0.45	0.83	2.62E-01	-0.23	0.70	1.00E-02	-0.56	0.96	1.33E-01	-0.33	0.65	3357203	137205	3290412	150202	3307336	156374	3273487	143333
RP_POS_383_39987a11_668	RP	POS	11.67	383.3999				7.83E-01	-0.06	0.71	2.62E-01	-0.23	0.66	4.52E-01	-0.17	0.50	8.08E-01	0.06	0.46	3350525	1530608	3264448	1523008	3435966	1576985	3092929	1462713
HILIC_NEG_125_87303a3_06	HILIC	NEG	3.06	125.8730				5.30E-01	0.10	1.01	2.62E-01	0.25	1.02	2.00E-01	0.22	0.69	9.02E-01	-0.03	1.14	801742	117257	820187	206309	796945	232911	843429	175058
RP_POS_280_93927a15_444	RP	POS	15.44	280.9393				9.61E-01	-0.01	0.46	2.62E-01	-0.23	0.68	5.81E-01	-0.13	0.32	5.96E-01	0.11	0.34	6614987	292829	6611959	341894	6650458	295224	6573460	382082
RP_POS_173_96126a15_422	RP	POS	15.42	173.9613				8.83E-02	0.35	0.59	2.63E-01	0.22	0.68	2.92E-02	0.46	0.94	3.25E-01	0.24	0.42	4631038	485715	4801959	480751	4747803	570002	4856114	368879
HILIC_POS_133_03194a4_625	HILIC	POS	4.625	133.0319				7.83E-01	-0.04	0.52	2.63E-01	0.26	0.68	6.93E-01	0.09	0.21	7.42E-02	-0.16	1.02	2668298	520529	2620479	1472587	2454070	523631	2786887	2012604
RP_NEG_326_98926a8_592	RP	NEG	8.59	326.9893				1.33E-01	-0.30	0.89	2.63E-01	-0.23	0.85	5.76E-02	-0.42	1.01	4.08E-01	-0.19	0.55	6474006	1728619	5935025	1772397	6134313	1911110	5735737	1616633
RP_NEG_207_93219a1_036	RP	NEG	1.04	207.9322				7.20E-01	0.06	0.56	2.63E-01	-0.24	0.87	7.88E-01	-0.05	0.35	3.90E-01	0.18	0.80	2170278	1001855	2249427	1303700	2395986	1355735	2102869	1245833
RP_POS_585_27057a5_914	RP	POS	5.91	585.2706				1.91E-01	0.20	0.75	2.63E-01	0.25	1.10	1.36E-01	0.32	0.60	6.27E-01	0.08	0.93	2444194	1670059	3010744	3129859	2658598	2298833	3362890	3775479
RP_POS_431_75452a13_207	RP	POS	13.21	431.7545				4.83E-04	0.64	1.12	2.64E-01	0.23	0.89	1.09E-03	0.76	1.18	4.01E-03	0.53	1.11	2788969	578699	3248629	718185	3167970	529934	3329288	864869
RP_NEG_357_0318a0_708	RP	NEG	0.71	357.0318				8.54E-02	0.28	0.64	2.64E-01	-0.24	0.71	3.95E-01	0.16	0.50	4.83E-02	0.40	0.78	5319215	1389998	5893464	2201430	6140392	2315286	5646536	2075212
HILIC_POS_292_20633a0_508	HILIC	POS	0.508	292.2063				1.23E-01	0.18	0.38	2.64E-01	0.26	0.67	1.83E-01	0.31	0.50	3.44E-02	0.05	1.15	78903	215404	871858	5078404	299205	668581	1444511	7140760
RP_POS_287_22226a8_909	RP	POS	8.91	287.2223				1.68E-01	0.28	0.65	2.64E-01	0.23	0.66	1.06E-01	0.39	0.73	4.25E-01	0.16	0.38	1681769	308549	1770290	321651	1734205	253881	1806375	376719
RP_NEG_634_33282a10_626	RP	NEG	10.63	634.3328				9.92E-02	-0.34	0.81	2.65E-01	-0.22	0.83	4.43E-02	-0.45	0.88	3.28E-01	-0.23	0.61	15087024	2679130	14172284	2695114	14474277	2851434	13870291	2521650
RP_NEG_187_13365a8_132	RP	NEG	8.13	187.1337				7.09E-03	0.45	1.45	2.65E-01	0.24	1.38	5.32E-03	0.57	1.31	8.50E-02	0.33	1.22	2180827	1385859	3073870	2107294	2837800	2023221	3309940	2182852
RP_POS_323_25583a10_415	RP	POS	10.42	323.2558				3.48E-02	-0.42	1.03	2.65E-01	0.22	0.97	1.56E-01	-0.31	0.84	1.83E-02	-0.54	1.00	3480368	429226	3289655	447741	3239519	456587	3339791	437531
RP_NEG_351_84293a15_713	RP	NEG	15.71	351.8429				1.22E-01	-0.30	0.54	2.65E-01	-0.23	0.81	6.46E-02	-0.41	0.71	3.83E-01	-0.19	0.45	1074609	176264	1016737	196415	1038728	186886	994746	205016
HILIC_POS_610_62384a10_707	HILIC	POS	10.707	610.6238				3.32E-01	-0.18	0.67	2.65E-01	-0.23	0.88	1.37E-01	-0.30	0.79	7.81E-01	-0.06	0.28	3868058	146995	3837196	179567	3857306	201569	3817086	153919
RP_POS_1069_62231a10_308	RP	POS	10.31	1069.6223				3.21E-03	0.48	1.10	2.65E-01	-0.24	0.86	5.76E-02	0.37	0.81	2.47E-03	0.60	1.23	828425	420060	1129732	658922	1203491	666458	1055972	649575
HILIC_POS_199_18056a4_009	HILIC	POS	4.009	199.1806				7.16E-01	0.07	0.72	2.65E-01	-0.23	0.81	8.44E-01	-0.04	0.08	4.13E-01	0.19	0.31	8065767	1702863	8194635	1838654	8400399	1931294	7988872	1736084
RP_POS_836_79102a0_494	RP	POS	0.49	836.7910				5.23E-09	-0.75	1.38	2.65E-01	0.24	1.22	2.58E-04	-0.63	1.34	8.21E-07	-0.87	1.58	1764025	201215	1270575	703344	1191878	692666	1349272	712078
RP_POS_283_26282a11_254	RP	POS	11.25	283.2628				8.17E-06	0.81	1.76	2.65E-01	0.22	1.16	2.61E-05	0.92	1.70	2.77E-04	0.70	1.66	6031591	2732758	8930803	3562920	8532112	3118667	9329495	3949352
RP_POS_711_54047a12_471	RP	POS	12.47	711.5405				5.08E-07	-1.19	2.03	2.66E-01	-0.18	0.66	1.57E-07	-1.28	2.11	7.89E-06	-1.10	1.73	2030299	731219	1200458	551453	1262152	627406	1138765	461519
RP_POS_271_16595a9_207	RP	POS	9.21	271.1660				6.31E-02	-0.33	0.62	2.66E-01	-0.23	0.82	3.48E-02	-0.45	0.76	2.83E-01	-0.22	0.53	1373061	45154	1354329	58778	1360900	56007	1347758	61279
RP_POS_281_91141a0_253	RP	POS	0.25	281.9114				6.52E-01	0.09	0.59	2.66E-01	-0.23	0.88	9.00E-01	-0.03	0.29	3.58E-01	0.20	0.78	1811780	215454	1832159	239594	1858943	239118	1805376	239460
RP_POS_615_42841a15_099	RP	POS	15.10	615.4284				3.34E-01	0.21	0.48	2.66E-01	-0.22	0.68	6.67E-01	0.10	0.32	1.82E-01	0.32	0.71	4218669	1647306	4536179	1456546	4698970	1442208	4373387	1467072
RP_POS_655_39435a10_925	RP	POS	10.93	655.3944				1.31E-02	0.29	0.88	2.66E-01	-0.25	1.09	2.68E-01	0.17	1.04	1.99E-02	0.42	1.03	745382	76957	902929	609792	971078	657001	834781	556912
RP_POS_141_05025a15_447	RP	POS	15.45	141.0503				1.85E-01	0.27	0.71	2.66E-01	-0.22	0.66	4.96E-01	0.16	0.52	8.61E-02	0.38	0.69	8891991	268572	8965651	275075	8996390	258239	8934912	290278

Supplementary table 1: Metabolomics results (in asceding order according to p-value from progressive ALD vs non-progressive ALD comparison, with molecular features with ID_level of 1-2 first)

								all_ALD_vs_control			Prog_ALD_vs_non-prog_ALD			Prog_ALD_vs_control_ALD			Non-prog_ALD_vs_control			Healthy_control		all_ALD		Non-prog_ALD		Progressive_ALD	
								t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA								
Feature_ID	RP_HILIC	POS_NEG	Average.Rt	Average.Mz	Metabolite.name	curated_MSMS	ID_level	p	d	VIP	p	d	VIP	p	d	VIP	p	d	VIP	Mean	SD	Mean	SD	Mean	SD	Mean	SD
RP_NEG_174_9864a3_09	RP	NEG	3.09	174.9864				1.06E-01	0.24	0.87	2.66E-01	0.25	0.96	7.86E-02	0.36	1.20	4.74E-01	0.12	0.38	856421	865133	1235205	1747948	1039933	1445005	1430476	2001784
HILIC_POS_165_05475a5_119	HILIC	POS	5.119	165.0548				3.06E-01	0.18	0.97	2.66E-01	0.24	1.14	1.81E-01	0.30	0.47	7.47E-01	0.06	0.47	1246033	326974	1321362	448033	1271318	369643	1371405	513630
RP_NEG_180_97296a15_463	RP	NEG	15.46	180.9730				3.21E-01	-0.23	0.53	2.67E-01	-0.21	0.67	1.68E-01	-0.33	0.57	6.24E-01	-0.13	0.40	4284418	196097	4246388	153781	4263556	171886	4229221	132791
RP_POS_470_13562a6_499	RP	POS	6.50	470.1356				6.25E-02	0.39	0.71	2.67E-01	-0.22	0.70	2.25E-01	0.28	0.61	3.08E-02	0.50	0.88	382730	282988	491591	276863	522464	274147	460718	278870
HILIC_POS_660_10303a0_575	HILIC	POS	0.575	660.1030				1.96E-06	0.60	1.28	2.67E-01	-0.25	0.93	8.13E-04	0.48	1.46	2.79E-04	0.72	1.45	57679	194484	487677	790007	575772	912530	399582	642192
RP_POS_210_08932a6_519	RP	POS	6.52	210.0893				7.84E-03	0.40	0.85	2.67E-01	-0.24	0.72	8.40E-02	0.28	0.65	1.29E-02	0.52	0.96	97861	267865	288650	520458	346661	603876	230639	419221
RP_NEG_343_99527a1_093	RP	NEG	1.09	343.9953				3.04E-01	-0.19	0.78	2.68E-01	-0.23	1.05	1.05E-01	-0.31	0.84	7.52E-01	-0.07	0.79	15146013	11612296	12558533	14199740	14141661	17052710	10975405	10557953
RP_POS_238_88387a15_367	RP	POS	15.37	238.8839				7.63E-01	-0.07	0.38	2.68E-01	0.22	0.72	8.41E-01	0.04	0.29	4.96E-01	-0.17	0.47	1515347	230563	1501452	207579	1478308	251903	1524596	150031
RP_POS_459_27994a4_885	RP	POS	4.89	459.2799				4.00E-01	0.19	1.19	2.68E-01	-0.21	1.24	7.14E-01	0.09	0.99	2.48E-01	0.30	1.13	499367	1608924	765571	1316260	912051	1490523	619090	1111300
RP_POS_209_1076a6_497	RP	POS	6.50	209.1076	Unknown	209.111(100)	4	2.26E-01	0.26	0.65	2.68E-01	-0.22	0.78	5.33E-01	0.15	0.48	1.15E-01	0.37	0.81	1770097	840520	1976419	793957	2064721	768444	1888118	816812
HILIC_NEG_356_99289a7_309	HILIC	NEG	7.309	356.9929				4.21E-01	0.15	0.50	2.68E-01	-0.23	0.68	8.53E-01	0.04	0.42	2.23E-01	0.27	0.55	616879	26265	621356	29885	624680	30657	618033	29019
RP_POS_393_2959a11_436	RP	POS	11.44	393.2959				3.58E-01	0.17	0.65	2.68E-01	-0.23	0.71	8.00E-01	0.05	0.24	2.00E-01	0.28	0.86	6947019	1073177	7162704	1356684	7313549	1488688	7011859	1206698
RP_POS_191_97168a0_254	RP	POS	0.25	191.9717				4.86E-01	0.15	0.57	2.69E-01	-0.22	0.75	8.62E-01	0.04	0.17	2.69E-01	0.26	0.85	18616359	3009671	19035946	2733330	19339585	2618356	18732306	2837379
HILIC_POS_110_07167a6_784	HILIC	POS	6.784	110.0717				6.42E-01	-0.09	0.89	2.69E-01	-0.23	0.98	3.22E-01	-0.20	0.66	8.93E-01	0.03	0.70	1791982	476991	1744238	579343	1808555	626783	1679921	526142
HILIC_NEG_391_66599a1_364	HILIC	NEG	1.364	391.6660				9.24E-06	0.72	1.13	2.69E-01	-0.23	0.70	3.24E-03	0.60	0.99	4.27E-06	0.83	1.56	394551	159460	575750	261645	604790	225457	546710	292851
RP_POS_533_84021a10_617	RP	POS	10.62	533.8402				1.67E-01	0.31	1.20	2.70E-01	-0.21	0.90	4.09E-01	0.21	0.78	8.03E-02	0.42	1.15	639490	216576	698944	180569	718975	161461	678913	197451
RP_POS_503_30569a5_107	RP	POS	5.11	503.3057				3.15E-02	0.37	1.20	2.70E-01	-0.23	1.26	1.68E-01	0.25	1.12	2.57E-02	0.49	1.24	339501	1052840	861264	1482542	1025712	1680229	696816	1249944
HILIC_NEG_178_85893a2_974	HILIC	NEG	2.974	178.8589				7.83E-01	0.06	0.29	2.70E-01	0.22	0.68	4.84E-01	0.17	0.28	8.17E-01	-0.05	0.54	620354	202228	631623	192779	610251	173978	652995	209488
HILIC_NEG_192_89981a2_966	HILIC	NEG	2.966	192.8998				4.54E-01	-0.17	0.52	2.70E-01	0.21	0.85	7.91E-01	-0.07	0.11	2.63E-01	-0.28	0.77	439253	209193	408504	170698	389604	166870	427404	174055
RP_POS_1008_80438a0_491	RP	POS	0.49	1008.8044				2.33E-09	0.73	1.36	2.70E-01	-0.24	1.22	1.25E-04	0.60	1.36	4.51E-06	0.85	1.53	547092	186360	1657454	1668729	1842205	1767774	1472703	1559314
RP_POS_623_29059a7_257	RP	POS	7.26	623.2906				1.68E-01	-0.25	0.76	2.71E-01	0.23	0.90	5.07E-01	-0.14	0.56	8.50E-02	-0.37	0.82	2063109	113019	2029037	140215	2013527	142845	2044548	137209
RP_POS_120_08019a4_72	RP	POS	4.72	120.0802				7.37E-06	0.53	1.30	2.71E-01	0.25	1.20	8.62E-04	0.65	1.36	2.41E-03	0.41	1.38	3388	4081	789833	1661609	605954	1331665	973711	1932847
RP_POS_938_77222a0_495	RP	POS	0.50	938.7722				7.05E-10	-0.76	1.40	2.71E-01	0.24	1.24	1.05E-04	-0.64	1.41	1.24E-06	-0.88	1.57	4202748	250427	3013693	1705357	2825149	1749198	3202238	1656379
RP_NEG_507_22452a9_349	RP	NEG	9.35	507.2245				5.00E-03	-0.76	1.29	2.71E-01	-0.17	0.72	2.26E-03	-0.85	1.38	1.68E-02	-0.68	0.97	1641740	1715614	693874	943453	798249	1093038	589499	762500
RP_NEG_199_00674a5_419	RP	NEG	5.42	199.0067				4.69E-03	0.51	0.88	2.71E-01	0.23	1.07	8.07E-03	0.63	1.01	2.35E-02	0.40	0.81	1967143	2655747	3666127	3416050	3287786	2254870	4044468	4266190
RP_POS_297_92844a15_499	RP	POS	15.50	297.9284				5.05E-03	-0.42	0.76	2.71E-01	-0.24	0.74	9.02E-03	-0.54	0.85	6.58E-02	-0.30	0.72	2953485	231693	2779186	449880	2828948	372801	2729425	514666
RP_POS_285_24213a10_12	RP	POS	10.12	285.2421				4.01E-03	-0.57	0.97	2.71E-01	-0.22	0.92	1.57E-03	-0.68	1.23	4.27E-02	-0.46	0.83	1377884	171498	1270861	188075	1291644	203724	1250078	170532
RP_POS_420_24771a13_061	RP	POS	13.06	420.2477				4.71E-01	0.17	0.70	2.72E-01	-0.20	0.70	7.81E-01	0.07	0.34	2.77E-01	0.27	0.65	4379667	1772236	4626103	1291043	4768736	1165230	4483470	1402968
RP_NEG_416_14499a11_256	RP	NEG	11.26	416.1450				1.43E-04	0.81	1.36	2.72E-01	-0.21	1.10	2.82E-03	0.70	1.31	4.63E-05	0.91	1.62	540108	213214	716482	203927	739015	174884	693948	228911
RP_POS_308_17563a4_697	RP	POS	4.70	308.1756				6.52E-03	0.37	0.69	2.72E-01	0.25	0.89	2.64E-02	0.50	0.75	3.27E-02	0.25	0.74	11972831	6988308	17952318	17731914	15990030	9721410	19914607	23084501
RP_POS_395_2146a11_254	RP	POS	11.25	395.2146				3.19E-05	0.77	1.72	2.72E-01	0.22	1.01	8.03E-05	0.88	1.62	6.61E-04	0.66	1.64	2149093	706864	2833955	885271	2736255	758303	2931656	994434
HILIC_POS_154_15887a0_658	HILIC	POS	0.658	154.1589				3.94E-04	-0.60	1.22	2.72E-01	-0.23	0.98	1.34E-03	-0.71	1.06	4.79E-03	-0.49	1.09	899175	77273	833181	114318	845805	86416	820558	136422
HILIC_POS_150_05835a0_846	HILIC	POS	0.846	150.0584				7.59E-02	0.34	0.76	2.72E-01	0.23	0.88	4.49E-02	0.45	0.82	2.79E-01	0.22	0.40	4900611	2100500	5704548	2455651	5433757	2244568	5975338	2644954
HILIC_NEG_200_85875a5_463	HILIC	NEG	5.463	200.8588				9.92E-01	0.00	0.31	2.72E-01	-0.22	0.90	6.31E-01	-0.11	0.21	6.40E-01	0.11	0.25	9341136	2227543	9336491	2144341	9572902	2105754	9100080	2177608
RP_POS_217_98738a0_734	RP	POS	0.73	217.9874				4.66E-10	0.79	1.30	2.73E-01	0.24	0.78	3.53E-06	0.91	1.48	8.63E-06	0.67	1.35	66391	105843	385856	433949	338037	372364	433676	486974
RP_POS_608_38519a0_621	HILIC	POS	0.621	608.3852				4.99E-06	0.55	1.27	2.73E-01	-0.25	0.98	3.00E-03	0.43	1.41	4.52E-04	0.67	1.48	283796	488878	2165207	3818752	2585986	4296828	1744427	3261790
HILIC_NEG_134_89474a5_507	HILIC	NEG	5.507	134.8947				3.57E-01	-0.18	0.37	2.73E-01	-0.23	0.59	1.80E-01	-0.29	0.61	7.76E-01	-0.06	0.11	13045942	4652863	12134719	5357519	12724209	5441938	11545229	5260030
RP_POS_154_04987a0_742	HILIC	POS	0.742	154.0499				5.81E-01	-0.10	0.39	2.74E-01	-0.23	0.69	3.22E-01	-0.21	0.35	9.12E-01	0.02	0.21	476541	233840	447472	323033	483014	289613	411930	352670
RP_NEG_1019_61267a10_324	RP	NEG	10.32	1019.6127				6.99E-08	0.91	1.61	2.74E-01	-0.22	0.94	1.57E-04	0.80	1.34	1.74E-08	1.02	1.90	2423631	623097	3285880	944260	3389819	750040	3181941	1103106
HILIC_POS_672_45221a0_505	HILIC	POS	0.505	672.4522				1.40E-06	0.60	1.32	2.74E-01	-0.24	1.00	9.46E-04	0.48	1.51	2.13E-04	0.72	1.49	68952	211629	580788	936796	683749	1063524	477826	787633
RP_POS_279_23181a9_786	RP	POS	9.79	279.2318				9.77E-01	0.00	0.58	2.74E-01	-0.24	1.01	5.34E-01	-0.11	0.28	5.62E-01	0.12	0.93	1361888	489485	1365144	744657	1446947	830725	1283342	645434
RP_POS_249_18524a9_207	RP	POS	9.21	249.1852	Unknown	249.1854(100), 193.1226(40)	4	7.82E-01	-0.06	0.52	2.74E-01	-0.22	0.82	4.64E-01	-0.17	0.40	8.27E-01	0.05	0.53	5435485	386150	5413824	371955	5454668	386246	5372979	356277
RP_POS_313_15506a4_72	RP	POS	4.72	313.1551				4.51E-06	0.54	1.30	2.75E-01	0.25	1.21	6.87E-04	0.67	1.37	1.80E-03	0.42	1.39	523713	187327	48808277	99464825	37883019	80018941	59733536	115506626
HILIC_POS_232_15456a1_608	HILIC	POS	1.608	232.1546				4.64E-01	0.11	0.41	2.75E-01	-0.24	0.87	9.62E-01	-0.01	0.25	1.97E-01	0.23	0.43	23363804	9482970	25157365	17700321	27100050	16498601	23214680	18790709
RP_POS_579_4317a11_163	RP	POS	11.16	579.4317				9.40E-01	0.01	0.71	2.75E-01	0.23	0.87	5.85E-01	0.13	0.62	6.03E-01	-0.10	0.65	360587	112488	362387	133266	347748	101614	377026	158492
RP_POS_305_24518a11_254	RP	POS	11.25	305.2452				1.69E-04	0.65	1.43	2.75E-01	0.23	0.81	4.30E-04	0.76	1.39	3.50E-03	0.54	1.40	6039101	2024758	7857317	2872254	7542027	2451177	8172607	3233714
RP_POS_621_39728a10_461	RP	POS	10.46	621.3973				2.67E-01	0.20	0.53	2.75E-01	0.23	0.67	1.47E-01	0.32	0.56	6.62E-01	0.09	0.46	1293196	333599	1374022	416109	1328371	383549	1419674	445493
RP_NEG_893_19366a9_609	RP	NEG	9.61	893.1937				7.26E-01	0.06	0.41	2.75E-01	-0.23	0.68	8.04E-01	-0.05	0.21	3.86E-01	0.18	0.39	4413301	266351	4433782	342419	4471342	332655	4396221	351221
HILIC_NEG_158_93901a4_724	HILIC	NEG	4.724	158.9390				4.53E-03	0.47	0.92	2.75E-01	0.23	0.96	5.08E-03	0.59	0.94	5.18E-02	0.36	0.68	384086	104174	454904	157580	437617	140644	472191	172566
HILIC_POS_150_05836a4_625	HILIC	POS	4.625	150.0584				5.17E-01	-0.09	0.63	2.75E-01	0.25	0.73	8.85E-01	0.03	0.10	5.35E-02	-0.21	1.01	16788197	3829498	16041205	9282394	15020105	4199033	17062306	12422736
RP_POS_744_58899a14_249	RP	POS	14.25	744.5890				6.06E-01	0.08	0.30	2.75E-01	0.24	0.87	3.39E-01	0.20	0.47	7.77E-01	-0.05	0.63	1211415	950749	1343410	1922176	1132588	1563676	1554233	2220165
HILIC_NEG_369_17435a0_555	HILIC	NEG	0.555	369.1744				7.84E-07	0.65	1.18	2.75E-01	0.24	0.62	1.69E-04	0.77	1.26	1.72E-04	0.53	1.27	162204	172140	476383	523124	419019	404359	533747	618612
HILIC_POS_630_41815a0_563	HILIC	POS	0.563	630.4182				1.30E-06	0.61	1.31	2.76E-01	-0.24	0.93	7.21E-04	0.49	1.48	2.05E-04	0.73	1.48	84499	280380	703338	1111912	825188	1270958	581487	923198
RP_POS_163_97667a15_627	RP	POS	15.63	163.9767				7.32E-02	0.38	0.98	2.76E-01	-0.21	0.79	2.37E-01	0.27	0.63	3.89E-02	0.49	1.23	182742344	70554324	208637375	66874731	215960302	68029777	201314449	65560959
RP_NEG_813_53955a12_329	RP	NEG	12.33	813.5396				3.98E-05	-0.89	1.57	2.76E-01	-0.20	0.67	3.62E-05	-0.99	1.56	3.94E-04	-0.79	1.56	2208645	435291	1817240	397918	1860807	361476	1773674	430546
RP_POS_513_84253a15_153	RP	POS	15.15	513.8425				9.71E-02	0.25	0.57	2.76E-01	-0.24	0.82	3.83E-01	0.12	0.46	9.62E-02	0.37	0.66	143736	305534	281094	617905	348827	770359	213360	410597
HILIC_POS_630_75275a0_563	HILIC	POS	0.563	630.7528				1.33E-06	0.61	1.30	2.76E-01	-0.24	0.93	7.08E-04	0.49	1.48	2.11E-04	0.73	1.47	87571	284809	715987	1130278	839717	1293855	592256	935854
RP_POS_397_22189a9_004	RP	POS	9.00	397.2219				4.32E-03	0.33	0.68	2.76E-01	0.25	0.75	3.48E-02	0.46	0.70	1.89E-02	0.21	0.84	18613	24123	1069134	3595727	674672	1910082	1463596	4707059
RP_POS_809_4859a10_617	RP	POS	10.62	809.4859				2.98E-02	0.48	1.19	2.76E-01	-0.21	0.83	1.34E-01	0.37	0.92	1.07E-02	0.58	1.26	816969	388142	988708	342159	1026152	276339	951264	396623
RP_POS_152_96854a0_252	RP	POS	0.25	152.9685				2.51E-01	0.24	0.63	2.77E-01	0.22	0.66	1.26E-01	0.35	0.58	5.74E-01	0.13	0.39	12391810	1874662	12830650	1810489	12632765	1900171	13028535	1712329
RP_POS_793_54272a12_766	RP	POS	12.77	793.5427				1.51E-01	-0.27	0.79	2.77E-01	0.23	0.68	4.71E-01	-0.15	0.46	7.25E-02	-0.38	0.82	1152355	301436	1058841	361086	1019377	352685	1098305	368593
RP_POS_358_27371a10_661	RP	POS	10.66	358.2737				2.83E-03	0.44	0.75	2.77E-01	-0.24	0.87	1.93E-02	0.32	0.89	1.26E-02	0.56	0.82	201090	169087	342518	353816	381268	449682	303768	218283
RP_POS_330_89917a15_378	RP	POS	15.38	330.8992				7.87E-01	0.05	0.44	2.77E-01	-0.22	0.78	7.85E-01	-0.06	0.36	4.51E-01	0.16	0.41	1435979	64881	1439657	72332	1447558	71351	1431755	73160
RP_POS_1039_6687a10_499	RP	POS	10.50	1039.6687				1.16E-02	0.50	1.00	2.77E-01	0.22	0.67	7.89E-03	0.61	1.13	6.46E-02	0.39	0.91	656682	419869	883024	448613	834031	411684	932017	481905
RP_POS_581_23883a11_804	RP	POS	11.80	581.2388				2.70E-02	-0.43	1.03	2.77E-01	0.22	1.26	1.99E-01	-0.32	0.61	3.78E-03	-0.54	1.37	1188999	803885	808109	893782	710267	465293	905952	1173865
RP_POS_481_26181a4_885	RP	POS	4.89	481.2618	Unknown	481.2611(100)	4	4.38E-01	0.18	1.21	2.77E-01	-0.20	1.23	7.44E-01	0.08	0.99	2.79E-01	0.28	1.13	872391	2775348	1292657	2177564	1530416	2466795	1054897	1838450
HILIC_POS_287_19641a3_509	HILIC	POS	3.509	287.1964				5.02E-03	0.40	0.76	2.77E-01	0.24	0.79	4.70E-03	0.52	1.03	1.23E-01	0.28	0.65	608796	891956	1352615	2069173	1126836	2066022	1578393	2068297
RP_POS_475_41516a15_1	RP	POS	15.10	475.4152				6.64E-01	-0.08	0.27	2.78E-01	0.23	0.69	8.59E-01	0.04	0.30	3.48E-01	-0.19	0.51	126642300	8654067	125813539	11247358	124586592	10973776	127040487	11493120
HILIC_POS_432_28073a0_616	HILIC	POS	0.616	432.2807				9.11E-01	-0.03	1.07	2.78E-01	-0.17	0.95	6.85E-01	-0.12	0.81	8.60E-01	0.05	1.03	2901037	8396778	2726715	4263452	3191978	4868243	2261452	3547314
RP_POS_363_22897a10_661	RP	POS	10.66	363.2290				2.09E-03	0.44	0.75	2.78E-01	-0.24	0.87	1.88E-02	0.32	0.86	1.04E-02	0.56	0.83	206282	158664	347673	350747	385952	438787	309394	230290
RP_POS_185_08087a6_347	RP	POS	6.35	185.0809				1.73E-03	0.52	0.87	2.78E-01	-0.23	0.69	4.28E-02	0.41	0.82	9.59E-04	0.64	1.12	267404	239489	448189	362633	487697	341378	408681	382054
RP_POS_584_25861a11_804	RP	POS	11.80	584.2586				2.42E-02	-0.45	1.11	2.79E-01	0.22	1.30	1.70E-01	-0.34	0.70	4.48E-03	-0.56	1.30	11009756	5898109	8183894	6328078	7493964	3895386	8873824	8047416
RP_POS_701_40918a13_574	RP	POS	13.57	701.4092				3.17E-01	-0.20	0.88	2.79E-01	-0.22	0.66	1.86E-01	-0.31	0.97	6.65E-01	-0.09	0.46	12983111	3625547	12234346	3716764	12638584	3298976	11830108	4085812
RP_POS_323_25592a10_222	RP	POS	10.22	323.2559				4.23E-01	0.14	0.92	2.79E-01	0.23	0.94	2.19E-01	0.26	0.81	9.00E-01	0.03	0.83	18358052	2328659	18776104	3148017	18433887	3072224	19118322	3216318
HILIC_POS_144_10199a0_55	HILIC	POS	0.55	144.1020				9.44E-02	-0.37	1.07	2.79E-01	-0.21	0.93	5.33E-02	-0.48	0.81	2.55E-01	-0.27	0.56	1444181	941566	1128694	802063	1215879	763252	1041509	837659
RP_POS_472_133a6_5	RP	POS	6.50	472.1330				6.27E-02	0.38	0.72	2.79E-01	-0.22	0.68	2.29E-01	0.27	0.62	3.08E-02	0.49	0.88	314682	227857	402734	228196	427534	222503	377933	233339
RP_NEG_558_33215a10_935	RP	NEG	10.94	558.3322				7.40E-02	-0.41	1.23	2.79E-01	-0.20	1.62	4.43E-02	-0.51	1.14	2.00E-01	-0.30	1.02	3461543	696853	3213050	573603	3275387	520479	3150713	621229
RP_POS_148_97342a0_256	RP	POS	0.26	148.9734				4.98E-01	0.12	0.49	2.80E-01	-0.23	0.81	9.69E-01	0.01	0.27	2.63E-01	0.24	0.44	3669786	349662	3721863	448247	3770562	456417	3673164	439085
RP_POS_405_12567a0_709	RP	POS	0.71	405.1257				4.76E-03	0.36	0.57	2.80E-01	0.24	0.84	1.94E-02	0.49	0.77	6.29E-02	0.24	0.69	404648	93855	507449	317050	472977	227133	541920	386106
HILIC_NEG_150_88943a2_956	HILIC	NEG	2.956	150.8894				7.86E-01	0.05	0.63	2.80E-01	-0.22	0.72	7.96E-01	-0.06	0.24	4.71E-01	0.16	0.27	724259	296133	740884	313617	774931	327832	706837	298125
RP_POS_476_30658a4_885	RP	POS	4.89	476.3066				4.64E-01	0.17	1.19	2.80E-01	-0.20	1.23	7.63E-01	0.07	0.98	3.00E-01	0.27	1.11	1532137	4804360	2215519	3638103	2610645	4139022	1820394	3048209
HILIC_POS_152_05397a4_625	HILIC	POS	4.625	152.0540				6.26E-01	-0.06	0.52	2.80E-01	0.25	0.67	8.01E-01	0.06	0.19	3.33E-02	-0.19	1.19	680362	127403	659375	365495	619539	116832	699210	503002
RP_POS_660_37354a9_783	RP	POS	9.78	660.3735				8.77E-05	0.51	1.13	2.80E-01	0.24	0.68	1.47E-03	0.63	1.20	8.99E-03	0.39	0.88	454675	489587	1215908	1668538	1034781	1395378	1397036	1900215
RP_POS_952_15094a0_485	RP	POS	0.49	952.1509				3.31E-08	0.68	1.22	2.80E-01	-0.24	1.08	7.09E-04	0.56	1.16	8.16E-06	0.80	1.46	164552	48361	347368	296151	379486	301508	315249	290153
RP_NEG_246_87759a15_577	RP	NEG	15.58	246.8776				1.14E-01	-0.35	0.81	2.81E-01	-0.21	0.86	6.06E-02	-0.46	0.76	3.01E-01	-0.25	0.79	1107433	48825	1091973	41781	1096502	41871	1087444	41617
RP_POS_1070_16028a10_617	RP	POS	10.62	1070.1603				5.38E-03	0.58	1.28	2.81E-01	-0.21	0.91	4.27E-02	0.47	0.99	2.14E-03	0.68	1.37	597416	372235	816353	366852	856119	329761	776587	399922
HILIC_NEG_413_20108a0_612	HILIC	NEG	0.612	413.2011				2.13E-01	0.23	0.42	2.81E-01	-0.22	0.67	5.52E-01	0.12	0.23	1.22E-01	0.35	0.65	119738	73448	139379	86811	148786	93754	129971	79094
RP_NEG_468_89688a0_497	RP	NEG	0.50	468.8969				2.23E-09	-0.74	1.37	2.81E-01	0.24	1.23	1.44E-04	-0.62	1.37	2.63E-06	-0.85	1.54	27259313	1164110	22644310	6803539	21907224	7046197	23381395	6539364

Supplementary table 1: Metabolomics results (in asceding order according to p-value from progressive ALD vs non-progressive ALD comparison, with molecular features with ID_level of 1-2 first)

								all_ALD_vs_control			Prog_ALD_vs_non-prog_ALD			Prog_ALD_vs_control_ALD			Non-prog_ALD_vs_control			Healthy_control		all_ALD		Non-prog_ALD		Progressive_ALD	
								t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA								
Feature_ID	RP_HILIC	POS_NEG	Average.Rt	Average.Mz	Metabolite.name	curated_MSMS	ID_level	p	d	VIP	p	d	VIP	p	d	VIP	p	d	VIP	Mean	SD	Mean	SD	Mean	SD	Mean	SD
HILIC_NEG_132_92361a5_059	HILIC	NEG	5.059	132.9236				1.86E-01	0.27	0.95	2.81E-01	0.22	1.16	9.42E-02	0.38	0.80	4.77E-01	0.16	0.39	4431598	1946750	4962663	1958205	4750542	2001079	5174784	1910822
RP_NEG_189_0022a4_572	RP	NEG	4.57	189.0022				7.81E-03	-0.57	0.90	2.81E-01	-0.21	0.73	6.16E-03	-0.67	1.00	3.44E-02	-0.46	0.81	14792443	10018793	9233360	9397618	10251207	7890881	8215513	10679535
RP_POS_328_23019a10_649	RP	POS	10.65	328.2302				5.42E-01	-0.08	0.48	2.82E-01	0.24	0.67	8.57E-01	0.04	0.40	5.94E-02	-0.20	0.74	3793398	375275	3718305	1032181	3606330	507999	3830280	1367072
RP_POS_199_01088a15_388	RP	POS	15.39	199.0109				1.80E-01	-0.31	1.05	2.82E-01	0.20	0.82	3.93E-01	-0.21	0.65	1.05E-01	-0.41	0.89	13579272	5564387	12107891	4456268	11625975	4698044	12589807	4192415
RP_POS_541_32935a10_617	RP	POS	10.62	541.3294				3.99E-02	0.48	1.24	2.82E-01	-0.20	1.06	1.41E-01	0.38	0.95	1.63E-02	0.58	1.29	644336	232351	739416	181161	759005	146779	719827	209717
RP_POS_497_39636a14_164	RP	POS	14.16	497.3964				3.89E-01	-0.15	0.50	2.82E-01	0.23	0.66	8.47E-01	-0.04	0.48	1.89E-01	-0.27	0.50	5858589	2063556	5466880	2668249	5178546	2555655	5755215	2771888
RP_POS_299_87692a15_557	RP	POS	15.56	299.8769				6.27E-01	0.08	0.67	2.83E-01	0.23	0.87	3.34E-01	0.20	0.49	8.81E-01	-0.03	0.79	5604776	189287	5625450	260528	5597338	256329	5653561	264231
RP_POS_1056_72791a0_494	RP	POS	0.49	1056.7279				4.06E-03	-0.61	1.18	2.83E-01	0.21	0.65	2.69E-02	-0.51	1.07	2.26E-03	-0.71	1.16	696197	91324	641021	86547	631683	86653	650358	86295
RP_POS_153_0405a0_71	RP	POS	0.71	153.0405				9.77E-05	0.46	1.07	2.83E-01	0.24	0.96	2.60E-03	0.58	1.29	1.38E-02	0.34	0.98	466901	137646	2147184	4131245	1701272	3414223	2593095	4734973
HILIC_NEG_134_89481a6_094	HILIC	NEG	6.094	134.8948				8.65E-01	-0.03	0.51	2.83E-01	-0.22	0.79	4.91E-01	-0.14	0.46	7.37E-01	0.08	0.65	16411299	8231395	16118769	9071617	17097525	10093399	15140012	7901659
RP_NEG_241_88274a15_787	RP	NEG	15.79	241.8827				5.73E-01	-0.13	0.32	2.83E-01	-0.20	0.72	3.62E-01	-0.23	0.45	9.15E-01	-0.03	0.23	4413221	2229062	4166507	1831506	4364074	1657849	3968941	1987251
RP_POS_338_2326a9_441	RP	POS	9.44	338.2326				4.68E-01	-0.14	0.32	2.83E-01	-0.22	1.00	2.77E-01	-0.25	0.47	8.81E-01	-0.03	0.32	5424028	355954	5369852	391804	5412104	341563	5327599	435712
RP_NEG_992_73187a0_497	RP	NEG	0.50	992.7319				9.80E-01	0.00	0.80	2.84E-01	-0.22	1.16	5.94E-01	-0.11	0.52	6.44E-01	0.11	0.85	1635281	291125	1633776	315052	1667715	334209	1599836	294099
RP_POS_546_3537a10_934	RP	POS	10.93	546.3537				3.41E-01	-0.22	0.88	2.84E-01	-0.20	1.35	2.03E-01	-0.32	0.67	6.32E-01	-0.12	0.78	124594877	29488688	119085380	23740978	121642029	22891328	116528732	24523830
RP_POS_436_37802a12_243	RP	POS	12.24	436.3780				6.82E-01	-0.07	0.36	2.84E-01	0.23	0.69	8.49E-01	0.04	0.29	3.92E-01	-0.19	0.57	1894481	179252	1878464	225024	1854228	243617	1902700	204345
RP_POS_177_99225a15_425	RP	POS	15.43	177.9923				7.50E-01	-0.07	0.53	2.84E-01	0.21	0.63	8.97E-01	0.03	0.29	4.80E-01	-0.17	0.61	8404975	987683	8343104	826835	8254116	852275	8432092	799207
HILIC_POS_388_25433a0_616	HILIC	POS	0.616	388.2543				7.08E-01	-0.11	1.05	2.84E-01	-0.15	0.93	5.41E-01	-0.19	0.78	9.01E-01	-0.04	0.97	4040543	12094460	3212323	5027059	3753533	5748979	2671113	4172511
RP_NEG_311_14078a4_717	RP	NEG	4.72	311.1408				4.56E-06	0.54	1.29	2.84E-01	0.24	1.20	7.13E-04	0.66	1.37	1.75E-03	0.42	1.38	71070	27630	7048569	14380514	5500865	11597653	8596273	16686062
RP_POS_154_99043a0_761	RP	POS	0.76	154.9904				7.12E-01	-0.07	0.67	2.84E-01	0.23	0.74	8.38E-01	0.04	0.36	3.79E-01	-0.18	0.89	1453946	623404	1404107	767578	1321557	713431	1486658	816998
RP_NEG_416_62344a15_584	RP	NEG	15.58	416.6234				7.69E-01	0.06	0.90	2.85E-01	-0.22	0.64	8.32E-01	-0.05	0.63	4.70E-01	0.17	0.64	764478	44643	767149	44532	771937	46329	762360	42585
RP_POS_315_25241a10_628	RP	POS	10.63	315.2524				2.97E-04	-0.76	1.49	2.85E-01	0.20	0.90	5.27E-03	-0.66	1.22	8.94E-05	-0.86	1.60	6568168	676228	6039467	649900	5969556	536922	6109378	745051
RP_POS_350_2121a10_65	RP	POS	10.65	350.2121				4.30E-01	-0.12	0.64	2.85E-01	0.24	0.69	9.98E-01	0.00	0.51	7.03E-02	-0.24	0.86	10293450	1610146	9959081	3118172	9622888	1609730	10295274	4101527
HILIC_NEG_176_83629a3_029	HILIC	NEG	3.029	176.8363				7.15E-01	-0.06	0.90	2.85E-01	-0.23	0.93	3.55E-01	-0.18	0.42	7.95E-01	0.05	0.22	733473	84896	726297	125632	739791	134439	712803	115945
HILIC_NEG_162_83916a2_962	HILIC	NEG	2.962	162.8392				3.02E-01	0.20	0.91	2.85E-01	0.22	1.31	1.90E-01	0.31	0.48	6.55E-01	0.09	0.76	40219423	14847426	43453346	16633875	41665674	13244773	45241017	19418348
RP_POS_1065_45972a0_484	RP	POS	0.48	1065.4597				5.87E-07	0.60	1.18	2.85E-01	-0.24	1.05	3.37E-03	0.48	1.07	4.12E-05	0.72	1.43	135135	20116	246986	207112	269223	209515	224750	204354
HILIC_NEG_136_89172a7_391	HILIC	NEG	7.391	136.8917				6.73E-01	-0.09	0.27	2.86E-01	0.21	1.04	9.34E-01	0.02	0.04	3.88E-01	-0.19	0.44	3552603	173237	3537745	169090	3519603	158325	3555888	178962
HILIC_POS_145_0972a0_825	HILIC	POS	0.825	145.0972				2.15E-01	0.15	0.41	2.86E-01	0.25	0.97	2.40E-01	0.27	0.36	5.92E-01	0.02	0.49	391085	143952	506338	888902	410504	181285	602172	1242904
RP_POS_616_25061a7_158	RP	POS	7.16	616.2506				6.55E-01	-0.08	0.81	2.86E-01	0.23	1.15	8.91E-01	0.03	0.42	3.09E-01	-0.19	0.88	613866	274340	587193	344077	550292	273458	624094	402039
RP_POS_786_50458a12_951	RP	POS	12.95	786.5046				9.72E-01	0.01	0.62	2.86E-01	0.22	0.65	6.32E-01	0.12	0.53	5.90E-01	-0.10	0.32	1477602	928505	1484383	1033914	1373477	702794	1595289	1280918
RP_POS_192_00853a15_423	RP	POS	15.42	192.0085				4.69E-01	-0.16	0.75	2.87E-01	-0.21	0.78	2.81E-01	-0.26	0.53	8.16E-01	-0.05	0.57	67503044	12583349	65686633	11111095	66876122	10578877	64497144	11603113
RP_NEG_276_8754a15_502	RP	NEG	15.50	276.8754				6.24E-01	-0.10	0.61	2.87E-01	-0.21	0.67	3.60E-01	-0.21	0.47	9.89E-01	0.00	0.43	1902240	58616	1896434	55990	1902427	58623	1890441	53140
RP_POS_457_27142a11_836	RP	POS	11.84	457.2714				8.39E-01	0.04	0.52	2.87E-01	-0.21	0.73	7.82E-01	-0.06	0.60	5.53E-01	0.15	0.66	22984509	15273211	23604806	13911694	25093381	16184894	22116232	11160072
RP_POS_303_09714a7_093	RP	POS	7.09	303.0971				8.62E-01	0.03	0.54	2.87E-01	0.22	0.80	5.00E-01	0.14	0.55	7.23E-01	-0.08	0.58	2089724	130317	2094524	150970	2078386	155823	2110662	145729
HILIC_POS_218_09216a4_125	HILIC	POS	4.125	218.0922				4.71E-02	-0.34	1.05	2.87E-01	-0.23	1.35	3.32E-02	-0.45	1.04	2.33E-01	-0.23	0.97	1182625	288583	1050010	414170	1094286	373627	1005734	450529
HILIC_POS_601_40167a0_553	HILIC	POS	0.553	601.4017				6.85E-07	0.60	1.32	2.88E-01	-0.24	0.94	1.00E-03	0.48	1.50	1.68E-04	0.72	1.53	71213	140532	650083	1069240	764325	1193838	535840	926281
RP_POS_558_5083a13_618	RP	POS	13.62	558.5083				7.61E-01	0.04	0.41	2.88E-01	0.24	0.72	4.74E-01	0.16	0.37	4.69E-01	-0.08	0.38	786552	90896	795270	236429	769955	114607	820584	313839
HILIC_NEG_183_93417a0_933	HILIC	NEG	0.933	183.9342				5.80E-01	0.11	0.98	2.88E-01	-0.22	0.90	9.98E-01	0.00	0.20	3.33E-01	0.22	0.44	2036152	370407	2079012	403894	2122109	417010	2035915	389747
RP_POS_231_14429a0_553	RP	POS	0.55	231.1443				6.55E-01	0.08	0.29	2.88E-01	0.22	0.66	3.73E-01	0.19	0.65	8.94E-01	-0.03	0.45	3219607	657719	3282771	789270	3198559	751694	3366983	824069
HILIC_NEG_129_01941a1_95	HILIC	NEG	1.95	129.0194				9.73E-03	0.31	0.75	2.88E-01	0.24	0.94	5.77E-02	0.43	0.58	5.59E-03	0.19	0.88	230584	97889	423893	714021	347423	261372	500363	974580
RP_NEG_824_80914a0_493	RP	NEG	0.49	824.8091				1.35E-09	-0.74	1.39	2.88E-01	0.23	1.24	1.28E-04	-0.63	1.40	1.96E-06	-0.86	1.57	7104532	405429	5268768	2682094	4982679	2756956	5554857	2601198
HILIC_POS_174_14867a0_728	HILIC	POS	0.728	174.1487				7.21E-06	-0.73	1.21	2.89E-01	-0.22	1.10	1.99E-05	-0.84	1.47	1.20E-03	-0.62	1.13	908916	88416	807122	144996	822584	144220	791660	145565
RP_NEG_510_25348a10_52	RP	NEG	10.52	510.2535				1.35E-02	0.32	0.68	2.89E-01	0.24	0.67	1.28E-02	0.44	0.79	2.46E-01	0.20	1.01	380733	670756	1033265	2318918	786020	2299567	1280510	2334896
RP_POS_309_90543a15_528	RP	POS	15.53	309.9054				1.15E-01	-0.34	0.68	2.89E-01	0.21	0.91	2.96E-01	-0.24	0.63	7.10E-02	-0.44	0.69	2028364	262133	1944587	240104	1918986	265245	1970188	211623
RP_POS_582_29559a10_306	RP	POS	10.31	582.2956				9.43E-02	0.35	0.91	2.89E-01	-0.21	1.17	3.04E-01	0.25	0.61	4.12E-02	0.45	0.99	515598	221630	591703	213842	614500	188429	568907	236270
RP_NEG_187_00662a4_573	RP	NEG	4.57	187.0066				7.42E-03	-0.57	0.91	2.89E-01	-0.20	0.72	6.03E-03	-0.67	1.00	3.20E-02	-0.47	0.82	286359818	195825419	177033456	182936609	196538117	152867067	157528795	208494244
RP_POS_231_15944a6_819	RP	POS	6.82	231.1594				1.87E-01	0.28	0.61	2.89E-01	0.21	0.69	1.11E-01	0.38	0.67	4.37E-01	0.17	0.50	990399	195624	1042740	183775	1023162	167348	1062318	198616
RP_POS_129_05473a0_615	RP	POS	0.62	129.0547				1.03E-01	0.32	0.62	2.89E-01	-0.22	0.92	3.58E-01	0.21	0.57	4.27E-02	0.43	0.79	1999115	508243	2174063	555940	2233288	487815	2114837	615894
RP_POS_305_15695a3_646	RP	POS	3.65	305.1570				5.53E-01	0.14	1.11	2.89E-01	-0.20	1.20	8.65E-01	0.04	0.96	3.66E-01	0.24	1.01	758111	1925593	979575	1464392	1135592	1671618	823557	1220109
RP_POS_575_41132a10_66	RP	POS	10.66	575.4113				8.39E-01	-0.05	0.34	2.89E-01	0.20	0.63	8.18E-01	0.06	0.24	5.58E-01	-0.15	0.29	24419619	1764021	24349186	1452315	24194532	1560760	24503839	1332929
HILIC_POS_652_41119a0_623	HILIC	POS	0.623	652.4112				1.65E-06	0.57	1.27	2.89E-01	-0.24	0.97	1.78E-03	0.45	1.43	2.89E-04	0.69	1.48	118176	148098	1598015	2893457	1906189	3234774	1289841	2501492
HILIC_POS_665_24457a0_562	HILIC	POS	0.562	665.2446				1.16E-02	-0.42	0.93	2.89E-01	0.23	0.79	1.69E-01	-0.31	0.46	1.49E-03	-0.54	1.24	394082	179947	286217	270203	257407	185982	315026	333506
RP_POS_499_82712a6_958	RP	POS	6.96	499.8271				2.45E-01	0.22	0.48	2.90E-01	-0.22	0.69	6.05E-01	0.10	0.31	1.43E-01	0.33	0.52	1489032	2879808	2213982	3505467	2587115	3822965	1840849	3150902
RP_NEG_243_19698a9_919	RP	NEG	9.92	243.1970				8.14E-05	0.63	1.56	2.90E-01	0.22	1.20	1.39E-04	0.75	1.53	6.06E-03	0.52	1.29	1762540	517509	2280772	857569	2189514	853318	2372029	860645
RP_NEG_915_12726a9_373	RP	NEG	9.37	915.1273				7.73E-01	-0.05	0.22	2.90E-01	-0.23	0.76	4.31E-01	-0.16	0.35	7.63E-01	0.06	0.32	3098493	200305	3085641	266566	3114007	262218	3057275	270490
RP_POS_166_98474a0_253	RP	POS	0.25	166.9847				5.05E-01	0.14	0.51	2.90E-01	-0.21	0.80	8.84E-01	0.03	0.18	2.86E-01	0.25	0.59	4109341	750370	4210755	721258	4287476	700726	4134034	740279
RP_POS_609_48181a11_254	RP	POS	11.25	609.4818				9.83E-05	0.64	1.61	2.90E-01	0.22	0.98	3.12E-04	0.75	1.52	3.75E-03	0.53	1.53	443656	273154	709986	437213	663503	392852	756469	476938
HILIC_POS_472_2753a0_622	HILIC	POS	0.622	472.2753				8.21E-06	0.53	1.19	2.91E-01	-0.24	0.99	3.84E-03	0.42	1.34	6.30E-04	0.65	1.37	73643	155534	742674	1400195	891388	1573998	593961	1199375
RP_POS_643_52637a11_609	RP	POS	11.61	643.5264				9.52E-01	0.01	0.31	2.91E-01	-0.23	0.74	5.34E-01	-0.10	0.50	5.83E-01	0.12	0.52	1277626	1724728	1301699	2576173	1575448	3150327	1027950	1825180
RP_POS_497_34442a11_439	RP	POS	11.44	497.3444				9.77E-01	0.00	0.50	2.91E-01	-0.24	0.87	2.76E-01	-0.11	0.53	6.05E-01	0.12	0.54	883918	1522696	895941	3257124	1243099	4493942	548784	996370
RP_NEG_746_51477a13_263	RP	NEG	13.26	746.5148				3.97E-01	-0.14	0.86	2.91E-01	0.23	0.67	9.23E-01	-0.02	0.57	7.34E-02	-0.25	0.77	1960546	1108378	1736504	1752908	1549872	776853	1923135	2352339
RP_NEG_434_8743a15_35	RP	NEG	15.35	434.8743				8.86E-01	-0.03	0.80	2.91E-01	-0.22	0.66	5.37E-01	-0.14	0.59	7.27E-01	0.08	0.42	1263246	63644	1261360	67154	1268482	69276	1254238	64874
RP_POS_825_03937a13_059	RP	POS	13.06	825.0394				6.32E-01	-0.11	0.56	2.92E-01	-0.20	0.66	4.07E-01	-0.21	0.65	9.77E-01	-0.01	0.22	745284	314020	715656	261843	743403	234771	687908	286067
HILIC_NEG_144_92349a7_354	HILIC	NEG	7.354	144.9235				1.78E-01	0.24	0.46	2.92E-01	-0.22	0.95	5.36E-01	0.13	0.42	8.46E-02	0.35	0.61	65578647	6796807	67607538	8808803	68540382	8453347	66674694	9139946
RP_POS_346_27386a10_907	RP	POS	10.91	346.2739				3.28E-02	0.30	1.42	2.92E-01	0.23	0.92	3.94E-02	0.42	1.12	2.28E-01	0.19	1.21	4359728	1855413	5503915	4157212	5063530	3379899	5944299	4806040
RP_NEG_399_18478a11_611	RP	NEG	11.61	399.1848				1.94E-01	0.29	0.69	2.92E-01	0.20	1.03	1.09E-01	0.39	0.79	4.31E-01	0.19	0.47	4431094	909857	4666183	768996	4584772	765939	4747593	771096
HILIC_POS_524_37213a1_213	HILIC	POS	1.213	524.3721				4.15E-01	-0.18	0.83	2.92E-01	-0.21	1.00	2.39E-01	-0.28	0.57	7.57E-01	-0.07	0.20	96686972	39647625	90224717	35647973	93998555	35825626	86450880	35425269
HILIC_POS_60_05658a2_199	HILIC	POS	2.199	60.0566				1.56E-01	0.23	0.53	2.92E-01	0.23	0.74	1.14E-01	0.35	0.66	4.93E-01	0.12	0.26	2728454	1737552	3321631	2776460	3027610	2171158	3615653	3268704
RP_NEG_307_85614a15_653	RP	NEG	15.65	307.8561				8.66E-01	0.05	0.34	2.92E-01	-0.17	0.76	8.92E-01	-0.04	0.20	6.53E-01	0.13	0.59	13118936	2060301	13183692	1113887	13301585	1231833	13065800	980322
RP_NEG_226_0179a5_127	RP	NEG	5.13	226.0179				2.66E-02	-0.56	0.86	2.92E-01	-0.18	0.73	8.56E-03	-0.65	1.26	9.99E-02	-0.47	0.62	2229501	3466674	720138	2328659	967327	3125082	472949	1032056
RP_NEG_654_31287a10_935	RP	NEG	10.94	654.3129				6.43E-02	-0.46	1.17	2.93E-01	-0.19	1.72	4.12E-02	-0.55	1.11	1.51E-01	-0.36	0.97	1531919	345533	1407077	241312	1432607	210385	1381548	268439
RP_POS_485_81046a0_249	RP	POS	0.25	485.8105				5.15E-01	0.13	0.54	2.93E-01	-0.21	0.84	9.16E-01	0.02	0.33	2.98E-01	0.24	0.50	426420	86352	438058	90455	447623	94007	428492	86643
RP_NEG_514_28558a11_611	RP	NEG	11.61	514.2856	Taurine conjugated sterol (BA 24:1;O4;T)	514.285(100)	3	9.41E-01	-0.01	0.64	2.93E-01	0.24	1.06	6.29E-01	0.11	0.36	1.25E-01	-0.13	0.70	71490334	52454357	70068203	168510691	52177520	58784236	87958886	230786501
RP_NEG_426_17337a11_254	RP	NEG	11.25	426.1734				4.95E-07	0.92	1.80	2.93E-01	0.21	1.15	2.61E-06	1.02	1.77	2.44E-05	0.81	1.71	968163	358246	1404778	462860	1355852	411055	1453704	508920
RP_NEG_309_17471a9_728	RP	NEG	9.73	309.1747				5.27E-01	0.08	0.37	2.93E-01	-0.24	0.66	3.97E-01	-0.04	0.45	3.92E-01	0.20	0.37	92722	82454	120713	416521	164945	582206	76482	86975
RP_POS_120_97947a15_395	RP	POS	15.40	120.9795				1.58E-01	-0.34	0.70	2.93E-01	-0.19	0.67	9.54E-02	-0.43	0.69	3.36E-01	-0.24	0.81	18656339	9120721	16136524	6860028	16860725	6417416	15412323	7268204
HILIC_POS_164_07384a0_686	HILIC	POS	0.686	164.0738				4.92E-02	-0.54	1.07	2.94E-01	-0.17	0.82	2.89E-02	-0.62	1.00	1.09E-01	-0.45	1.04	569518	477142	389758	264409	417665	271930	361852	256350
RP_POS_317_18521a11_161	RP	POS	11.16	317.1852				2.79E-01	0.19	1.00	2.94E-01	0.22	0.96	1.66E-01	0.30	0.91	6.86E-01	0.08	1.02	1286867	293606	1358415	400881	1316111	353020	1400719	443188
RP_NEG_391_177a8_105	RP	NEG	8.11	391.1770				1.79E-07	0.67	1.09	2.94E-01	0.23	0.86	8.93E-05	0.79	1.20	1.13E-04	0.56	1.22	802057	624926	2163460	2205205	1930703	1779792	2396218	2558687
RP_POS_1038_7074a0_497	RP	POS	0.50	1038.7074				7.28E-01	-0.07	0.76	2.94E-01	-0.21	1.14	4.45E-01	-0.18	0.54	8.87E-01	0.03	0.72	950384	226534	934404	219974	957598	216884	911209	222774
RP_POS_285_24225a9_662	RP	POS	9.66	285.2423				2.34E-04	0.47	0.87	2.94E-01	-0.23	0.70	7.76E-03	0.35	0.92	4.19E-03	0.59	1.03	1980557	240178	2335260	835369	2423427	1006019	2247093	618051
RP_POS_283_17508a3_646	RP	POS	3.65	283.1751				6.48E-01	0.11	1.11	2.94E-01	-0.19	1.19	9.52E-01	0.01	0.94	4.41E-01	0.21	1.01	731663	1838059	893308	1328400	1033335	1515057	753282	1109005
RP_POS_168_97989a10_442	RP	POS	10.44	168.9799				6.54E-01	-0.08	0.68	2.94E-01	-0.22	0.82	3.67E-01	-0.19	0.83	9.11E-01	0.02	0.45	4784737	1839261	4609556	2135015	4834497	2159011	4384614	2108319
RP_POS_213_18478a8_146	RP	POS	8.15	213.1848	Unknown	213.1843(100)	4	8.03E-01	-0.05	0.27	2.95E-01	0.21	1.07	8.11E-01	0.06	0.30	4.69E-01	-0.16	0.30	927242	82891	923000	85313	914016	75825	931984	93760
RP_POS_794_56537a13_194	RP	POS	13.19	794.5654				1.06E-03	0.62	1.09	2.95E-01	0.21	0.84	1.54E-03	0.72	1.16	8.80E-03	0.51	1.20	5328774	980661	6046503	1162890	5924104	962654	6168901	1332272
RP_POS_357_98346a0_708	RP	POS	0.71	357.9835				2.50E-01	-0.16	0.96	2.95E-01	-0.24	0.85	1.50E-01	-0.27	0.98	8.17E-01	-0.04	0.63	453015	72786	426070	194476	446530	175402	405609	211645
RP_POS_280_26352a9_982	RP	POS	9.98	280.2635				3.43E-01	-0.27	0.93	2.95E-01	-0.16	0.73	2.35E-01	-0.35	0.76	5.18E-01	-0.19	0.64	3241208	5397621	2290669	2645329	2568860	2755833	2012478	2527011
RP_POS_379_28146a10_809	RP	POS	10.81	379.2815				1.73E-01	-0.27	0.62	2.95E-01	0.21	0.76	4.59E-01	-0.16	0.60	9.28E-02	-0.38	0.71	1341896	319243	1250707	342836	1214664	345633	1286750	339643

Supplementary table 1: Metabolomics results (in asceding order according to p-value from progressive ALD vs non-progressive ALD comparison, with molecular features with ID_level of 1-2 first)

							all_ALD_vs_control			Prog_ALD_vs_non-prog_ALD			Prog_ALD_vs_control_ALD			Non-prog_ALD_vs_control			Healthy_control		all_ALD		Non-prog_ALD		Progressive_ALD	
							t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA								
Feature_ID	RP_HILIC	POS_NEG	Average.Rt	Average.Mz	Metabolite.name	curated_MSMS	ID_level	p	d	VIP	p	d	VIP	p	d	VIP	p	d	VIP	Mean	SD	Mean	SD	Mean	SD	Mean	SD
RP_POS_343_20035a11_253	RP	POS	11.25	343.2004				8.57E-06	0.76	1.71	2.95E-01	0.21	0.96	3.48E-05	0.86	1.64	5.20E-04	0.65	1.65	2397454	1143517	3652171	1684726	3475034	1544564	3829308	1812406
HILIC_NEG_116_9285a6_274	HILIC	NEG	6.274	116.9285				1.51E-02	-0.50	0.82	2.96E-01	-0.21	0.73	9.71E-03	-0.60	0.94	7.33E-02	-0.39	0.86	20866262	7714338	16919155	7816611	17740838	7367448	16097473	8233381
RP_POS_255_23166a10_135	RP	POS	10.14	255.2317				4.78E-01	0.13	0.48	2.96E-01	-0.22	0.81	9.20E-01	0.02	0.39	2.50E-01	0.24	0.82	3495172	344173	3547970	419870	3592070	404280	3503870	434475
RP_POS_388_30533a8_356	RP	POS	8.36	388.3053				3.18E-08	0.87	1.44	2.96E-01	0.21	0.71	1.84E-06	0.97	1.56	1.19E-05	0.76	1.52	502599	199343	803238	352849	766192	311524	840284	389484
RP_POS_499_82727a4_275	RP	POS	4.28	499.8273				6.69E-03	0.43	0.86	2.96E-01	-0.22	0.75	8.19E-02	0.32	0.67	6.65E-03	0.55	1.08	1537956	2070261	2933673	3444578	3295248	3629766	2572098	3245053
RP_POS_219_1738a11_631	RP	POS	11.63	219.1738				1.68E-01	0.22	0.45	2.96E-01	0.23	0.74	1.17E-01	0.34	0.79	5.33E-01	0.11	0.79	1344116	250541	1426950	399152	1385041	340059	1468858	450191
HILIC_NEG_285_70767a1_362	HILIC	NEG	1.362	285.7077				2.21E-10	0.86	1.58	2.96E-01	-0.22	0.58	1.02E-04	0.75	1.35	2.93E-09	0.97	2.15	1569135	218244	2063103	603802	2126495	513718	1999710	681532
HILIC_NEG_132_92357a7_947	HILIC	NEG	7.947	132.9236				6.98E-04	-0.69	1.12	2.96E-01	0.20	0.74	7.48E-03	-0.59	1.01	5.00E-04	-0.79	1.24	2518491	857702	1886068	890306	1792670	907668	1979466	871666
RP_POS_145_96626a0_254	RP	POS	0.25	145.9663				9.19E-01	0.02	0.31	2.97E-01	-0.20	0.77	7.44E-01	-0.08	0.27	6.01E-01	0.12	0.70	931766	171625	935238	150581	951021	145496	919455	155352
HILIC_POS_155_1179a0_509	HILIC	POS	0.509	155.1179				3.75E-01	0.12	0.55	2.97E-01	0.24	0.73	2.78E-01	0.24	0.36	9.88E-01	0.00	0.79	3269715	767147	3488737	2054867	3272919	1212389	3704555	2639353
HILIC_POS_302_23184a0_782	HILIC	POS	0.782	302.2318				8.83E-04	-0.63	1.12	2.97E-01	-0.21	0.66	3.51E-04	-0.74	1.40	1.71E-02	-0.53	0.99	4079151	1801492	2742413	2111349	2963714	2325728	2521112	1870189
HILIC_NEG_335_05005a4_723	HILIC	NEG	4.723	335.0501				3.24E-04	0.57	0.99	2.97E-01	0.22	1.09	1.60E-03	0.68	1.02	5.48E-03	0.46	0.95	573128	293875	843976	505473	790966	394708	896986	595559
RP_NEG_327_12787a10_705	RP	NEG	10.71	327.1279				3.73E-05	0.67	1.53	2.98E-01	0.22	1.05	2.19E-04	0.78	1.47	1.44E-03	0.56	1.49	591380	265300	868665	432002	823486	370027	913844	485772
RP_POS_408_78662a0_247	RP	POS	0.25	408.7866				1.52E-01	0.29	0.74	2.98E-01	-0.21	1.01	4.04E-01	0.19	0.49	8.35E-02	0.40	0.90	870139	116487	904714	118836	917136	120757	892291	116769
HILIC_NEG_100_93336a3_013	HILIC	NEG	3.013	100.9334				8.62E-01	0.03	0.75	2.99E-01	0.22	0.83	5.42E-01	0.14	0.54	7.16E-01	-0.07	0.35	14962814	1932130	15033536	2180222	14805685	1852528	15261387	2462912
HILIC_POS_357_23569a0_626	HILIC	POS	0.626	357.2357				5.96E-07	0.60	1.30	2.99E-01	-0.23	0.96	1.05E-03	0.48	1.47	1.69E-04	0.71	1.51	34881	67440	577302	1010881	682898	1122787	471707	883861
RP_POS_956_79181a0_494	RP	POS	0.49	956.7918				1.80E-03	0.41	1.04	2.99E-01	0.23	1.22	8.00E-03	0.52	1.11	4.95E-02	0.29	1.13	297991	145541	466653	462551	418333	384610	514973	528756
RP_POS_464_37384a11_924	RP	POS	11.92	464.3738				3.88E-01	-0.19	0.57	2.99E-01	0.20	0.92	7.07E-01	-0.09	0.82	2.20E-01	-0.29	0.70	14263605	3682074	13634971	3119134	13309270	2903044	13960672	3318491
HILIC_POS_205_09724a4_123	HILIC	POS	4.123	205.0972				9.14E-03	-0.44	1.10	2.99E-01	-0.22	1.40	8.85E-03	-0.55	1.11	7.69E-02	-0.33	0.99	59863888	12115387	52441111	17642531	54282521	15978957	50599700	19147401
RP_POS_985_58789a10_833	RP	POS	10.83	985.5879				5.36E-03	0.40	0.90	2.99E-01	-0.23	0.78	1.09E-01	0.28	0.83	6.34E-03	0.51	0.94	527895	102548	611251	231147	635366	237938	587136	223936
HILIC_POS_136_04829a1_231	HILIC	POS	1.231	136.0483				4.45E-07	-1.12	2.01	2.99E-01	-0.18	0.68	1.01E-06	-1.21	1.86	2.43E-06	-1.03	2.26	11797176	2504055	8906274	2192958	9135288	1585136	8677260	2663941
RP_POS_168_98042a10_573	RP	POS	10.57	168.9804				2.45E-01	0.25	0.50	3.00E-01	-0.20	0.72	5.40E-01	0.15	0.64	1.31E-01	0.35	0.89	4994556	1497949	5346559	1393189	5491801	1326207	5201317	1455915
RP_NEG_330_8735a15_437	RP	NEG	15.44	330.8735				2.09E-01	0.25	1.11	3.00E-01	-0.21	0.66	4.96E-01	0.15	0.58	1.23E-01	0.36	0.89	5236428	181482	5283623	187420	5303159	199976	5264087	173782
RP_NEG_187_13371a8_491	RP	NEG	8.49	187.1337				8.65E-01	-0.03	0.31	3.00E-01	0.22	0.68	7.41E-01	0.08	0.55	4.29E-01	-0.14	0.52	2206998	991002	2170164	1248571	2039888	818224	2300440	1563825
HILIC_POS_148_0966a5_642	HILIC	POS	5.642	148.0966				8.89E-01	-0.03	0.38	3.00E-01	-0.21	0.93	5.45E-01	-0.13	0.22	7.14E-01	0.08	0.29	6044489	821804	6020454	912194	6115463	893384	5925444	929848
RP_POS_389_33871a10_269	RP	POS	10.27	389.3387				4.76E-01	-0.13	0.74	3.00E-01	0.22	0.81	9.41E-01	-0.02	0.57	1.90E-01	-0.24	0.66	1742021	138079	1720247	180530	1701424	130782	1739071	219136
RP_POS_451_22906a9_064	RP	POS	9.06	451.2291				4.13E-02	0.35	0.61	3.00E-01	0.22	0.61	2.21E-02	0.46	0.90	2.31E-01	0.24	0.39	248330	152273	319604	212799	297461	216168	341748	209193
HILIC_POS_696_43726a0_625	HILIC	POS	0.625	696.4373				1.15E-06	0.59	1.30	3.00E-01	-0.23	0.96	1.26E-03	0.48	1.47	2.10E-04	0.71	1.49	91861	284711	1073699	1840704	1265275	2050506	882123	1601891
RP_POS_181_07217a2_184	RP	POS	2.18	181.0722				5.37E-04	-0.99	1.96	3.01E-01	0.14	0.64	1.70E-03	-0.92	1.47	2.64E-04	-1.06	1.94	36654466	33362472	13413503	15922434	11755866	12843110	15071139	18484281
RP_POS_346_17944a10_704	RP	POS	10.70	346.1794				7.01E-03	0.55	1.30	3.01E-01	0.20	1.14	7.19E-03	0.65	1.24	2.97E-02	0.45	1.18	347350	84906	395909	86204	386941	66763	404877	101944
RP_POS_300_20166a3_646	RP	POS	3.65	300.2017				5.73E-01	0.13	1.11	3.01E-01	-0.19	1.19	8.77E-01	0.04	0.96	3.85E-01	0.23	1.01	1048455	2587250	1330937	1947753	1533307	2205367	1128567	1648539
RP_POS_436_85858a0_512	RP	POS	0.51	436.8586				1.68E-03	-0.57	0.91	3.01E-01	0.21	0.73	3.54E-02	-0.46	0.73	5.10E-04	-0.68	1.17	537387	136249	440059	174120	421971	145183	458148	198767
HILIC_POS_371_23099a5_476	HILIC	POS	5.476	371.2400				2.33E-02	0.43	0.80	3.02E-01	-0.21	1.14	1.30E-01	0.33	0.65	1.26E-02	0.54	1.06	8788594	1505346	9529598	1744992	9710766	1717142	9348431	1771039
RP_POS_327_23157a10_512	RP	POS	10.51	327.2316				9.48E-01	0.01	0.33	3.02E-01	-0.22	0.80	5.70E-01	-0.10	0.31	5.77E-01	0.12	0.44	285038	465782	292039	691107	363834	806129	220244	551945
HILIC_NEG_155_86568a0_55	HILIC	NEG	0.55	155.8657				1.66E-03	-0.44	0.75	3.02E-01	0.23	0.68	9.60E-02	-0.33	0.57	5.65E-04	-0.56	1.53	531076	64321	470476	150127	454884	126304	486068	170550
RP_POS_439_33917a11_029	RP	POS	11.03	439.3392				9.14E-01	0.02	0.75	3.02E-01	0.22	0.86	5.30E-01	0.13	0.56	6.54E-01	-0.09	0.71	1172449	166816	1176475	227112	1152905	225778	1200045	228260
RP_POS_414_18463a10_907	RP	POS	10.91	414.1846				5.11E-02	0.29	1.36	3.02E-01	0.23	0.93	4.48E-02	0.40	1.10	3.00E-01	0.17	1.13	676704	305198	837991	614246	774238	540167	901743	679868
RP_POS_262_01343a0_734	RP	POS	0.73	262.0134				1.64E-10	0.81	1.32	3.02E-01	0.22	0.70	1.74E-06	0.92	1.54	7.36E-06	0.70	1.35	419971	702232	2655820	2958214	2348902	2633011	2962737	3248948
RP_POS_351_18411a10_704	RP	POS	10.70	351.1841				8.07E-03	0.50	1.42	3.02E-01	0.21	1.26	8.27E-03	0.60	1.35	4.60E-02	0.39	1.24	1859945	328776	2051985	392612	2011247	328604	2092723	447288
RP_POS_615_49524a14_758	RP	POS	14.76	615.4952				6.27E-01	0.06	0.67	3.02E-01	0.24	0.64	4.31E-01	0.18	0.51	5.42E-01	-0.05	0.41	2529641	1601048	2797725	4713439	2306908	1610890	3288542	6465277
RP_POS_382_203a10_864	RP	POS	10.86	382.2030				1.40E-02	-0.52	1.06	3.02E-01	-0.20	0.68	1.06E-02	-0.62	1.09	5.56E-02	-0.42	0.83	895418	358207	712383	339326	747580	292439	677187	380245
HILIC_POS_212_99937a4_797	HILIC	POS	4.797	212.9994				6.46E-01	0.08	0.25	3.02E-01	-0.22	0.92	8.92E-01	-0.03	0.13	3.26E-01	0.19	0.51	735406	91286	744762	122866	757505	109566	732020	134774
RP_POS_547_35443a10_933	RP	POS	10.93	547.3544				3.00E-01	-0.24	0.88	3.02E-01	-0.20	1.31	1.82E-01	-0.33	0.66	5.69E-01	-0.14	0.78	37404844	8342901	35703754	6783383	36407090	6529454	35000417	7023126
HILIC_NEG_227_96104a4_083	HILIC	NEG	4.083	227.9610				1.98E-08	0.83	1.29	3.03E-01	0.21	0.75	9.67E-06	0.94	1.39	2.12E-06	0.73	1.59	223837	69010	336245	139441	321789	104416	350702	167198
RP_POS_282_27908a9_95	RP	POS	9.95	282.2791				8.10E-02	0.37	0.68	3.03E-01	-0.20	0.72	2.16E-01	0.27	0.68	5.75E-02	0.47	0.79	994951	1164145	1410731	1103041	1525030	1284949	1296432	883444
HILIC_POS_675_54468a0_973	HILIC	POS	0.973	675.5447				2.75E-01	-0.21	0.40	3.03E-01	0.21	0.88	6.43E-01	-0.10	0.25	1.36E-01	-0.32	0.73	1906876	456087	1801466	514828	1748173	479141	1854758	547845
RP_POS_485_36041a11_953	RP	POS	11.95	485.3604				5.78E-01	-0.12	0.79	3.03E-01	-0.20	0.79	3.44E-01	-0.22	0.75	9.42E-01	-0.02	0.37	1226047	514914	1168507	475615	1217721	490863	1119293	459506
HILIC_NEG_259_83914a7_667	HILIC	NEG	7.667	259.8391				2.23E-01	0.21	0.80	3.03E-01	0.22	0.90	1.20E-01	0.32	0.61	6.12E-01	0.10	0.55	16907338	999653	17182764	1379533	17040031	1351350	17325497	1406179
HILIC_POS_86_06067a0_846	HILIC	POS	0.846	86.0607				9.82E-02	0.30	0.69	3.03E-01	0.22	0.87	6.79E-02	0.41	0.70	3.16E-01	0.20	0.37	1226379	479405	1400119	594856	1338554	508207	1461685	670015
HILIC_NEG_134_89478a2_172	HILIC	NEG	2.172	134.8948				3.26E-01	0.19	0.71	3.03E-01	-0.21	0.86	7.04E-01	0.08	0.14	1.79E-01	0.29	0.49	41380174	8919999	43240109	10166663	44291521	10311338	42188698	10012580
RP_POS_349_05902a9_047	RP	POS	9.05	349.0590				4.08E-04	-0.73	1.17	3.04E-01	-0.20	0.78	1.26E-04	-0.83	1.46	7.27E-03	-0.63	0.97	4829366	284132	4611447	283883	4640814	326936	4582081	232759
RP_NEG_1010_75519a0_495	RP	NEG	0.50	1010.7552				1.10E-02	-0.61	1.04	3.04E-01	-0.18	0.89	5.64E-03	-0.70	1.11	4.27E-02	-0.51	0.86	958220	119289	897300	89503	906553	93668	888046	85068
HILIC_POS_377_23315a0_631	HILIC	POS	0.631	377.2332				1.21E-06	0.58	1.26	3.04E-01	-0.23	0.95	1.34E-03	0.46	1.43	2.83E-04	0.69	1.47	39732	38516	1152518	2150814	1374906	2413383	930130	1849611
HILIC_NEG_100_93346a5_429	HILIC	NEG	5.429	100.9335				4.20E-01	0.15	0.41	3.04E-01	-0.22	0.74	8.34E-01	0.04	0.09	2.47E-01	0.26	0.44	57875088	5266951	58788230	6320484	59441498	6849085	58134962	5738589
RP_POS_766_53705a12_414	RP	POS	12.41	766.5371				1.21E-02	-0.48	1.13	3.05E-01	-0.21	0.77	7.53E-03	-0.58	1.10	8.04E-02	-0.37	0.72	1281220	594426	955175	697305	1027119	689375	883232	704692
RP_POS_553_46045a14_159	RP	POS	14.16	553.4605				6.67E-01	-0.09	0.71	3.05E-01	0.20	0.66	9.63E-01	0.01	0.67	4.02E-01	-0.19	0.49	18095576	8680458	17342052	8177348	16498481	7844041	18185623	8492436
RP_POS_231_92145a15_584	RP	POS	15.58	231.9215				8.17E-02	-0.36	0.63	3.05E-01	0.20	0.80	2.69E-01	-0.26	0.46	3.96E-02	-0.46	0.94	1435525	72288	1409523	71599	1402138	66715	1416908	76126
HILIC_POS_64_01662a5_463	HILIC	POS	5.463	64.0166				6.52E-01	-0.08	0.52	3.05E-01	0.21	0.78	9.20E-01	0.02	0.07	3.55E-01	-0.19	0.72	7856481	737740	7785386	870920	7695584	801353	7875188	934804
RP_POS_294_11188a8_017	RP	POS	8.02	294.1119				2.46E-01	0.13	0.64	3.05E-01	-0.24	0.63	2.59E-02	0.02	0.85	2.76E-01	0.25	0.68	373575	51618	856920	4138351	1285568	5848232	428271	156881
RP_POS_250_21394a10_188	RP	POS	10.19	250.2139				7.99E-03	0.32	0.70	3.05E-01	0.23	0.90	5.60E-02	0.44	0.79	8.17E-04	0.21	1.20	1021630	296998	1447656	1489291	1293514	408814	1601799	2065338
RP_NEG_291_08377a1_096	RP	NEG	1.10	291.0838				2.57E-01	-0.19	0.62	3.05E-01	0.22	0.74	7.00E-01	-0.08	0.48	1.01E-01	-0.30	0.82	5584995	4298072	4469558	6136559	3836974	5142981	5102142	6986868
RP_POS_166_08627a1_451	RP	POS	1.45	166.0863		120.0814(100), 166.0854(5)		1.24E-02	0.41	0.78	3.05E-01	0.22	0.74	1.91E-02	0.52	0.89	6.88E-02	0.30	0.87	223131323	45762898	250530596	70309489	243278780	51699440	257782412	84897458
RP_POS_513_84259a13_501	RP	POS	13.50	513.8426				3.31E-01	-0.32	1.14	3.06E-01	-0.10	1.05	2.63E-01	-0.37	0.93	4.21E-01	-0.27	0.87	329834	885536	173403	245269	198662	263462	148144	225449
RP_NEG_224_06241a6_687	RP	NEG	6.69	224.0624				2.62E-01	-0.22	0.57	3.06E-01	-0.21	0.74	1.35E-01	-0.33	0.59	5.99E-01	-0.12	0.57	43447679	47223729	32443507	49654946	37552673	52424272	27334341	46690138
RP_POS_520_33258a5_108	RP	POS	5.11	520.3326				9.06E-02	0.32	1.17	3.06E-01	-0.21	1.21	2.90E-01	0.21	1.06	6.32E-02	0.42	1.19	1102384	3321698	2321378	3975916	2730546	4479529	1912211	3395670
HILIC_NEG_112_98571a0_699	HILIC	NEG	0.699	112.9857				5.23E-03	0.51	0.93	3.06E-01	-0.21	0.71	4.39E-02	0.41	0.78	4.50E-03	0.62	1.06	2215024	880774	2767025	1106644	2880876	1173672	2653174	1034580
RP_NEG_494_95416a11_391	RP	NEG	11.39	494.9542				9.67E-02	-0.44	0.77	3.06E-01	-0.17	0.69	5.30E-02	-0.53	0.91	2.07E-01	-0.36	0.55	498497	540630	326953	317621	359639	365276	294267	261186
HILIC_POS_240_11488a0_537	HILIC	POS	0.537	240.1149				2.57E-01	0.13	0.36	3.06E-01	-0.24	0.65	6.61E-01	0.02	0.24	2.76E-01	0.25	0.46	222785	675327	794891	4875252	1298648	6856430	291134	701920
RP_NEG_326_98907a8_022	RP	NEG	8.02	326.9891				8.37E-01	-0.04	0.34	3.06E-01	0.21	0.93	7.64E-01	0.07	0.44	5.10E-01	-0.15	0.32	7674438	432180	7655767	479089	7606516	483468	7705019	474388
HILIC_NEG_118_92428a1_049	HILIC	NEG	1.049	118.9243				4.58E-02	0.37	0.94	3.07E-01	0.21	0.85	3.00E-02	0.47	1.11	2.00E-01	0.26	0.58	1241464	298683	1372916	371213	1334766	347422	1411066	393368
RP_POS_293_2085a9_962	RP	POS	9.96	293.2085				5.38E-01	0.10	0.82	3.07E-01	0.22	0.86	3.24E-01	0.21	0.73	9.60E-01	-0.01	0.84	4050410	512919	4124653	785476	4043916	651814	4205390	899095
RP_POS_251_12733a8_624	RP	POS	8.62	251.1273				2.82E-01	-0.21	0.56	3.07E-01	0.21	0.75	6.41E-01	-0.10	0.45	1.47E-01	-0.31	0.81	1508601	102044	1485446	113617	1473781	109364	1497110	117656
RP_POS_529_42969a14_264	RP	POS	14.26	529.4297				4.98E-01	0.11	0.79	3.07E-01	0.22	0.71	3.47E-01	0.22	0.63	9.67E-01	-0.01	0.47	1319481	973830	1482657	1670351	1310728	894578	1654585	2185518
RP_POS_809_52618a13_068	RP	POS	13.07	809.5262				5.78E-01	-0.11	0.41	3.07E-01	-0.21	0.76	3.37E-01	-0.21	0.74	9.99E-01	0.00	0.45	3850035	831532	3752048	955720	3850162	921814	3653934	987955
RP_POS_295_15152a8_666	RP	POS	8.67	295.1515				5.91E-01	0.09	0.57	3.07E-01	-0.22	0.77	9.28E-01	-0.02	0.23	3.71E-01	0.20	0.65	535638	270959	568412	374248	606842	445665	529983	285219
RP_POS_646_50574a13_498	RP	POS	13.50	646.5057				7.04E-01	0.05	0.30	3.08E-01	0.23	0.70	4.56E-01	0.17	0.37	5.87E-01	-0.06	0.43	1362345	175387	1382571	431301	1338222	222851	1426920	567592
RP_POS_320_25583a9_549	RP	POS	9.55	320.2558				3.47E-01	-0.25	0.85	3.08E-01	-0.17	0.73	2.23E-01	-0.34	0.74	5.55E-01	-0.17	0.50	12733378	18478700	9462041	10678342	10557130	11742655	8366952	9489137
HILIC_NEG_200_85883a4_752	HILIC	NEG	4.752	200.8588				5.65E-01	-0.09	0.70	3.08E-01	-0.23	1.28	1.81E-01	-0.20	0.47	9.02E-01	0.03	0.48	2222442	475320	2150681	917898	2244904	1132601	2056459	633534
RP_POS_599_45178a15_291	RP	POS	15.29	599.4518				7.04E-01	-0.07	0.55	3.08E-01	0.21	0.84	8.64E-01	0.04	0.51	3.98E-01	-0.18	0.58	1320400	264768	1298659	323805	1265495	314164	1331824	333010
HILIC_NEG_201_80212a0_553	HILIC	NEG	0.553	201.8021				5.56E-01	0.12	0.44	3.08E-01	-0.21	0.79	9.35E-01	0.02	0.06	3.48E-01	0.22	0.55	167655	76838	176904	76890	184781	84764	169028	68069
RP_POS_199_01123a10_571	RP	POS	10.57	199.0112				1.80E-02	-0.46	0.84	3.08E-01	0.21	0.66	9.43E-02	-0.36	0.69	1.11E-02	-0.57	0.88	3746455	1015468	3231919	1112036	3118082	1137214	3345757	1085718
HILIC_POS_371_23969a2_454	HILIC	POS	2.454	371.2397				8.93E-12	0.89	1.68	3.09E-01	-0.21	0.63	3.31E-06	0.78	1.62	6.85E-08	1.00	1.85	1777068	866726	4199206	2843454	4489852	2934870	3908559	2747654
RP_POS_355_26318a9_325	RP	POS	9.33	355.2632				2.67E-01	-0.32	0.63	3.09E-01	0.15	0.62	4.19E-01	-0.24	0.40	1.78E-01	-0.39	0.60	1390023	2710964	829593	1320139	694673	1176509	964512	1449061
HILIC_POS_678_5061a0_621	HILIC	POS	0.621	678.5061				1.16E-01	0.33	0.72	3.09E-01	0.20	0.62	6.91E-02	0.43	0.76	3.15E-01	0.22	0.56	309194	328616	415462	322838	382484	304882	448439	339711
RP_NEG_404_16357a11_612	RP	NEG	11.61	404.1636				1.41E-01	-0.30	0.66	3.10E-01	0.20	0.80	3.54E-01	-0.20	0.60	9.04E-02	-0.40	0.64	1057256	135243	1016269	134507	1002536	149063	1030002	118105
RP_NEG_297_15421a14_115	RP	NEG	14.12	297.1542				6.18E-01	0.10	0.77	3.10E-01	-0.21	0.61	9.71E-01	-0.01	0.34	3.80E-01	0.20	0.79	3865716	3080697	4187289	3400573	4534015	3713974	3840563	3053660
HILIC_POS_379_24896a0_627	HILIC	POS	0.627	379.2490				7.95E-07	0.59	1.28	3.11E-01	-0.23	0.95	1.37E-03	0.48	1.45	1.75E-04	0.70	1.49	107340	265999	1827398	3237860	2157421	3558338	1497374	2880517
RP_POS_159_07649a0_548	RP	POS	0.55	159.0765				7.47E-08	0.80	1.46	3.11E-01	0.21	1.24	1.31E-06	0.91	1.71	1.51E-04	0.69	1.31	523431	112199	697331	226357	674276	227657	720386	224962

Supplementary table 1: Metabolomics results (in asceding order according to p-value from progressive ALD vs non-progressive ALD comparison, with molecular features with ID_level of 1-2 first)

								all_ALD_vs_control			Prog_ALD_vs_non-prog_ALD			Prog_ALD_vs_control_ALD			Non-prog_ALD_vs_control			Healthy_control		all_ALD		Non-prog_ALD		Progressive_ALD	
								t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA								
Feature_ID	RP_HILIC	POS_NEG	Average.Rt	Average.Mz	Metabolite.name	curated_MSMS	ID_level	p	d	VIP	p	d	VIP	p	d	VIP	p	d	VIP	Mean	SD	Mean	SD	Mean	SD	Mean	SD
HILIC_NEG_202_92894a4_723	HILIC	NEG	4.723	202.9289				2.78E-03	0.50	0.95	3.11E-01	0.21	0.93	3.98E-03	0.61	0.98	3.20E-02	0.40	0.74	776072	201482	920131	301223	889454	267044	950808	331797
RP_POS_306_89014a15_428	RP	POS	15.43	306.8901				7.30E-01	-0.06	0.50	3.11E-01	0.21	0.95	8.21E-01	0.04	0.33	4.42E-01	-0.17	0.38	1427678	262184	1407923	333278	1373988	365515	1441859	297428
RP_POS_553_4566a14_506	RP	POS	14.51	553.4566				1.07E-01	-0.31	0.91	3.11E-01	0.21	1.11	3.56E-01	-0.20	0.81	5.31E-02	-0.41	0.77	48825141	9486894	45557893	10868619	44451576	10319505	46664209	11387471
RP_POS_168_00809a15_535	RP	POS	15.54	168.0081				1.42E-01	-0.22	0.69	3.11E-01	-0.22	0.63	1.49E-01	-0.34	0.73	3.85E-01	-0.11	0.40	15293475	401970	15141319	741064	15216973	360160	15065666	983954
HILIC_POS_616_07721a0_558	HILIC	POS	0.558	616.0772				2.20E-06	0.61	1.32	3.12E-01	-0.22	0.92	1.01E-03	0.50	1.46	2.04E-04	0.72	1.48	112703	395621	865655	1348583	1002858	1510408	728452	1163924
RP_POS_764_55566a13_498	RP	POS	13.50	764.5557				2.75E-03	-0.72	1.13	3.12E-01	-0.18	0.69	1.67E-03	-0.81	1.26	1.16E-02	-0.63	0.94	8036668	3251149	6054464	2413342	6299856	2347402	5809071	2476714
RP_NEG_325_18509a15_122	RP	NEG	15.12	325.1851				1.97E-01	-0.29	0.72	3.12E-01	-0.19	0.88	9.15E-02	-0.39	0.81	4.47E-01	-0.20	0.68	12919409	12908775	9632116	10484607	10699066	12702568	8565167	7643225
RP_POS_556_44165a10_542	RP	POS	10.54	556.4417				2.93E-01	-0.34	0.55	3.12E-01	-0.12	0.85	2.24E-01	-0.39	0.61	3.95E-01	-0.28	0.46	1948360	939418	1767925	315437	1799965	326314	1735885	304066
RP_POS_640_31744a7_257	RP	POS	7.26	640.3174				2.29E-01	-0.23	0.76	3.12E-01	0.21	0.88	5.72E-01	-0.12	0.64	1.23E-01	-0.33	0.83	2675866	157177	2635226	185896	2616354	184419	2654097	187305
HILIC_NEG_257_98438a0_836	HILIC	NEG	0.836	257.9844				5.53E-01	-0.11	0.87	3.12E-01	-0.21	0.95	3.31E-01	-0.22	0.48	9.85E-01	0.00	0.34	362291	96867	349916	117574	361853	107150	337979	127112
RP_NEG_347_22183a10_979	RP	NEG	10.98	347.2218				2.91E-02	0.40	1.41	3.13E-01	-0.21	1.38	1.73E-01	0.29	1.16	1.41E-02	0.50	1.33	1723361	565129	1997709	717011	2070492	674194	1924925	757200
HILIC_POS_128_08195a1_176	HILIC	POS	1.176	128.0820				7.07E-03	-0.59	1.07	3.13E-01	0.19	0.85	4.52E-02	-0.50	0.74	2.47E-03	-0.69	1.40	493914	185809	390677	162653	374162	128704	407192	190605
RP_POS_368_21869a10_271	RP	POS	10.27	368.2187				3.99E-01	-0.14	0.55	3.13E-01	0.22	0.70	8.76E-01	-0.03	0.34	1.88E-01	-0.25	0.58	803711	79619	788115	118377	776108	107919	800122	127950
HILIC_POS_145_10857a3_119	HILIC	POS	3.119	145.1086				3.49E-01	0.14	0.34	3.13E-01	0.22	0.77	2.48E-01	0.25	0.58	8.61E-01	0.03	0.20	44780	135668	79116	275331	51162	193741	107070	337685
RP_NEG_503_13342a8_946	RP	NEG	8.95	503.1334				9.97E-02	0.24	0.54	3.13E-01	-0.22	0.67	3.64E-01	0.13	0.49	1.04E-01	0.36	0.73	892004	1647038	1624337	3312249	1960455	4095884	1288219	2271354
RP_NEG_195_81081a0_705	RP	NEG	0.71	195.8108				9.24E-01	0.02	0.18	3.14E-01	-0.21	0.63	6.73E-01	-0.09	0.56	5.37E-01	0.12	0.46	11294700	6551197	11432137	8593553	12302522	8060052	10561753	9093676
RP_NEG_339_68536a15_599	RP	NEG	15.60	339.6854				2.12E-01	-0.26	0.61	3.14E-01	0.20	0.68	4.98E-01	-0.16	0.35	1.14E-01	-0.36	0.70	1106465	58805	1091410	58251	1085511	56190	1097308	60227
HILIC_POS_158_04041a3_695	HILIC	POS	3.695	158.0404				2.49E-02	-0.38	0.87	3.14E-01	0.21	0.87	1.91E-01	-0.28	0.90	1.04E-02	-0.49	0.97	1419441	445660	1186710	643274	1121563	576221	1251858	703814
HILIC_POS_202_14378a0_507	HILIC	POS	0.507	202.1438				1.53E-02	0.41	0.90	3.14E-01	-0.21	0.91	1.30E-01	0.30	0.91	1.03E-02	0.51	1.03	354152	368130	566174	554819	622283	555417	510065	554091
RP_POS_365_23407a12_207	RP	POS	12.21	365.2341				2.39E-02	-0.43	0.94	3.14E-01	0.21	0.70	1.24E-01	-0.33	0.77	1.39E-02	-0.54	0.96	795978	250946	673613	286208	644671	285714	702556	286635
RP_NEG_287_77679a15_612	RP	NEG	15.61	287.7768				2.72E-01	-0.24	0.64	3.14E-01	-0.19	0.92	1.60E-01	-0.34	0.68	5.44E-01	-0.15	0.48	804361	42323	795102	36668	798810	36585	791395	36744
RP_POS_501_37546a10_88	RP	POS	10.88	501.3755				1.48E-02	-0.45	0.86	3.15E-01	0.21	0.94	8.42E-02	-0.35	0.82	1.23E-02	-0.55	0.96	35382046	1689049	34469542	2087119	34258618	2267891	34680467	1888626
RP_POS_367_20316a10_908	RP	POS	10.91	367.2032				2.56E-03	0.40	1.41	3.15E-01	0.23	0.76	1.43E-02	0.51	1.11	3.23E-02	0.29	1.38	558731	298576	874222	879549	785249	632458	963195	1070907
RP_NEG_567_53644a11_61	RP	NEG	11.61	567.5364				9.22E-02	-0.33	0.86	3.15E-01	-0.21	1.03	3.53E-02	-0.43	0.90	3.35E-01	-0.23	0.77	1987478	722046	1729746	796987	1810319	922099	1649174	647937
RP_POS_514_28741a6_081	RP	POS	6.08	514.2874				9.10E-01	-0.02	0.37	3.15E-01	0.21	0.67	7.11E-01	0.08	0.37	5.19E-01	-0.13	0.44	6643007	384299	6633675	465777	6586602	385463	6680748	534060
HILIC_NEG_312_8367a4_109	HILIC	NEG	4.109	312.8367				3.16E-01	-0.24	0.42	3.15E-01	0.18	0.93	5.56E-01	-0.15	0.24	1.95E-01	-0.33	0.62	1309384	653151	1182948	466760	1135817	454551	1230079	478568
RP_POS_256_89368a15_369	RP	POS	15.37	256.8937				4.20E-02	-0.30	0.56	3.16E-01	0.22	0.60	2.07E-01	-0.18	0.61	5.82E-02	-0.41	0.80	1443884	87488	1394252	185198	1375554	225741	1412950	132756
RP_NEG_164_83542a15_575	RP	NEG	15.58	164.8354				1.84E-01	-0.25	0.69	3.16E-01	-0.21	0.74	7.30E-02	-0.36	0.79	5.23E-01	-0.15	0.37	1002364	39939	991010	46386	995691	54115	986330	37068
HILIC_NEG_389_66833a1_364	HILIC	NEG	1.364	389.6683				7.95E-06	0.73	1.15	3.16E-01	-0.21	0.67	2.52E-03	0.63	1.01	3.75E-06	0.83	1.58	397473	166445	586339	266461	613213	225021	559465	302231
RP_POS_504_84506a0_512	RP	POS	0.51	504.8451				6.89E-03	-0.54	0.86	3.16E-01	0.20	0.72	5.79E-02	-0.44	0.69	2.47E-03	-0.64	1.07	362962	115921	295996	121942	283701	102232	308290	138864
RP_POS_1078_62793a10_315	RP	POS	10.32	1078.6279				1.15E-01	-0.34	0.90	3.16E-01	-0.19	1.24	6.14E-02	-0.44	0.85	3.05E-01	-0.25	0.70	279830	176807	223583	157831	239477	164671	207690	150658
RP_POS_468_38907a10_454	RP	POS	10.45	468.3891				1.30E-01	-0.32	0.72	3.17E-01	0.20	0.78	3.43E-01	-0.22	0.56	7.19E-02	-0.42	0.73	5938201	449365	5799612	425560	5756787	418866	5842437	432096
RP_POS_633_45349a10_925	RP	POS	10.93	633.4535				7.57E-01	-0.06	0.68	3.17E-01	0.21	0.75	8.59E-01	0.04	0.63	4.19E-01	-0.16	0.66	10173631	1278169	10091257	1391697	9951163	1090947	10231352	1637971
RP_NEG_231_9321a13_392	RP	NEG	13.39	231.9321				4.66E-01	0.16	0.34	3.17E-01	-0.20	1.05	8.06E-01	0.06	0.27	2.72E-01	0.26	0.45	4703084	2417512	5056291	2193848	5276838	2055607	4835744	2323656
RP_POS_822_48035a11_627	RP	POS	11.63	822.4804				6.23E-01	0.08	0.37	3.17E-01	0.22	0.60	3.78E-01	0.19	0.60	8.98E-01	-0.02	0.48	1903409	488069	1958131	697984	1887946	596144	2028317	786680
RP_POS_482_32376a10_824	RP	POS	10.82	482.3238				8.80E-02	0.33	1.09	3.17E-01	0.21	1.03	6.60E-02	0.43	0.87	2.61E-01	0.22	0.95	1649781	661959	1891799	759765	1815408	617255	1968190	879405
RP_POS_868_73798a0_498	RP	POS	0.50	868.7380				8.48E-01	-0.04	0.84	3.17E-01	-0.20	1.21	5.38E-01	-0.14	0.71	7.95E-01	0.06	0.79	421896	211170	413653	206707	434422	212674	392884	200542
RP_POS_1024_77905a0_495	RP	POS	0.50	1024.7791				6.54E-05	0.51	1.12	3.18E-01	0.22	1.21	1.64E-03	0.62	1.22	6.41E-03	0.40	1.20	135812	101785	307752	375613	269999	311609	345505	430164
HILIC_POS_315_0802a7_651	HILIC	POS	7.651	315.0802				4.58E-01	-0.12	0.67	3.18E-01	-0.22	0.79	2.33E-01	-0.23	0.57	9.74E-01	-0.01	0.52	1308620	132963	1284060	231057	1307272	235205	1260848	226810
RP_POS_289_84821a15_571	RP	POS	15.57	289.8482				1.39E-01	-0.29	0.56	3.18E-01	0.20	0.60	4.06E-01	-0.19	0.57	6.60E-02	-0.39	0.78	1550015	61933	1530727	67053	1523990	60749	1537464	72808
HILIC_POS_402_23318a1_841	HILIC	POS	1.841	402.2332				8.16E-01	0.05	1.03	3.18E-01	-0.19	0.82	8.66E-01	-0.04	0.87	5.76E-01	0.15	1.02	911225	2908824	1043114	2274474	1271748	2710602	814480	1731472
RP_POS_185_12868a2_461	RP	POS	2.46	185.1287				6.89E-03	0.46	0.78	3.18E-01	0.21	0.60	1.20E-02	0.57	1.01	3.87E-02	0.36	0.99	5189311	2205195	6584921	3167099	6266636	2337935	6903206	3820086
RP_POS_449_35907a11_735	RP	POS	11.74	449.3591				1.45E-01	-0.24	0.83	3.18E-01	0.22	0.97	4.84E-01	-0.13	0.82	9.06E-02	-0.35	0.80	835676	161298	779626	252166	754313	268667	804939	234485
RP_POS_335_21921a10_71	RP	POS	10.71	335.2192				2.15E-05	0.50	0.96	3.18E-01	-0.23	0.93	5.55E-03	0.39	0.99	1.31E-03	0.61	1.13	56340	36739	428434	831976	511975	944217	344893	701931
RP_POS_405_25052a11_609	RP	POS	11.61	405.2505				6.30E-03	-0.58	1.12	3.18E-01	0.19	1.06	3.14E-02	-0.49	1.07	4.39E-03	-0.68	1.06	15418712	1748978	14420808	1635606	14256735	1723692	14584881	1542386
RP_POS_160_13333a2_502	RP	POS	2.50	160.1333	Isomer of pregabalin	142.122(100), 160.1333(35), 118.0564(65), 97.1012(35)	3	4.07E-02	0.24	0.57	3.18E-01	0.23	0.78	1.16E-01	0.36	0.62	3.07E-02	0.13	0.71	2967642	4363342	9767942	31919587	6553358	10125879	12982526	43987393
RP_POS_572_36804a11_004	RP	POS	11.00	572.3680	LPC 20:1 [M+Na]+	104.1073(100), 513.2985(50), 572.3693(25), 86.0964(14), 146.982(20)		6.66E-01	-0.09	0.70	3.19E-01	0.20	1.16	9.81E-01	0.01	0.45	4.01E-01	-0.19	0.78	1627412	739051	1563512	678124	1495534	600995	1631490	747303
RP_POS_780_55072a13_286	RP	POS	13.29	780.5507				5.17E-01	-0.16	0.64	3.19E-01	-0.18	0.68	3.05E-01	-0.25	0.62	8.00E-01	-0.07	0.80	26423790	37649344	21750102	25938187	24354069	33278139	19146135	15428445
HILIC_POS_87_09223a3_609	HILIC	POS	3.609	87.0922				1.11E-02	0.48	1.23	3.19E-01	0.20	0.68	8.02E-03	0.58	1.11	6.91E-02	0.38	0.91	7004067	3420421	8902125	3997668	8501725	3826190	9302525	4161963
RP_POS_320_25598a9_387	RP	POS	9.39	320.2560				3.02E-01	-0.28	0.90	3.19E-01	-0.16	0.70	1.96E-01	-0.36	0.76	4.87E-01	-0.20	0.54	5958485	9220387	4167163	5179436	4685915	5630438	3648411	4685036
RP_POS_401_26797a10_444	RP	POS	10.44	401.2680				2.25E-01	0.23	0.58	3.19E-01	0.20	0.60	1.30E-01	0.34	0.61	5.39E-01	0.13	0.50	887168	260385	953945	291364	924772	282295	983119	300151
RP_POS_749_53638a13_57	RP	POS	13.57	749.5364				9.78E-01	0.01	0.34	3.19E-01	0.21	0.72	6.07E-01	0.11	0.23	6.53E-01	-0.10	0.46	6352534	546255	6355687	636954	6291923	660862	6419451	612098
HILIC_POS_200_12828a1_024	HILIC	POS	1.024	200.1283				3.18E-01	0.12	0.47	3.20E-01	-0.23	0.55	6.69E-01	0.00	0.17	3.20E-01	0.23	0.51	12002	21981	2199058	21771948	4388166	30788454	9950	19609
RP_NEG_241_75818a15_587	RP	NEG	15.59	241.7582				1.03E-01	-0.31	0.66	3.20E-01	-0.21	0.70	4.91E-02	-0.41	0.77	3.51E-01	-0.21	0.39	16182151	509474	16003768	591284	16062908	633717	15944627	545558
HILIC_NEG_162_83911a3_004	HILIC	NEG	3.004	162.8391				9.26E-01	-0.02	0.93	3.20E-01	0.21	1.12	7.11E-01	0.09	0.36	5.34E-01	-0.12	0.30	53873330	11249888	53650459	13279140	52322403	10488805	54978514	15577398
RP_POS_679_43933a10_703	RP	POS	10.70	679.4393				2.84E-01	-0.19	0.71	3.20E-01	0.21	0.66	6.90E-01	-0.08	0.42	1.58E-01	-0.29	0.61	2398591	444075	2291103	613419	2229810	627843	2352395	598658
RP_POS_265_25256a10_652	RP	POS	10.65	265.2526				2.72E-03	-0.58	1.04	3.20E-01	0.20	0.86	2.26E-02	-0.48	0.99	2.40E-03	-0.68	1.09	875806	121295	795842	139147	781941	147003	809744	130822
RP_POS_872_82965a0_492	RP	POS	0.49	872.8297				1.73E-08	0.68	1.33	3.20E-01	-0.22	1.20	2.14E-04	0.57	1.35	2.45E-05	0.79	1.49	51818	56305	1751620	2767651	2028079	2997991	1475160	2516382
RP_POS_413_32385a13_01	RP	POS	13.01	413.3239				1.02E-01	-0.33	0.77	3.20E-01	-0.20	0.98	5.48E-02	-0.43	1.09	3.09E-01	-0.23	0.49	2492759	862201	2199429	888750	2288182	912164	2110676	864727
HILIC_POS_401_26199a0_63	HILIC	POS	0.63	401.2620				4.18E-07	0.60	1.29	3.21E-01	-0.22	0.93	8.80E-04	0.49	1.44	1.51E-04	0.71	1.51	53209	46685	1774020	3173415	2090889	3506165	1457152	2801525
HILIC_POS_375_32144a0_797	HILIC	POS	0.797	375.3214				6.88E-02	0.37	0.63	3.21E-01	0.20	0.72	4.27E-02	0.47	0.79	2.21E-01	0.27	0.58	4114822	1698331	4760234	1751381	4585405	1656896	4935064	1841082
RP_POS_259_13058a8_457	RP	POS	8.46	259.1306	Unknown	259.1289(100)	4	7.49E-01	0.07	0.51	3.21E-01	-0.20	0.65	8.77E-01	-0.03	0.34	4.79E-01	0.17	0.53	3283847	314546	3304418	314285	3335778	334419	3273059	292785
RP_POS_374_15546a4_997	RP	POS	5.00	374.1555				3.22E-03	0.43	0.90	3.21E-01	0.22	0.78	7.04E-03	0.54	1.05	5.16E-02	0.32	0.65	11740831	8739604	18878557	17964085	17087351	15705645	20669762	19969664
RP_NEG_338_7814a15_4	RP	NEG	15.40	338.7814				3.59E-01	0.25	1.03	3.21E-01	-0.16	0.60	5.33E-01	0.17	0.52	2.59E-01	0.33	0.74	800222	84279	814697	45405	819225	51949	810170	37748
RP_POS_398_75006a13_491	RP	POS	13.49	398.7501				2.32E-02	-0.47	0.81	3.21E-01	-0.20	0.66	1.28E-02	-0.56	1.00	1.05E-01	-0.37	0.57	763900	314374	614524	315023	645916	321343	583132	308596
RP_POS_741_52795a12_763	RP	POS	12.76	741.5280				1.01E-02	-0.52	0.95	3.22E-01	0.20	0.60	6.27E-02	-0.42	0.76	5.30E-03	-0.62	1.01	1045317	400414	826089	417828	784464	398291	867714	436523
RP_POS_406_16394a4_275	RP	POS	4.28	406.1639				3.55E-01	-0.12	0.51	3.22E-01	0.22	0.91	9.62E-01	-0.01	0.65	7.32E-02	-0.23	1.09	10015070	1503626	9539208	4387842	9101834	3017479	9976582	5422513
RP_POS_166_98486a10_671	RP	POS	10.67	166.9849				5.13E-01	0.15	0.46	3.22E-01	-0.19	1.02	8.38E-01	0.05	0.30	3.13E-01	0.24	0.51	11827814	3009170	12217619	2569826	12473430	2436743	11961809	2696576
HILIC_POS_446_25934a1_81	HILIC	POS	1.81	446.2593				4.89E-01	0.14	1.01	3.22E-01	-0.20	0.80	8.61E-01	0.03	0.93	3.28E-01	0.24	1.05	487544	1516476	706085	1634250	868928	1978324	543241	1195061
RP_POS_279_19138a0_543	RP	POS	0.54	279.1914				1.50E-06	0.71	1.25	3.22E-01	0.21	0.63	6.82E-05	0.81	1.40	2.09E-04	0.60	1.27	457517	150421	665593	310463	634680	261738	696506	352541
HILIC_POS_160_13326a1_725	HILIC	POS	1.725	160.1333				3.22E-01	0.11	0.74	3.22E-01	0.23	0.83	3.23E-01	0.23	0.59	1.87E-02	0.00	1.03	106422	40865	5277106	51935307	81943	50791	10472270	73447362
RP_POS_223_09433a15_227	RP	POS	15.23	223.0943				2.67E-01	-0.22	0.45	3.22E-01	-0.20	0.72	1.37E-01	-0.32	0.60	5.94E-01	-0.12	0.50	19516373	8720914	17518760	8941550	18408634	9761004	16628887	8039965
RP_POS_139_12296a0_71	RP	POS	0.71	139.1230				1.15E-01	0.29	0.70	3.22E-01	0.21	0.64	6.67E-02	0.39	0.81	3.79E-01	0.18	0.31	340208	26126	349287	33241	345980	32540	352593	33931
RP_POS_158_96167a0_808	RP	POS	0.81	158.9617				8.64E-01	0.03	0.28	3.22E-01	0.20	0.83	5.37E-01	0.13	0.28	7.83E-01	-0.07	0.27	3943593	1568852	3998357	1581817	3840994	1736732	4155721	1410170
RP_NEG_414_20816a11_611	RP	NEG	11.61	414.2082				3.64E-01	-0.17	0.60	3.22E-01	0.20	0.86	7.28E-01	-0.07	0.56	2.23E-01	-0.28	0.79	512618	74407	498339	83968	489987	91355	506692	75875
RP_POS_441_29758a12_243	RP	POS	12.24	441.2976				9.85E-01	0.00	0.51	3.23E-01	0.20	0.78	6.91E-01	0.10	0.43	6.42E-01	-0.10	0.25	24240382	11358774	24197671	11021875	23102060	9777012	25293282	12140963
HILIC_NEG_157_90117a3_943	HILIC	NEG	3.943	157.9012				5.11E-01	0.12	0.41	3.23E-01	-0.21	0.58	9.24E-01	0.02	0.16	2.89E-01	0.23	0.70	1500579	454936	1564590	537357	1617971	530069	1511210	544618
RP_POS_253_09706a5_577	RP	POS	5.58	253.0971	Isomer of Carbamazepine-10,11-epoxide	180.0811(100), 210.092(95), 253.0961(35), 182.0972(20)	3	3.21E-01	0.11	0.75	3.23E-01	-0.23	0.78	7.38E-01	0.00	0.62	3.23E-01	0.23	0.83	15296	9290	1080549	10677040	2146509	15099863	14590	9290
HILIC_POS_139_123a0_555	HILIC	POS	0.555	139.1230				1.22E-02	-0.54	1.41	3.23E-01	0.19	0.71	5.54E-02	-0.45	0.79	7.15E-03	-0.64	1.27	9208154	2908793	7702753	2644977	7440061	2639786	7965445	2650524
RP_POS_770_50848a13_248	RP	POS	13.25	770.5085				8.79E-01	0.03	0.93	3.23E-01	0.21	0.61	5.67E-01	0.13	0.70	6.25E-01	-0.08	0.45	1151829	393749	1165580	571765	1108706	378224	1222453	714736
RP_POS_362_3053a10_423	RP	POS	10.42	362.3053				9.82E-01	0.00	0.36	3.23E-01	-0.22	0.76	5.17E-01	-0.11	0.30	6.34E-01	0.10	0.44	985226	1271596	978299	1999698	1176982	2351013	779615	1572057
RP_POS_303_23187a10_423	RP	POS	10.42	303.2319				5.84E-01	0.09	0.40	3.23E-01	-0.22	0.77	8.85E-01	-0.02	0.26	3.74E-01	0.19	0.52	2063618	3036834	2477401	5281206	3002229	6377067	1952573	3888749
RP_POS_130_96298a15_441	RP	POS	15.44	130.9630				4.76E-01	-0.14	0.46	3.23E-01	0.20	0.59	8.71E-01	-0.04	0.34	2.50E-01	-0.24	0.59	13152164	2240326	12817394	2464870	12572715	2150617	13062073	2743689
HILIC_POS_133_09724a7_152	HILIC	POS	7.152	133.0972				1.38E-05	0.56	1.07	3.24E-01	0.22	0.83	9.53E-04	0.67	1.15	1.13E-03	0.46	1.16	2275957	1130709	4184652	3720640	3815254	2874278	4554050	4407821
RP_NEG_876_82288a0_486	RP	NEG	0.49	876.8229				6.29E-03	0.36	1.07	3.24E-01	0.22	1.26	1.21E-02	0.47	1.12	1.19E-01	0.25	1.13	2978744	521078	3473876	1525995	3322474	1396292	3625277	1645732
RP_POS_513_84302a11_759	RP	POS	11.76	513.8430				3.35E-01	0.11	0.38	3.24E-01	-0.23	0.75	9.26E-01	0.00	0.48	3.27E-01	0.23	0.44	120824	75876	236275	1184469	354308	1666407	118241	170936

Supplementary table 1: Metabolomics results (in asceding order according to p-value from progressive ALD vs non-progressive ALD comparison, with molecular features with ID_level of 1-2 first)

							all_ALD_vs_control			Prog_ALD_vs_non-prog_ALD			Prog_ALD_vs_control_ALD			Non-prog_ALD_vs_control			Healthy_control		all_ALD		Non-prog_ALD		Progressive_ALD	
							t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA								
Feature_ID	RP_HILIC	POS_NEG	Average.Rt	Average.Mz	Metabolite.name	curated_MSMS	ID_level	p	d	VIP	p	d	VIP	p	d	VIP	p	d	VIP	Mean	SD	Mean	SD	Mean	SD	Mean	SD
RP_POS_760_57599a10_906	RP	POS	10.91	760.5760				9.63E-03	-0.55	1.10	3.24E-01	0.19	1.17	5.84E-02	-0.45	0.82	4.06E-03	-0.64	1.13	821463	234389	694846	222587	672765	193462	716927	248353
RP_POS_594_5993a11_168	RP	POS	11.17	594.5993				3.34E-07	0.83	1.63	3.24E-01	-0.20	1.02	1.96E-04	0.73	1.40	1.07E-06	0.93	1.73	995419	275750	1362556	451008	1407283	430226	1317828	470947
RP_POS_414_30035a11_183	RP	POS	11.18	414.3004				2.97E-01	0.19	0.84	3.24E-01	0.21	0.86	1.76E-01	0.29	0.71	6.67E-01	0.09	0.53	573976	787096	752477	974186	655909	913985	849046	1031041
HILIC_POS_194_02217a4_624	HILIC	POS	4.624	194.0222				5.36E-01	-0.08	0.61	3.24E-01	0.22	0.66	9.05E-01	0.03	0.26	5.33E-02	-0.20	1.34	701766	118164	678785	306020	648358	122711	709211	415042
HILIC_NEG_99_92564a7_352	HILIC	NEG	7.352	99.9256				1.83E-03	-0.48	0.74	3.25E-01	-0.21	0.63	3.81E-03	-0.59	0.94	3.06E-02	-0.38	0.76	2845993	312809	2594241	557568	2649436	495671	2539046	613353
RP_POS_445_2924Sa10_448	RP	POS	10.45	445.2925				1.48E-01	0.29	0.62	3.25E-01	-0.20	0.73	3.94E-01	0.19	0.59	7.99E-02	0.39	0.82	1253569	442019	1386394	454907	1431411	441309	1341377	468204
RP_POS_317_91235a15_381	RP	POS	15.38	317.9124				6.05E-01	0.11	0.32	3.25E-01	0.20	0.70	3.48E-01	0.21	0.53	9.79E-01	0.01	0.31	1519909	210055	1542167	211872	1521198	233172	1563135	188226
RP_POS_351_22906a10_907	RP	POS	10.91	351.2291				1.14E-02	0.35	1.43	3.25E-01	0.22	0.87	2.22E-02	0.46	1.15	1.13E-01	0.24	1.25	24316962	9844275	31811351	23410049	29494786	19215358	34127915	26964109
RP_POS_337_1821a11_243	RP	POS	11.24	337.1821				1.59E-03	0.57	1.34	3.25E-01	0.20	1.03	2.73E-03	0.67	1.33	1.37E-02	0.46	1.18	1062878	280616	1266301	369172	1229774	307864	1302828	421727
RP_POS_266_17313a11_608	RP	POS	11.61	266.1731				4.61E-02	-0.37	0.86	3.25E-01	0.20	0.78	1.71E-01	-0.27	0.65	3.62E-02	-0.48	0.93	1038459	115026	988574	136731	975051	153516	1002097	117608
RP_NEG_563_505a11_254	RP	NEG	11.25	563.5050				5.36E-07	0.74	1.61	3.25E-01	0.21	1.00	1.20E-05	0.84	1.61	3.40E-04	0.63	1.53	615472	525315	1379439	1093283	1271355	1047337	1487522	1137617
HILIC_NEG_524_27826a1_681	HILIC	NEG	1.681	524.2783				1.69E-02	0.39	0.73	3.25E-01	-0.21	0.74	1.39E-01	0.29	0.51	1.25E-02	0.50	0.93	368779	135812	447223	214035	468382	217136	426064	210938
RP_NEG_194_08148a8_528	RP	NEG	8.53	194.0815				4.72E-01	-0.18	0.63	3.25E-01	-0.17	1.03	3.07E-01	-0.27	0.65	7.31E-01	-0.09	0.31	940301	55991	932617	37758	936349	40656	928884	34629
RP_POS_265_2532a11_254	RP	POS	11.25	265.2532				5.20E-06	0.84	1.74	3.25E-01	0.19	1.11	1.78E-05	0.94	1.70	1.49E-04	0.74	1.65	1130437	499262	1668336	627500	1606306	562037	1730366	686885
RP_POS_553_45984a11_162	RP	POS	11.16	553.4598				2.32E-01	-0.22	0.63	3.26E-01	0.21	0.67	5.72E-01	-0.12	0.52	1.38E-01	-0.32	0.58	16752261	2299267	16153222	2859754	15870696	3007816	16435747	2704336
RP_NEG_158_9778a15_298	RP	NEG	15.30	158.9778				7.68E-01	-0.05	0.61	3.26E-01	-0.21	0.61	4.35E-01	-0.16	0.52	8.23E-01	0.05	0.34	16106937	445085	16078494	551229	16132931	600635	16024056	497089
HILIC_NEG_195_741a3_034	HILIC	NEG	3.034	195.7410				4.83E-02	0.25	0.88	3.26E-01	0.22	0.79	2.38E-02	0.36	1.14	4.42E-01	0.14	0.79	564134	33568	590594	118692	578879	127956	602309	108675
RP_POS_386_15237a9_047	RP	POS	9.05	386.1524				5.66E-04	-0.74	1.15	3.26E-01	-0.18	0.81	2.48E-04	-0.83	1.38	6.21E-03	-0.65	0.96	5526114	352143	5267055	325605	5299181	358818	5234929	288694
HILIC_POS_399_24649a0_634	HILIC	POS	0.634	399.2465				3.16E-06	0.57	1.29	3.27E-01	-0.22	0.94	1.88E-03	0.46	1.46	3.82E-04	0.68	1.47	275972	752339	2558223	4462126	2998264	4981767	2118182	3874828
RP_POS_478_38898a11_841	RP	POS	11.84	478.3890				7.94E-01	0.06	0.40	3.27E-01	0.19	0.69	5.45E-01	0.15	0.40	8.90E-01	-0.03	0.69	100295351	48353140	102763084	39176963	98902968	36396108	106623201	41784043
HILIC_NEG_266_91565a0_882	HILIC	NEG	0.882	266.9157				1.11E-01	0.30	0.98	3.27E-01	0.20	0.89	7.18E-02	0.40	0.72	3.30E-01	0.20	0.50	597745	143978	647112	167957	630564	153873	663661	180994
RP_NEG_327_25452a11_254	RP	NEG	11.25	327.2545				4.19E-07	0.76	1.65	3.27E-01	0.21	0.99	9.62E-06	0.86	1.63	2.15E-04	0.65	1.58	1313397	713322	2334412	1409898	2195529	1336591	2473295	1479983
RP_NEG_283_70932a15_59	RP	NEG	15.59	283.7093				6.08E-01	0.10	1.36	3.27E-01	-0.20	0.66	9.86E-01	0.00	0.71	3.61E-01	0.20	1.23	1108952	46577	1114019	53458	1119284	54113	1108754	52811
RP_NEG_236_84775a15_584	RP	NEG	15.58	236.8478				2.37E-03	-0.60	1.17	3.27E-01	-0.19	0.60	1.62E-03	-0.70	1.17	2.05E-02	-0.51	1.08	811981	33912	789639	36443	793228	36479	786051	36419
RP_POS_376_29688a11_67	RP	POS	11.67	376.2969				9.90E-01	0.00	0.64	3.27E-01	-0.20	0.61	6.56E-01	-0.10	0.42	6.72E-01	0.10	0.36	13177311	7518375	13157454	7562627	13901924	7560889	12412983	7566751
RP_POS_303_22903a10_978	RP	POS	10.98	303.2290				1.59E-02	0.41	1.29	3.27E-01	-0.21	1.38	1.26E-01	0.30	1.07	1.07E-02	0.51	1.22	15885900	6220578	19406387	9102218	20302344	9065929	18510431	9141238
RP_POS_327_19391a15_431	RP	POS	15.43	327.1939				6.57E-01	-0.10	1.12	3.28E-01	0.19	0.75	9.76E-01	-0.01	0.55	4.29E-01	-0.19	1.00	3726197	1527680	3593091	1251160	3469956	1239492	3716227	1263118
HILIC_POS_586_72632a0_549	HILIC	POS	0.549	586.7263				1.22E-06	0.62	1.34	3.28E-01	-0.22	0.92	7.73E-04	0.51	1.49	1.58E-04	0.73	1.51	51994	192930	443592	689094	511425	766966	375758	601469
HILIC_NEG_331_65601a1_363	HILIC	NEG	1.363	331.6560				1.03E-07	0.85	1.36	3.28E-01	-0.20	0.67	2.84E-04	0.75	1.20	5.59E-08	0.95	1.86	3690301	966896	5060858	1640536	5222326	1339627	4899391	1894686
RP_NEG_243_06291a1_341	RP	NEG	1.34	243.0629				9.64E-01	-0.01	0.60	3.28E-01	-0.21	0.85	5.87E-01	-0.11	0.57	6.39E-01	0.10	0.67	630810	207656	628725	277394	656011	275700	601438	279169
HILIC_POS_181_05247a1_514	HILIC	POS	1.514	181.0525				7.59E-01	0.06	1.00	3.28E-01	0.20	0.99	4.90E-01	0.16	0.26	8.25E-01	-0.04	0.62	439946	122061	447916	142575	433897	117335	461936	164016
RP_POS_200_0401a0_507	RP	POS	0.51	200.0401				5.95E-05	0.51	1.18	3.28E-01	-0.22	1.25	7.05E-03	0.40	1.23	1.38E-03	0.62	1.30	369954	88360	518725	322411	550423	363080	487026	275938
RP_POS_481_81564a0_246	RP	POS	0.25	481.8156				9.46E-02	0.28	0.61	3.29E-01	0.21	0.67	7.87E-02	0.39	0.87	3.16E-01	0.18	0.70	360651	161201	423163	235020	400094	188863	446233	273570
RP_POS_1090_71948a0_495	RP	POS	0.50	1090.7195				2.34E-06	-0.61	1.29	3.29E-01	0.21	1.20	4.34E-03	-0.51	1.26	2.88E-05	-0.72	1.44	975786	96328	798201	316465	767164	304105	829237	328480
RP_NEG_369_17453a8_265	RP	NEG	8.27	369.1745				2.20E-06	0.60	1.19	3.29E-01	0.22	0.89	5.28E-04	0.71	1.17	3.20E-04	0.49	1.14	6204431	5410227	18006186	21767943	15869603	16636370	20142769	25908915
HILIC_POS_136_07585a5_119	HILIC	POS	5.119	136.0759				4.50E-01	0.14	0.91	3.30E-01	0.21	1.13	2.80E-01	0.24	0.42	8.69E-01	0.03	0.41	1024089	328094	1078783	426094	1037015	372180	1120552	474066
RP_POS_412_77649a13_998	RP	POS	14.00	412.7765				7.32E-01	0.08	0.52	3.30E-01	0.19	0.73	4.86E-01	0.17	0.51	9.40E-01	-0.02	0.35	7984122	2201254	8132935	1880596	7948657	1834160	8317213	1926659
RP_NEG_375_13141a10_705	RP	NEG	10.71	375.1314				4.45E-03	0.51	1.29	3.30E-01	0.20	1.01	5.70E-03	0.61	1.28	3.19E-02	0.41	1.11	611554	78494	662289	102251	652267	87650	672311	115050
HILIC_NEG_100_9334a4_163	HILIC	NEG	4.163	100.9334				9.82E-02	0.36	1.03	3.30E-01	0.19	1.24	4.94E-02	0.46	1.03	2.75E-01	0.27	0.64	30886573	8241287	33636684	7316750	32919861	8025474	34353507	6534930
RP_POS_635_41174a10_704	RP	POS	10.70	635.4117				1.02E-01	-0.31	0.65	3.30E-01	0.20	0.58	3.33E-01	-0.21	0.41	5.33E-02	-0.41	0.76	3441277	731524	3186075	832084	3104628	794430	3267522	868447
HILIC_NEG_144_92345a6_105	HILIC	NEG	6.105	144.9235				3.11E-01	0.22	0.88	3.30E-01	0.19	0.78	1.76E-01	0.31	0.89	6.08E-01	0.12	0.64	33409287	11600986	35763732	10422230	34743913	11151485	36783550	9642843
RP_NEG_249_04369a0_928	HILIC	NEG	0.928	249.0437				1.10E-05	0.61	0.97	3.31E-01	-0.21	1.23	6.42E-03	0.50	0.86	4.52E-05	0.71	1.29	128933	128624	310565	324566	342313	307626	278817	340802
HILIC_NEG_115_0207a1_299	HILIC	NEG	1.299	115.0207				3.39E-08	0.87	1.53	3.31E-01	0.20	0.84	1.13E-06	0.97	1.57	2.13E-05	0.77	1.43	2376320	696803	3424191	1232072	3303689	1160807	3544693	1299951
RP_NEG_457_59796a15_583	RP	NEG	15.58	457.5980				1.35E-02	-0.49	0.97	3.31E-01	-0.19	0.65	7.50E-03	-0.59	1.00	7.63E-02	-0.40	0.86	953162	39982	932130	42305	936265	43732	927995	40848
RP_POS_217_10445a13_011	RP	POS	13.01	217.1045				2.00E-01	-0.25	0.44	3.31E-01	-0.20	0.59	1.11E-01	-0.35	0.61	4.93E-01	-0.15	0.64	3545696	959569	3287750	1042013	3389558	1060614	3185943	1023567
HILIC_POS_368_27975a0_643	HILIC	POS	0.643	368.2798				6.85E-01	-0.07	0.69	3.31E-01	-0.21	1.05	3.29E-01	-0.18	0.37	8.90E-01	0.03	0.44	4305974	2180921	4109357	2906060	4393538	3521941	3825175	2119868
RP_NEG_413_65027a15_582	RP	NEG	15.58	413.6503				1.43E-01	-0.32	0.63	3.31E-01	-0.19	0.66	7.79E-02	-0.42	0.78	3.49E-01	-0.23	0.54	902561	43816	889697	38364	893444	40836	885951	35741
RP_POS_457_34958a10_941	RP	POS	10.94	457.3496				7.61E-01	-0.06	0.48	3.32E-01	0.19	0.63	8.94E-01	0.03	0.21	4.85E-01	-0.16	0.58	37691034	6894199	37270225	6438854	36641673	6088736	37898777	6773832
HILIC_NEG_234_82024a5_49	HILIC	NEG	5.49	234.8202				7.77E-01	-0.06	0.19	3.32E-01	0.19	0.85	8.97E-01	0.03	0.20	5.17E-01	-0.16	0.25	995247	381658	973888	328162	941856	327313	1005920	329166
RP_POS_832_81879a0_472	RP	POS	0.47	832.8188				2.10E-09	-0.80	1.41	3.32E-01	0.21	1.17	8.57E-05	-0.70	1.42	3.46E-07	-0.91	1.58	374691	56000	253427	159968	237815	155947	269039	163967
RP_POS_300_20163a3_417	RP	POS	3.42	300.2016				5.33E-01	0.14	1.13	3.32E-01	-0.18	1.17	8.26E-01	0.05	0.98	3.62E-01	0.24	1.03	1272570	3157781	1656291	2486877	1899026	2779140	1413557	2156726
RP_POS_564_18536a2_724	RP	POS	2.72	564.1854				9.71E-01	0.01	0.64	3.32E-01	0.22	0.70	6.06E-01	0.11	0.75	4.59E-01	-0.10	0.31	2597582	621137	2603716	1276617	2478951	818071	2728482	1609893
RP_NEG_858_8031a0_492	RP	NEG	0.49	858.8031				1.92E-09	-0.76	1.40	3.32E-01	0.21	1.22	1.49E-04	-0.66	1.39	7.71E-07	-0.87	1.59	2042237	215060	1443516	843226	1361263	828123	1525768	858474
RP_NEG_207_10272a7_77	RP	NEG	7.77	207.1027				9.16E-02	-0.35	0.82	3.32E-01	0.19	0.64	2.52E-01	-0.25	0.49	6.04E-02	-0.45	0.99	3118403	139285	3069911	137602	3056491	149249	3083331	124949
RP_POS_561_81549a10_932	RP	POS	10.93	561.8155				1.81E-03	-0.69	1.38	3.32E-01	-0.18	1.05	9.53E-04	-0.78	1.41	1.20E-02	-0.60	1.29	401387	165319	293759	142931	307692	151100	279826	134344
RP_NEG_300_99033a7_983	RP	NEG	7.98	300.9903				1.21E-01	-0.32	0.70	3.32E-01	-0.19	0.61	6.35E-02	-0.42	0.71	3.37E-01	-0.22	0.58	2758449	164911	2705958	161695	2721712	172018	2690205	150755
RP_POS_261_14609a9_687	RP	POS	9.69	261.1461				7.05E-01	-0.06	0.92	3.33E-01	0.21	0.61	8.56E-01	0.04	0.55	2.68E-01	-0.17	0.96	1522653	731212	1457688	1119732	1348348	615085	1567027	1459609
HILIC_POS_336_05252a3_077	HILIC	POS	3.077	336.0525				3.40E-01	0.13	1.21	3.33E-01	-0.22	0.98	9.13E-01	0.02	1.22	1.85E-01	0.24	1.32	846890	51577	862979	140914	876705	143745	849253	138099
HILIC_NEG_393_664a1_364	HILIC	NEG	1.364	393.6640				5.17E-05	0.66	1.04	3.33E-01	-0.20	0.66	7.46E-03	0.56	0.89	1.94E-05	0.76	1.46	138553	57918	197377	92365	206377	76552	188377	105883
RP_POS_499_82706a4_05	RP	POS	4.05	499.8271				7.33E-01	-0.08	0.36	3.33E-01	0.18	0.65	9.66E-01	0.01	0.23	4.84E-01	-0.17	0.32	2389612	2254460	2240524	1742035	2070814	1502396	2410234	1953287
RP_NEG_519_40698a13_286	RP	NEG	13.29	519.4070				2.56E-01	-0.22	0.75	3.33E-01	0.20	0.60	6.03E-01	-0.12	0.60	1.21E-01	-0.32	0.67	9940443	3036539	9213031	3380984	8883735	2857407	9542326	3835274
RP_POS_383_16611a10_907	RP	POS	10.91	383.1661				1.93E-01	0.19	1.35	3.33E-01	0.22	0.93	1.31E-01	0.30	1.04	6.25E-01	0.08	1.11	269289	143151	320044	293637	291458	264133	348631	320579
RP_POS_585_33899a14_949	RP	POS	14.95	585.3390				6.29E-03	0.42	0.76	3.33E-01	0.21	0.59	1.64E-02	0.53	0.82	3.83E-02	0.32	0.72	1574142	354467	1822851	632141	1761267	444715	1884435	775789
RP_POS_392_7319a12_532	RP	POS	12.53	392.7319				5.76E-01	0.11	0.74	3.33E-01	0.20	0.58	3.68E-01	0.21	0.75	9.55E-01	0.01	0.15	1365859	606190	1436285	646190	1373401	572833	1499169	712346
RP_NEG_428_98193a7_73	RP	NEG	7.73	428.9819				6.37E-01	-0.10	0.33	3.34E-01	0.19	0.59	9.95E-01	0.00	0.61	4.17E-01	-0.19	0.36	3564715	399051	3526448	388647	3488683	429227	3564212	343554
RP_POS_357_27859a9_205	RP	POS	9.21	357.2786				3.23E-01	0.17	0.77	3.34E-01	0.21	0.61	2.35E-01	0.28	0.66	6.92E-01	0.07	0.80	321338	328986	394793	455274	350507	315010	439078	561734
HILIC_POS_616_41132a0_558	HILIC	POS	0.558	616.4113				1.88E-06	0.62	1.32	3.34E-01	-0.21	0.90	8.57E-04	0.51	1.48	2.04E-04	0.72	1.49	64024	227343	501257	778031	576846	870151	425668	673940
HILIC_NEG_134_89471a4_164	HILIC	NEG	4.164	134.8947				8.76E-01	0.03	0.47	3.34E-01	0.19	1.05	6.00E-01	0.13	0.59	7.91E-01	-0.06	0.10	15674454	8198277	15929230	7368484	15213953	6674571	16644507	8006444
RP_POS_369_19876a11_161	RP	POS	11.16	369.1988				7.03E-01	0.07	0.70	3.35E-01	0.20	0.81	4.43E-01	0.17	0.64	8.70E-01	-0.03	0.67	2024818	338334	2052856	423419	2011767	368973	2093945	471848
RP_NEG_473_40158a13_286	RP	NEG	13.29	473.4016				1.28E-01	-0.29	0.80	3.35E-01	0.20	0.60	3.97E-01	-0.19	0.65	5.86E-02	-0.39	0.78	8303750	2414554	7521820	2736230	7256319	2386443	7787321	3047578
HILIC_NEG_327_65942a1_363	HILIC	NEG	1.363	327.6594				5.24E-08	0.86	1.38	3.35E-01	-0.20	0.67	2.11E-04	0.76	1.22	3.03E-08	0.96	1.89	1038917	266597	1429415	459916	1474046	373520	1384784	532711
RP_POS_270_31525a9_493	RP	POS	9.49	270.3153				2.38E-02	-0.39	0.63	3.35E-01	0.20	0.81	1.45E-01	-0.29	0.55	1.66E-02	-0.50	0.86	4543385	139763	4470995	192972	4452281	196800	4489709	189185
RP_POS_816_58881a13_364	RP	POS	13.36	816.5888				5.75E-06	-1.06	1.92	3.35E-01	0.16	0.77	3.88E-05	-0.98	1.72	4.73E-06	-1.14	1.73	1724399	714124	1011929	560797	957543	596192	1066315	523379
RP_NEG_325_1853a13_304	RP	NEG	13.30	325.1853				8.25E-02	-0.37	0.85	3.35E-01	-0.19	0.79	4.43E-02	-0.46	0.99	2.45E-01	-0.27	0.76	3320122	1607737	2750150	1504858	2895997	1581560	2604303	1425015
RP_POS_276_22968a10_361	RP	POS	10.36	276.2297				9.01E-04	0.44	0.82	3.35E-01	0.22	0.80	1.50E-02	0.55	0.87	1.36E-03	0.34	1.19	4358031	1868580	6481515	5303065	5966096	2502410	6996934	7072108
RP_NEG_211_91734a14_271	RP	NEG	14.27	211.9173				4.70E-01	0.11	0.34	3.35E-01	0.22	0.60	3.50E-01	0.21	0.33	9.93E-01	0.00	0.22	3070320	342154	3137077	694526	3069600	363928	3204553	912601
HILIC_POS_421_25961a0_637	HILIC	POS	0.637	421.2596				3.33E-06	0.56	1.26	3.35E-01	-0.22	0.92	2.38E-03	0.45	1.41	4.26E-04	0.66	1.47	217463	495500	2876585	5339902	3394146	5919659	2359025	4692760
RP_NEG_371_15314a11_165	RP	NEG	11.17	371.1531				5.90E-02	0.37	0.96	3.35E-01	0.20	0.81	2.97E-02	0.47	1.04	2.25E-01	0.27	0.78	2159901	190959	2236239	207316	2216153	221021	2256325	192778
HILIC_POS_150_11253a2_738	HILIC	POS	2.738	150.1125				4.49E-01	0.09	0.39	3.35E-01	-0.22	0.59	1.49E-01	-0.02	0.62	3.89E-01	0.20	0.46	1098098	1223094	2406489	17068293	4068025	24133212	744954	743416
RP_NEG_484_79187a15_482	RP	NEG	15.48	484.7919				7.22E-01	0.08	0.29	3.35E-01	-0.19	0.72	9.42E-01	-0.02	0.51	4.91E-01	0.17	0.36	1066176	36179	1068741	32084	1071850	36189	1065632	27394
RP_POS_246_94275a15_334	RP	POS	15.33	246.9428				5.08E-01	-0.14	0.30	3.35E-01	-0.19	0.59	2.96E-01	-0.23	0.51	8.60E-01	-0.04	0.17	5323682	262283	5288404	253866	5312987	274104	5263820	232045
RP_POS_336_25073a8_177	RP	POS	8.18	336.2507				2.70E-01	-0.32	0.89	3.35E-01	-0.14	0.68	1.86E-01	-0.39	0.79	4.06E-01	-0.25	0.57	1383834	3565404	654282	1616159	810845	1864837	497719	1322727
RP_POS_940_81738a0_492	RP	POS	0.49	940.8174				1.74E-08	0.68	1.33	3.36E-01	-0.21	1.19	2.31E-04	0.57	1.33	2.30E-05	0.78	1.47	136366	88113	1687426	2523809	1931492	2711549	1443359	2322747
RP_POS_512_26837a10_18	RP	POS	10.18	512.2684				7.99E-01	0.05	0.64	3.36E-01	0.19	0.68	5.59E-01	0.15	0.96	8.32E-01	-0.04	0.18	500786	631030	533326	609927	474254	386223	592398	771572
HILIC_POS_358_20712a1_886	HILIC	POS	1.886	358.2071				8.56E-01	0.04	1.03	3.36E-01	-0.18	0.82	8.61E-01	-0.04	0.84	6.24E-01	0.13	1.02	1151390	3853231	1285586	2760679	1552593	3159680	1018578	2295466
RP_POS_305_15692a3_416	RP	POS	3.42	305.1569				5.06E-01	0.15	1.13	3.36E-01	-0.18	1.17	8.00E-01	0.06	0.98	3.42E-01	0.24	1.03	849850	2124908	1126792	1729185	1293943	1924938	959640	1509561
RP_POS_348_28711a10_813	RP	POS	10.81	348.2871				6.36E-16	1.11	1.93	3.37E-01	0.19	1.12	4.69E-11	1.20	2.09	1.16E-08	1.01	1.93	449351	209055	1060366	545344	1007694	549556	1113039	541475
RP_POS_239_16339a8_915	RP	POS	8.92	239.1634				3.77E-01	0.16	0.83	3.37E-01	-0.20	0.80	7.83E-01	0.06	0.73	2.11E-01	0.26	0.79	1436749	63126	1448999	80868	1456807	80169	1441191	81617

Supplementary table 1: Metabolomics results (in asceding order according to p-value from progressive ALD vs non-progressive ALD comparison, with molecular features with ID_level of 1-2 first)

							all_ALD_vs_control			Prog_ALD_vs_non-prog_ALD			Prog_ALD_vs_control_ALD			Non-prog_ALD_vs_control			Healthy_control		all_ALD		Non-prog_ALD		Progressive_ALD	
							t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA								
Feature_ID	RP_HILIC	POS_NEG	Average.Rt	Average.Mz	Metabolite.name	curated_MSMS	ID_level	p	d	VIP	p	d	VIP	p	d	VIP	p	d	VIP	Mean	SD	Mean	SD	Mean	SD	Mean	SD
HILIC_POS_188_07077a4_123	HILIC	POS	4.123	188.0708				1.44E-02	-0.42	1.08	3.37E-01	-0.20	1.38	1.33E-02	-0.52	1.04	9.56E-02	-0.32	0.94	26792506	6022675	23374865	8520295	24197467	7848557	22552262	9148311
HILIC_POS_604_35382a0_624	HILIC	POS	0.624	604.3538				3.88E-06	0.56	1.26	3.37E-01	-0.21	0.94	2.19E-03	0.45	1.43	4.39E-04	0.67	1.44	196267	567447	2054840	3692037	2411123	4109836	1698557	3223455
HILIC_NEG_329_65723a1_363	HILIC	NEG	1.363	329.6572				5.90E-08	0.86	1.38	3.37E-01	-0.20	0.67	2.16E-04	0.76	1.22	3.57E-08	0.96	1.88	3243892	843056	4471389	1449083	4611248	1181190	4331531	1675533
RP_POS_283_17505a3_416	RP	POS	3.42	283.1751				5.47E-01	0.14	1.13	3.37E-01	-0.18	1.17	8.37E-01	0.05	0.98	3.74E-01	0.23	1.03	873987	2181736	1130273	1714320	1295628	1910406	964917	1494093
RP_POS_441_29712a10_979	RP	POS	10.98	441.2971				1.80E-01	0.26	1.19	3.37E-01	0.20	0.96	1.06E-01	0.36	1.06	4.48E-01	0.17	1.10	5749136	1046442	6043449	1131027	5934390	1113011	6152507	1149559
RP_NEG_910_81549a0_492	RP	NEG	0.49	910.8155				2.46E-03	0.40	1.05	3.38E-01	0.21	1.22	8.00E-03	0.51	1.13	6.35E-02	0.29	1.12	623598	231093	870404	686604	804208	612097	936601	754231
HILIC_NEG_266_94656a4_723	HILIC	NEG	4.723	266.9466				2.98E-04	0.61	1.02	3.38E-01	0.20	1.02	1.01E-03	0.71	1.09	4.39E-03	0.51	1.00	880323	314143	1154929	466349	1109974	389318	1199884	532642
RP_POS_784_58264a14_255	RP	POS	14.26	784.5826				4.16E-02	0.38	0.72	3.38E-01	0.20	0.60	2.72E-02	0.47	0.86	1.83E-01	0.28	0.53	976841	734213	1306169	907876	1218698	882013	1393640	933670
RP_POS_912_76477a0_496	RP	POS	0.50	912.7648				4.40E-10	-0.77	1.41	3.38E-01	0.21	1.21	6.87E-05	-0.66	1.45	1.09E-06	-0.87	1.58	1441379	95038	1023037	588792	966314	598024	1079759	579852
RP_POS_388_26947a10_24	RP	POS	10.24	388.2695				1.30E-06	0.57	1.14	3.38E-01	-0.21	1.05	3.07E-03	0.47	1.09	1.39E-04	0.68	1.34	14234	10316	244928	447261	287981	468060	201876	425798
RP_NEG_466_81677a15_466	RP	NEG	15.47	466.8168				1.91E-01	0.25	0.96	3.38E-01	-0.20	0.67	4.86E-01	0.15	0.46	1.09E-01	0.35	0.86	3349992	83279	3373248	95976	3382485	96170	3364011	95854
RP_POS_261_1308a3_194	RP	POS	3.19	261.1308				4.23E-02	0.32	1.11	3.38E-01	-0.21	1.13	2.21E-01	0.21	1.12	4.20E-02	0.42	1.12	519602	556322	805657	981998	900196	1099660	711119	849016
RP_POS_499_12787a10_7	RP	POS	10.70	499.1279				3.46E-01	0.21	0.68	3.38E-01	-0.19	0.83	6.31E-01	0.11	0.47	2.17E-01	0.30	0.68	759582	198253	796926	175563	813823	182199	780029	168804
RP_POS_432_2804a4_635	RP	POS	4.64	432.2804				8.82E-01	0.04	1.18	3.39E-01	-0.16	1.18	8.93E-01	-0.04	0.92	6.83E-01	0.12	1.03	2095189	6498818	2274467	3603006	2621146	4017775	1927787	3136948
RP_NEG_458_1452a11_604	RP	NEG	11.60	458.1452				1.88E-01	-0.26	0.90	3.39E-01	0.19	0.74	4.36E-01	-0.16	0.70	1.26E-01	-0.36	0.81	570461	68824	551540	73218	544496	81551	558584	63871
HILIC_NEG_158_8468a2_961	HILIC	NEG	2.961	158.8468				3.37E-03	0.48	0.92	3.39E-01	-0.20	0.61	1.76E-02	0.38	0.91	1.02E-02	0.58	0.87	2114957	451000	2437128	709811	2505460	884104	2368796	476212
RP_NEG_362_9422a15_284	RP	NEG	15.28	362.9422				7.76E-01	-0.06	0.54	3.39E-01	-0.19	0.68	4.84E-01	-0.15	0.44	8.68E-01	0.04	0.41	2236432	115073	2229741	116223	2240912	124630	2218569	107258
RP_POS_492_21271a11_804	RP	POS	11.80	492.2127				1.24E-02	-0.49	1.20	3.39E-01	0.19	1.31	1.07E-01	-0.39	0.79	2.59E-03	-0.58	1.41	865896	411292	643924	458627	599775	298261	688072	576223
RP_POS_419_73749a12_695	RP	POS	12.70	419.7375				1.83E-02	0.49	0.95	3.39E-01	-0.19	0.70	9.15E-02	0.39	0.83	8.98E-03	0.58	0.99	1040611	560830	1317691	556926	1371185	508814	1264196	601608
RP_POS_546_45386a14_267	RP	POS	14.27	546.4539				9.52E-01	-0.01	0.10	3.40E-01	0.19	0.67	7.08E-01	0.08	0.23	6.63E-01	-0.11	0.27	8845072	1684714	8824738	1580311	8672943	1821904	8976532	1295908
RP_POS_708_51147a13_57	RP	POS	13.57	708.5115				6.19E-01	0.09	0.57	3.40E-01	0.20	0.75	3.65E-01	0.19	0.49	9.76E-01	-0.01	0.49	15397712	976833	15501536	1156716	15390502	1181554	15612571	1132281
RP_POS_318_96899a0_538	RP	POS	0.54	318.9690				1.66E-01	0.20	1.03	3.40E-01	-0.21	1.02	5.63E-01	0.10	0.80	1.19E-01	0.31	1.21	901786	311940	1018695	631787	1079337	693707	958054	563669
RP_POS_413_2868a10_591	RP	POS	10.59	413.2868				2.05E-02	-0.51	1.27	3.40E-01	0.18	0.72	8.77E-02	-0.42	0.89	9.70E-03	-0.60	1.25	801094	133291	737979	117618	726690	103721	749267	130124
RP_NEG_243_82039a0_769	RP	NEG	0.77	243.8204				2.65E-08	0.90	1.42	3.40E-01	-0.19	0.65	7.22E-05	0.81	1.27	3.23E-08	1.00	1.80	2638166	1808750	5300353	2950159	5583510	2534711	5017195	3316037
RP_POS_404_7883a13_996	RP	POS	14.00	404.7883				1.80E-01	-0.30	0.56	3.40E-01	0.18	0.90	4.09E-01	-0.21	0.50	9.57E-02	-0.39	0.68	2998319	924680	2750625	797363	2674120	700530	2827129	884230
HILIC_POS_648_37988a0_625	HILIC	POS	0.625	648.3799				6.64E-06	0.55	1.27	3.40E-01	-0.21	0.94	2.99E-03	0.45	1.43	5.01E-04	0.66	1.44	216672	597348	1816356	3221992	2125255	3563507	1507456	2842711
RP_POS_840_77875a11_247	RP	POS	11.25	840.7788				2.61E-02	0.36	1.30	3.40E-01	-0.21	0.94	1.93E-01	0.26	0.91	1.44E-02	0.47	1.42	407869	201493	515785	316548	546126	298871	485445	333537
HILIC_POS_293_09729a7_328	HILIC	POS	7.328	293.0973				7.36E-01	-0.07	0.44	3.41E-01	-0.19	0.71	4.45E-01	-0.17	0.31	9.20E-01	0.02	0.63	1253348	169252	1241816	162422	1257388	188492	1226245	131439
HILIC_POS_224_12793a5_92	HILIC	POS	5.92	224.1279				1.88E-01	-0.24	0.84	3.41E-01	0.20	0.75	5.01E-01	-0.15	0.67	1.01E-01	-0.34	0.86	6085658	1207008	5741688	1457172	5602277	1395333	5881100	1517702
HILIC_POS_338_04959a3_077	HILIC	POS	3.077	338.0496				5.12E-01	0.09	1.25	3.41E-01	-0.22	1.00	9.08E-01	-0.02	1.29	2.73E-01	0.20	1.36	1650713	99334	1672165	275152	1698488	279438	1645843	271041
HILIC_POS_465_28586a0_645	HILIC	POS	0.645	465.2859				1.53E-06	0.59	1.29	3.41E-01	-0.21	0.93	1.37E-03	0.48	1.47	2.58E-04	0.69	1.48	181331	548544	1978690	3405720	2304553	3766781	1652826	3004865
RP_POS_329_00464a8_121	RP	POS	8.12	329.0046				4.07E-01	-0.18	0.44	3.41E-01	0.19	0.99	7.19E-01	-0.08	0.36	2.57E-01	-0.27	0.63	2610845	556389	2517955	514887	2468702	536504	2567209	492787
RP_NEG_231_93253a13_214	RP	NEG	13.21	231.9325				5.52E-01	0.10	0.58	3.41E-01	-0.20	0.68	9.98E-01	0.00	0.60	2.83E-01	0.20	0.64	4997471	569758	5074874	812811	5152621	723082	4997127	894216
RP_POS_207_11032a2_819	RP	POS	2.82	207.1103				1.23E-02	0.43	0.71	3.42E-01	0.20	0.59	1.83E-02	0.53	0.94	5.85E-02	0.33	0.97	855318	377594	1074305	530754	1023518	399142	1125093	636058
RP_POS_344_22794a4_023	RP	POS	4.02	344.2279				9.43E-01	-0.02	1.13	3.42E-01	-0.14	1.16	7.52E-01	-0.09	0.88	8.65E-01	0.05	0.94	2393705	7272461	2297301	3510994	2633049	3924846	1961554	3044875
RP_POS_144_94791a15_379	RP	POS	15.38	144.9479				8.65E-01	-0.02	0.36	3.42E-01	0.21	0.64	4.78E-01	0.08	0.50	5.65E-01	-0.13	0.33	9936004	248222	9923819	567721	9869434	752620	9978203	280568
HILIC_NEG_199_97797a1_299	HILIC	NEG	1.299	199.9780				9.89E-04	0.64	1.12	3.42E-01	0.19	1.21	1.20E-03	0.74	1.15	7.90E-03	0.55	1.05	670042	201956	816366	223999	794977	200617	837754	245345
RP_POS_298_64755a10_621	RP	POS	10.62	298.6476				3.01E-02	0.50	1.32	3.43E-01	-0.18	0.84	1.03E-01	0.41	0.99	1.54E-02	0.59	1.36	2231465	500185	2449259	404984	2487906	363722	2410612	442753
RP_NEG_369_17462a10_264	RP	NEG	10.26	369.1746				5.62E-01	-0.10	0.30	3.43E-01	-0.21	0.63	2.07E-01	-0.20	0.48	9.73E-01	0.01	0.34	37525595	41165307	31901289	63701153	37989775	80917285	25812804	39689135
RP_POS_199_13039a13_111	RP	POS	13.11	199.1304				3.20E-01	0.20	0.61	3.43E-01	0.19	0.63	1.97E-01	0.29	0.62	6.46E-01	0.10	0.51	16411721	1887142	16803827	2030290	16610204	1919960	16997450	2136709
RP_POS_385_16687a10_907	RP	POS	10.91	385.1669				2.80E-02	0.31	1.45	3.43E-01	0.21	0.88	3.54E-02	0.42	1.15	1.99E-01	0.21	1.26	2702308	1095272	3391866	2418902	3161135	2095077	3622596	2706214
HILIC_POS_72_08161a1_413	HILIC	POS	1.413	72.0816				6.66E-01	-0.09	0.53	3.43E-01	-0.19	0.76	3.95E-01	-0.18	0.40	9.73E-01	0.01	0.12	4748363	2121062	4560781	2144282	4765278	2395925	4356284	1861163
RP_NEG_652_29156a10_62	RP	NEG	10.62	652.2916				2.49E-02	0.52	1.20	3.43E-01	-0.17	0.88	8.89E-02	0.43	0.93	1.22E-02	0.61	1.26	2139649	421652	2329188	332979	2360927	288984	2297448	372083
RP_POS_144_08063a2_893	RP	POS	2.89	144.0806				3.63E-04	-0.61	1.24	3.43E-01	-0.20	1.07	1.13E-03	-0.71	1.29	4.96E-03	-0.51	1.17	1798409	281614	1557180	412342	1596483	345526	1517877	470087
RP_POS_349_18307a4_023	RP	POS	4.02	349.1831				9.56E-01	-0.02	1.13	3.43E-01	-0.14	1.17	7.63E-01	-0.09	0.89	8.51E-01	0.06	0.94	1158872	3632450	1122089	1775508	1291235	1978326	952944	1548233
RP_POS_280_26349a9_535	RP	POS	9.54	280.2635				3.00E-01	-0.26	0.77	3.43E-01	-0.17	0.75	1.74E-01	-0.34	0.79	5.23E-01	-0.18	0.44	18839932	26869384	13519613	17704912	15207792	21714695	11831435	12489230
RP_POS_395_17786a6_811	RP	POS	6.81	395.1779				3.06E-03	-0.44	0.99	3.44E-01	0.21	0.93	7.12E-02	-0.34	0.80	3.08E-03	-0.55	1.20	1455194	70202	1398791	138544	1385600	135032	1411983	142099
HILIC_NEG_215_03293a4_979	HILIC	NEG	4.979	215.0329				4.42E-01	0.13	0.57	3.44E-01	0.21	0.71	2.99E-01	0.23	0.41	8.82E-01	0.03	0.62	13244423	7673216	14621422	11566480	13519454	8871889	15723391	13751675
RP_POS_311_18518a8_277	RP	POS	8.28	311.1852				2.18E-01	-0.29	0.55	3.44E-01	-0.18	0.62	1.19E-01	-0.38	0.65	4.44E-01	-0.20	0.45	877940	114163	850355	89136	858841	101931	841869	74269
HILIC_POS_147_11279a7_097	HILIC	POS	7.097	147.1128				1.97E-02	0.31	1.00	3.44E-01	-0.21	0.88	2.28E-01	0.20	1.06	2.39E-02	0.41	1.07	14267022	5462863	18771378	16452010	20337036	17246561	17205720	15633767
HILIC_NEG_173_92601a5_428	HILIC	NEG	5.428	173.9260				7.20E-01	0.09	0.37	3.45E-01	-0.17	0.92	9.94E-01	0.00	0.15	4.93E-01	0.17	0.37	910305	214060	925119	159248	940254	149755	909984	168354
HILIC_NEG_101_02424a1_261	HILIC	NEG	1.261	101.0242				6.76E-01	-0.07	0.37	3.45E-01	0.20	1.28	8.89E-01	0.03	0.32	3.06E-01	-0.17	0.78	396942	243659	373441	358892	339302	252397	407579	440629
RP_POS_499_82724a5_744	RP	POS	5.74	499.8272				3.24E-01	0.19	0.82	3.45E-01	0.20	0.89	2.21E-01	0.29	0.45	6.47E-01	0.09	0.53	1343048	1942658	1749448	2212086	1539181	1783699	1959716	2571906
RP_POS_504_30881a10_416	RP	POS	10.42	504.3088				1.53E-05	0.73	1.35	3.45E-01	-0.19	0.59	2.62E-03	0.63	1.18	8.28E-06	0.82	1.54	629460	245854	892653	370774	927877	317053	857430	417969
HILIC_NEG_144_92343a0_546	HILIC	NEG	0.546	144.9234				2.01E-03	-0.53	1.08	3.46E-01	0.20	0.80	6.48E-02	-0.43	0.62	1.63E-04	-0.63	1.50	7976709	1181274	7110499	1724025	6946738	1049181	7274261	2202197
RP_POS_1002_79565a0_489	RP	POS	0.49	1002.7957				3.13E-08	0.67	1.31	3.46E-01	-0.21	1.15	3.58E-04	0.56	1.31	2.40E-05	0.77	1.48	100836	29160	283580	301150	312122	318919	255038	282598
RP_POS_239_16414a9_687	RP	POS	9.69	239.1641				7.39E-01	-0.05	0.93	3.46E-01	0.21	0.59	8.37E-01	0.05	0.56	2.98E-01	-0.16	0.98	5916523	2889268	5688946	4507735	5260925	2548486	6116966	5846826
HILIC_POS_59_06129a4_279	HILIC	POS	4.279	59.0613				1.77E-02	-0.41	0.68	3.46E-01	0.20	0.77	1.18E-01	-0.31	0.75	1.46E-02	-0.51	0.82	3577961	440521	3334247	634885	3274131	661128	3394364	608210
HILIC_POS_195_11279a0_525	HILIC	POS	0.525	195.1128				1.59E-01	0.24	0.73	3.46E-01	-0.20	0.78	5.25E-01	0.14	0.30	5.80E-02	0.34	0.91	289874	128992	331555	183555	348943	144934	314167	215522
RP_POS_707_49231a10_656	RP	POS	10.66	707.4923				7.41E-01	0.06	0.44	3.46E-01	0.19	0.55	4.58E-01	0.16	0.44	8.87E-01	-0.03	0.26	7801772	587954	7842320	639215	7781812	663698	7902827	614461
RP_POS_325_21387a10_423	RP	POS	10.42	325.2139				6.57E-01	0.07	0.39	3.47E-01	-0.21	0.74	8.44E-01	-0.03	0.26	4.23E-01	0.17	0.51	2350974	3616247	2743473	6062134	3317654	7190184	2169292	4677323
HILIC_NEG_333_6528a1_364	HILIC	NEG	1.364	333.6528				1.27E-07	0.84	1.34	3.47E-01	-0.19	0.67	3.16E-04	0.75	1.19	7.00E-08	0.94	1.85	1704784	450149	2338569	766824	2411156	622758	2265982	888516
HILIC_POS_534_29486a1_319	HILIC	POS	1.319	534.2949				1.11E-06	0.81	1.29	3.47E-01	-0.19	0.72	8.94E-04	0.72	1.08	1.94E-07	0.91	2.00	4110254	421389	4629690	645522	4690799	481035	4568581	776457
RP_NEG_1036_75708a0_493	RP	NEG	0.49	1036.7571				1.05E-02	-0.44	0.81	3.47E-01	0.20	1.13	1.12E-01	-0.34	0.75	4.29E-03	-0.54	1.17	938065	114611	869751	163537	854280	141202	885223	183325
RP_NEG_245_00291a7_878	RP	NEG	7.88	245.0029				8.72E-01	-0.03	0.72	3.47E-01	-0.19	0.63	5.66E-01	-0.13	0.26	7.69E-01	0.06	0.75	1782739	180236	1776700	194283	1795069	191772	1758331	196968
RP_POS_542_37183a14_267	RP	POS	14.27	542.3718				4.34E-01	0.11	0.43	3.47E-01	0.21	0.61	3.26E-01	0.21	0.49	9.84E-01	0.00	0.33	11582253	1610416	11962139	3919897	11591090	2462790	12333187	4969755
HILIC_POS_308_18564a0_952	HILIC	POS	0.952	308.1856				4.82E-01	0.09	0.57	3.47E-01	-0.21	0.71	8.78E-01	-0.01	0.31	3.84E-01	0.20	0.48	420597	1022977	667099	2987975	950392	4078919	383807	1112129
HILIC_NEG_158_93893a5_428	HILIC	NEG	5.428	158.9389				3.26E-02	0.38	1.03	3.48E-01	0.20	0.64	3.07E-02	0.48	1.05	1.39E-01	0.28	0.82	1052471	77759	1089951	103218	1080205	87975	1099697	116585
HILIC_POS_159_14922a1_89	HILIC	POS	1.89	159.1492				2.85E-04	0.49	0.93	3.48E-01	-0.21	0.85	1.85E-02	0.38	0.82	1.89E-03	0.59	1.20	477780	792147	1454963	2212976	1663756	2391276	1246169	2021707
RP_NEG_259_00073a7_439	RP	NEG	7.44	259.0007				5.26E-02	-0.40	0.74	3.48E-01	-0.19	0.82	3.74E-02	-0.49	0.76	1.62E-01	-0.31	0.91	2587834	347826	2447851	346677	2480542	313687	2415160	377150
HILIC_NEG_348_99936a7_428	HILIC	NEG	7.428	348.9994				7.50E-04	-0.50	1.24	3.48E-01	0.20	0.92	2.70E-02	-0.40	1.28	1.70E-03	-0.60	1.37	1350066	55283	1298296	112767	1287664	116548	1308928	108986
RP_POS_327_19333a10_423	RP	POS	10.42	327.1933				9.77E-01	0.01	0.42	3.49E-01	-0.19	0.59	6.98E-01	-0.09	0.41	6.87E-01	0.10	0.38	3487950	1870837	3498847	1732044	3662158	1955666	3335536	1477199
HILIC_NEG_157_90067a2_172	HILIC	NEG	2.172	157.9007				4.43E-01	0.15	0.60	3.49E-01	-0.19	0.68	8.05E-01	0.06	0.12	2.62E-01	0.25	0.56	2734750	681036	2843520	732588	2912553	715468	2774487	750135
RP_NEG_173_98596a0_708	RP	NEG	0.71	173.9860				4.16E-01	-0.21	0.58	3.49E-01	0.16	0.60	6.45E-01	-0.13	0.52	2.65E-01	-0.29	0.58	1153194	2611992	750421	1622826	597346	1192254	903495	1962545
HILIC_POS_284_1644a0_537	HILIC	POS	0.537	284.1644				7.29E-01	0.04	0.64	3.49E-01	0.22	1.17	5.10E-01	0.15	0.21	3.75E-01	-0.06	0.31	717727	77309	729351	305968	700417	97507	758285	421813
RP_POS_418_20691a4_223	RP	POS	4.22	418.2069				8.52E-01	-0.04	0.84	3.49E-01	0.18	0.91	8.43E-01	0.05	0.56	6.00E-01	-0.13	0.60	861324	529401	841924	437407	800730	472991	883117	399212
RP_POS_434_26779a11_609	RP	POS	11.61	434.2678				2.39E-03	-0.54	1.08	3.49E-01	0.19	0.92	2.13E-02	-0.45	1.01	3.22E-03	-0.64	1.13	7896847	614100	7470254	805667	7394446	881837	7546061	722551
RP_POS_722_52661a13_921	RP	POS	13.92	722.5266				6.00E-01	0.11	0.71	3.50E-01	-0.19	0.72	9.61E-01	0.01	0.22	3.91E-01	0.20	0.83	3636690	1772841	3827919	1827229	3999809	1987420	3656030	1653945
RP_POS_441_29764a10_448	RP	POS	10.45	441.2976				1.36E-01	0.28	0.53	3.50E-01	0.19	0.55	8.93E-02	0.38	0.67	3.69E-01	0.19	0.54	1010321	474902	1162282	551944	1110414	511196	1214150	590500
RP_POS_378_24072a9_634	RP	POS	9.63	378.2407				3.36E-01	0.18	0.81	3.51E-01	-0.20	0.84	7.16E-01	0.08	0.60	1.68E-01	0.28	0.57	598657	243469	649083	291122	676414	250655	621752	326927
RP_POS_654_32996a10_563	RP	POS	10.56	654.3300				1.48E-04	-0.70	1.14	3.51E-01	0.19	0.70	8.50E-03	-0.60	0.96	2.60E-05	-0.79	1.48	645823	73195	581728	92532	573035	66638	590422	112713
RP_POS_437_23547a4_635	RP	POS	4.64	437.2355				9.22E-01	0.03	1.17	3.51E-01	-0.15	1.18	8.69E-01	-0.05	0.91	7.31E-01	0.10	1.01	1090951	3540832	1154949	1860456	1329483	2062839	980414	1635774
HILIC_POS_171_18561a5_337	HILIC	POS	5.337	171.1856				9.24E-01	-0.02	0.61	3.51E-01	-0.20	0.81	5.69E-01	-0.12	0.53	6.85E-01	0.08	0.30	124689065	30988225	124026764	42499357	128008197	42740563	120045331	42310111
RP_POS_564_18542a3_001	RP	POS	3.00	564.1854				3.87E-01	0.11	0.37	3.52E-01	0.21	0.73	3.11E-01	0.22	0.65	9.46E-01	0.01	0.85	1804749	261162	1883373	779811	1810189	467815	1956556	999420
HILIC_POS_350_01508a7_373	HILIC	POS	7.373	350.0151				4.45E-02	0.34	0.74	3.52E-01	-0.20	0.56	1.75E-01	0.24	0.49	4.47E-02	0.44	0.75	14093749	1244262	14672930	1786348	14840322	2069157	14505537	1452103
RP_NEG_279_03925a0_71	RP	NEG	0.71	279.0393				8.06E-01	0.03	0.76	3.52E-01	-0.21	0.80	6.14E-01	-0.07	0.87	4.98E-01	0.14	0.68	1963262	425043	1996741	1134731	2103094	1350109	1890387	869269
RP_NEG_357_89819a15_4	RP	NEG	15.40	357.8982				5.50E-01	0.11	0.40	3.52E-01	-0.19	0.56	9.33E-01	0.02	0.32	3.44E-01	0.21	0.70	840949	33136	845143	37812	848683	39764	841602	35805
RP_POS_688_51788a10_457	RP	POS	10.46	688.5179				2.47E-01	-0.23	0.45	3.52E-01	-0.19	1.18	1.37E-01	-0.32	0.59	5.59E-01	-0.13	0.38	1951993	396841	1855395	434633	1896090	455814	1814700	412942

Supplementary table 1: Metabolomics results (in asceding order according to p-value from progressive ALD vs non-progressive ALD comparison, with molecular features with ID_level of 1-2 first)

							all_ALD_vs_control			Prog_ALD_vs_non-prog_ALD			Prog_ALD_vs_control_ALD			Non-prog_ALD_vs_control			Healthy_control		all_ALD		Non-prog_ALD		Progressive_ALD	
							t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA								
Feature_ID	RP_HILIC	POS_NEG	Average.Rt	Average.Mz	Metabolite.name	curated_MSMS	ID_level	p	d	VIP	p	d	VIP	p	d	VIP	p	d	VIP	Mean	SD	Mean	SD	Mean	SD	Mean	SD
RP_POS_283_1752a10_66	RP	POS	10.66	283.1752				6.71E-01	-0.10	0.32	3.52E-01	0.17	0.56	9.56E-01	-0.01	0.27	4.62E-01	-0.19	0.33	1216117	425769	1181041	322707	1150836	323709	1211245	322111
RP_POS_415_25375a4_635	RP	POS	4.64	415.2538				9.63E-01	0.01	1.17	3.52E-01	-0.15	1.17	8.35E-01	-0.06	0.91	7.73E-01	0.09	1.00	713349	2364871	733441	1207712	846430	1339539	620451	1061359
RP_NEG_241_82358a0_769	RP	NEG	0.77	241.8236				2.33E-08	0.91	1.43	3.52E-01	-0.19	0.64	6.70E-05	0.81	1.27	3.07E-08	1.00	1.81	3766699	2543991	7538179	4176664	7928941	3583711	7147417	4700048
RP_POS_321_21899a11_252	RP	POS	11.25	321.2190				3.62E-03	0.49	1.37	3.53E-01	0.20	0.87	5.70E-03	0.59	1.28	3.38E-02	0.39	1.31	975896	307158	1189403	460156	1146386	404945	1232419	509953
HILIC_POS_220_11758a1_026	HILIC	POS	1.026	220.1176				8.73E-05	0.57	1.04	3.53E-01	0.20	0.79	5.75E-04	0.67	1.16	6.75E-03	0.46	0.93	341051	96788	451642	211198	431903	196362	471381	225313
RP_POS_560_32739a5_008	RP	POS	5.01	560.3274				1.11E-06	0.58	1.27	3.53E-01	-0.21	1.21	1.11E-03	0.48	1.37	3.06E-04	0.68	1.36	41174	88098	1020440	1880823	1196105	2099227	844775	1636292
RP_NEG_312_85175a15_493	RP	NEG	15.49	312.8518				7.45E-01	0.08	0.73	3.53E-01	-0.16	0.55	9.99E-01	0.00	0.32	5.46E-01	0.16	0.68	3177622	146334	3186696	97670	3195816	106438	3177576	88175
HILIC_NEG_173_92616a0_918	HILIC	NEG	0.918	173.9262				3.00E-07	-1.05	1.76	3.53E-01	-0.17	1.13	8.21E-07	-1.14	1.79	4.00E-06	-0.97	1.80	1132842	359366	703044	367462	737349	319867	668740	409995
HILIC_POS_615_74255a0_558	HILIC	POS	0.558	615.7426				7.07E-07	0.60	1.32	3.53E-01	-0.21	0.88	6.83E-04	0.50	1.52	2.26E-04	0.71	1.52	91643	202518	824036	1346057	949683	1508973	698389	1162541
RP_POS_204_9791a1_46	RP	POS	1.46	204.9791				2.67E-11	0.89	1.48	3.53E-01	0.19	0.59	1.74E-07	0.99	1.71	1.81E-06	0.80	1.46	742842	696435	2454327	1996461	2268034	1870348	2640620	2117552
RP_NEG_136_90892a15_534	RP	NEG	15.53	136.9089				1.21E-01	-0.29	0.60	3.54E-01	0.19	0.55	3.64E-01	-0.19	0.41	7.40E-02	-0.38	0.73	1996624	346646	1879904	420824	1840658	427502	1919150	414606
RP_NEG_327_82883a15_602	RP	NEG	15.60	327.8288				7.00E-02	-0.36	0.67	3.54E-01	0.19	0.60	2.25E-01	-0.27	0.64	4.20E-02	-0.46	0.90	736640	29333	725523	30486	722680	30383	728365	30630
RP_POS_586_4201a11_625	RP	POS	11.63	586.4201				1.15E-06	-1.21	1.94	3.54E-01	-0.14	0.72	5.95E-07	-1.28	1.95	6.88E-06	-1.14	1.73	395307	190258	189553	127941	201479	134841	177626	120828
RP_POS_271_2056a8_793	RP	POS	8.79	271.2056				2.21E-01	0.23	0.88	3.54E-01	0.19	0.72	1.48E-01	0.32	0.69	5.18E-01	0.13	0.49	644003	834388	865002	1011132	770739	901829	959266	1110950
HILIC_POS_258_16983a1_179	HILIC	POS	1.179	258.1698				9.91E-03	0.44	0.87	3.54E-01	0.20	1.00	1.24E-02	0.54	1.06	6.57E-02	0.34	0.65	470625	236110	613578	343226	581587	299150	645570	382666
RP_POS_821_37671a7_55	RP	POS	7.55	821.3767				8.61E-01	0.04	0.76	3.55E-01	0.18	0.76	5.87E-01	0.13	0.68	8.28E-01	-0.05	0.78	4111118	304763	4121736	270006	4096608	276805	4146864	263409
HILIC_NEG_155_95197a1_3	HILIC	NEG	1.3	155.9520				6.36E-07	0.88	1.37	3.55E-01	0.18	0.94	2.11E-06	0.97	1.59	6.70E-05	0.79	1.36	1516015	280105	1857910	381095	1822452	376749	1893367	385908
HILIC_POS_560_32776a0_623	HILIC	POS	0.623	560.3278				2.51E-06	0.57	1.25	3.55E-01	-0.21	0.93	1.74E-03	0.46	1.43	3.78E-04	0.67	1.42	123817	410676	1663566	3013297	1943701	3341593	1383430	2649307
RP_POS_672_52209a10_874	RP	POS	10.87	672.5221				3.96E-02	-0.41	0.79	3.56E-01	-0.19	1.05	2.36E-02	-0.50	0.87	1.58E-01	-0.31	0.89	2497813	350060	2344918	379132	2380133	386046	2309703	372631
HILIC_POS_443_27264a0_64	HILIC	POS	0.64	443.2726				1.43E-06	0.59	1.29	3.56E-01	-0.21	0.92	1.27E-03	0.48	1.48	2.55E-04	0.69	1.47	233349	792506	2771209	4786529	3215880	5282794	2326538	4240027
RP_NEG_269_87726a15_537	RP	NEG	15.54	269.8773				7.71E-02	-0.37	0.69	3.56E-01	-0.18	0.65	4.83E-02	-0.46	0.75	2.21E-01	-0.28	0.55	724025	31635	712534	30467	715364	29844	709704	31119
RP_POS_295_927a15_508	RP	POS	15.51	295.9270				2.12E-01	0.24	0.67	3.56E-01	-0.19	0.57	5.13E-01	0.14	0.30	1.19E-01	0.34	0.67	30503925	2699607	31219095	3057346	31502959	2937066	30935231	3177214
RP_POS_237_22136a9_676	RP	POS	9.68	237.2214				1.57E-03	0.54	1.13	3.56E-01	0.19	0.74	2.84E-03	0.64	1.16	1.72E-02	0.44	1.20	1147946	142031	1254156	204395	1235181	180506	1273132	226031
RP_POS_548_50385a14_506	RP	POS	14.51	548.5039				9.63E-02	-0.30	0.59	3.56E-01	0.19	0.91	3.27E-01	-0.21	0.41	5.70E-02	-0.40	0.78	11455996	2027344	10711833	2569768	10473397	2550240	10950269	2592765
RP_NEG_146_93753a15_49	RP	NEG	15.49	146.9375				7.28E-01	-0.07	0.40	3.56E-01	-0.18	0.60	4.60E-01	-0.16	0.36	9.33E-01	0.02	0.22	19249309	408198	19220512	396426	19257299	432220	19183726	357686
RP_POS_393_20914a4_35	RP	POS	4.35	393.2091				8.56E-01	-0.05	1.16	3.56E-01	-0.13	1.16	6.95E-01	-0.12	0.88	9.73E-01	0.01	0.96	1362662	4510098	1212557	1935835	1392198	2141211	1032917	1709019
RP_POS_478_3891a11_092	RP	POS	11.09	478.3891				5.12E-01	-0.15	0.38	3.56E-01	-0.18	0.63	3.13E-01	-0.24	0.49	8.16E-01	-0.06	0.36	2546981	1402013	2366035	1165385	2474195	1331757	2257875	972886
RP_POS_569_43256a12_896	RP	POS	12.90	569.4326				1.53E-01	0.26	0.53	3.56E-01	-0.19	0.80	4.41E-01	0.16	0.36	8.98E-02	0.35	0.75	2784842	1131680	3142339	1454878	3277274	1451447	3007405	1460370
RP_NEG_328_88159a15_384	RP	NEG	15.38	328.8816				8.16E-01	0.05	0.77	3.57E-01	-0.19	0.58	8.28E-01	-0.05	0.50	5.48E-01	0.14	0.54	2098398	66858	2101607	69393	2108036	76101	2095178	62074
RP_POS_368_87076a0_514	RP	POS	0.51	368.8708				1.17E-03	-0.59	0.93	3.57E-01	0.19	0.66	2.59E-02	-0.50	0.76	3.72E-04	-0.69	1.21	590464	147161	481798	186604	464507	150412	499089	217069
RP_POS_894_74231a0_497	RP	POS	0.50	894.7423				6.07E-01	-0.10	0.84	3.57E-01	-0.19	1.15	3.62E-01	-0.19	0.67	9.97E-01	0.00	0.86	794731	163410	776655	197036	794902	202732	758407	191464
RP_NEG_229_054a7_908	RP	NEG	7.91	229.0540				4.78E-01	-0.23	0.59	3.57E-01	-0.11	0.60	3.79E-01	-0.28	0.53	6.02E-01	-0.17	0.60	4037867	14166722	2207799	4802103	2652885	5807574	1762713	3529701
RP_POS_371_26544a12_763	RP	POS	12.76	371.2654				1.55E-02	-0.48	0.97	3.57E-01	0.19	0.58	7.78E-02	-0.38	0.72	1.05E-02	-0.57	1.01	734181	224900	617755	243954	595174	246606	640335	241632
RP_POS_631_46283a11_253	RP	POS	11.25	631.4628				8.80E-06	0.67	1.63	3.58E-01	0.20	0.79	1.26E-04	0.77	1.55	9.29E-04	0.57	1.51	397602	286639	750389	558931	698679	504455	802098	609304
RP_NEG_560_3338a10_933	RP	NEG	10.93	560.3338				6.32E-02	-0.42	1.23	3.58E-01	-0.17	1.72	4.74E-02	-0.50	1.15	1.54E-01	-0.33	1.06	953715	181688	885914	154005	900159	129381	871668	175402
RP_POS_545_34137a10_618	RP	POS	10.62	545.3414				8.03E-03	0.59	1.36	3.58E-01	-0.17	1.00	4.32E-02	0.50	1.06	3.43E-03	0.68	1.43	34441648	8739047	39200571	7524687	39896638	6209811	38504503	8651404
HILIC_POS_132_10207a3_434	HILIC	POS	3.43	132.1021	132.1016(100)		4	7.54E-03	0.31	0.75	3.58E-01	0.21	1.09	6.64E-02	0.42	0.79	9.79E-05	0.21	1.29	5190960	4076476	17045259	42901384	13063159	12387045	21027359	59437522
RP_POS_209_15349a9_002	RP	POS	9.00	209.1535				1.94E-02	-0.49	0.98	3.58E-01	0.18	0.83	8.56E-02	-0.40	0.96	1.12E-02	-0.58	1.11	1658536	99645	1609969	97307	1600973	93569	1618964	101046
RP_POS_920_74915a0_496	RP	POS	0.50	920.7492				2.62E-01	-0.24	0.66	3.58E-01	-0.18	0.77	1.69E-01	-0.33	0.56	5.09E-01	-0.15	0.54	1078877	107064	1054803	95985	1063676	91040	1045931	100823
RP_POS_581_50049a10_582	RP	POS	10.58	581.5005				9.00E-04	0.58	0.92	3.58E-01	-0.19	0.60	2.06E-02	0.48	0.83	5.98E-04	0.67	1.24	1004899	676894	1532345	942386	1619443	869945	1445247	1010951
RP_POS_415_15228a9_931	RP	POS	9.93	415.1523				2.01E-01	-0.42	0.69	3.59E-01	0.10	0.83	2.66E-01	-0.37	0.52	1.56E-01	-0.47	0.65	1046204	2460353	471251	704281	406180	527373	536322	845803
HILIC_NEG_265_00073a4_789	HILIC	NEG	4.789	265.0007				9.69E-01	0.01	1.07	3.59E-01	-0.19	1.02	6.84E-01	-0.09	0.77	6.08E-01	0.10	0.98	634219	183921	635755	228790	656850	208293	614660	247918
RP_POS_271_22681a10_12	RP	POS	10.12	271.2268				1.86E-02	-0.42	0.80	3.59E-01	-0.19	0.91	1.15E-02	-0.52	0.99	1.18E-01	-0.33	0.86	2017122	202341	1910177	262059	1934324	271028	1886030	253191
RP_POS_553_45679a15_1	RP	POS	15.10	553.4568				2.17E-01	0.24	0.54	3.59E-01	-0.19	0.55	5.10E-01	0.14	0.28	1.31E-01	0.33	0.75	945541564	105691166	973242877	120215347	984319139	121786788	962166615	118810758
HILIC_POS_692_40607a0_627	HILIC	POS	0.627	692.4061				2.91E-06	0.57	1.27	3.60E-01	-0.20	0.93	2.01E-03	0.46	1.45	3.77E-04	0.67	1.45	129792	367949	1437295	2570890	1674156	2832655	1200435	2283728
HILIC_POS_125_98631a7_963	HILIC	POS	7.963	125.9863				1.39E-05	-0.66	1.28	3.60E-01	0.20	0.89	2.81E-03	-0.56	1.34	5.41E-05	-0.75	1.40	7039179	1594833	5136261	3071742	4853327	3017714	5419194	3129504
RP_POS_345_1944a11_159	RP	POS	11.16	345.1944				4.91E-02	-0.35	0.83	3.60E-01	0.19	0.90	2.15E-01	-0.26	0.69	3.11E-02	-0.45	0.88	5107982	316093	4968784	412643	4930790	411560	5006777	414363
RP_NEG_366_68091a15_577	RP	NEG	15.58	366.6809				3.42E-01	-0.20	0.56	3.60E-01	-0.18	0.55	2.11E-01	-0.29	0.60	6.30E-01	-0.11	0.39	1091836	52786	1081755	48303	1086200	49368	1077309	47290
RP_NEG_176_81676a15_521	RP	NEG	15.52	176.8168				9.07E-01	0.02	0.51	3.60E-01	-0.19	0.58	7.25E-01	-0.07	0.34	6.08E-01	0.12	0.37	1582931	66770	1584582	75938	1591570	84259	1577594	66721
RP_POS_329_24725a10_907	RP	POS	10.91	329.2473				2.41E-03	0.40	1.42	3.60E-01	0.20	0.71	1.23E-02	0.50	1.11	3.98E-02	0.30	1.36	6981151	3109192	10297581	9199493	9450870	7377909	11144292	10728088
RP_NEG_822_62433a10_957	RP	NEG	10.96	822.6243				4.48E-03	-0.63	1.27	3.60E-01	-0.17	1.30	2.54E-03	-0.72	1.28	2.33E-02	-0.55	1.15	1228851	345253	1026047	297297	1053394	312975	998699	281238
HILIC_POS_175_11884a7_095	HILIC	POS	7.095	175.1188				1.33E-02	0.31	1.07	3.60E-01	-0.21	0.87	1.92E-01	0.21	1.06	2.41E-02	0.41	1.14	1089128	337624	1468772	1388042	1596456	1489167	1341088	1281308
RP_POS_806_56732a13_58	RP	POS	13.58	806.5673				2.03E-09	1.02	1.64	3.61E-01	0.18	0.58	8.95E-08	1.11	1.72	4.37E-07	0.93	1.69	6305859	4776515	13787870	7098897	13135265	6404915	14440475	7741126
RP_NEG_213_99808a3_294	RP	NEG	3.29	213.9981				1.28E-01	-0.34	0.75	3.61E-01	-0.17	0.54	8.45E-02	-0.43	0.85	2.86E-01	-0.25	0.51	1189256	796658	947101	676960	1009326	634812	884876	717645
RP_NEG_1043_6123a10_313	RP	NEG	10.31	1043.6123				3.87E-03	0.48	1.10	3.61E-01	-0.19	0.61	5.00E-02	0.38	0.84	4.11E-03	0.57	1.11	1657101	503007	2009843	785951	2082041	799406	1937645	773534
RP_NEG_297_15356a13_293	RP	NEG	13.29	297.1536				8.72E-02	-0.39	0.82	3.61E-01	-0.17	0.75	4.69E-02	-0.48	0.92	2.28E-01	-0.30	0.84	8085243	6181641	5981073	5040443	6444005	5576648	5518140	4449074
RP_POS_184_98494a0_895	RP	POS	0.90	184.9849				5.05E-01	0.14	0.40	3.61E-01	-0.18	0.58	8.43E-01	0.04	0.60	3.27E-01	0.23	0.37	5632422	2854956	6023003	2883349	6287768	3045716	5758238	2716177
RP_NEG_203_00211a3_478	RP	NEG	3.48	203.0021				7.96E-01	0.05	0.44	3.61E-01	0.19	0.84	5.47E-01	0.14	0.57	8.48E-01	-0.04	0.46	591385	525807	619214	537396	569858	443632	668570	617821
RP_POS_249_1824a8_323	RP	POS	8.32	249.1824				7.67E-01	-0.06	0.36	3.61E-01	0.19	0.73	8.89E-01	0.03	0.17	4.77E-01	-0.15	0.35	1046312	57232	1042822	59000	1037404	51327	1048239	65868
RP_POS_604_45929a13_499	RP	POS	13.50	604.4593				9.62E-01	-0.01	0.27	3.61E-01	0.21	0.60	6.69E-01	0.10	0.28	3.94E-01	-0.11	0.34	1857812	226164	1854790	497995	1808993	286718	1900587	643873
RP_NEG_273_82733a15_561	RP	NEG	15.56	273.8273				7.01E-02	-0.34	0.83	3.62E-01	-0.19	0.79	3.24E-02	-0.44	0.93	2.72E-01	-0.25	0.68	1126384	49729	1106906	58561	1112281	65275	1101532	51079
HILIC_POS_478_29205a1_683	HILIC	POS	1.683	478.2921				4.04E-02	0.40	0.65	3.62E-01	-0.18	0.69	1.85E-01	0.31	0.48	1.59E-02	0.50	0.94	429527	218170	524352	235604	545980	189093	502724	274664
RP_POS_317_16113a10_704	RP	POS	10.70	317.1611				1.93E-02	0.45	1.26	3.62E-01	0.19	1.15	1.82E-02	0.54	1.25	7.81E-02	0.36	1.11	871834	173519	959458	196365	941442	168941	977473	220685
HILIC_NEG_476_27966a1_827	HILIC	NEG	1.827	476.2797				3.92E-02	0.41	0.66	3.62E-01	-0.18	0.69	1.79E-01	0.32	0.49	1.57E-02	0.50	0.94	751125	371858	913311	396752	949700	319748	876923	461622
RP_NEG_893_19354a9_697	RP	NEG	9.70	893.1935				6.65E-01	-0.09	0.61	3.62E-01	-0.18	0.57	4.22E-01	-0.18	0.54	9.87E-01	0.00	0.39	9315105	678664	9254932	684352	9317660	707018	9192203	662063
RP_POS_127_95573a15_424	RP	POS	15.42	127.9557				4.87E-01	-0.12	0.61	3.62E-01	0.20	0.71	9.10E-01	-0.02	0.16	3.35E-01	-0.22	0.86	3511963	337285	3458136	488528	3413342	582556	3502929	372456
RP_POS_870_78503a0_496	RP	POS	0.50	870.7850				1.73E-09	-0.73	1.39	3.62E-01	0.20	1.21	9.67E-05	-0.63	1.43	4.68E-06	-0.83	1.54	7117044	279013	5160484	2922236	4892782	3045733	5428187	2798296
RP_POS_343_33795a10_978	RP	POS	10.98	343.3380				6.19E-02	0.34	1.24	3.62E-01	-0.19	1.29	2.50E-01	0.24	0.98	3.57E-02	0.43	1.15	7367961	2381456	8352164	3021870	8628959	2919907	8075369	3125306
RP_POS_341_20868a9_419	RP	POS	9.42	341.2087				6.25E-01	0.07	0.31	3.62E-01	-0.20	0.70	8.09E-01	-0.03	0.24	4.33E-01	0.17	0.40	446878	782097	555807	1742754	715683	2200018	395931	1115404
RP_POS_723_46436a10_697	RP	POS	10.70	723.4644				5.16E-01	-0.12	0.60	3.62E-01	-0.19	0.74	3.16E-01	-0.22	0.44	8.95E-01	-0.03	0.55	1459921	357227	1410590	414116	1448516	412185	1372664	416716
HILIC_POS_586_39197a0_549	HILIC	POS	0.549	586.3920				1.48E-06	0.61	1.34	3.62E-01	-0.20	0.90	9.83E-04	0.51	1.51	1.91E-04	0.71	1.51	64760	191302	477330	743214	545399	817856	409262	661560
RP_POS_478_38882a13_804	RP	POS	13.80	478.3888				6.40E-01	0.11	0.50	3.63E-01	0.17	0.68	4.27E-01	0.20	0.71	9.21E-01	0.03	0.98	6981058	1835529	7147343	1388830	7020228	1557992	7274457	1198644
HILIC_POS_116_62675a4_87	HILIC	POS	4.87	116.6268				8.26E-01	-0.06	0.57	3.63E-01	-0.15	0.68	6.29E-01	-0.13	0.60	9.46E-01	0.02	0.36	395912	421989	378434	251973	401481	240018	355387	263787
RP_POS_504_30576a10_932	RP	POS	10.93	504.3058				4.71E-02	0.35	1.13	3.64E-01	0.19	1.00	4.81E-02	0.44	0.94	1.68E-01	0.25	0.97	2167674	545146	2413785	745185	2345666	592375	2481904	872672
RP_POS_281_17172a8_909	RP	POS	8.91	281.1717				1.61E-01	0.28	0.66	3.64E-01	0.18	0.54	1.21E-01	0.37	0.71	3.58E-01	0.19	0.43	2832056	472488	2969384	487706	2924806	389871	3013962	569661
RP_POS_149_02342a9_524	RP	POS	9.52	149.0234				4.47E-01	0.10	0.37	3.64E-01	0.21	0.62	3.75E-01	0.21	0.49	9.95E-01	0.00	0.30	2077763	89182	2099783	241759	2077629	85815	2121937	331242
RP_POS_161_98148a0_252	RP	POS	0.25	161.9815				2.55E-01	-0.21	0.39	3.64E-01	0.19	0.58	5.89E-01	-0.11	0.51	1.54E-01	-0.30	0.57	1198635	167991	1156942	209115	1137854	212468	1176030	206070
RP_NEG_201_0378a0_716	RP	NEG	0.72	201.0378				1.62E-06	0.69	1.25	3.64E-01	0.19	1.03	1.47E-04	0.78	1.36	1.46E-04	0.59	1.25	1420772	423937	2033624	953317	1946554	765725	2120693	1111021
HILIC_POS_340_04672a3_077	HILIC	POS	3.077	340.0467				6.38E-01	0.06	1.23	3.64E-01	-0.21	0.96	8.27E-01	-0.04	1.26	3.51E-01	0.17	1.31	1309586	81787	1321700	212645	1341105	214192	1302295	211452
RP_NEG_203_88559a15_54	RP	NEG	15.54	203.8856				2.52E-01	0.34	0.82	3.64E-01	-0.13	0.56	3.69E-01	0.28	0.49	1.81E-01	0.40	0.65	1214055	248054	1266710	108252	1276586	93838	1256833	121127
RP_NEG_334_8707a15_435	RP	NEG	15.44	334.8707				1.23E-01	0.26	0.56	3.64E-01	-0.20	0.77	3.82E-01	0.16	0.51	9.59E-02	0.36	0.77	1626978	310500	1739481	467559	1782137	522786	1696825	405791
RP_POS_327_20126a4_023	RP	POS	4.02	327.2013				9.33E-01	-0.02	1.12	3.65E-01	-0.14	1.15	7.54E-01	-0.09	0.88	8.86E-01	0.04	0.93	898870	2870324	854204	1360865	978248	1509394	730160	1196674
HILIC_POS_182_0811a5_12	HILIC	POS	5.12	182.0811				3.88E-01	0.15	0.90	3.65E-01	0.19	1.05	2.64E-01	0.25	0.40	7.72E-01	0.05	0.45	9533681	2842971	10085600	3890895	9730976	3229157	10440223	4461276
HILIC_POS_418_20605a0_952	HILIC	POS	0.952	418.2061				6.25E-01	0.11	0.43	3.65E-01	0.18	0.58	3.83E-01	0.19	0.45	9.47E-01	0.02	0.37	1067199	609187	1126725	550600	1076540	639694	1176911	445152
RP_POS_533_34515a10_456	RP	POS	10.46	533.3452				5.98E-01	-0.10	0.65	3.65E-01	-0.19	0.71	3.50E-01	-0.19	1.10	9.98E-01	0.00	0.33	2405439	637367	2332300	797364	2404934	842097	2259665	751440
RP_POS_478_38867a13_234	RP	POS	13.23	478.3887				7.21E-01	0.08	0.56	3.65E-01	-0.18	0.70	9.63E-01	-0.01	0.32	4.76E-01	0.17	0.44	3445168	776846	3500517	696669	3563957	654653	3437077	737440
RP_POS_419_31384a11_88	RP	POS	11.88	419.3138				2.81E-01	-0.23	0.67	3.66E-01	0.18	0.67	5.60E-01	-0.14	0.57	1.67E-01	-0.32	0.61	123651172	17731410	119767466	16887345	118231123	16155484	121303809	17617270
RP_POS_369_38385a11_668	RP	POS	11.67	369.3839				8.93E-01	-0.03	0.64	3.66E-01	-0.18	0.54	6.01E-01	-0.12	0.43	7.81E-01	0.06	0.41	961605	460588	948955	461063	990878	468615	907033	454214

Supplementary table 1: Metabolomics results (in asceding order according to p-value from progressive ALD vs non-progressive ALD comparison, with molecular features with ID_level of 1-2 first)

							all_ALD_vs_control			Prog_ALD_vs_non-prog_ALD			Prog_ALD_vs_control_ALD			Non-prog_ALD_vs_control			Healthy_control		all_ALD		Non-prog_ALD		Progressive_ALD	
							t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA								
Feature_ID	RP_HILIC	POS_NEG	Average.Rt	Average.Mz	Metabolite.name	curated_MSMS	ID_level	p	d	VIP	p	d	VIP	p	d	VIP	p	d	VIP	Mean	SD	Mean	SD	Mean	SD	Mean	SD
RP_POS_152_0222a0_55	RP	POS	0.55	152.0222				3.03E-12	-1.02	1.69	3.66E-01	-0.18	1.22	6.52E-10	-1.11	1.93	6.13E-07	-0.93	1.57	1046139	172718	675109	361684	707979	380908	642238	342060
RP_POS_645_27142a7_257	RP	POS	7.26	645.2714				4.43E-01	-0.15	0.68	3.67E-01	0.19	0.78	8.08E-01	-0.05	0.48	2.70E-01	-0.24	0.73	13524142	780964	13397150	895882	13315801	898113	13478500	895252
HILIC_POS_190_14349a0_778	HILIC	POS	0.778	190.1435				7.98E-01	-0.05	0.44	3.67E-01	0.19	0.68	8.52E-01	0.04	0.17	4.92E-01	-0.14	0.41	728452	65523	724948	72074	718402	62010	731494	81011
HILIC_POS_478_29379a1_923	HILIC	POS	1.923	478.2938				4.34E-02	0.40	0.66	3.67E-01	-0.18	0.69	1.95E-01	0.30	0.47	1.72E-02	0.49	0.93	3611661	1787673	4379115	1952083	4556433	1559387	4201797	2281045
RP_POS_195_11301a2_973	RP	POS	2.97	195.1130				1.45E-01	0.24	0.55	3.67E-01	-0.19	0.60	5.10E-01	0.14	0.39	5.18E-02	0.34	0.83	1459927	579357	1658863	882346	1738952	687028	1578775	1043005
RP_POS_182_02362a15_525	RP	POS	15.53	182.0236				8.59E-01	-0.03	0.62	3.67E-01	-0.20	0.69	5.29E-01	-0.13	0.65	7.11E-01	0.07	0.52	37098319	4194219	36919095	6766250	37532707	6379948	36305484	7143280
RP_POS_996_72632a0_497	RP	POS	0.50	996.7263				7.19E-01	-0.07	0.89	3.67E-01	-0.19	1.06	4.61E-01	-0.16	0.48	8.94E-01	0.03	0.99	672657	115033	663759	138593	676323	131281	651194	145777
HILIC_NEG_99_92569a0_927	HILIC	NEG	0.927	99.9257				1.50E-04	0.57	1.03	3.67E-01	-0.19	1.21	1.76E-02	0.47	0.77	1.31E-04	0.66	1.31	3109827	713741	3853462	1407940	3981078	1245452	3725845	1555846
RP_POS_296_29483a11_056	RP	POS	11.06	296.2948				8.58E-06	0.56	1.00	3.68E-01	0.20	1.01	3.56E-03	0.66	1.04	1.91E-07	0.46	1.68	556433	219023	992301	855981	914562	349651	1070040	1160074
RP_POS_315_68723a5_488	RP	POS	5.49	315.6872				1.34E-06	0.58	1.31	3.68E-01	-0.20	1.23	1.56E-03	0.48	1.37	2.53E-04	0.68	1.41	93807	154215	876661	1501926	1012618	1638575	740704	1354603
RP_NEG_723_08893a9_125	RP	NEG	9.13	723.0889				7.85E-01	0.06	0.14	3.68E-01	0.17	1.20	5.51E-01	0.15	0.43	9.18E-01	-0.02	0.24	5074091	437122	5097582	364652	5064587	347986	5130577	381235
RP_POS_822_63617a14_714	RP	POS	14.71	822.6362				5.56E-04	-0.83	1.38	3.68E-01	0.16	0.70	2.77E-03	-0.75	1.20	3.51E-04	-0.91	1.51	2313009	1319226	1368688	979579	1280073	961536	1457304	999079
RP_POS_564_41315a14_947	RP	POS	14.95	564.4132				1.19E-02	0.34	0.76	3.69E-01	0.20	0.57	4.87E-02	0.44	0.77	3.64E-02	0.24	0.71	2112685	235805	2308872	646239	2250313	349548	2367430	845334
RP_POS_181_98769a15_655	RP	POS	15.66	181.9877				3.89E-01	-0.19	0.51	3.69E-01	0.17	0.69	6.74E-01	-0.10	0.82	2.35E-01	-0.28	0.77	44699056	24310836	40545603	20779994	38666588	18391101	42424618	22956276
HILIC_POS_445_28815a0_637	HILIC	POS	0.637	445.2882				5.39E-07	0.60	1.29	3.70E-01	-0.20	0.89	9.84E-04	0.50	1.45	1.77E-04	0.70	1.50	39187	70759	997864	1784670	1158943	1949402	836786	1606853
RP_POS_189_0437a15_341	RP	POS	15.34	189.0437				1.47E-01	-0.31	0.50	3.70E-01	-0.18	0.59	9.57E-02	-0.40	0.65	3.32E-01	-0.22	0.40	1834353	576377	1664958	529148	1712711	505601	1617206	552651
RP_POS_385_17462a11_161	RP	POS	11.16	385.1746				4.35E-01	0.14	0.84	3.70E-01	0.19	0.86	2.74E-01	0.23	0.76	8.36E-01	0.04	0.89	1133408	201575	1168708	274269	1143960	256314	1193456	291609
RP_POS_794_06061a13_275	RP	POS	13.28	794.0606				9.29E-01	0.02	0.68	3.70E-01	-0.18	0.62	7.59E-01	-0.07	0.24	6.56E-01	0.11	0.80	2881867	924184	2898307	854921	2975445	924873	2821169	780488
RP_POS_244_92317a0_497	RP	POS	0.50	244.9232				1.23E-08	-0.69	1.35	3.70E-01	0.20	1.20	2.19E-04	-0.59	1.38	1.60E-05	-0.79	1.50	8774874	178586	7375669	2237170	7173865	2359240	7577474	2112552
RP_POS_199_13052a13_33	RP	POS	13.33	199.1305				7.40E-01	0.06	0.35	3.70E-01	0.19	0.86	4.62E-01	0.16	0.49	8.98E-01	-0.03	0.62	21467623	5849341	21875979	6566084	21284158	6960148	22467800	6160221
RP_POS_380_89728a0_497	RP	POS	0.50	380.8973				1.34E-08	-0.70	1.35	3.70E-01	0.20	1.19	1.92E-04	-0.60	1.37	1.47E-05	-0.79	1.51	2402346	98306	2002052	629612	1945318	664889	2058787	593521
RP_POS_401_34161a10_636	RP	POS	10.64	401.3416				7.57E-03	-0.53	0.93	3.70E-01	-0.18	1.00	5.62E-03	-0.62	1.06	4.44E-02	-0.44	0.82	601005	297203	430268	322108	459281	318567	401256	326224
HILIC_POS_423_27502a0_633	HILIC	POS	0.633	423.2750				4.57E-07	0.60	1.30	3.70E-01	-0.20	0.90	8.54E-04	0.50	1.46	1.64E-04	0.70	1.51	69910	172716	1440487	2524328	1667877	2761723	1213097	2267570
RP_POS_617_50989a11_165	RP	POS	11.17	617.5099				6.37E-01	-0.10	0.54	3.71E-01	-0.17	0.59	4.13E-01	-0.19	0.52	9.43E-01	-0.02	0.72	1178129	2206071	972081	1895385	1142796	2094136	801366	1677320
HILIC_POS_342_04358a3_078	HILIC	POS	3.078	342.0436				6.32E-01	0.06	1.26	3.71E-01	-0.20	0.95	8.36E-01	-0.04	1.30	3.51E-01	0.17	1.40	542570	33034	547635	87883	555542	88488	539729	87445
RP_POS_548_36963a10_647	RP	POS	10.65	548.3696				9.27E-02	0.37	0.89	3.71E-01	-0.17	0.74	2.53E-01	0.28	0.65	4.91E-02	0.45	0.96	1385468	464818	1543192	412185	1580276	361698	1506109	457852
RP_POS_431_27673a9_325	RP	POS	9.33	431.2767	Unknown	431.2795(100)	4	2.59E-01	-0.33	0.65	3.71E-01	0.13	0.57	3.86E-01	-0.26	0.43	1.84E-01	-0.39	0.59	1268391	2591023	724099	1221984	614172	1098872	834026	1335958
HILIC_POS_601_0672a0_553	HILIC	POS	0.553	601.0672				8.92E-07	0.62	1.33	3.71E-01	-0.20	0.89	6.56E-04	0.52	1.51	1.78E-04	0.72	1.51	101167	274338	734874	1125280	836103	1248183	633645	989686
RP_NEG_165_97849a6_183	RP	NEG	6.18	165.9785				4.40E-02	0.38	0.97	3.71E-01	-0.18	0.73	1.46E-01	0.29	0.84	3.97E-02	0.47	0.97	1472406	1268511	2026848	1494970	2161306	1705566	1892390	1252848
HILIC_POS_467_30136a0_64	HILIC	POS	0.64	467.3014				8.41E-07	0.61	1.32	3.72E-01	-0.20	0.90	1.01E-03	0.51	1.48	1.65E-04	0.71	1.51	52250	201635	630997	1053894	725647	1147798	536347	953063
RP_POS_326_30536a10_432	RP	POS	10.43	326.3054				4.14E-01	-0.24	0.91	3.72E-01	-0.13	0.66	3.12E-01	-0.31	0.73	5.61E-01	-0.18	0.57	1527235	3353051	1022680	1471704	1154799	1615403	890560	1315627
RP_POS_223_09459a10_449	RP	POS	10.45	223.0946				8.56E-01	0.03	0.48	3.72E-01	-0.19	0.57	7.86E-01	-0.06	0.61	5.68E-01	0.13	0.36	6877871	2433436	6971085	2757821	7218608	2897192	6723562	2616793
RP_POS_345_2171a8_422	RP	POS	8.42	345.2171				8.46E-01	0.04	0.35	3.72E-01	0.18	0.68	6.01E-01	0.13	0.45	8.41E-01	-0.05	0.42	6693103	8824097	7034989	7917610	6324431	6816223	7745547	8897481
HILIC_POS_325_19104a0_671	HILIC	POS	0.671	325.1910				4.71E-02	0.28	0.58	3.72E-01	0.20	0.55	6.56E-02	0.38	0.59	2.35E-01	0.18	0.60	2101175	2462352	3548010	5750117	3031855	4556444	4064164	6745188
RP_POS_195_12299a2_163	RP	POS	2.16	195.1230				1.29E-01	0.22	0.92	3.72E-01	-0.20	0.91	4.94E-01	0.12	1.01	9.91E-02	0.32	0.93	5297949	558634	5540107	1239301	5651273	1322136	5428941	1153175
RP_POS_388_25406a4_35	RP	POS	4.35	388.2541				8.46E-01	-0.06	1.16	3.73E-01	-0.12	1.15	6.92E-01	-0.12	0.88	9.89E-01	0.00	0.96	2799419	8989331	2479782	3829582	2823230	4229584	2136335	3391251
RP_POS_225_14847a9_418	RP	POS	9.42	225.1485				1.89E-01	-0.36	0.88	3.73E-01	-0.14	0.68	1.36E-01	-0.43	0.70	3.00E-01	-0.29	0.61	1128600	1454227	769142	772892	838418	719267	699866	824485
RP_POS_765_05273a12_788	RP	POS	12.79	765.0527				2.75E-07	-1.21	1.98	3.73E-01	-0.14	0.56	2.33E-07	-1.28	1.96	1.65E-06	-1.14	1.82	787922	355373	371844	271075	396112	253767	347576	287861
RP_NEG_216_85312a15_604	RP	NEG	15.60	216.8531				1.24E-01	-0.33	0.79	3.74E-01	-0.18	0.89	7.64E-02	-0.41	0.72	3.07E-01	-0.24	0.68	4171689	176254	4116494	165920	4131339	167721	4101649	164440
RP_NEG_183_01538a0_715	RP	NEG	0.72	183.0154				1.50E-02	0.42	0.86	3.74E-01	-0.19	0.56	1.16E-01	0.33	0.81	9.25E-03	0.51	0.88	1229092	284114	1389401	402145	1425382	379884	1353421	424013
RP_POS_659_28522a10_563	RP	POS	10.56	659.2852				2.95E-05	-0.77	1.20	3.74E-01	0.18	0.62	2.98E-03	-0.68	1.00	5.14E-06	-0.85	1.61	4239253	334294	3912636	424328	3874634	302654	3950637	518880
RP_POS_198_90514a15_579	RP	POS	15.58	198.9051				2.91E-01	0.19	0.42	3.74E-01	0.19	1.06	1.77E-01	0.28	0.67	6.51E-01	0.09	0.23	2414862	71438	2431663	94896	2423175	93611	2440152	96354
RP_NEG_291_16144a9_711	RP	NEG	9.71	291.1614				2.41E-02	-0.50	0.86	3.74E-01	-0.17	0.52	1.32E-02	-0.58	0.98	9.09E-02	-0.41	0.68	4859605	185452	4774244	163554	4788875	176415	4759614	149955
RP_NEG_325_18533a9_212	RP	NEG	9.21	325.1853				5.74E-01	0.12	0.65	3.74E-01	-0.18	0.57	8.98E-01	0.03	0.43	3.84E-01	0.21	0.57	2803658	2687851	3110185	2588699	3341527	2749334	2878843	2423103
RP_POS_378_20523a10_704	RP	POS	10.70	378.2052				1.52E-03	0.57	1.43	3.75E-01	0.18	1.23	3.28E-03	0.67	1.39	9.84E-03	0.48	1.33	3550605	571112	3963713	735173	3898023	587910	4029403	858804
RP_POS_272_90616a15_366	RP	POS	15.37	272.9062				5.52E-01	0.13	0.53	3.75E-01	-0.17	0.55	8.65E-01	0.04	0.40	3.62E-01	0.22	0.56	5350950	374051	5395498	342018	5426039	339888	5364956	344836
RP_POS_980_7533a0_494	RP	POS	0.49	980.7533				8.25E-10	-0.83	1.42	3.75E-01	0.19	1.18	4.98E-05	-0.73	1.43	1.83E-07	-0.92	1.62	1044401	123932	770559	349925	739322	336992	801795	363097
RP_POS_392_70184a6_811	RP	POS	6.81	392.7018				7.33E-05	-0.64	1.16	3.75E-01	0.19	0.99	3.70E-03	-0.54	1.11	2.33E-04	-0.73	1.26	1060119	59158	1000414	98243	991644	101508	1009183	95076
RP_NEG_374_90674a0_511	RP	NEG	0.51	374.9067				8.63E-06	0.54	1.25	3.75E-01	-0.20	1.21	4.08E-03	0.44	1.22	5.20E-04	0.64	1.40	592560	139054	979667	793978	1050523	858722	908811	725272
RP_POS_358_25861a6_961	RP	POS	6.96	358.2586				3.62E-01	0.14	0.66	3.75E-01	0.20	0.98	2.96E-01	0.24	0.57	7.74E-01	0.04	0.65	593683	374876	682354	705248	619348	422032	745359	904814
RP_POS_614_3399a10_82	RP	POS	10.82	614.3399				2.18E-03	-0.73	1.30	3.76E-01	-0.16	1.19	1.50E-03	-0.81	1.28	8.61E-03	-0.65	1.22	612442	237384	463839	177155	479619	173987	448059	180633
RP_POS_758_77081a0_498	RP	POS	0.50	758.7708				3.60E-01	-0.15	1.02	3.76E-01	-0.19	1.25	1.93E-01	-0.25	0.90	7.83E-01	-0.06	1.07	904416	238762	853237	360930	885385	385305	821089	335606
RP_POS_199_01111a10_782	RP	POS	10.78	199.0111				2.93E-01	0.21	0.59	3.76E-01	0.18	0.77	1.96E-01	0.30	0.77	5.82E-01	0.12	0.35	3372214	1225740	3640897	1311215	3524169	1194861	3757626	1420618
HILIC_POS_394_31628a1_392	HILIC	POS	1.392	394.3163				4.67E-10	-0.95	1.59	3.76E-01	0.18	0.74	6.49E-06	-0.86	1.48	1.49E-08	-1.04	1.96	3084092	547042	2102444	1046154	2009350	989986	2195537	1101569
HILIC_POS_115_51926a4_869	HILIC	POS	4.869	115.5193				7.05E-01	-0.10	0.68	3.76E-01	-0.14	0.71	5.41E-01	-0.18	0.69	9.10E-01	-0.03	0.42	411404	491250	376659	269424	400630	262587	352688	276651
RP_POS_171_03413a15_643	RP	POS	15.64	171.0341				8.05E-01	-0.05	0.45	3.76E-01	0.18	0.58	8.55E-01	0.04	0.26	5.40E-01	-0.14	0.53	9373077	3953912	9171926	4110599	8806259	4235159	9537592	3991168
HILIC_POS_359_00687a7_33	HILIC	POS	7.33	359.0069				1.87E-01	-0.26	0.48	3.77E-01	0.18	0.61	4.19E-01	-0.17	0.32	1.33E-01	-0.35	0.72	1892525	60172	1875820	65697	1869980	73358	1881660	57178
RP_POS_304_21173a4_577	RP	POS	4.58	304.2117				1.92E-01	0.23	0.60	3.77E-01	-0.19	0.86	5.11E-01	0.14	0.45	1.09E-01	0.33	0.85	4151538	1875113	4697311	2481721	4917775	2383595	4476847	2581251
RP_POS_473_25107a10_168	RP	POS	10.17	473.2511				2.22E-01	0.21	0.58	3.77E-01	-0.19	0.56	5.24E-01	0.12	0.36	1.61E-01	0.31	0.60	3884701	2837849	4660685	3817629	4999797	4303680	4321573	3269506
HILIC_POS_203_05261a5_066	HILIC	POS	5.066	203.0526				9.92E-03	0.39	1.01	3.77E-01	0.19	0.65	2.02E-02	0.49	0.98	6.92E-02	0.30	0.65	37832831	19741937	51194848	36951906	47911842	29811059	54477853	42989039
HILIC_POS_155_15425a0_604	HILIC	POS	0.604	155.1543				7.47E-01	0.06	0.65	3.77E-01	-0.19	0.66	8.35E-01	-0.04	0.36	5.01E-01	0.15	0.66	2703331	1084961	2781793	1480834	2913351	1730438	2650236	1183535
HILIC_POS_164_12817a2_534	HILIC	POS	2.534	164.1282				5.44E-02	0.23	0.90	3.78E-01	0.20	1.03	1.25E-01	0.34	0.89	1.61E-01	0.13	0.70	629493	413072	1057497	2078569	872605	1096162	1242389	2730885
RP_POS_1043_60645a10_324	RP	POS	10.32	1043.6065				3.27E-08	0.96	1.63	3.78E-01	-0.17	0.75	1.76E-05	0.88	1.52	6.56E-08	1.05	1.77	658682	229096	978637	323026	1007303	296554	949972	348138
RP_NEG_240_89978a15_555	RP	NEG	15.56	240.8998				7.61E-01	-0.06	0.49	3.78E-01	-0.18	0.78	4.77E-01	-0.15	0.49	9.02E-01	0.03	0.60	586441	30363	584534	31811	587357	35802	581712	27323
RP_POS_393_23022a11_376	RP	POS	11.38	393.2302				3.51E-03	-0.53	1.06	3.78E-01	0.18	1.12	2.53E-02	-0.44	0.96	4.44E-03	-0.63	1.07	1086721	160861	980990	202414	963038	220694	998942	182798
RP_NEG_285_70731a15_59	RP	NEG	15.59	285.7073				1.36E-02	-0.50	0.86	3.78E-01	-0.18	0.69	7.81E-03	-0.58	1.01	7.28E-02	-0.41	0.66	2876459	104040	2821867	109408	2831568	116040	2812166	102603
RP_POS_394_35257a10_656	RP	POS	10.66	394.3526				2.39E-01	0.23	0.75	3.78E-01	-0.18	0.84	5.11E-01	0.15	0.38	1.51E-01	0.32	0.68	4635830	783611	4827987	827432	4901337	845394	4754638	810919
RP_NEG_592_2666a10_301	RP	NEG	10.30	592.2666				7.90E-02	0.32	1.10	3.78E-01	0.18	0.68	5.05E-02	0.42	1.01	2.70E-01	0.23	0.81	684152	303286	800742	372765	767706	372795	833777	373551
RP_POS_767_36609a6_81	RP	POS	6.81	767.3661				5.03E-01	-0.12	0.72	3.78E-01	0.19	0.64	9.07E-01	-0.03	0.48	2.65E-01	-0.21	0.64	829605	46160	822764	60322	817418	50460	828110	68900
RP_POS_564_84271a0_496	RP	POS	0.50	564.8427				3.85E-07	-0.64	1.33	3.78E-01	0.19	1.22	1.24E-03	-0.55	1.34	3.24E-05	-0.74	1.47	568662	60894	428113	239248	406919	242182	449307	236809
HILIC_POS_189_07329a4_839	HILIC	POS	4.839	189.0733				2.29E-02	-0.49	0.72	3.79E-01	0.17	0.68	1.06E-01	-0.40	0.66	8.87E-03	-0.57	1.05	2032131	451692	1820515	417103	1783553	312516	1857476	501045
RP_POS_613_33984a5_488	RP	POS	5.49	613.3398				1.72E-06	0.57	1.30	3.79E-01	-0.20	1.23	1.80E-03	0.47	1.36	2.89E-04	0.67	1.40	133953	210521	1217521	2104804	1403892	2289617	1031151	1907244
HILIC_POS_59_06127a0_798	HILIC	POS	0.798	59.0613				3.49E-03	0.56	1.11	3.79E-01	0.18	0.56	3.57E-03	0.65	1.10	2.32E-02	0.47	1.26	2530050	1237529	3322601	1411927	3197636	1319346	3447566	1501738
RP_POS_374_22043a11_163	RP	POS	11.16	374.2204				7.88E-01	0.04	0.73	3.79E-01	-0.19	0.90	7.71E-01	-0.06	0.58	4.68E-01	0.14	0.71	1119852	67709	1124426	120111	1135049	120643	1113803	119844
RP_POS_163_11165a15_1	RP	POS	15.10	163.1117				1.97E-01	-0.24	0.49	3.79E-01	0.18	0.57	4.58E-01	-0.15	0.41	1.37E-01	-0.33	0.65	2994978	654584	2813735	770489	2745607	842245	2881863	693233
RP_POS_270_90982a15_367	RP	POS	15.37	270.9098				3.91E-01	-0.18	0.49	3.80E-01	-0.17	0.57	2.46E-01	-0.27	0.54	6.87E-01	-0.09	0.25	9623866	262725	9578368	246197	9600111	253829	9556625	238891
RP_POS_608_38464a5_488	RP	POS	5.49	608.3846				1.61E-06	0.57	1.30	3.80E-01	-0.20	1.22	1.64E-03	0.48	1.36	2.92E-04	0.67	1.39	240985	348221	2015189	3433736	2318336	3747376	1712042	3096987
RP_NEG_658_39166a10_977	RP	NEG	10.98	658.3917				1.34E-02	0.44	1.37	3.80E-01	-0.18	1.26	8.93E-02	0.35	1.10	1.02E-02	0.53	1.35	709373	514260	997755	680872	1057826	679630	937684	683648
RP_POS_198_99181a2_815	RP	POS	2.82	198.9918				3.67E-02	-0.41	0.90	3.81E-01	0.18	0.69	1.38E-01	-0.32	0.63	2.60E-02	-0.50	0.94	1383362	107136	1335649	117684	1325271	121398	1346027	114124
RP_NEG_614_34729a10_544	RP	NEG	10.54	614.3473				1.82E-06	0.73	1.32	3.81E-01	-0.18	0.62	1.82E-03	0.63	1.16	1.41E-06	0.82	1.59	1069365	359871	1541490	680344	1601510	564217	1481469	780698
RP_POS_285_2428a9_579	RP	POS	9.58	285.2428				8.47E-01	0.04	0.61	3.81E-01	-0.18	0.81	8.26E-01	-0.05	0.32	5.86E-01	0.13	0.95	9174747	1302166	9225910	1294500	9340056	1384432	9111764	1201007
RP_POS_159_09175a2_49	RP	POS	2.49	159.0918				1.00E-03	-0.57	1.16	3.81E-01	-0.18	1.09	2.69E-03	-0.66	1.22	8.38E-03	-0.48	1.09	4834970	829933	4192917	1164360	4295625	950537	4090208	1346881
RP_POS_875_52356a10_849	RP	POS	10.85	875.5236				6.38E-03	0.33	1.00	3.81E-01	-0.20	1.00	9.53E-02	0.23	0.99	2.56E-02	0.43	1.17	1095491	221937	1422212	1109281	1520023	1277715	1324401	913259
RP_POS_129_03055a15_433	RP	POS	15.43	129.0306				4.32E-02	-0.25	0.81	3.81E-01	0.20	0.57	2.66E-01	-0.15	0.70	7.75E-02	-0.35	0.65	10747379	388698	10377168	1676963	10229363	1977161	10524973	1314552
RP_POS_308_2948a10_438	RP	POS	10.44	308.2948				3.84E-01	-0.26	0.94	3.81E-01	-0.12	0.67	2.93E-01	-0.32	0.75	5.14E-01	-0.20	0.60	695596	1662815	429317	684083	489581	763789	369053	595571
HILIC_POS_151_09654a0_631	HILIC	POS	0.631	151.0965				2.77E-01	0.15	1.04	3.81E-01	-0.20	0.78	7.17E-01	0.05	1.12	2.25E-01	0.25	1.05	2893203	413883	3026780	978718	3113004	1158119	2940556	760863
RP_POS_242_92581a0_497	RP	POS	0.50	242.9258				1.44E-08	-0.68	1.35	3.81E-01	0.19	1.20	1.97E-04	-0.59	1.38	2.15E-05	-0.78	1.50	107015456	1892214	90070285	27288855	87668177	29051033	92472392	25471995
HILIC_POS_342_26398a0_675	HILIC	POS	0.675	342.2640				1.15E-03	0.49	0.88	3.81E-01	0.19	0.89	1.21E-03	0.58	1.38	4.09E-02	0.39	0.66	9775791	5362729	14471909	10355478	13560414	10979477	15383404	9716783

Supplementary table 1: Metabolomics results (in asceding order according to p-value from progressive ALD vs non-progressive ALD comparison, with molecular features with ID_level of 1-2 first)

							all_ALD_vs_control			Prog_ALD_vs_non-prog_ALD			Prog_ALD_vs_control_ALD			Non-prog_ALD_vs_control			Healthy_control		all_ALD		Non-prog_ALD		Progressive_ALD	
							t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA								
Feature_ID	RP_HILIC	POS_NEG	Average.Rt	Average.Mz	Metabolite.name	curated_MSMS	ID_level	p	d	VIP	p	d	VIP	p	d	VIP	p	d	VIP	Mean	SD	Mean	SD	Mean	SD	Mean	SD
RP_POS_499_82715a4_636	RP	POS	4.64	499.8272				1.41E-01	0.26	0.81	3.81E-01	-0.19	0.56	4.02E-01	0.16	0.38	1.02E-01	0.35	1.05	2041841	2195504	2774153	3032552	3041084	3278705	2507222	2772202
HILIC_NEG_219_94669a0_601	HILIC	NEG	0.601	219.9467				9.41E-02	0.20	0.98	3.82E-01	-0.20	0.60	4.89E-01	0.09	0.55	1.17E-01	0.30	0.47	40349	43907	126086	501477	170237	573964	81935	417944
RP_POS_592_33734a10_543	RP	POS	10.54	592.3373				1.88E-05	0.66	1.27	3.82E-01	-0.19	0.65	5.54E-03	0.57	1.08	1.05E-05	0.76	1.50	449895	183222	658587	331632	687781	274574	629393	380885
RP_POS_352_24582a11_161	RP	POS	11.16	352.2458				4.21E-01	-0.14	0.71	3.82E-01	0.19	0.79	8.28E-01	-0.04	0.60	2.64E-01	-0.23	0.70	3130669	329156	3069834	476256	3027936	497308	3111732	455381
HILIC_POS_487_29883a0_649	HILIC	POS	0.649	487.2988				2.07E-06	0.57	1.27	3.82E-01	-0.20	0.90	2.11E-03	0.47	1.44	3.23E-04	0.66	1.47	87462	171106	1405922	2600957	1634707	2822458	1177137	2365360
RP_POS_239_14896a3_195	RP	POS	3.20	239.1490				2.61E-02	0.34	1.11	3.82E-01	-0.19	1.10	1.51E-01	0.25	1.13	3.28E-02	0.44	1.12	584605	634946	947809	1150871	1049047	1285202	846571	1001688
HILIC_POS_516_3017a0_622	HILIC	POS	0.622	516.3017				4.29E-06	0.56	1.23	3.82E-01	-0.20	0.91	2.25E-03	0.46	1.41	4.92E-04	0.65	1.40	93364	289640	1060144	1932928	1230081	2130413	890207	1717868
HILIC_POS_130_08641a7_097	HILIC	POS	7.097	130.0864				1.57E-02	0.32	0.99	3.82E-01	-0.20	0.85	1.83E-01	0.22	1.04	2.33E-02	0.42	1.05	4470529	1532178	5766457	4548236	6166110	4787947	5366803	4306354
RP_POS_371_31427a11_436	RP	POS	11.44	371.3143				3.01E-01	0.19	0.76	3.83E-01	-0.18	0.67	6.37E-01	0.09	0.27	2.04E-01	0.28	0.97	2212226	366438	2296048	476200	2337866	520762	2254230	428251
RP_POS_257_22641a10_168	RP	POS	10.17	257.2264				2.01E-01	0.22	0.58	3.83E-01	-0.19	0.55	4.91E-01	0.13	0.37	1.57E-01	0.31	0.60	2580999	1942076	3149323	2767805	3392374	3199151	2906272	2263341
RP_POS_221_9818a1_461	RP	POS	1.46	221.9818				4.30E-12	0.93	1.51	3.83E-01	0.18	0.55	6.84E-08	1.02	1.75	5.25E-07	0.84	1.51	1370598	1232794	4509008	3480095	4203592	3268464	4814424	3687283
RP_POS_217_10535a2_162	RP	POS	2.16	217.1054				4.40E-03	0.39	1.03	3.83E-01	-0.19	0.99	7.39E-02	0.29	1.07	1.18E-02	0.48	1.10	6769392	734236	7450259	1956204	7621908	2138661	7278609	1759990
RP_NEG_209_06641a0_618	RP	NEG	0.62	209.0664				8.24E-02	0.34	0.57	3.83E-01	-0.18	0.67	2.51E-01	0.25	0.51	5.56E-02	0.43	0.74	1959333	638080	2195481	716237	2258311	738238	2132652	695276
RP_POS_441_29492a11_162	RP	POS	11.16	441.2949				8.76E-01	-0.03	0.69	3.83E-01	0.19	0.83	7.57E-01	0.06	0.65	5.59E-01	-0.12	0.76	12264324	1254280	12221011	1638110	12077350	1618885	12364673	1660923
RP_NEG_344_98062a9_044	RP	NEG	9.04	344.9806				8.52E-01	0.03	0.58	3.83E-01	-0.19	0.56	7.20E-01	-0.06	0.80	5.67E-01	0.13	0.64	3330433	590924	3356061	887701	3433910	1036639	3278211	710719
RP_NEG_144_99081a15_809	RP	NEG	15.81	144.9908				5.76E-01	0.12	0.51	3.84E-01	0.17	0.91	3.81E-01	0.20	0.79	8.94E-01	0.03	0.28	2469556	1418739	2629762	1346082	2511794	1341123	2747731	1354194
HILIC_POS_154_15897a5_539	HILIC	POS	5.539	154.1590				6.45E-01	0.09	0.24	3.84E-01	-0.18	0.57	9.86E-01	0.00	0.22	4.45E-01	0.18	0.32	9757287	3912442	10128554	4061803	10484453	4569626	9772655	3491877
HILIC_NEG_387_67157a1_364	HILIC	NEG	1.364	387.6716				2.16E-05	0.69	1.09	3.84E-01	-0.18	0.61	3.55E-03	0.60	0.97	1.53E-05	0.78	1.48	142405	59670	206481	95778	214870	82413	198092	107697
RP_POS_654_29541a10_501	RP	POS	10.50	654.2954				2.64E-01	0.23	0.61	3.84E-01	-0.17	0.57	5.21E-01	0.15	0.47	1.73E-01	0.32	0.76	360753	264334	421035	257601	443590	267472	398481	247975
RP_NEG_583_25793a11_808	RP	NEG	11.81	583.2579				3.52E-02	-0.46	1.24	3.84E-01	0.17	1.08	1.44E-01	-0.37	0.83	1.29E-02	-0.54	1.26	2288042	1034923	1842659	937907	1760492	639204	1924827	1164016
RP_POS_121_25214a11_666	RP	POS	11.67	121.2521				9.36E-01	0.02	0.66	3.85E-01	-0.18	0.51	7.44E-01	-0.07	0.41	6.44E-01	0.10	0.41	310202	199039	313515	208633	331756	214041	295273	203596
HILIC_POS_132_10208a5_139	HILIC	POS	5.139	132.1021				2.21E-01	0.16	0.30	3.85E-01	0.20	0.66	2.04E-01	0.26	0.39	6.69E-01	0.06	0.42	1572690	1197522	2130851	4011601	1779879	3069119	2481822	4779480
HILIC_NEG_229_9762a0_935	HILIC	NEG	0.935	229.9762				7.86E-02	0.26	1.09	3.85E-01	-0.19	0.55	3.92E-01	0.17	0.28	4.46E-02	0.36	0.95	139660	64306	169976	127353	181102	118956	158849	135518
RP_NEG_343_995a0_727	RP	NEG	0.73	343.9950				4.23E-03	-0.51	1.04	3.85E-01	0.18	0.99	3.91E-02	-0.42	0.96	3.99E-03	-0.60	1.10	64905340	30457928	44985010	40409038	41456549	40919664	48513472	39990972
RP_POS_438_26651a11_668	RP	POS	11.67	438.2665				7.54E-01	-0.06	0.74	3.85E-01	-0.18	0.53	4.94E-01	-0.15	0.47	9.11E-01	0.03	0.56	872603	501739	840243	521607	885775	546645	794711	496636
RP_POS_373_25851a10_242	RP	POS	10.24	373.2585				3.47E-05	0.49	0.97	3.86E-01	-0.20	0.89	1.17E-02	0.39	0.95	1.10E-03	0.59	1.13	31261	41821	637087	1395010	758816	1482047	515357	1305802
RP_POS_848_55518a13_871	RP	POS	13.87	848.5552				7.31E-01	-0.07	0.43	3.86E-01	0.17	0.65	9.49E-01	0.02	0.46	4.62E-01	-0.16	0.36	4601133	1583809	4490415	1548234	4355267	1261207	4625563	1793058
RP_NEG_864_50781a10_374	RP	NEG	10.37	864.5078				4.32E-01	-0.20	0.49	3.86E-01	-0.15	0.57	3.08E-01	-0.27	0.44	6.50E-01	-0.12	0.44	573983	541223	492515	370538	524833	349104	460198	391656
RP_POS_373_21109a10_905	RP	POS	10.91	373.2111				3.89E-03	0.42	1.52	3.86E-01	0.19	0.91	9.83E-03	0.52	1.29	4.79E-02	0.33	1.31	1386144	515825	1798108	1057571	1705877	922140	1890339	1179846
RP_POS_544_33722a10_618	RP	POS	10.62	544.3372				7.37E-03	0.60	1.37	3.86E-01	-0.16	1.00	3.90E-02	0.52	1.07	3.28E-03	0.68	1.44	123112936	30617396	139975438	26296057	142268080	21437014	137682795	30443465
RP_POS_344_3147a10_174	RP	POS	10.17	344.3147				7.41E-01	-0.06	0.83	3.86E-01	0.18	0.90	8.88E-01	0.03	0.66	5.04E-01	-0.15	0.77	791305	146214	780974	172229	765961	194301	795986	147370
RP_POS_569_31427a5_307	RP	POS	5.31	569.3143				4.93E-05	0.52	1.28	3.87E-01	-0.19	1.21	7.79E-03	0.42	1.31	1.04E-03	0.61	1.37	308473	728500	1551338	2663031	1783282	2880071	1319393	2433844
RP_POS_232_88356a0_245	RP	POS	0.25	232.8836				3.23E-01	-0.20	0.61	3.87E-01	0.17	0.52	6.03E-01	-0.11	0.31	2.18E-01	-0.29	0.49	1286054	198416	1245794	199614	1228413	213963	1263174	184683
RP_POS_697_65625a11_668	RP	POS	11.67	697.6563				9.15E-01	0.02	0.65	3.87E-01	-0.18	0.51	7.67E-01	-0.07	0.38	6.38E-01	0.11	0.45	8445427	7699970	8613782	7785204	9291529	8227857	7936035	7336258
HILIC_POS_342_21198a1_952	HILIC	POS	1.952	342.2120				5.77E-01	0.12	1.07	3.88E-01	-0.17	0.80	8.81E-01	0.03	0.95	4.02E-01	0.20	1.09	409437	1149912	538424	1064207	630815	1176542	446033	941549
HILIC_POS_314_14551a2_457	HILIC	POS	2.457	314.1455				2.70E-02	0.26	0.79	3.88E-01	0.20	0.72	6.76E-02	0.36	0.58	1.96E-01	0.17	0.98	663980	100146	814540	648063	758250	494070	870831	773286
RP_NEG_180_98903a6_159	RP	NEG	6.16	180.9890				4.27E-01	-0.17	0.46	3.88E-01	0.17	0.96	7.10E-01	-0.09	0.38	2.75E-01	-0.26	0.47	2568087	1569836	2319781	1377394	2200273	1312468	2439289	1442715
RP_POS_161_98148a15_55	RP	POS	15.55	161.9815				9.70E-01	0.01	0.68	3.89E-01	-0.18	0.51	7.11E-01	-0.08	0.27	6.79E-01	0.10	0.55	6099346	176234	6100717	185312	6116785	199152	6084649	170861
RP_POS_591_35822a5_488	RP	POS	5.49	591.3582				1.85E-06	0.57	1.30	3.89E-01	-0.19	1.22	1.78E-03	0.48	1.36	3.11E-04	0.67	1.39	82616	148745	816352	1428572	940197	1554667	692507	1294217
HILIC_POS_694_42188a1_064	HILIC	POS	1.064	694.4219				5.07E-06	0.55	1.25	3.89E-01	-0.19	0.88	2.71E-03	0.45	1.41	5.52E-04	0.64	1.43	141933	414098	1879634	3541611	2186666	3886876	1572602	3168880
RP_POS_809_55432a10_857	RP	POS	10.86	809.5543				2.60E-02	-0.45	0.96	3.89E-01	-0.17	0.71	1.53E-02	-0.53	0.92	1.12E-01	-0.36	0.64	1240480	409988	1047930	427587	1084989	451561	1010870	403340
HILIC_POS_328_24811a0_735	HILIC	POS	0.735	328.2481				1.80E-01	-0.26	0.55	3.89E-01	-0.18	0.69	1.26E-01	-0.35	0.55	4.20E-01	-0.17	0.39	5011964	2250409	4370724	2554391	4592116	2339891	4149331	2758236
RP_POS_591_45923a11_254	RP	POS	11.25	591.4592				1.76E-01	0.20	0.40	3.89E-01	-0.19	0.76	4.66E-01	0.11	0.48	1.75E-01	0.30	0.50	468318	507166	650918	995435	737272	1234759	564563	679821
RP_NEG_213_91519a14_266	RP	NEG	14.27	213.9152				5.38E-01	0.12	0.37	3.89E-01	0.18	0.53	3.71E-01	0.21	0.40	8.79E-01	0.03	0.26	932672	203779	958902	223330	939550	191544	978255	251629
RP_POS_185_97462a15_577	RP	POS	15.58	185.9746				7.51E-01	0.06	0.30	3.89E-01	0.18	0.66	4.92E-01	0.15	0.39	8.57E-01	-0.04	0.48	6442882	236397	6459587	315387	6432278	289483	6486895	340067
HILIC_POS_182_0578a3_508	HILIC	POS	3.508	182.0578				7.13E-01	0.06	0.53	3.90E-01	0.19	0.65	4.55E-01	0.16	0.56	8.80E-01	-0.03	0.49	3316569	3714409	3628531	5297071	3170172	5007140	4086890	5584831
HILIC_POS_217_15443a5_486	HILIC	POS	5.486	217.1544				2.56E-01	0.21	0.54	3.90E-01	0.18	0.64	1.95E-01	0.30	0.47	5.43E-01	0.11	0.32	442754	397742	541976	506802	498099	404101	585852	593053
RP_POS_272_79459a0_522	RP	POS	0.52	272.7946				2.39E-06	-0.67	1.24	3.90E-01	0.19	1.04	1.10E-03	-0.58	1.18	4.07E-05	-0.76	1.39	952906	125315	773967	284611	749341	289611	798593	280263
RP_POS_721_50726a10_916	RP	POS	10.92	721.5073				9.13E-01	-0.02	0.47	3.90E-01	0.17	0.56	7.88E-01	0.06	0.34	6.14E-01	-0.11	0.67	4515185	744058	4498646	743165	4434345	636846	4562948	837764
HILIC_POS_313_15457a1_741	HILIC	POS	1.741	313.1546				3.94E-05	0.49	1.27	3.90E-01	0.19	0.80	2.42E-03	0.59	1.40	4.69E-03	0.39	1.26	317630	1517230	6850919	14980073	5555309	12382939	8146528	17222715
RP_POS_794_56494a13_421	RP	POS	13.42	794.5649				4.27E-06	-0.97	1.62	3.90E-01	0.16	0.78	5.05E-05	-0.90	1.62	5.79E-06	-1.05	1.55	4917386	1450683	3413720	1392928	3293361	1463715	3534079	1322147
HILIC_POS_371_24088a4_125	HILIC	POS	4.125	371.2409				5.13E-02	-0.35	1.03	3.90E-01	-0.18	1.21	3.97E-02	-0.44	0.82	1.92E-01	-0.26	0.74	8676778	1308859	8111091	1662743	8254730	1571336	7967452	1753468
RP_POS_395_24033a10_242	RP	POS	10.24	395.2403				4.20E-05	0.48	0.94	3.91E-01	-0.19	0.87	1.18E-02	0.39	0.93	1.33E-03	0.58	1.11	126714	155119	2006401	4376863	2384429	4687029	1628373	4055236
RP_POS_428_31177a11_669	RP	POS	11.67	428.3118				9.67E-01	-0.01	0.75	3.91E-01	-0.17	0.52	6.75E-01	-0.10	0.45	7.31E-01	0.08	0.48	1294721	826488	1287806	833062	1359744	841716	1215869	826499
HILIC_POS_141_13866a0_558	HILIC	POS	0.558	141.1387				1.74E-02	-0.51	1.01	3.91E-01	0.17	0.87	7.45E-02	-0.43	0.76	9.52E-03	-0.59	1.20	2605241	1134441	2047868	1050553	1957170	953036	2138567	1142269
RP_POS_347_17102a6_444	RP	POS	6.44	347.1710				7.42E-01	0.05	0.26	3.91E-01	0.19	0.53	5.08E-01	0.15	0.40	7.90E-01	-0.04	0.24	969401	90613	976740	154374	963402	111367	990079	188104
RP_POS_371_22751a4_35	RP	POS	4.35	371.2275				8.41E-01	-0.06	1.16	3.91E-01	-0.12	1.14	6.94E-01	-0.12	0.88	9.98E-01	0.00	0.95	930910	3130440	815662	1318949	929513	1442956	701811	1185825
RP_POS_318_16489a5_488	RP	POS	5.49	318.1649				1.44E-06	0.58	1.31	3.91E-01	-0.19	1.23	1.76E-03	0.48	1.37	2.48E-04	0.67	1.41	62407	110726	642034	1116684	738414	1203646	545655	1025522
HILIC_NEG_141_92368a2_899	HILIC	NEG	2.899	141.9237				3.10E-01	0.19	1.00	3.91E-01	0.18	0.90	2.10E-01	0.28	0.49	6.23E-01	0.10	0.21	2139793	447490	2237131	529142	2191473	484344	2282789	571710
RP_POS_837_55939a13_871	RP	POS	13.87	837.5594				3.25E-02	-0.51	0.99	3.91E-01	0.15	0.94	9.83E-02	-0.44	0.71	1.67E-02	-0.59	1.02	1089498	833585	736411	615458	683302	500790	789519	713274
HILIC_POS_501_27377a1_309	HILIC	POS	1.309	501.2738				6.61E-01	0.10	0.19	3.91E-01	-0.17	0.58	9.57E-01	0.01	0.02	4.60E-01	0.18	0.29	339895	270992	363461	237440	383933	246665	342989	228489
RP_POS_551_26941a7_093	RP	POS	7.09	551.2694				5.83E-01	-0.11	0.54	3.92E-01	0.18	0.62	9.38E-01	-0.02	0.35	3.68E-01	-0.19	0.63	48020240	2581354	47721069	2910749	47470238	2833635	47971900	2993317
HILIC_POS_165_06361a0_721	HILIC	POS	0.721	165.0636				1.02E-02	0.31	0.57	3.92E-01	-0.20	0.61	3.95E-03	0.21	1.29	7.25E-02	0.40	0.56	724697	976053	2665318	7216777	3289142	9808853	2041494	2866850
RP_POS_532_89423a0_493	RP	POS	0.49	532.8942				3.74E-08	0.66	1.33	3.92E-01	-0.19	1.20	3.09E-04	0.56	1.35	3.87E-05	0.75	1.47	20505	11620	531698	856270	605485	914305	457911	796425
HILIC_POS_199_18044a2_224	HILIC	POS	2.224	199.1804				9.47E-01	-0.01	0.75	3.92E-01	0.18	0.81	7.41E-01	0.08	0.12	6.25E-01	-0.10	0.51	6660003	1584603	6637899	1779813	6484593	1571452	6791205	1970454
RP_POS_631_2738a11_805	RP	POS	11.81	631.2738				9.33E-03	-0.53	1.24	3.92E-01	0.17	1.30	6.91E-02	-0.44	0.82	2.97E-03	-0.61	1.34	1105632	490867	834351	509093	790467	368227	878235	619774
HILIC_POS_185_12846a0_617	HILIC	POS	0.617	185.1285				4.26E-01	0.15	0.84	3.92E-01	0.18	0.80	3.16E-01	0.24	0.44	7.34E-01	0.07	0.34	7601618	4198668	8305292	4679431	7902083	3358432	8708502	5712282
RP_POS_329_18701a5_652	RP	POS	5.65	329.1870	Tiapride OR propentofylline [M+Na]+	329.1549(100)	3	4.19E-07	0.60	1.31	3.93E-01	-0.19	1.22	8.32E-04	0.51	1.38	1.62E-04	0.70	1.41	24547	36226	488581	854334	562063	929484	415099	774409
RP_POS_319_22433a9_813	RP	POS	9.81	319.2243				1.75E-04	0.59	1.22	3.93E-01	0.18	1.07	4.70E-04	0.68	1.19	8.16E-03	0.49	1.28	1079467	489582	1558357	867879	1483735	857299	1632979	880610
RP_POS_170_06018a2_892	RP	POS	2.89	170.0602				8.73E-04	-0.57	1.19	3.93E-01	-0.18	1.04	2.45E-03	-0.66	1.22	8.35E-03	-0.48	1.13	863228	151376	743379	218986	762211	183585	724547	249922
RP_NEG_637_14545a9_358	RP	NEG	9.36	637.1455				6.53E-01	-0.09	0.52	3.93E-01	-0.18	0.60	4.33E-01	-0.17	0.46	9.89E-01	0.00	0.36	12037800	694724	11971506	798381	12040140	752501	11902871	843779
RP_POS_441_33472a12_241	RP	POS	12.24	441.3347				3.16E-01	-0.18	0.46	3.93E-01	0.18	0.52	6.36E-01	-0.09	0.34	2.22E-01	-0.27	0.67	11424113	872913	11233456	1087372	11139962	1212118	11326950	949640
HILIC_POS_294_20639a0_882	HILIC	POS	0.882	294.2064				3.41E-01	0.13	0.40	3.93E-01	-0.19	1.18	7.42E-01	0.03	0.19	3.24E-01	0.23	0.49	1966910	991032	2261714	2538518	2480502	3438003	2042927	1049813
HILIC_NEG_236_81744a7_68	HILIC	NEG	7.68	236.8174				4.95E-01	-0.14	0.44	3.93E-01	-0.17	0.67	3.00E-01	-0.22	0.40	8.36E-01	-0.05	0.26	1570791	306721	1527244	327582	1555388	356494	1499101	296826
RP_POS_199_13036a12_612	RP	POS	12.61	199.1304				8.49E-01	-0.04	0.26	3.93E-01	0.17	0.54	8.47E-01	0.05	0.33	5.59E-01	-0.13	0.42	13103385	6453003	12852375	6420033	12300933	5283418	13403816	7398630
RP_POS_822_53723a13_399	RP	POS	13.40	822.5372				4.44E-01	-0.17	0.58	3.94E-01	-0.16	0.60	3.05E-01	-0.26	0.59	7.02E-01	-0.09	0.48	5648181	2001473	5347519	1624869	5486879	1584516	5208159	1668519
RP_NEG_580_28802a9_952	RP	NEG	9.95	580.2880				1.22E-02	0.41	0.94	3.94E-01	-0.18	0.60	1.14E-01	0.32	0.75	7.67E-03	0.51	0.92	2131770	679259	2541058	1051391	2631122	971921	2450994	1127927
RP_POS_203_1499a0_58	RP	POS	0.58	203.1499				1.41E-04	0.53	1.03	3.95E-01	0.19	1.09	8.36E-04	0.63	1.21	1.14E-02	0.44	0.99	1114551	214448	1366756	517497	1322456	498510	1411055	537172
RP_POS_340_17786a5_652	RP	POS	5.65	340.1779				4.69E-07	0.60	1.31	3.95E-01	-0.19	1.22	9.42E-04	0.51	1.38	1.63E-04	0.70	1.41	60702	57833	913789	1578996	1048951	1710138	778628	1440655
HILIC_POS_161_20377a4_843	HILIC	POS	4.843	161.2038				5.05E-01	0.13	0.37	3.95E-01	-0.18	0.79	8.54E-01	0.04	0.07	3.02E-01	0.22	0.45	1407660	1045904	1553784	1152556	1652415	1027337	1455153	1268309
RP_POS_121_84098a11_668	RP	POS	11.67	121.8410				9.71E-01	0.01	0.69	3.95E-01	-0.17	0.50	7.23E-01	-0.08	0.40	6.80E-01	0.09	0.46	1469135	865737	1475650	897151	1552406	918210	1398894	878096
RP_NEG_640_2915a10_935	RP	NEG	10.94	640.2915				4.57E-02	-0.48	1.25	3.95E-01	-0.15	1.78	3.46E-02	-0.55	1.20	1.04E-01	-0.40	1.04	1545548	285551	1432776	213221	1451019	188420	1414533	235952
RP_POS_547_33252a5_307	RP	POS	5.31	547.3325				6.22E-05	0.51	1.28	3.95E-01	-0.19	1.20	8.56E-03	0.42	1.30	1.16E-03	0.61	1.37	181608	458401	932174	1621582	1070861	1749970	793487	1486967
HILIC_NEG_144_92352a5_425	HILIC	NEG	5.425	144.9235				4.84E-01	0.16	0.47	3.95E-01	0.16	0.52	3.39E-01	0.24	0.39	7.38E-01	0.08	0.20	78702047	16832977	80999235	13209473	79870259	12667049	82128211	13765394
RP_POS_840_58612a13_563	RP	POS	13.56	840.5861				2.63E-07	-1.29	2.28	3.96E-01	0.12	0.92	1.28E-06	-1.23	1.91	1.51E-07	-1.35	2.13	3077395	1055933	1845785	696657	1786263	673903	1905307	720549
RP_POS_270_79749a0_522	RP	POS	0.52	270.7975				9.93E-06	-0.64	1.21	3.96E-01	0.18	1.01	2.30E-03	-0.55	1.13	8.55E-05	-0.73	1.37	681256	97086	556351	208305	538558	210196	574145	206977
RP_POS_668_86829a0_493	RP	POS	0.49	668.8683				4.37E-08	0.66	1.33	3.96E-01	-0.19	1.20	3.41E-04	0.56	1.36	4.14E-05	0.75	1.48	103229	67913	3202947	5222909	3649065	5566211	2756830	4870873

Supplementary table 1: Metabolomics results (in asceding order according to p-value from progressive ALD vs non-progressive ALD comparison, with molecular features with ID_level of 1-2 first)

							all_ALD_vs_control			Prog_ALD_vs_non-prog_ALD			Prog_ALD_vs_control_ALD			Non-prog_ALD_vs_control			Healthy_control		all_ALD		Non-prog_ALD		Progressive_ALD	
							t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA								
Feature_ID	RP_HILIC	POS_NEG	Average.Rt	Average.Mz	Metabolite.name	curated_MSMS	ID_level	p	d	VIP	p	d	VIP	p	d	VIP	p	d	VIP	Mean	SD	Mean	SD	Mean	SD	Mean	SD
HILIC_POS_224_1277a4_785	HILIC	POS	4.785	224.1277			1.34E-01	0.30	0.53	3.96E-01	0.17	0.64	1.15E-01	0.38	0.72	2.92E-01	0.21	0.48	5097065	2077323	5748815	2218046	5559235	1644341	5938396	2676314
RP_POS_373_2251a11_608	RP	POS	11.61	373.2251			1.33E-02	-0.50	0.93	3.96E-01	0.17	0.88	4.67E-02	-0.41	0.87	1.45E-02	-0.58	0.96	5362390	494177	5102503	518036	5058254	597144	5146753	426171
RP_POS_525_3913a11_606	RP	POS	11.61	525.3913			8.74E-02	-0.34	0.72	3.96E-01	-0.17	0.79	6.75E-02	-0.43	0.78	2.31E-01	-0.25	0.69	671560	430491	516933	458593	556057	407723	477809	505514
RP_POS_159_98203a15_424	RP	POS	15.42	159.9820			8.70E-01	0.03	0.56	3.97E-01	-0.18	0.56	7.87E-01	-0.06	0.36	5.78E-01	0.12	0.37	52987851	1377154	53036189	1635687	53175672	1642262	52896706	1633652
RP_NEG_701_15576a9_437	RP	NEG	9.44	701.1558			3.39E-01	-0.20	0.58	3.97E-01	-0.17	0.63	2.28E-01	-0.28	0.57	6.17E-01	-0.11	0.32	11600312	713865	11460580	708278	11520968	670839	11400192	745712
RP_POS_310_91199a0_497	RP	POS	0.50	310.9120			1.72E-08	-0.68	1.35	3.97E-01	0.19	1.20	2.08E-04	-0.59	1.38	2.41E-05	-0.77	1.50	22879308	474248	19090713	6132902	18567833	6518664	19613592	5739479
RP_POS_570_4556a10_66	RP	POS	10.66	570.4556			2.87E-01	-0.21	0.44	3.98E-01	0.17	0.52	5.63E-01	-0.13	0.45	1.87E-01	-0.30	0.58	8813500	635418	8673479	656879	8617595	671324	8729362	644000
HILIC_POS_340_24741a0_705	HILIC	POS	0.705	340.2474			1.40E-01	-0.28	0.87	3.98E-01	0.17	0.76	3.90E-01	-0.20	0.32	7.25E-02	-0.37	0.99	1574065	629784	1375788	716881	1314797	623795	1436779	801007
HILIC_POS_274_87381a2_979	HILIC	POS	2.979	274.8738			1.33E-02	-0.44	1.22	3.98E-01	0.18	0.84	8.27E-02	-0.35	1.20	1.21E-02	-0.53	1.27	909655	183560	805881	248006	784787	255731	826974	240754
RP_POS_320_25577a9_62	RP	POS	9.62	320.2558			4.65E-01	-0.19	0.78	3.98E-01	-0.14	0.59	3.35E-01	-0.26	0.66	6.66E-01	-0.12	0.46	23687273	31944474	19284390	19294343	20925207	20522920	17643573	18040400
RP_NEG_437_1618a10_386	RP	NEG	10.39	437.1618			6.87E-01	-0.06	0.52	3.98E-01	0.19	0.52	9.09E-01	0.03	0.20	2.33E-01	-0.16	0.64	575439	658981	511634	1068366	420509	378101	602759	1464991
RP_POS_600_88123a0_493	RP	POS	0.49	600.8812			4.77E-08	0.65	1.34	3.98E-01	-0.19	1.21	3.11E-04	0.56	1.37	4.89E-05	0.75	1.48	121910	81009	2576044	4147778	2928662	4455852	2223427	3827644
HILIC_POS_156_07663a6_786	HILIC	POS	6.786	156.0766			5.73E-01	-0.10	0.93	3.98E-01	-0.18	0.88	3.48E-01	-0.19	0.68	9.51E-01	-0.01	0.75	65527446	16948440	63445251	21305605	65256267	22574580	61634236	20020398
RP_POS_321_24002a9_95	RP	POS	9.95	321.2400			2.23E-13	0.97	1.60	3.98E-01	0.17	1.12	2.64E-08	1.06	1.71	8.57E-08	0.89	1.71	1400509	560514	3006711	1694439	2862723	1569361	3150700	1815389
RP_NEG_532_30115a10_51	RP	NEG	10.51	532.3012			4.51E-01	-0.14	0.76	3.99E-01	0.18	0.55	8.12E-01	-0.06	0.48	2.42E-01	-0.23	0.91	1476994	512321	1394894	590540	1344716	466192	1445072	694347
RP_NEG_306_91946a0_512	RP	NEG	0.51	306.9195			3.02E-04	0.47	1.20	3.99E-01	-0.19	1.17	2.21E-02	0.37	1.13	2.36E-03	0.56	1.35	1167266	276269	1555903	925452	1634474	981748	1477332	868318
RP_POS_337_06329a0_706	RP	POS	0.71	337.0633			6.27E-02	0.29	0.62	3.99E-01	0.18	0.54	8.13E-02	0.38	0.75	2.06E-01	0.20	0.56	1622814	613776	1909858	1069295	1819007	771195	2000709	1303277
RP_NEG_756_82141a0_495	RP	NEG	0.50	756.8214			4.36E-09	-0.72	1.38	3.99E-01	0.19	1.21	1.36E-04	-0.62	1.42	7.39E-06	-0.81	1.53	9705174	497250	7243781	3755315	6925099	3893851	7562463	3622602
HILIC_POS_118_12287a0_85	HILIC	POS	0.85	118.1229			4.01E-01	-0.16	0.80	4.00E-01	0.17	0.83	7.30E-01	-0.07	0.13	2.60E-01	-0.25	0.46	779583	136283	755391	154027	742341	157666	768441	150755
RP_NEG_584_23071a9_952	RP	NEG	9.95	584.2307			9.71E-03	0.42	0.91	4.00E-01	-0.18	0.59	1.08E-01	0.32	0.75	6.22E-03	0.51	0.93	621677	195598	746594	321989	773864	294699	719323	348001
RP_POS_467_37024a11_422	RP	POS	11.42	467.3702			7.40E-01	0.06	0.59	4.00E-01	0.18	0.67	4.87E-01	0.15	0.39	8.74E-01	-0.03	0.58	1282666	170534	1295255	228869	1275874	213422	1314637	243958
HILIC_NEG_183_93422a4_804	HILIC	NEG	4.804	183.9342			7.01E-01	0.08	0.54	4.00E-01	0.17	0.79	4.74E-01	0.16	0.49	9.81E-01	-0.01	0.18	1784860	624434	1833678	616585	1781477	623563	1885880	611328
RP_POS_163_98772a10_57	RP	POS	10.57	163.9877			2.01E-01	-0.26	0.46	4.00E-01	0.17	0.67	4.43E-01	-0.18	0.38	1.21E-01	-0.35	0.60	1999837	565473	1851412	561883	1803841	527465	1898983	595845
RP_NEG_815_5556a12_771	RP	NEG	12.77	815.5556			6.16E-02	-0.36	0.84	4.00E-01	0.17	0.53	2.10E-01	-0.27	0.61	3.99E-02	-0.45	0.85	2047809	548500	1828301	621962	1775671	612582	1880931	632975
RP_POS_700_81635a0_495	RP	POS	0.50	700.8164			1.62E-09	-0.74	1.40	4.00E-01	0.18	1.20	9.55E-05	-0.65	1.43	3.10E-06	-0.83	1.54	2919679	199753	2083849	1223297	1980347	1248478	2187351	1201205
HILIC_POS_609_40076a1_277	HILIC	POS	1.277	609.4008			8.42E-01	0.04	0.57	4.00E-01	-0.17	0.56	8.62E-01	-0.04	0.24	5.93E-01	0.13	0.21	587688	241343	597336	223861	616273	224328	578400	224044
RP_POS_287_63608a9_952	RP	POS	9.95	287.6361			5.49E-03	0.44	0.95	4.01E-01	-0.18	0.59	7.48E-02	0.35	0.80	5.04E-03	0.53	0.97	763114	254052	941173	436155	978057	420464	904290	452525
HILIC_POS_310_20111a0_87	HILIC	POS	0.87	310.2011			8.88E-01	0.03	0.35	4.01E-01	0.17	0.59	6.26E-01	0.11	0.29	7.87E-01	-0.06	0.10	5735845	3940701	5851151	4161313	5499512	3687422	6202791	4597501
RP_POS_605_40082a10_894	RP	POS	10.89	605.4008			8.54E-01	0.04	0.62	4.01E-01	-0.17	0.50	8.20E-01	-0.05	0.44	5.89E-01	0.12	0.42	1760541	598175	1783328	640286	1837385	664924	1729270	616613
RP_POS_335_22266a5_652	RP	POS	5.65	335.2227			4.55E-07	0.60	1.31	4.01E-01	-0.19	1.20	8.57E-04	0.51	1.37	1.72E-04	0.70	1.41	52537	59483	785043	1353180	899273	1470402	670812	1229166
HILIC_NEG_200_85867a7_393	HILIC	NEG	7.393	200.8587			8.45E-01	-0.03	0.14	4.01E-01	-0.18	0.78	5.48E-01	-0.12	0.26	7.59E-01	0.06	0.14	2288403	63362	2285518	96014	2293622	90289	2277413	101683
RP_POS_194_11745a0_71	RP	POS	0.71	194.1175			4.98E-01	0.12	0.63	4.01E-01	0.18	0.53	3.28E-01	0.21	0.46	8.80E-01	0.03	0.62	2735834	286458	2779134	384244	2746706	359006	2811561	408985
RP_POS_149_99751a15_465	RP	POS	15.47	149.9975			9.33E-01	-0.02	0.43	4.02E-01	0.18	0.57	7.61E-01	0.07	0.50	5.90E-01	-0.10	0.46	4235858	2028721	4199562	2380663	3998557	1782136	4400567	2862221
RP_POS_199_13007a11_221	RP	POS	11.22	199.1301			4.02E-01	-0.21	0.38	4.02E-01	-0.15	0.50	2.79E-01	-0.28	0.57	6.18E-01	-0.13	0.36	3023113	1381721	2801286	953371	2881702	997820	2720869	909692
RP_POS_413_22025a10_874	RP	POS	10.87	413.2203			7.52E-02	0.32	0.69	4.02E-01	0.18	0.64	5.51E-02	0.41	0.83	2.49E-01	0.24	0.63	475587	221101	562449	279419	538893	268742	586005	290497
RP_POS_308_29471a10_994	RP	POS	10.99	308.2947			2.25E-07	0.70	1.13	4.02E-01	0.18	1.01	2.80E-04	0.79	1.20	2.08E-06	0.61	1.56	963779	455970	1786217	1268631	1679157	806303	1893278	1605670
RP_NEG_583_2572a5_909	RP	NEG	5.91	583.2572			4.87E-01	0.11	0.84	4.02E-01	0.18	1.11	3.38E-01	0.20	0.56	9.10E-01	0.02	1.00	813993	504715	899012	829194	829134	697604	968890	944743
RP_POS_564_35895a5_307	RP	POS	5.31	564.3590			5.56E-05	0.52	1.28	4.02E-01	-0.19	1.20	8.08E-03	0.42	1.31	1.12E-03	0.61	1.37	537874	1185658	2517612	4260139	2876455	4589932	2158769	3916334
HILIC_NEG_252_95584a4_801	HILIC	NEG	4.801	252.9558			3.00E-01	0.21	0.45	4.03E-01	0.17	0.52	1.64E-01	0.29	0.61	6.11E-01	0.12	0.28	418551	226581	467578	242385	447165	276786	487992	203073
RP_NEG_134_8931a15_597	RP	NEG	15.60	134.8931			7.12E-02	-0.25	0.72	4.03E-01	0.19	0.52	3.29E-01	-0.16	0.56	7.73E-02	-0.35	0.68	2178780	96282	2126899	228681	2107644	253304	2146154	201837
HILIC_POS_466_24567a0_8	HILIC	POS	0.8	466.2457			5.98E-01	-0.12	0.66	4.03E-01	0.16	0.56	8.65E-01	-0.04	0.37	4.28E-01	-0.20	0.70	554349	335229	519763	270589	496991	287718	542535	253163
RP_POS_298_27411a9_809	RP	POS	9.81	298.2741			4.89E-01	-0.19	0.83	4.03E-01	-0.13	0.62	3.65E-01	-0.26	0.69	6.69E-01	-0.12	0.49	5359624	9141841	4178540	4929263	4593025	5283649	3764054	4563287
HILIC_NEG_289_06821a1_415	HILIC	NEG	1.415	289.0682			6.84E-01	0.07	0.80	4.03E-01	-0.18	0.68	9.37E-01	-0.02	0.64	4.33E-01	0.16	0.91	402580	125942	413930	165650	427855	162839	400006	168901
RP_POS_320_2561a9_752	RP	POS	9.75	320.2561			1.82E-01	-0.42	1.17	4.04E-01	-0.10	0.68	1.40E-01	-0.47	0.90	2.53E-01	-0.36	0.87	8866798	14428682	5315752	5309435	5761788	5616213	4869715	5000764
RP_NEG_405_1579a11_168	RP	NEG	11.17	405.1579			5.15E-01	0.13	0.44	4.04E-01	-0.17	0.73	8.53E-01	0.04	0.57	3.27E-01	0.21	0.61	818166	101213	831942	110640	841232	106224	822651	115206
RP_POS_319_20282a10_978	RP	POS	10.98	319.2028			6.33E-03	0.45	1.32	4.04E-01	-0.18	1.22	7.00E-02	0.36	1.10	5.90E-03	0.54	1.31	1893302	869571	2472156	1381864	2588106	1354666	2356206	1412625
RP_NEG_437_16223a10_264	RP	NEG	10.26	437.1622			4.50E-01	-0.20	0.48	4.05E-01	-0.14	0.56	3.34E-01	-0.27	0.39	6.42E-01	-0.13	0.38	1580309	2020108	1291881	1241793	1396001	1171385	1187760	1311985
HILIC_POS_243_18253a1_504	HILIC	POS	1.504	243.1825			4.77E-02	0.27	0.65	4.05E-01	0.19	0.98	8.84E-02	0.36	0.73	1.83E-01	0.18	0.65	186502	174864	295612	449585	257894	305546	333331	558674
RP_POS_578_41718a11_375	RP	POS	11.38	578.4172			1.86E-01	-0.36	0.69	4.05E-01	0.14	1.31	2.97E-01	-0.29	0.52	1.37E-01	-0.42	0.75	590542	522300	459839	298597	434816	321350	484861	274948
RP_POS_647_45752a14_19	RP	POS	14.19	647.4575			2.87E-01	0.16	0.40	4.05E-01	-0.18	0.50	6.93E-01	0.07	0.49	2.00E-01	0.25	0.49	613956	332150	705005	614883	756525	659303	653485	569017
RP_POS_812_50983a10_932	RP	POS	10.93	812.5098			2.30E-02	-0.54	1.19	4.05E-01	-0.15	1.43	1.61E-02	-0.62	1.13	6.22E-02	-0.47	1.07	524087	279490	397664	208125	415098	203588	380229	213185
RP_POS_260_87869a0_251	RP	POS	0.25	260.8787			4.88E-01	-0.15	0.36	4.05E-01	-0.16	1.04	3.38E-01	-0.23	0.51	7.60E-01	-0.07	0.41	2401412	309481	2358773	268448	2381260	257811	2336286	279465
HILIC_POS_334_08151a5_462	HILIC	POS	5.462	334.0815			2.75E-01	-0.24	0.43	4.05E-01	-0.16	0.77	1.94E-01	-0.32	0.53	4.97E-01	-0.16	0.28	1649494	280050	1588306	248626	1609128	227208	1567484	269040
HILIC_NEG_311_14035a1_689	HILIC	NEG	1.689	311.1404			5.83E-06	0.54	1.27	4.05E-01	0.19	0.81	1.08E-03	0.63	1.42	1.54E-03	0.44	1.32	14755	21704	919717	1888425	761571	1573423	1077864	2162955
RP_POS_565_28265a5_011	RP	POS	5.01	565.2827			1.05E-06	0.58	1.25	4.05E-01	-0.19	1.17	1.19E-03	0.49	1.34	2.92E-04	0.67	1.35	20801	16875	1149072	2167009	1330447	2374123	967697	1945273
RP_POS_324_21762a9_441	RP	POS	9.44	324.2176			2.63E-01	-0.21	0.42	4.05E-01	-0.17	0.96	1.92E-01	-0.29	0.54	5.48E-01	-0.12	0.39	1189472	79108	1170255	96977	1178371	84336	1162138	108416
RP_POS_265_25317a10_223	RP	POS	10.22	265.2532			5.99E-01	0.10	0.79	4.06E-01	0.18	0.81	3.90E-01	0.18	0.67	9.69E-01	0.01	0.77	1927666	258824	1957354	325330	1930133	317148	1984574	334281
RP_POS_522_79742a10_501	RP	POS	10.50	522.7974			2.30E-01	-0.27	0.74	4.06E-01	0.16	0.50	4.30E-01	-0.19	0.45	1.57E-01	-0.35	0.81	5254167	1277593	4949860	1074395	4859977	1109686	5039742	1041305
RP_POS_635_38452a5_652	RP	POS	5.65	635.3845			4.26E-07	0.60	1.31	4.06E-01	-0.19	1.21	8.68E-04	0.51	1.37	1.60E-04	0.70	1.41	25616	40237	551214	968365	632220	1047724	470208	885144
RP_POS_265_25269a10_555	RP	POS	10.56	265.2527			8.25E-04	-0.61	1.13	4.06E-01	0.17	0.88	8.46E-03	-0.53	1.04	1.30E-03	-0.70	1.21	573411	78483	513633	99008	505354	105736	521913	92116
HILIC_POS_178_08606a3_645	HILIC	POS	3.645	178.0861			4.87E-01	-0.14	0.58	4.06E-01	-0.17	0.65	3.10E-01	-0.22	0.39	8.13E-01	-0.05	0.50	1510811	637908	1418969	672503	1475161	704175	1362776	641439
RP_NEG_473_34885a11_551	RP	NEG	11.55	473.3489			9.28E-01	0.01	0.43	4.06E-01	-0.19	0.69	2.39E-01	-0.08	0.68	6.49E-01	0.11	0.51	1498030	2399004	1577353	7679098	2221434	10774020	933272	1488083
RP_POS_342_2637a7_887	RP	POS	7.89	342.2637			1.02E-03	0.54	1.08	4.06E-01	0.18	0.80	2.96E-03	0.62	1.09	1.24E-02	0.45	1.12	2334194	1064954	3197757	1701354	3055638	1484217	3339875	1898463
HILIC_POS_338_14975a0_767	HILIC	POS	0.767	338.1498			3.00E-01	-0.14	0.46	4.07E-01	0.19	0.62	7.85E-01	-0.05	0.13	1.78E-01	-0.24	0.57	23502841	5253831	21829798	13114692	20735472	12806548	22924124	13455436
HILIC_POS_158_11755a2_288	HILIC	POS	2.288	158.1176			9.93E-05	0.56	1.01	4.07E-01	0.18	0.75	2.10E-03	0.65	1.10	1.59E-03	0.47	1.08	602706	193419	821938	422417	786666	316021	857210	508041
RP_POS_790_53522a12_745	RP	POS	12.75	790.5352			3.61E-03	-0.65	1.43	4.07E-01	-0.15	0.70	3.11E-03	-0.72	1.46	1.45E-02	-0.57	1.13	2652343	1002110	2047963	866012	2120154	810070	1975772	921092
RP_POS_801_55127a11_626	RP	POS	11.63	801.5513			5.85E-01	0.09	0.24	4.07E-01	0.18	0.60	4.09E-01	0.18	0.44	9.75E-01	0.01	0.60	1248305	322797	1288141	449063	1250693	366411	1325588	519916
RP_POS_844_77747a0_497	RP	POS	0.50	844.7775			1.17E-09	-0.74	1.41	4.08E-01	0.18	1.21	8.64E-05	-0.65	1.45	2.84E-06	-0.83	1.55	1900977	106398	1374887	768209	1310887	782921	1438887	755651
HILIC_POS_139_12299a0_691	HILIC	POS	0.691	139.1230			7.80E-01	0.05	0.28	4.08E-01	0.17	0.69	5.13E-01	0.14	0.25	8.95E-01	-0.03	0.57	10813460	4101948	11052672	4450385	10681908	4808706	11423435	4075764
RP_NEG_502_27188a9_951	RP	NEG	9.95	502.2719			8.86E-03	0.42	0.92	4.08E-01	-0.18	0.58	9.99E-02	0.33	0.75	5.73E-03	0.51	0.94	763663	250047	924277	405151	958015	369549	890538	439038
HILIC_POS_163_08652a0_637	HILIC	POS	0.637	163.0865			5.87E-06	0.74	1.41	4.08E-01	0.17	0.93	1.05E-04	0.83	1.31	1.52E-04	0.66	1.62	106882	229515	370693	364241	340356	298958	401031	420472
RP_POS_382_0553a0_615	RP	POS	0.62	382.0553			2.13E-07	0.66	1.25	4.08E-01	-0.18	1.09	1.17E-04	0.56	1.39	1.52E-04	0.75	1.37	121924	72534	297258	292522	321617	335477	272900	243164
RP_NEG_552_3316a10_583	RP	NEG	10.58	552.3316			5.31E-01	-0.13	0.81	4.08E-01	-0.17	1.03	3.53E-01	-0.21	0.62	8.51E-01	-0.04	0.44	822133	339462	778345	349680	807442	349540	749248	350915
RP_POS_326_24545a9_368	RP	POS	9.37	326.2455			4.54E-01	0.13	0.58	4.08E-01	-0.18	0.59	8.36E-01	0.04	0.32	3.32E-01	0.22	0.69	481269	72452	493834	107391	502774	126933	484893	83821
RP_POS_242_13062a5_147	RP	POS	5.15	242.1306			8.95E-02	0.22	0.48	4.08E-01	-0.19	0.50	1.06E-01	0.12	0.91	1.80E-01	0.31	0.59	4313454	5782156	8298012	20925564	10044481	28938390	6551543	6406211
RP_POS_810_53583a13_196	RP	POS	13.20	810.5358			2.16E-02	0.44	0.80	4.09E-01	0.17	0.85	1.48E-02	0.52	0.97	1.04E-01	0.35	0.67	902399	352399	1078214	409435	1044182	421069	1112246	398790
RP_POS_341_30478a11_172	RP	POS	11.17	341.3048			8.43E-01	0.03	0.35	4.09E-01	0.18	0.60	5.64E-01	0.12	0.48	7.49E-01	-0.06	0.41	340018	228346	350732	357924	320975	308245	380489	402506
RP_POS_313_20966a5_487	RP	POS	5.49	313.2097			1.22E-06	0.58	1.31	4.09E-01	-0.18	1.21	1.45E-03	0.49	1.37	2.49E-04	0.67	1.41	30253	65228	350655	611552	401457	660822	299853	560064
HILIC_POS_118_65714a3_687	HILIC	POS	3.687	118.6571			8.11E-02	0.32	0.60	4.09E-01	0.17	0.93	7.92E-02	0.40	0.73	2.19E-01	0.23	0.56	933980	729841	1215323	925795	1138375	721931	1292271	1094722
RP_POS_806_50671a11_625	RP	POS	11.63	806.5067			5.61E-01	0.10	0.24	4.09E-01	0.18	0.56	3.93E-01	0.19	0.40	9.54E-01	0.01	0.60	8558296	2482543	8887983	3552612	8592993	2923583	9182973	4095699
RP_POS_795_57495a13_395	RP	POS	13.40	795.5750			9.49E-01	0.01	0.37	4.10E-01	-0.16	0.53	7.77E-01	-0.07	0.49	6.85E-01	0.10	0.50	6249705	2125244	6276952	1942936	6438081	1895964	6115824	1994838
HILIC_NEG_153_86877a7_393	HILIC	NEG	7.393	153.8688			8.72E-01	0.03	0.35	4.10E-01	0.17	0.49	5.95E-01	0.12	0.33	7.73E-01	-0.06	0.35	512517	34526	513735	43638	510117	39766	517353	47322
RP_POS_897_53479a10_842	RP	POS	10.84	897.5348			6.50E-03	0.33	0.72	4.10E-01	-0.19	0.73	7.40E-02	0.24	0.73	3.08E-02	0.43	0.92	1493480	186034	1749307	863234	1820858	1017738	1677756	677728
RP_NEG_204_06639a4_894	RP	NEG	4.89	204.0664			4.12E-02	0.30	0.69	4.10E-01	-0.18	0.55	2.39E-01	0.21	0.53	4.15E-02	0.39	0.76	5045142	1622025	5952670	3327455	6228241	3487007	5677098	3171069
HILIC_NEG_512_29919a1_357	HILIC	NEG	1.357	512.2992			7.69E-04	0.52	0.78	4.10E-01	-0.18	0.46	2.64E-02	0.43	0.73	1.03E-03	0.61	1.12	292043	104089	383942	190200	399693	181411	368190	199184
RP_POS_1003_66943a10_378	RP	POS	10.38	1003.6694			3.98E-03	0.50	1.13	4.10E-01	-0.17	0.79	4.26E-02	0.41	0.93	3.82E-03	0.58	1.15	209535	182278	332446	259042	353894	255608	310997	263250
RP_POS_337_70026a5_652	RP	POS	5.65	337.7003			4.23E-07	0.60	1.31	4.10E-01	-0.18	1.21	8.47E-04	0.51	1.38	1.63E-04	0.69	1.41	116241	103518	1510693	2568714	1723386	2780029	1297999	2347415
HILIC_NEG_134_8947a5_136	HILIC	NEG	5.136	134.8947			6.41E-01	-0.09	0.28	4.11E-01	0.17	0.62	9.82E-01	0.00	0.07	4.31E-01	-0.18	0.29	21413138	5229450	20901292	5840275	20417792	6023230	21384792	5670743

Supplementary table 1: Metabolomics results (in asceding order according to p-value from progressive ALD vs non-progressive ALD comparison, with molecular features with ID_level of 1-2 first)

								all_ALD_vs_control			Prog_ALD_vs_non-prog_ALD			Prog_ALD_vs_control_ALD			Non-prog_ALD_vs_control			Healthy_control		all_ALD		Non-prog_ALD		Progressive_ALD	
								t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA								
Feature_ID	RP_HILIC	POS_NEG	Average.Rt	Average.Mz	Metabolite.name	curated_MSMS	ID_level	p	d	VIP	p	d	VIP	p	d	VIP	p	d	VIP	Mean	SD	Mean	SD	Mean	SD	Mean	SD
HILIC_NEG_132_90036a2_172	HILIC	NEG	2.172	132.9004				8.32E-01	0.04	0.68	4.11E-01	-0.17	0.78	8.30E-01	-0.05	0.25	5.41E-01	0.13	0.38	1937252	416730	1956242	506534	1998178	470408	1914307	541772
RP_POS_303_23172a10_099	RP	POS	10.10	303.2317				1.82E-01	0.18	0.36	4.11E-01	-0.19	0.58	4.52E-01	0.09	0.31	2.12E-01	0.28	0.47	274350	336741	413488	847349	483749	1096251	343228	488686
HILIC_POS_526_29309a1_766	HILIC	POS	1.766	526.2931				9.28E-03	0.41	0.76	4.11E-01	-0.18	0.65	8.56E-02	0.32	0.58	1.08E-02	0.50	0.92	1709479	595411	2097593	1011574	2181307	1038361	2013878	987396
RP_NEG_272_79538a0_521	RP	NEG	0.52	272.7954				2.37E-04	0.46	1.23	4.11E-01	-0.18	1.19	2.00E-02	0.37	1.19	2.58E-03	0.55	1.36	588669	89107	734966	353086	764182	377556	705750	328015
RP_POS_413_26755a11_391	RP	POS	11.39	413.2676				3.25E-01	-0.20	0.42	4.11E-01	0.17	0.63	6.28E-01	-0.12	0.32	1.78E-01	-0.28	0.57	17359831	1716024	17012375	1737848	16868572	1377687	17156178	2040011
RP_POS_154_96451a0_252	RP	POS	0.25	154.9645				4.78E-01	0.15	0.56	4.11E-01	-0.17	0.53	7.69E-01	0.06	0.47	3.41E-01	0.23	0.45	5229781	846198	5352132	833695	5421065	933798	5283200	722914
HILIC_POS_144_10196a3_375	HILIC	POS	3.375	144.1020				2.72E-01	0.13	0.52	4.12E-01	0.19	1.09	3.29E-01	0.23	0.55	4.40E-01	0.04	0.26	2318099	1660782	3680564	11988581	2686416	2639895	4674713	16774960
RP_POS_388_35327a12_166	RP	POS	12.17	388.3533				6.05E-01	-0.11	0.63	4.12E-01	-0.16	0.50	4.04E-01	-0.19	0.44	9.14E-01	-0.03	0.40	2582677	1628830	2411418	1588491	2542481	1656686	2280355	1522642
HILIC_NEG_348_00107a7_352	HILIC	NEG	7.352	348.0011				4.77E-03	0.51	1.35	4.12E-01	-0.17	0.78	4.34E-02	0.43	0.81	3.67E-03	0.60	1.22	4680394	120731	4757456	155221	4770255	148739	4744658	161930
RP_POS_647_16553a11_289	RP	POS	11.29	647.1655				1.20E-01	0.28	0.73	4.12E-01	-0.17	0.59	3.44E-01	0.19	0.57	8.82E-02	0.36	0.76	323768	115834	364021	153088	376643	161037	351399	145231
HILIC_NEG_315_04202a7_428	HILIC	NEG	7.428	315.0420				4.38E-01	0.16	0.64	4.12E-01	0.16	0.66	2.78E-01	0.25	0.92	7.31E-01	0.08	0.43	2236241	327497	2287528	308599	2262084	336249	2312973	279330
RP_POS_652_41095a5_652	RP	POS	5.65	652.4110				5.03E-07	0.60	1.31	4.12E-01	-0.18	1.20	9.41E-04	0.51	1.37	1.75E-04	0.69	1.41	102878	103001	1414059	2432944	1614644	2629442	1213475	2227815
HILIC_POS_387_21365a4_123	HILIC	POS	4.123	387.2137				1.71E-04	-0.73	1.27	4.13E-01	-0.16	1.16	2.13E-04	-0.81	1.30	2.29E-03	-0.65	1.08	2118595	403160	1778799	455753	1816352	450055	1741246	462853
RP_POS_371_24298a10_241	RP	POS	10.24	371.2430				7.78E-07	0.59	1.17	4.13E-01	-0.18	1.05	1.93E-03	0.50	1.16	1.34E-04	0.68	1.35	19823	20367	480736	873010	552655	908606	408816	838885
RP_POS_419_35239a13_194	RP	POS	13.19	419.3524				3.81E-01	0.17	0.56	4.13E-01	0.17	0.48	2.55E-01	0.26	0.76	6.89E-01	0.09	0.18	2079618	375172	2148563	412597	2114583	399031	2182543	427042
RP_POS_430_31641a10_241	RP	POS	10.24	430.3164				4.43E-05	0.48	0.93	4.14E-01	-0.19	0.85	1.24E-02	0.39	0.93	1.34E-03	0.57	1.12	60073	27101	423867	850123	493784	900742	353949	799284
RP_POS_217_10449a10_574	RP	POS	10.57	217.1045				2.85E-01	0.22	0.34	4.14E-01	-0.16	0.62	5.57E-01	0.14	0.27	1.76E-01	0.30	0.57	2447967	854992	2635486	853881	2705656	791816	2565317	914375
RP_POS_358_30698a11_37	RP	POS	11.37	358.3070				8.11E-01	-0.05	0.64	4.14E-01	-0.16	0.49	5.67E-01	-0.13	0.39	8.91E-01	0.03	0.38	5874941	4038103	5679290	3896612	5999423	3976975	5359157	3827736
HILIC_POS_203_15015a6_49	HILIC	POS	6.49	203.1502				1.17E-02	0.40	0.96	4.14E-01	0.18	0.91	1.40E-02	0.49	0.83	9.03E-02	0.32	0.97	4339940	1164806	5064532	1919528	4906879	1829473	5222185	2011634
RP_POS_288_92123a15_367	RP	POS	15.37	288.9212				4.45E-01	-0.11	0.46	4.14E-01	-0.18	0.58	2.77E-01	-0.20	0.56	9.01E-01	-0.02	0.44	3677011	119596	3652756	235742	3672116	233791	3633395	238453
RP_NEG_217_95235a15_411	RP	NEG	15.41	217.9524				1.63E-01	-0.32	0.58	4.14E-01	-0.15	0.67	1.06E-01	-0.40	0.65	3.24E-01	-0.25	0.40	3954239	235739	3889431	185938	3904698	193271	3874164	178947
HILIC_POS_502_29175a1_798	HILIC	POS	1.798	502.2918				1.09E-06	0.86	1.47	4.15E-01	-0.16	0.52	3.54E-04	0.78	1.25	3.84E-07	0.94	2.05	2472246	831657	3464108	1139951	3557723	889687	3370492	1347616
RP_POS_627_26117a7_407	RP	POS	7.41	627.2612				6.08E-01	-0.10	0.44	4.15E-01	-0.17	0.71	4.11E-01	-0.18	0.39	9.51E-01	-0.01	0.46	733701	80747	724909	92930	732536	88266	717283	97667
RP_POS_278_96878a15_333	RP	POS	15.33	278.9688				2.65E-01	-0.20	0.49	4.15E-01	-0.17	0.49	1.51E-01	-0.29	0.63	5.98E-01	-0.11	0.42	3564740	156008	3526493	199809	3542887	217084	3510098	181627
RP_NEG_594_37946a11_007	RP	NEG	11.01	594.3795				2.83E-01	-0.26	0.79	4.15E-01	0.15	1.37	4.81E-01	-0.19	0.60	1.87E-01	-0.33	0.89	3339423	1508839	3026355	1088258	2937086	978263	3115625	1191435
RP_POS_679_4101a5_803	RP	POS	5.80	679.4101				2.40E-07	0.62	1.31	4.15E-01	-0.18	1.21	5.93E-04	0.52	1.39	1.32E-04	0.71	1.42	7439	5099	304010	534419	347838	579993	260181	486543
RP_POS_818_56506a13_297	RP	POS	13.30	818.5651				1.83E-02	-0.52	1.18	4.15E-01	-0.16	0.58	2.03E-02	-0.59	1.28	4.38E-02	-0.44	0.90	3616139	1848442	2722022	1644407	2856938	1172545	2587105	2012789
RP_POS_203_13878a0_684	RP	POS	0.68	203.1388				1.05E-04	0.59	1.00	4.15E-01	0.17	0.86	1.78E-04	0.68	1.34	9.72E-03	0.50	1.09	430713	319145	764122	602502	714760	643623	813484	560537
RP_POS_657_36591a5_652	RP	POS	5.65	657.3659				5.08E-07	0.60	1.31	4.16E-01	-0.18	1.21	9.32E-04	0.51	1.38	1.79E-04	0.69	1.41	48269	62041	855449	1498507	978126	1619914	732772	1371874
RP_POS_778_63098a11_673	RP	POS	11.67	778.6310				9.72E-01	-0.01	0.63	4.16E-01	-0.16	0.50	6.97E-01	-0.09	0.43	7.38E-01	0.08	0.34	1711107	776341	1705602	788285	1770036	770888	1641167	807915
RP_NEG_331_95239a6_868	RP	NEG	6.87	331.9524				1.15E-01	-0.31	0.66	4.17E-01	-0.17	1.12	2.87E-01	-0.22	0.72	8.83E-02	-0.39	0.81	1009174	120201	969047	133059	958172	145028	979922	120400
HILIC_NEG_115_92066a6_088	HILIC	NEG	6.088	115.9207				7.45E-01	0.07	0.55	4.17E-01	-0.17	0.51	9.39E-01	-0.02	0.23	5.15E-01	0.15	0.46	43726613	15548990	44767057	16067253	46078526	16386407	43455587	15797383
RP_POS_410_76077a12_818	RP	POS	12.82	410.7608				9.16E-07	-1.13	1.82	4.17E-01	-0.14	0.71	6.91E-07	-1.20	1.90	8.30E-06	-1.06	1.63	1930606	694086	1162637	563565	1208602	578402	1116672	550303
RP_POS_287_62479a10_042	RP	POS	10.04	287.6248				8.14E-02	0.33	0.83	4.18E-01	-0.17	0.72	2.66E-01	0.25	0.73	4.58E-02	0.42	0.95	813292	591854	1034362	678147	1089665	612211	979060	740343
RP_POS_151_00529a10_57	RP	POS	10.57	151.0053				4.08E-01	-0.18	0.28	4.18E-01	0.16	0.54	6.78E-01	-0.10	0.31	2.68E-01	-0.26	0.50	2427937	845722	2288156	754304	2226656	708368	2349656	800035
HILIC_POS_158_11763a0_523	HILIC	POS	0.523	158.1176				1.07E-02	-0.75	1.81	4.18E-01	-0.11	0.55	7.16E-03	-0.81	1.29	2.08E-02	-0.70	1.38	1075992	934789	616613	408656	649934	449928	583291	364290
RP_POS_136_98964a15_443	RP	POS	15.44	136.9896				2.67E-01	-0.31	0.81	4.18E-01	0.13	0.65	3.90E-01	-0.24	0.45	2.04E-01	-0.37	0.76	56498037	15830334	53199800	8513440	52505817	9376941	53893783	7584627
RP_POS_178_05885a0_511	RP	POS	0.51	178.0589				4.25E-04	0.45	1.13	4.18E-01	-0.18	1.14	1.99E-02	0.36	1.17	4.16E-03	0.54	1.22	551215	95271	683654	325068	710142	357629	657166	290111
RP_POS_159_09187a2_894	RP	POS	2.89	159.0919				9.77E-04	-0.57	1.20	4.18E-01	-0.17	1.14	2.96E-03	-0.65	1.21	7.75E-03	-0.48	1.14	4293800	715548	3735947	1019954	3819065	838578	3652828	1176660
RP_POS_307_17932a5_031	RP	POS	5.03	307.1793				1.11E-04	-0.68	1.17	4.18E-01	-0.17	0.96	2.68E-03	-0.60	1.16	2.30E-04	-0.76	1.28	732353	223225	528090	305814	503193	313536	552987	298970
RP_POS_186_03168a6_397	RP	POS	6.40	186.0317				2.82E-03	0.50	1.03	4.18E-01	-0.17	0.53	2.84E-02	0.41	0.92	5.03E-03	0.58	1.04	1782015	1022357	2520693	1576030	2648979	1697810	2392406	1449927
RP_POS_546_35272a11_255	RP	POS	11.26	546.3527				1.02E-01	0.29	1.09	4.18E-01	-0.17	0.77	3.46E-01	0.20	0.77	5.51E-02	0.38	1.15	743497	386417	885078	513572	926885	457619	843271	565608
RP_POS_318_1962a5_652	RP	POS	5.65	318.1962				4.66E-07	0.60	1.31	4.19E-01	-0.18	1.21	9.21E-04	0.51	1.38	1.67E-04	0.69	1.41	31422	40038	628781	1105419	718754	1191599	538808	1016077
RP_POS_554_46222a10_89	RP	POS	10.89	554.4622				3.13E-02	-0.41	0.84	4.19E-01	0.17	0.77	1.44E-01	-0.32	0.79	1.82E-02	-0.49	0.91	1278546	503005	1043257	590578	995207	539228	1091308	639690
HILIC_POS_314_18082a1_952	HILIC	POS	1.952	314.1808				5.93E-01	0.11	1.07	4.19E-01	-0.16	0.78	8.80E-01	0.03	0.94	4.25E-01	0.19	1.09	986896	2800652	1287326	2587377	1497821	2827024	1076831	2333061
RP_POS_820_52234a13_07	RP	POS	13.07	820.5223				5.05E-02	0.45	0.96	4.19E-01	-0.15	0.62	1.47E-01	0.37	0.69	2.73E-02	0.52	1.10	13444793	4231741	15102329	3475204	15385099	2896897	14819559	3980622
RP_POS_349_18936a10_704	RP	POS	10.70	349.1894				1.74E-03	0.58	1.41	4.19E-01	0.17	1.25	3.76E-03	0.66	1.36	9.47E-03	0.50	1.30	5223812	849553	5823329	1053397	5737617	848829	5909041	1227369
RP_POS_367_33591a11_469	RP	POS	11.47	367.3359				1.92E-01	0.19	0.41	4.19E-01	0.18	0.76	1.70E-01	0.28	0.55	5.42E-01	0.10	0.51	554999	402095	702963	873613	631906	730758	774019	998831
HILIC_POS_389_31216a2_202	HILIC	POS	2.202	389.3122				2.00E-01	0.24	0.60	4.19E-01	0.17	0.69	1.49E-01	0.32	0.62	4.51E-01	0.15	0.31	750926	380369	857122	468813	819010	421658	895235	513124
RP_NEG_390_87552a15_346	RP	NEG	15.35	390.8755				2.49E-01	-0.17	0.42	4.19E-01	-0.18	0.48	1.76E-01	-0.26	0.55	6.61E-01	-0.08	0.48	985786	33432	975166	70128	980866	67060	969465	73300
RP_POS_854_56519a13_087	RP	POS	13.09	854.5652				1.72E-04	-0.77	1.29	4.19E-01	0.15	0.49	2.68E-03	-0.70	1.12	9.39E-05	-0.85	1.51	4277939	1715366	2865073	1736594	2723953	1514077	3006193	1939069
RP_POS_211_13051a5_596	RP	POS	5.60	211.1305				3.57E-01	0.12	0.32	4.19E-01	-0.18	0.59	7.43E-01	0.03	0.91	3.60E-01	0.21	0.45	501578	469594	662289	1528322	786842	2104910	537736	506850
RP_POS_223_0945a0_483	RP	POS	0.48	223.0945				8.61E-05	0.50	1.10	4.19E-01	-0.18	1.09	1.29E-02	0.41	0.96	1.13E-03	0.59	1.34	10239488	419209	10937623	1553415	11063782	1619777	10811464	1489726
RP_NEG_297_24411a10_172	RP	NEG	10.17	297.2441				3.69E-01	-0.17	0.68	4.20E-01	-0.17	0.86	2.30E-01	-0.25	0.62	6.95E-01	-0.09	0.66	7523201	1045103	7322803	1216722	7421617	1271790	7223989	1163469
RP_NEG_830_59357a13_934	RP	NEG	13.93	830.5936				1.88E-01	0.26	0.61	4.20E-01	0.17	0.53	1.30E-01	0.34	0.58	4.22E-01	0.17	0.77	33932084	36296333	44018880	40277783	40747963	38850357	47289798	41791423
RP_POS_279_15961a9_524	RP	POS	9.52	279.1596				8.96E-01	0.02	0.48	4.20E-01	0.17	0.58	6.19E-01	0.11	0.39	7.53E-01	-0.06	0.63	5436020	890101	5461445	1145459	5368444	1027058	5554445	1256357
RP_NEG_160_97664a15_333	RP	NEG	15.33	160.9766				7.34E-01	-0.05	0.47	4.20E-01	0.18	0.79	8.25E-01	0.03	0.74	5.33E-01	-0.14	0.27	5167386	205302	5150513	335854	5123222	426979	5177804	209922
RP_POS_548_50323a13_808	RP	POS	13.81	548.5032				9.84E-02	-0.39	0.83	4.20E-01	-0.15	0.54	6.97E-02	-0.46	0.77	2.06E-01	-0.31	0.88	3616660	1168686	3236091	899375	3309031	867141	3163150	933524
RP_NEG_400_14725a11_254	RP	NEG	11.25	400.1473				4.36E-07	0.95	1.86	4.20E-01	0.15	1.17	2.66E-06	1.03	1.80	1.00E-05	0.88	1.76	1383508	874304	2438477	1050269	2353294	936526	2523659	1156180
RP_POS_283_26273a10_55	RP	POS	10.55	283.2627				1.58E-01	-0.30	0.76	4.20E-01	0.16	0.82	3.48E-01	-0.22	0.67	1.08E-01	-0.38	0.72	3986005	597238	3813953	574734	3767351	583425	3860555	567947
RP_POS_271_65848a10_326	RP	POS	10.33	271.6585				1.14E-02	-0.60	1.21	4.20E-01	-0.15	0.69	9.26E-03	-0.67	1.21	3.19E-02	-0.53	1.11	1301359	318745	1139315	242409	1158966	222011	1119665	262006
RP_POS_299_16107a9_095	RP	POS	9.10	299.1611				8.39E-01	0.03	1.19	4.21E-01	-0.17	0.50	7.77E-01	-0.05	0.26	5.69E-01	0.12	1.73	2097000	74843	2100519	110452	2109465	122311	2091573	97595
RP_POS_351_20013a5_802	RP	POS	5.80	351.2001				3.04E-07	0.61	1.31	4.21E-01	-0.18	1.21	6.86E-04	0.52	1.39	1.46E-04	0.70	1.41	23678	21520	567575	989323	647606	1070675	487545	904476
RP_POS_696_84479a0_471	RP	POS	0.47	696.8448				9.02E-09	-0.77	1.38	4.21E-01	0.17	1.15	1.29E-04	-0.68	1.40	1.57E-06	-0.85	1.54	640156	94556	441604	276293	419259	271264	463949	282188
RP_POS_553_46021a11_608	RP	POS	11.61	553.4602				3.34E-02	-0.43	0.89	4.22E-01	0.16	0.56	1.18E-01	-0.35	0.68	2.29E-02	-0.51	0.90	34948724	6605442	32009001	6696254	31467794	6594837	32550207	6819464
RP_POS_315_19354a9_788	RP	POS	9.79	315.1935		315.1942(100)	4	6.07E-03	-0.48	0.82	4.22E-01	0.17	0.70	4.84E-02	-0.40	0.73	6.30E-03	-0.57	1.06	11775237	382337	11533379	523876	11491087	532930	11575672	516555
RP_POS_379_17502a7_472	RP	POS	7.47	379.1750				5.02E-09	0.72	1.33	4.22E-01	0.18	1.00	2.35E-05	0.81	1.45	3.12E-05	0.63	1.31	147543	219395	965287	1234314	865638	1084750	1064936	1371571
RP_POS_512_26782a10_067	RP	POS	10.07	512.2678				3.34E-02	0.27	0.61	4.22E-01	0.18	0.61	7.25E-02	0.36	0.67	1.85E-01	0.18	0.48	398483	332134	677434	1157191	583993	888237	770874	1377943
RP_NEG_341_26999a10_614	RP	NEG	10.61	341.2700				1.11E-02	-0.57	0.94	4.23E-01	0.15	0.50	3.87E-02	-0.49	0.80	8.25E-03	-0.64	1.06	989217	303762	831617	258074	810809	262224	852424	254791
HILIC_POS_284_16989a0_779	HILIC	POS	0.779	284.1699				9.86E-01	0.00	0.69	4.23E-01	0.16	0.91	7.03E-01	0.09	0.19	7.17E-01	-0.08	0.70	1312448	282060	1313513	306671	1288805	293958	1338220	319932
RP_POS_356_26138a8_862	RP	POS	8.86	356.2614				4.67E-01	-0.15	0.74	4.23E-01	0.16	0.50	7.83E-01	-0.06	0.54	2.94E-01	-0.23	0.60	673375	335814	622853	351516	594531	318047	651175	383221
RP_POS_348_28723a9_95	RP	POS	9.95	348.2872				4.10E-01	-0.22	0.84	4.23E-01	-0.13	0.63	2.94E-01	-0.29	0.71	5.94E-01	-0.15	0.46	2186612	3685317	1614161	2187161	1790324	2455824	1437998	1889594
HILIC_POS_371_2402a4_905	HILIC	POS	4.905	371.2402				6.84E-01	-0.08	0.73	4.24E-01	0.16	0.80	9.99E-01	0.00	0.10	4.48E-01	-0.16	0.52	16179012	4475135	15803439	4645359	15429363	4101445	16177516	5147007
HILIC_NEG_225_06306a0_753	HILIC	NEG	0.753	225.0631				4.56E-01	0.12	0.39	4.24E-01	-0.17	0.48	8.67E-01	0.03	0.21	2.72E-01	0.21	0.38	217075	227964	257859	365690	287302	347021	228416	384701
RP_POS_802_79736a0_496	RP	POS	0.50	802.7974				5.80E-09	-0.70	1.38	4.24E-01	0.18	1.21	1.49E-04	-0.61	1.42	1.10E-05	-0.79	1.52	9102383	302261	6672755	3785922	6367965	3938693	6977544	3640883
RP_POS_187_05771a0_611	RP	POS	0.61	187.0577				1.47E-05	0.60	1.19	4.24E-01	-0.17	1.08	2.21E-03	0.51	1.21	3.65E-04	0.68	1.33	10114806	2764816	14000443	7092792	14570634	7643182	13430253	6523828
RP_NEG_230_99678a4_547	RP	NEG	4.55	230.9968				3.72E-01	-0.25	0.54	4.25E-01	-0.13	0.54	2.53E-01	-0.31	0.60	5.44E-01	-0.19	0.36	2228117	7869453	916326	4137257	1249654	5591436	582997	1758470
RP_POS_249_15567a0_577	RP	POS	0.58	249.1557				4.49E-03	0.45	0.72	4.25E-01	-0.17	0.84	9.51E-02	0.36	0.65	1.05E-03	0.53	1.12	699030	362901	959680	623455	1009806	458691	909555	754851
RP_POS_219_08257a0_505	RP	POS	0.51	219.0826				2.13E-06	0.57	1.26	4.25E-01	-0.18	1.18	1.67E-03	0.48	1.28	3.93E-04	0.66	1.38	293135	76827	720527	840157	788023	915900	653031	760240
HILIC_POS_330_33624a0_527	HILIC	POS	0.527	330.3362				7.72E-03	-0.51	1.20	4.25E-01	0.16	0.63	4.70E-02	-0.43	0.76	6.03E-03	-0.59	1.13	2578483	618235	2219360	707723	2162526	694924	2276193	722810
RP_POS_637_30396a10_563	RP	POS	10.56	637.3040				1.37E-03	-0.56	0.90	4.25E-01	0.17	0.53	3.19E-02	-0.47	0.74	4.88E-04	-0.64	1.20	4729034	312310	4494675	436813	4459579	345289	4529770	513583
RP_POS_286_09607a0_709	RP	POS	0.71	286.0961				5.21E-12	0.85	1.57	4.25E-01	0.17	0.63	2.46E-06	0.94	1.56	1.44E-07	0.76	1.75	33986	39078	261600	285782	238652	233825	284547	330546
RP_POS_609_30902a5_216	RP	POS	5.22	609.3090				1.16E-06	0.58	1.27	4.25E-01	-0.18	1.15	1.02E-03	0.49	1.35	3.58E-04	0.67	1.35	49921	137935	1554405	2895771	1786868	3198497	1321943	2569327
RP_POS_363_78888a0_248	RP	POS	0.25	363.7889				9.90E-01	0.00	0.40	4.25E-01	-0.15	0.53	7.61E-01	-0.07	0.32	7.43E-01	0.08	0.46	733346	90174	733577	76131	739687	76549	727468	75989
RP_POS_281_24738a10_978	RP	POS	10.98	281.2474				6.87E-03	0.45	1.37	4.25E-01	-0.17	1.31	6.37E-02	0.36	1.11	7.44E-03	0.53	1.35	2913320	1288584	3752262	1989551	3911869	2003967	3592655	1982305
RP_NEG_212_91109a15_628	RP	NEG	15.63	212.9111				3.26E-02	-0.45	0.99	4.26E-01	-0.16	0.61	2.82E-02	-0.53	0.90	9.26E-02	-0.37	0.90	3533319	146832	3468531	139643	3479718	124246	3457343	153967
RP_POS_459_14725a4_851	RP	POS	4.85	459.1473				5.68E-01	0.10	0.54	4.26E-01	-0.17	0.56	9.38E-01	0.02	0.45	3.88E-01	0.19	0.55	3185617	1563567	3385611	2119312	3555288	2289887	3215933	1942238
RP_POS_343_22437a9_959	RP	POS	9.96	343.2244				3.85E-07	0.61	1.11	4.26E-01	0.18	1.14	2.59E-04	0.69	1.29	4.09E-04	0.52	1.18	126002	98539	1406824	2349748	1218689	2034373	1594959	2635224

Supplementary table 1: Metabolomics results (in asceding order according to p-value from progressive ALD vs non-progressive ALD comparison, with molecular features with ID_level of 1-2 first)

							all_ALD_vs_control			Prog_ALD_vs_non-prog_ALD			Prog_ALD_vs_control_ALD			Non-prog_ALD_vs_control			Healthy_control		all_ALD		Non-prog_ALD		Progressive_ALD	
							t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA								
Feature_ID	RP_HILIC	POS_NEG	Average.Rt	Average.Mz	Metabolite.name	curated_MSMS	ID_level	p	d	VIP	p	d	VIP	p	d	VIP	p	d	VIP	Mean	SD	Mean	SD	Mean	SD	Mean	SD
RP_POS_406_74686a15_468	RP	POS	15.47	406.7469				2.25E-01	-0.27	0.51	4.27E-01	-0.15	0.55	1.44E-01	-0.35	0.62	4.29E-01	-0.20	0.48	528851	292735	458414	245054	478013	263741	438814	225799
RP_POS_320_96732a0_54	RP	POS	0.54	320.9673				6.75E-03	0.40	1.05	4.27E-01	-0.18	0.93	8.44E-02	0.31	0.86	1.09E-02	0.48	1.08	485622	171043	615197	358922	643900	371312	586494	347456
HILIC_NEG_137_0356a0_698	HILIC	NEG	0.698	137.0356				2.03E-01	-0.42	0.79	4.27E-01	0.08	0.72	2.59E-01	-0.38	0.53	1.65E-01	-0.46	0.76	291395	546760	164085	159951	151300	139001	176871	178985
RP_NEG_291_89606a3_706	RP	NEG	3.71	291.8961				1.43E-01	0.23	0.81	4.27E-01	0.17	0.78	1.37E-01	0.32	0.61	3.88E-01	0.15	0.39	973443	335971	1094567	565554	1049365	453361	1139768	660700
RP_POS_262_0134a4_851	RP	POS	4.85	262.0134				5.44E-01	0.11	0.50	4.27E-01	-0.17	0.58	9.05E-01	0.02	0.39	3.74E-01	0.19	0.55	619442	263692	654830	345575	682436	373006	627224	317164
RP_POS_696_43671a5_802	RP	POS	5.80	696.4367				3.31E-07	0.61	1.31	4.27E-01	-0.18	1.20	7.35E-04	0.52	1.38	1.49E-04	0.70	1.41	37785	32219	849197	1481211	967514	1598326	730880	1359977
RP_POS_217_10542a2_646	RP	POS	2.65	217.1054				2.18E-02	0.33	0.99	4.27E-01	-0.18	0.96	1.42E-01	0.24	1.06	3.76E-02	0.42	1.02	3031424	392533	3292604	883365	3363150	991580	3222059	763677
RP_POS_362_19077a5_803	RP	POS	5.80	362.1908		362.1882(100)	4	2.74E-07	0.61	1.32	4.28E-01	-0.18	1.21	6.91E-04	0.52	1.39	1.31E-04	0.70	1.42	57988	36804	1070222	1833186	1216567	1972625	923877	1689606
RP_POS_415_15228a10_047	RP	POS	10.05	415.1523				6.80E-01	-0.11	0.97	4.28E-01	0.13	0.69	8.89E-01	-0.04	0.66	4.93E-01	-0.18	0.71	1027246	2109955	863638	1265204	762424	582051	964853	1695423
RP_POS_521_17102a8_801	RP	POS	8.80	521.1710				6.49E-01	0.08	0.53	4.28E-01	0.17	1.06	4.53E-01	0.17	0.40	9.92E-01	0.00	0.59	530683	417700	572465	536670	529650	470877	615279	597027
RP_POS_359_71323a5_802	RP	POS	5.80	359.7132				2.49E-07	0.61	1.32	4.28E-01	-0.18	1.21	6.45E-04	0.53	1.39	1.27E-04	0.70	1.42	122139	67732	1922799	3247945	2181872	3498668	1663726	2989301
RP_NEG_227_90456a1_2	RP	NEG	1.20	227.9046				6.53E-10	0.86	1.40	4.28E-01	0.17	0.48	4.40E-06	0.94	1.47	3.55E-07	0.78	1.57	1257487	637342	2555823	1575633	2430201	1256241	2681445	1845416
HILIC_POS_176_06584a4_005	HILIC	POS	4.005	176.0658				6.06E-01	0.10	0.86	4.29E-01	-0.17	0.99	9.54E-01	0.01	0.37	3.78E-01	0.18	0.49	1293195	354642	1332572	427953	1366658	382557	1298486	470430
RP_NEG_584_80707a0_5	RP	NEG	0.50	584.8071				7.41E-02	-0.25	1.04	4.29E-01	-0.18	1.26	3.67E-02	-0.34	1.06	4.08E-01	-0.16	1.12	1093179	280308	945643	651892	997562	732062	893725	563190
RP_POS_570_3551a10_543	RP	POS	10.54	570.3551				1.58E-06	0.74	1.37	4.29E-01	-0.17	0.66	1.31E-03	0.66	1.20	1.33E-06	0.83	1.62	2348124	874428	3481075	1586321	3607388	1305210	3354762	1829767
HILIC_NEG_112_45235a4_235	HILIC	NEG	4.235	112.4524				6.33E-01	0.08	0.17	4.29E-01	0.17	0.53	4.19E-01	0.17	0.28	9.77E-01	-0.01	0.22	195485	94159	205934	140337	194770	133965	217097	146936
RP_NEG_876_5777a13_086	RP	NEG	13.09	876.5777				4.98E-03	-0.56	0.97	4.30E-01	0.16	0.56	3.93E-02	-0.49	0.75	2.19E-03	-0.64	1.30	3171060	1176866	2462746	1236157	2364472	1000675	2561021	1437461
RP_POS_528_30829a10_353	RP	POS	10.35	528.3083				1.72E-14	1.06	1.83	4.30E-01	0.16	0.58	1.84E-08	1.14	1.82	2.35E-10	0.98	1.92	272476	135331	632490	337662	605660	274672	659321	391719
RP_POS_495_29913a11_442	RP	POS	11.44	495.2991				5.00E-01	-0.11	0.49	4.30E-01	0.17	0.58	9.14E-01	-0.02	0.34	2.59E-01	-0.20	0.51	700343	95427	684944	152478	672836	122784	697052	177760
RP_POS_340_20917a5_802	RP	POS	5.80	340.2092				3.31E-07	0.61	1.31	4.31E-01	-0.18	1.20	7.55E-04	0.52	1.38	1.46E-04	0.70	1.41	62551	36430	1083096	1862977	1230812	2004881	935379	1717009
RP_POS_318_11911a0_708	RP	POS	0.71	318.1191				5.22E-12	0.84	1.52	4.31E-01	0.17	0.94	5.53E-06	0.93	1.59	2.27E-08	0.76	1.76	245805	193042	2064494	2306718	1881544	1733273	2247443	2770910
RP_POS_173_0784a10_278	RP	POS	10.28	173.0784				1.16E-01	-0.38	0.72	4.31E-01	-0.14	0.51	7.28E-02	-0.45	0.78	2.41E-01	-0.31	0.49	2152454	936419	1864709	685118	1918997	757737	1810421	606771
RP_NEG_860_84863a0_485	RP	NEG	0.49	860.8486				5.24E-08	0.65	1.34	4.31E-01	-0.17	1.21	2.84E-04	0.56	1.38	5.84E-05	0.74	1.47	648428	195092	4576199	6658434	5103451	7157275	4048947	6146574
RP_POS_355_31992a10_845	RP	POS	10.85	355.3199				1.51E-03	-0.67	1.17	4.31E-01	0.15	0.86	8.12E-03	-0.60	1.08	1.45E-03	-0.75	1.23	388247	187848	261782	177668	247716	184647	275847	171107
RP_POS_401_26208a6_067	RP	POS	6.07	401.2621				1.32E-07	0.63	1.33	4.31E-01	-0.18	1.20	4.56E-04	0.54	1.40	9.40E-05	0.72	1.43	50680	23815	916367	1522063	1036835	1638694	795900	1402032
HILIC_POS_217_08221a6_558	HILIC	POS	6.558	217.0822				1.09E-05	-0.63	1.22	4.32E-01	0.17	0.78	7.95E-04	-0.55	1.30	3.49E-04	-0.72	1.30	16670473	716484	15737996	1581951	15612820	1775921	15863172	1367604
RP_POS_357_23578a5_802	RP	POS	5.80	357.2358				2.56E-07	0.61	1.32	4.32E-01	-0.18	1.20	6.33E-04	0.53	1.39	1.33E-04	0.70	1.42	59687	37544	1047017	1783149	1188063	1923363	905970	1638354
RP_POS_878_77179a0_495	RP	POS	0.50	878.7718				7.74E-09	-0.72	1.36	4.32E-01	0.17	1.17	1.45E-04	-0.64	1.40	6.63E-06	-0.81	1.50	1503989	106843	1182227	482976	1144034	494160	1220420	473415
RP_POS_256_17572a2_88	RP	POS	2.88	256.1757				3.97E-02	0.32	1.13	4.32E-01	-0.17	1.09	1.83E-01	0.24	1.15	4.46E-02	0.41	1.11	342573	418543	557684	717838	614452	783156	500916	648990
RP_POS_253_21599a10_12	RP	POS	10.12	253.2160				1.38E-02	-0.46	1.05	4.32E-01	-0.16	0.87	8.32E-03	-0.54	1.08	8.33E-02	-0.38	0.91	1057294	104825	1000681	124514	1010526	135494	990836	112994
RP_POS_701_39203a5_802	RP	POS	5.80	701.3920				3.44E-07	0.61	1.31	4.32E-01	-0.18	1.20	7.60E-04	0.52	1.38	1.51E-04	0.69	1.41	16912	16432	528324	935215	602215	1007096	454433	861231
RP_POS_722_52863a13_57	RP	POS	13.57	722.5286				6.77E-01	0.08	0.58	4.32E-01	0.16	0.72	4.62E-01	0.16	0.45	9.85E-01	0.00	0.59	115565539	6644884	116156608	7860387	115535662	7652134	116777553	8092605
RP_POS_343_33734a0_645	RP	POS	0.65	343.3373				1.80E-02	0.39	0.66	4.32E-01	0.17	0.56	2.19E-02	0.48	1.02	9.73E-02	0.31	0.61	1325969	415661	1559653	629629	1509920	575278	1609385	681881
RP_POS_900_57135a13_874	RP	POS	13.87	900.5714				5.66E-01	-0.12	0.50	4.33E-01	-0.16	0.50	4.12E-01	-0.20	0.79	8.45E-01	-0.04	0.34	4951605	1280559	4803260	1204316	4898266	1065532	4708255	1332882
RP_POS_831_56866a13_209	RP	POS	13.21	831.5687				1.03E-03	0.62	1.10	4.33E-01	0.16	0.83	2.48E-03	0.70	1.10	5.21E-03	0.54	1.13	14229130	2595757	16133328	3076765	15890587	2438190	16376069	3614020
RP_POS_531_21985a9_327	RP	POS	9.33	531.2199				1.19E-03	-0.86	1.43	4.34E-01	-0.12	0.56	6.75E-04	-0.92	1.51	4.01E-03	-0.80	1.14	682866	621129	277546	364601	306273	418032	248819	303554
HILIC_POS_146_08121a0_757	HILIC	POS	0.757	146.0812				3.66E-02	0.30	0.66	4.34E-01	0.17	0.93	8.58E-02	0.38	0.59	9.83E-02	0.21	1.01	3143512	646919	3537018	1468708	3421140	850222	3652896	1899460
RP_POS_146_06017a2_893	RP	POS	2.89	146.0602	fragment of tryptophan	118.0653(100), 146.0602(70)		9.05E-04	-0.56	1.20	4.34E-01	-0.16	1.06	2.99E-03	-0.65	1.21	7.53E-03	-0.48	1.14	3813068	629651	3313821	922995	3386534	765530	3241107	1060377
RP_POS_487_35938a13_1	RP	POS	13.10	487.3594				2.58E-01	-0.23	1.02	4.34E-01	-0.16	0.76	1.98E-01	-0.31	0.92	4.85E-01	-0.15	0.47	3466741	644682	3315133	678400	3368565	572683	3261700	772045
HILIC_NEG_183_93423a2_172	HILIC	NEG	2.172	183.9342				6.33E-01	0.09	0.74	4.34E-01	-0.16	1.00	9.74E-01	0.01	0.31	4.11E-01	0.17	0.30	1584656	337330	1619173	402927	1650864	377644	1587481	428193
RP_POS_512_41718a10_466	RP	POS	10.47	512.4172				2.35E-02	-0.41	0.74	4.35E-01	0.16	0.55	1.10E-01	-0.33	0.68	2.06E-02	-0.49	0.82	6712401	1065194	6172413	1370912	6064640	1408727	6280185	1337512
RP_POS_862_75934a11_249	RP	POS	11.25	862.7593				5.47E-07	0.90	1.43	4.35E-01	-0.15	1.12	4.19E-05	0.82	1.39	2.14E-06	0.98	1.57	539317	216052	803063	286316	825569	288645	780557	285092
HILIC_POS_330_26425a0_677	HILIC	POS	0.677	330.2643				1.61E-01	-0.31	0.84	4.35E-01	-0.15	0.51	1.11E-01	-0.38	0.74	3.31E-01	-0.23	0.78	1180520	704051	982744	618366	1031309	618154	934179	620990
RP_POS_201_11195a0_655	RP	POS	0.66	201.1120				6.94E-01	-0.08	0.65	4.35E-01	-0.16	0.60	4.72E-01	-0.16	0.48	9.90E-01	0.00	0.54	5116814	2158714	4944104	2119267	5110483	2301974	4777724	1928385
HILIC_POS_120_08116a3_927	HILIC	POS	3.927	120.0812				2.20E-02	0.34	0.85	4.35E-01	0.17	0.86	4.64E-02	0.43	0.83	9.34E-02	0.26	0.75	19270995	4758082	22192173	9330102	21459226	6901939	22925119	11275861
RP_POS_302_64917a10_508	RP	POS	10.51	302.6492				3.23E-01	-0.22	0.47	4.36E-01	0.15	0.81	5.70E-01	-0.14	0.35	2.06E-01	-0.29	0.49	1777343	563829	1666262	495137	1627415	433739	1705110	551466
RP_NEG_806_78931a0_497	RP	NEG	0.50	806.7893				5.70E-03	-0.42	1.13	4.36E-01	-0.17	1.24	7.14E-03	-0.50	1.17	7.89E-02	-0.33	1.15	1245076	224160	1078812	435668	1112975	443412	1044649	429523
RP_POS_149_9973a15_526	RP	POS	15.53	149.9973				1.36E-01	-0.21	0.43	4.36E-01	-0.18	0.92	1.99E-01	-0.30	0.43	2.59E-01	-0.12	0.56	13467734	427905	13279173	1001367	13357867	423746	13200479	1354156
HILIC_POS_59_06128a1_435	HILIC	POS	1.435	59.0613				5.42E-01	-0.15	0.33	4.36E-01	0.14	0.65	7.61E-01	-0.08	0.15	3.97E-01	-0.22	0.35	3094350	1683639	2897416	1174535	2805446	1136145	2989386	1216195
RP_POS_736_85577a0_492	RP	POS	0.49	736.8558				4.56E-08	0.65	1.33	4.36E-01	-0.17	1.19	3.44E-04	0.57	1.36	4.33E-05	0.74	1.47	47203	32873	2756798	4573230	3114847	4830395	2398749	4319879
RP_POS_596_32703a5_034	RP	POS	5.03	596.3270				6.25E-05	-0.70	1.20	4.37E-01	0.16	0.97	1.79E-03	-0.62	1.19	1.50E-04	-0.78	1.29	1037668	305983	745227	425005	711972	433426	778483	418126
RP_POS_328_23022a8_387	RP	POS	8.39	328.2302				3.42E-01	0.17	0.92	4.37E-01	0.16	0.70	2.53E-01	0.25	0.79	6.53E-01	0.09	0.62	429070	209130	473052	272875	451701	238980	494403	303971
HILIC_POS_216_1707a0_549	HILIC	POS	0.549	216.1707				1.89E-01	0.16	0.71	4.37E-01	0.18	0.64	2.01E-01	0.25	0.68	6.26E-01	0.07	0.42	42336	44228	84114	306595	60128	250667	108100	354839
RP_POS_468_29572a10_167	RP	POS	10.17	468.2957				2.12E-01	0.22	0.57	4.37E-01	-0.17	0.48	4.72E-01	0.13	0.38	1.76E-01	0.30	0.58	766881	595169	936342	837292	1001825	962489	870859	693750
RP_NEG_979_1394a9_433	RP	NEG	9.43	979.1394				3.15E-01	-0.18	0.43	4.37E-01	-0.16	0.53	1.92E-01	-0.26	0.52	6.42E-01	-0.10	0.30	2109212	179131	2069834	225434	2087446	242216	2052222	208271
RP_NEG_642_39667a10_978	RP	NEG	10.98	642.3967				3.97E-02	0.38	1.30	4.38E-01	-0.16	1.29	1.54E-01	0.30	1.05	2.97E-02	0.46	1.24	550387	387832	725064	470342	761802	468918	688326	473622
RP_POS_245_22583a10_592	RP	POS	10.59	245.2258				1.61E-03	0.54	1.09	4.38E-01	-0.16	0.50	2.41E-02	0.46	0.84	1.74E-03	0.62	1.33	2001641	982174	2735539	1420262	2846402	1374178	2624677	1470377
HILIC_POS_242_1306a0_571	HILIC	POS	0.571	242.1306				6.56E-01	0.06	0.20	4.38E-01	-0.18	0.57	5.54E-01	-0.03	0.24	5.35E-01	0.14	0.25	3821115	5819860	5013616	24628067	6942772	34558464	3084459	4855836
HILIC_POS_298_18573a2_143	HILIC	POS	2.143	298.1857				1.29E-01	0.24	1.07	4.38E-01	-0.17	0.77	3.79E-01	0.16	1.09	1.14E-01	0.33	1.16	529810	1102347	940712	1837358	1084049	2025524	797375	1635844
RP_POS_477_10349a0_714	RP	POS	0.71	477.1035				3.45E-07	-0.75	1.35	4.38E-01	-0.16	0.97	5.74E-06	-0.83	1.54	3.23E-04	-0.67	1.16	734475	109415	572735	226679	590407	232939	555063	221172
RP_POS_327_20135a3_84	RP	POS	3.84	327.2014				9.79E-01	-0.01	1.17	4.38E-01	-0.12	1.12	8.13E-01	-0.07	0.92	8.56E-01	0.05	0.97	848505	2697793	835269	1390128	943643	1491603	726896	1286662
RP_NEG_329_95615a6_867	RP	NEG	6.87	329.9562				7.08E-01	-0.07	0.54	4.38E-01	-0.16	0.53	4.78E-01	-0.15	0.49	9.83E-01	0.00	0.26	1629969	180440	1615955	191811	1630907	206239	1601002	177039
HILIC_NEG_125_92897a2_904	HILIC	NEG	2.904	125.9290				8.66E-01	0.03	0.83	4.39E-01	0.16	0.73	6.17E-01	0.11	0.54	8.17E-01	-0.05	0.56	353987	123609	358415	141751	347367	129808	369463	153289
HILIC_POS_267_14407a0_779	HILIC	POS	0.779	267.1441				9.27E-01	0.02	0.68	4.39E-01	0.16	0.98	6.62E-01	0.10	0.21	7.76E-01	-0.06	0.71	707310	153860	710255	169110	697092	164707	723418	174063
HILIC_POS_171_18555a7_963	HILIC	POS	7.963	171.1856				3.03E-01	-0.20	0.94	4.39E-01	0.16	0.71	5.92E-01	-0.12	0.86	1.96E-01	-0.28	0.93	12442063	5532206	11236390	6239030	10750922	6020157	11721858	6474728
RP_NEG_407_28094a9_323	RP	NEG	9.32	407.2809				2.28E-01	-0.35	0.67	4.39E-01	0.12	0.52	3.33E-01	-0.29	0.48	1.71E-01	-0.40	0.59	1511360	2881898	863929	1387538	755987	1301040	971871	1474222
RP_POS_344_22815a3_84	RP	POS	3.84	344.2282				9.92E-01	0.00	1.16	4.39E-01	-0.12	1.12	8.26E-01	-0.06	0.92	8.44E-01	0.06	0.97	2240728	6960080	2228276	3587470	2507367	3859707	1949185	3308509
RP_NEG_400_90952a0_497	RP	NEG	0.50	400.9095				9.32E-09	-0.70	1.37	4.40E-01	0.17	1.21	1.31E-04	-0.61	1.41	1.74E-05	-0.78	1.49	23696054	885846	19276695	6925414	18738368	7312959	19815022	6544519
RP_POS_151_00688a10_441	RP	POS	10.44	151.0069				9.83E-01	0.00	0.20	4.40E-01	-0.16	0.91	7.10E-01	-0.08	0.46	7.41E-01	0.07	0.39	2493847	964558	2489509	1012083	2568124	1021827	2410895	1006372
RP_POS_523_42706a10_932	RP	POS	10.93	523.4271				1.30E-03	0.58	1.27	4.40E-01	-0.16	0.82	7.51E-03	0.50	1.16	3.40E-03	0.66	1.24	1816740	402154	2112442	520162	2152863	605678	2072022	420094
RP_NEG_369_17471a9_317	RP	NEG	9.32	369.1747				6.22E-01	0.09	0.42	4.40E-01	-0.16	0.73	9.48E-01	0.01	0.24	4.01E-01	0.17	0.52	21903621	20525151	24041686	23231594	25846267	20716994	22237104	25584929
RP_POS_300_63419a10_303	RP	POS	10.30	300.6342				3.50E-03	0.62	1.07	4.40E-01	-0.15	0.75	2.11E-02	0.55	0.88	2.06E-03	0.70	1.16	3035176	821832	3539181	767773	3598815	684447	3479546	845728
RP_POS_311_21945a15_428	RP	POS	15.43	311.2195				3.39E-01	0.21	0.44	4.40E-01	-0.15	0.55	5.48E-01	0.13	0.40	2.65E-01	0.28	0.49	4081353	1707244	4407108	1512634	4524653	1796823	4289564	1168779
HILIC_POS_146_11758a0_54	HILIC	POS	0.54	146.1176				7.03E-04	0.40	0.80	4.40E-01	0.18	0.73	1.37E-02	0.49	0.83	1.56E-02	0.31	1.00	126090	231931	1042774	2592072	841424	2000952	1244124	3080300
RP_NEG_397_16895a11_254	RP	NEG	11.25	397.1690				5.24E-06	0.94	1.73	4.41E-01	0.14	0.92	1.00E-05	1.01	1.73	6.28E-05	0.86	1.60	2459205	762682	3247609	777900	3187296	731897	3307922	824324
RP_NEG_449_25485a10_207	RP	NEG	10.21	449.2549				1.46E-01	0.25	0.60	4.41E-01	-0.17	0.49	3.71E-01	0.16	0.41	1.31E-01	0.33	0.61	8069828	5812790	10033347	8555557	10696624	9765294	9370070	7185411
RP_POS_235_08502a15_34	RP	POS	15.34	235.0850				4.97E-01	0.11	0.50	4.41E-01	-0.17	0.54	8.98E-01	0.03	0.24	2.34E-01	0.20	0.78	11979427	681640	12088015	1037542	12168505	717632	12007526	1283253
RP_POS_380_33536a10_442	RP	POS	10.44	380.3354				6.31E-02	-0.37	0.73	4.42E-01	0.16	0.54	1.91E-01	-0.29	0.58	4.55E-02	-0.44	0.80	2378559	184206	2306094	200072	2290604	200676	2321584	200285
HILIC_POS_270_15451a2_143	HILIC	POS	2.143	270.1545				1.27E-01	0.24	1.07	4.42E-01	-0.17	0.76	3.79E-01	0.16	1.08	1.14E-01	0.33	1.16	334050	725220	607937	1234040	703493	1359108	512381	1100445
RP_POS_295_22433a9_732	RP	POS	9.73	295.2243				5.99E-05	0.56	1.23	4.42E-01	0.17	1.00	2.87E-04	0.64	1.35	9.32E-03	0.48	1.31	2743421	337578	3164977	819495	3101536	847595	3228419	793863
RP_POS_360_32272a11_668	RP	POS	11.67	360.3227				9.88E-01	0.00	0.67	4.42E-01	-0.16	0.45	7.38E-01	-0.08	0.40	7.22E-01	0.08	0.43	167119332	90839775	167391291	93145444	174601691	95184903	160180891	91449127
RP_POS_604_35376a5_214	RP	POS	5.21	604.3538				1.27E-06	0.58	1.26	4.42E-01	-0.17	1.14	1.10E-03	0.49	1.34	3.71E-04	0.66	1.35	60212	142813	1630994	3036159	1866005	3335282	1395984	2718057
RP_POS_210_10927a11_237	RP	POS	11.24	210.1093				2.31E-03	0.62	1.47	4.42E-01	0.15	1.06	3.11E-03	0.70	1.37	1.04E-02	0.55	1.46	1211059	376221	1456977	384870	1427190	335532	1486764	429976
RP_POS_441_29498a13_284	RP	POS	13.28	441.2950				6.06E-03	0.47	0.96	4.42E-01	-0.16	0.54	3.81E-02	0.39	0.97	9.79E-03	0.55	0.90	16740766	5414424	20213941	7716251	20811034	8512736	19616849	6863084
RP_NEG_227_90456a1_708	RP	NEG	1.71	227.9046				1.82E-10	0.84	1.39	4.42E-01	0.16	0.48	5.10E-06	0.92	1.43	3.47E-07	0.76	1.56	829499	435834	1913806	1363546	1808287	1100568	2019325	1588234
RP_POS_407_24576a11_609	RP	POS	11.61	407.2458				1.24E-03	-0.65	1.20	4.42E-01	0.15	0.90	7.09E-03	-0.58	1.20	1.63E-03	-0.73	1.12	5287001	488041	4945338	510431	4905868	552696	4984807	466632
RP_POS_296_25833a8_177	RP	POS	8.18	296.2583	Unknown	296.2584(40), 279.2303(100), 57.0706(65)	4	2.99E-01	-0.30	0.87	4.42E-01	-0.11	0.53	2.26E-01	-0.36	0.73	4.20E-01	-0.24	0.56	1928762	5205807	923300	2502143	1116739	2723839	729861	2270141
RP_POS_1042_79785a0_491	RP	POS	0.49	1042.7979				5.59E-08	0.65	1.33	4.42E-01	-0.17	1.18	2.97E-04	0.56	1.36	5.99E-05	0.74	1.47	177520	95906	1916221	2954153	2144571	3165372	1687871	2739735

Supplementary table 1: Metabolomics results (in asceding order according to p-value from progressive ALD vs non-progressive ALD comparison, with molecular features with ID_level of 1-2 first)

							all_ALD_vs_control			Prog_ALD_vs_non-prog_ALD			Prog_ALD_vs_control_ALD			Non-prog_ALD_vs_control			Healthy_control		all_ALD		Non-prog_ALD		Progressive_ALD	
							t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA								
Feature_ID	RP_HILIC	POS_NEG	Average.Rt	Average.Mz	Metabolite.name	curated_MSMS	ID_level	p	d	VIP	p	d	VIP	p	d	VIP	p	d	VIP	Mean	SD	Mean	SD	Mean	SD	Mean	SD
RP_POS_224_0347a15_418	RP	POS	15.42	224.0347				9.27E-01	-0.02	0.94	4.42E-01	-0.16	0.50	6.59E-01	-0.10	0.63	7.97E-01	0.06	0.82	4611895	1761378	4578713	1821154	4719453	1949095	4437974	1691597
RP_POS_492_44131a13_202	RP	POS	13.20	492.4413				8.92E-01	0.03	0.69	4.43E-01	0.15	0.55	6.26E-01	0.11	0.44	8.39E-01	-0.05	0.62	11299326	2356664	11364535	2325872	11184915	2663668	11544154	1941337
RP_NEG_413_20081a8_909	RP	NEG	8.91	413.2008				5.80E-01	0.11	0.81	4.43E-01	-0.15	0.69	8.74E-01	0.04	0.56	4.08E-01	0.19	0.55	11700856	8773011	12693261	8778456	13370683	8981796	12015840	8607326
RP_POS_339_3363a10_586	RP	POS	10.59	339.3363				1.93E-02	0.53	0.93	4.43E-01	-0.14	0.49	6.20E-02	0.46	0.73	1.30E-02	0.60	1.15	2016425	766396	2379579	638165	2428809	611774	2330349	666038
RP_NEG_415_2081a10_979	RP	NEG	10.98	415.2081				1.29E-02	0.46	1.46	4.43E-01	-0.16	1.44	7.68E-02	0.39	1.24	8.76E-03	0.54	1.37	1396106	454112	1644876	547239	1687091	510512	1602662	583775
HILIC_NEG_315_04208a6_094	HILIC	NEG	6.094	315.0421				3.15E-02	-0.42	0.82	4.43E-01	-0.16	0.70	2.93E-02	-0.50	0.82	1.02E-01	-0.35	0.69	5661000	1432405	5004660	1562817	5125218	1415130	4884102	1703638
RP_POS_217_14349a9_529	RP	POS	9.53	217.1435				1.50E-01	-0.32	0.58	4.44E-01	-0.15	0.58	1.08E-01	-0.40	0.64	2.98E-01	-0.25	0.53	2196728	114323	2163970	96436	2171403	93278	2156537	99880
RP_NEG_200_91951a15_4	RP	NEG	15.40	200.9195				1.58E-01	-0.21	0.42	4.44E-01	0.17	0.60	3.23E-01	-0.12	0.41	2.07E-01	-0.29	0.44	1139997	42702	1123264	90334	1116285	120151	1130242	44174
RP_POS_348_7225a5_802	RP	POS	5.80	348.7225				2.94E-07	0.61	1.31	4.44E-01	-0.17	1.20	6.84E-04	0.53	1.38	1.43E-04	0.70	1.42	25662	20091	573490	995178	650172	1070195	496808	918505
HILIC_NEG_132_92345a7_666	HILIC	NEG	7.666	132.9235				3.84E-01	0.19	0.88	4.44E-01	-0.15	0.48	6.29E-01	0.11	0.34	2.73E-01	0.26	0.61	1069669	192258	1103151	173025	1116481	178849	1089821	167740
RP_NEG_646_42749a11_253	RP	NEG	11.25	646.4275				7.26E-07	0.92	1.80	4.44E-01	0.15	1.15	4.83E-06	0.99	1.76	1.87E-05	0.84	1.70	2452822	1083124	3739111	1350598	3635047	1220950	3843176	1473986
RP_POS_481_28397a11_489	RP	POS	11.49	481.2840				5.66E-02	-0.33	0.57	4.44E-01	0.16	0.45	2.41E-01	-0.25	0.43	3.34E-02	-0.41	0.79	526642	55868	502324	77504	496357	69933	508291	84693
RP_POS_264_84393a0_515	RP	POS	0.52	264.8439				3.94E-03	-0.46	0.96	4.44E-01	-0.16	1.02	3.84E-03	-0.54	1.09	5.68E-02	-0.38	0.92	568118	148564	461034	248843	480185	262660	441883	235309
HILIC_NEG_131_08253a6_345	HILIC	NEG	6.345	131.0825				3.62E-04	0.57	0.99	4.44E-01	0.16	0.80	9.34E-04	0.65	1.11	9.57E-03	0.49	0.88	234234	60974	289276	102026	281425	99928	297128	104496
HILIC_POS_302_19565a1_102	HILIC	POS	1.102	302.1957				7.49E-01	0.06	0.56	4.44E-01	-0.16	0.77	9.17E-01	-0.02	0.24	4.96E-01	0.14	0.25	408900	166005	420478	208512	436525	195991	404432	221142
RP_POS_362_22229a5_94	RP	POS	5.94	362.2223				2.23E-07	0.62	1.32	4.44E-01	-0.17	1.20	5.75E-04	0.53	1.39	1.28E-04	0.70	1.42	69280	28292	1160883	1960790	1311760	2112011	1010006	1805771
HILIC_POS_264_19559a0_581	HILIC	POS	0.581	264.1956				2.99E-02	0.25	0.57	4.45E-01	0.18	0.52	5.66E-02	0.34	0.70	2.77E-01	0.16	0.51	14587	40521	779391	3470889	512377	3199247	1046405	3736218
RP_POS_303_03918a4_851	RP	POS	4.85	303.0392				8.40E-01	0.04	0.48	4.45E-01	-0.16	0.57	8.34E-01	-0.04	0.44	5.97E-01	0.12	0.51	1196369	355243	1211797	428635	1244771	466152	1178824	389472
RP_NEG_412_19138a11_611	RP	NEG	11.61	412.1914				2.04E-01	-0.24	0.72	4.45E-01	0.16	0.46	4.57E-01	-0.16	0.74	1.43E-01	-0.32	0.61	851755	150532	810501	180677	796607	184765	824396	177264
RP_POS_301_14099a9_524	RP	POS	9.52	301.1410				4.51E-02	-0.35	0.75	4.45E-01	0.16	0.72	2.39E-01	-0.27	0.68	1.41E-02	-0.43	0.87	12669261	1023583	12204709	1383175	12098229	960847	12311189	1708515
RP_POS_247_96416a15_591	RP	POS	15.59	247.9642				2.45E-01	-0.22	0.72	4.45E-01	0.16	0.48	4.87E-01	-0.14	0.43	1.84E-01	-0.30	0.68	2516660	57447	2502494	65067	2497492	71123	2507495	58688
RP_POS_209_0331a15_349	RP	POS	15.35	209.0331				2.77E-01	0.20	0.47	4.45E-01	0.16	0.82	1.82E-01	0.28	0.51	5.83E-01	0.12	0.58	979964	336063	1060485	430845	1027381	439902	1093589	423430
RP_NEG_120_08125a2_202	RP	POS	2.20	120.0813		120.0814(100), 103.0546(10)	4	2.47E-01	0.18	0.69	4.45E-01	0.17	0.78	2.25E-01	0.26	0.71	5.46E-01	0.10	0.86	7565021	1231404	7922595	2164019	7756229	1614883	8088960	2607144
RP_POS_548_50409a15_099	RP	POS	15.10	548.5041				3.47E-03	-0.41	0.85	4.45E-01	-0.17	0.82	9.65E-03	-0.50	1.01	5.22E-02	-0.33	0.83	235363565	12925260	224169039	29776778	226456339	27537092	221881740	31975609
RP_POS_197_1004a0_507	RP	POS	0.51	197.1004				1.92E-05	0.51	1.21	4.45E-01	-0.17	1.16	5.34E-03	0.43	1.20	1.08E-03	0.60	1.34	256403	71286	497705	525004	538011	567894	457399	480691
RP_POS_181_0584a0_705	RP	POS	0.71	181.0584				8.46E-02	-0.28	0.52	4.46E-01	-0.16	0.64	4.01E-02	-0.37	0.77	3.46E-01	-0.20	0.58	472384	99792	431463	154311	443311	177321	419614	127986
HILIC_NEG_209_00409a0_579	HILIC	NEG	0.579	209.0041				1.09E-02	-0.60	1.23	4.46E-01	-0.14	0.63	7.26E-03	-0.67	1.12	3.48E-02	-0.54	1.16	1069671	365107	882919	275559	904054	290728	861785	260732
RP_NEG_238_93163a0_513	RP	NEG	0.51	238.9316				3.34E-02	0.31	1.05	4.46E-01	-0.17	1.05	2.22E-01	0.22	0.93	3.41E-02	0.39	1.18	1096573	231661	1236639	505520	1275378	508803	1197900	504355
RP_POS_290_84647a0_5	RP	POS	0.50	290.8465				9.34E-02	-0.25	1.02	4.47E-01	-0.17	1.26	5.71E-02	-0.33	1.02	4.09E-01	-0.16	1.08	1245877	390205	1065495	812378	1127725	879854	1003265	742522
RP_POS_373_21341a5_94	RP	POS	5.94	373.2134				1.88E-07	0.62	1.32	4.47E-01	-0.17	1.20	5.28E-04	0.54	1.40	1.17E-04	0.71	1.42	19901	12865	501096	858239	566800	923369	435393	791681
RP_POS_268_26334a10_621	RP	POS	10.62	268.2633				1.05E-02	0.31	0.70	4.47E-01	0.17	0.78	8.44E-02	0.40	0.74	2.17E-04	0.22	1.32	1972569	737353	3026071	3838067	2731276	1031849	3320866	5340420
RP_POS_541_87433a14_263	RP	POS	14.26	541.8743				2.65E-02	0.28	0.61	4.47E-01	0.17	0.54	9.32E-02	0.36	0.63	7.48E-02	0.19	0.69	863594	428016	1295390	1768223	1159911	1027855	1430868	2285409
RP_POS_299_25806a10_8	RP	POS	10.80	299.2581				8.55E-02	-0.31	0.96	4.47E-01	0.16	0.98	2.64E-01	-0.23	0.82	6.84E-02	-0.39	0.97	1678991	219328	1594401	291023	1572147	303379	1616656	279405
RP_NEG_621_13031a0_621	RP	NEG	0.62	621.1303				8.93E-03	-0.42	1.04	4.47E-01	-0.16	1.15	6.68E-03	-0.50	1.12	9.84E-02	-0.33	1.04	1740852	505815	1410052	855895	1475500	926832	1344605	782500
RP_POS_521_25671a4_783	RP	POS	4.78	521.2567				4.38E-06	0.55	1.25	4.47E-01	-0.17	1.15	2.15E-03	0.47	1.33	6.01E-04	0.64	1.33	42061	152277	689532	1310134	789690	1431729	589375	1182205
RP_NEG_258_05649a6_707	RP	NEG	6.71	258.0565				2.14E-01	-0.41	0.73	4.47E-01	-0.08	0.50	1.77E-01	-0.45	0.68	2.68E-01	-0.37	0.57	931131	2325865	402564	678632	454433	712309	350695	646225
RP_POS_319_01111a4_851	RP	POS	4.85	319.0111				6.54E-01	0.08	0.51	4.48E-01	-0.16	0.58	9.85E-01	0.00	0.41	4.66E-01	0.16	0.55	1443364	601001	1501256	722874	1556489	791555	1446023	650362
RP_NEG_419_24155a11_61	RP	NEG	11.61	419.2416				3.49E-02	-0.40	0.77	4.48E-01	-0.16	0.80	2.54E-02	-0.48	0.83	1.38E-01	-0.32	0.63	1809943	181134	1726995	212803	1743241	218670	1710750	207701
RP_POS_211_09361a6_035	RP	POS	6.04	211.0936	Sinapyl alcohol	211.0952(100)	3	2.04E-01	0.21	0.73	4.48E-01	-0.17	0.75	5.30E-01	0.12	0.71	1.39E-01	0.29	0.78	1707395	247860	1783362	399990	1813888	397018	1752836	404628
RP_POS_369_29678a10_881	RP	POS	10.88	369.2968				1.74E-05	-0.64	1.24	4.48E-01	0.16	1.11	1.59E-03	-0.56	1.24	2.15E-04	-0.72	1.32	22115357	948812	20972146	1908801	20826511	2019415	21117780	1800021
RP_POS_381_72653a5_94	RP	POS	5.94	381.7265				1.81E-07	0.62	1.32	4.49E-01	-0.17	1.20	5.08E-04	0.54	1.40	1.17E-04	0.71	1.42	138710	48554	1963179	3249256	2210725	3498567	1715633	2994288
RP_POS_309_65762a5_03	RP	POS	5.03	309.6576				6.12E-05	-0.70	1.20	4.50E-01	0.15	0.96	1.62E-03	-0.63	1.20	1.56E-04	-0.78	1.29	2097156	614675	1510234	847456	1445762	868427	1574705	829681
RP_POS_384_20401a5_94	RP	POS	5.94	384.2040				2.04E-07	0.62	1.32	4.50E-01	-0.17	1.20	5.77E-04	0.54	1.40	1.17E-04	0.70	1.42	66714	27120	1055019	1768572	1189537	1895933	920502	1639524
RP_POS_189_97673a0_256	RP	POS	0.26	189.9767				6.37E-01	0.11	0.23	4.50E-01	-0.14	0.83	8.82E-01	0.04	0.21	4.59E-01	0.18	0.34	746618	161743	761484	127382	771168	115351	751800	138875
RP_POS_239_14914a2_881	RP	POS	2.88	239.1491				3.83E-02	0.32	1.13	4.50E-01	-0.17	1.08	1.78E-01	0.24	1.14	4.57E-02	0.40	1.11	1063313	1137495	1661574	2015794	1814812	2195794	1508336	1827662
RP_POS_249_10088a15_34	RP	POS	15.34	249.1009				6.24E-01	-0.10	0.85	4.50E-01	-0.15	0.79	4.34E-01	-0.18	0.95	9.02E-01	-0.03	0.62	1778786	467876	1732629	435957	1765766	466655	1699491	404955
RP_POS_348_03409a4_852	RP	POS	4.85	348.0341				7.03E-01	0.07	0.49	4.50E-01	-0.16	0.57	9.66E-01	-0.01	0.43	4.99E-01	0.15	0.51	770786	343310	798923	415366	830491	449908	767355	379643
RP_POS_212_20049a10_847	RP	POS	10.85	212.2005				8.34E-06	0.74	1.20	4.50E-01	0.16	0.92	2.97E-04	0.81	1.19	4.92E-05	0.66	1.47	537510	193050	754150	302074	731180	204231	777120	376261
RP_POS_463_23245a9_325	RP	POS	9.33	463.2325				3.95E-03	-0.78	1.26	4.50E-01	-0.12	0.51	2.43E-03	-0.84	1.32	1.08E-02	-0.72	1.01	1308208	1328933	550687	751127	607736	849563	493637	641480
RP_POS_497_39575a12_129	RP	POS	12.13	497.3958				5.48E-01	-0.14	0.47	4.51E-01	-0.14	0.68	4.08E-01	-0.21	0.44	7.85E-01	-0.07	0.52	2629099	1232391	2484439	987203	2559386	923810	2409491	1050781
HILIC_POS_371_23969a5_648	HILIC	POS	5.648	371.2397				4.36E-01	-0.14	0.98	4.51E-01	-0.16	0.85	3.00E-01	-0.22	0.73	7.57E-01	-0.06	0.66	9874219	1921444	9550454	2343195	9728312	2288011	9372595	2406994
RP_POS_245_17462a7_475	RP	POS	7.48	245.1746				8.92E-01	-0.03	0.59	4.51E-01	0.14	0.72	8.67E-01	0.04	0.32	6.80E-01	-0.10	0.53	1256930	271149	1249726	220262	1233009	227555	1266443	213704
RP_POS_429_37354a12_328	RP	POS	12.33	429.3735				9.18E-01	0.02	0.81	4.51E-01	-0.15	0.49	8.22E-01	-0.05	0.73	6.62E-01	0.10	0.33	2714370	715477	2729288	690776	2781719	612250	2676858	763952
RP_POS_417_23962a6_184	RP	POS	6.18	417.2396				2.01E-07	0.62	1.32	4.51E-01	-0.17	1.20	5.34E-04	0.54	1.40	1.23E-04	0.70	1.42	9363	13867	266425	459397	301273	494431	231576	423624
HILIC_POS_166_08627a3_928	HILIC	POS	3.928	166.0863				3.88E-02	0.31	0.87	4.51E-01	0.17	0.86	6.44E-02	0.39	0.79	1.50E-01	0.23	0.71	108521868	26189660	122946764	51070096	119071175	39527769	126822354	60633646
RP_POS_255_23077a9_676	RP	POS	9.68	255.2308				2.41E-03	0.52	1.10	4.51E-01	0.16	0.70	4.73E-03	0.60	1.10	1.88E-02	0.45	1.15	5288328	638355	5742396	901912	5674012	809267	5810779	989463
RP_POS_189_12393a0_706	RP	POS	0.71	189.1239				3.60E-02	0.35	0.86	4.51E-01	0.16	1.04	4.45E-02	0.43	0.87	1.35E-01	0.27	0.74	584983	117720	642981	174799	629727	148693	656236	198154
RP_POS_478_38843a13_49	RP	POS	13.49	478.3884				2.18E-01	0.25	1.47	4.51E-01	-0.15	0.50	4.29E-01	0.17	0.71	1.63E-01	0.32	1.53	7453897	2606556	8118046	2687050	8321637	2891334	7914455	2478594
HILIC_NEG_241_75836a1_358	HILIC	NEG	1.358	241.7584				5.97E-06	0.56	1.04	4.52E-01	0.17	0.52	6.35E-04	0.65	1.11	1.66E-03	0.48	1.28	383958	65251	532532	291919	510427	258607	554636	322952
RP_NEG_228_9903a5_938	RP	NEG	5.94	228.9903				5.25E-01	-0.12	0.62	4.52E-01	-0.16	0.60	3.50E-01	-0.20	0.62	8.58E-01	-0.04	0.29	1919086	1004131	1781184	1225530	1873939	1260802	1688430	1194704
RP_POS_765_98492a10_507	RP	POS	10.51	765.9849				1.55E-02	-0.53	1.07	4.52E-01	0.14	0.57	5.15E-02	-0.46	0.84	1.20E-02	-0.60	1.05	4928357	1396242	4235378	1237048	4141814	1252617	4328942	1226739
HILIC_NEG_197_80801a0_552	HILIC	NEG	0.552	197.8080				5.76E-01	0.12	0.41	4.52E-01	-0.15	0.72	8.50E-01	0.04	0.07	4.26E-01	0.19	0.56	1864056	859299	1961273	823300	2023551	909037	1898994	731584
RP_POS_406_21732a6_067	RP	POS	6.07	406.2173				1.66E-07	0.62	1.33	4.52E-01	-0.17	1.21	5.20E-04	0.54	1.41	1.06E-04	0.71	1.43	52135	22293	906659	1516616	1021358	1624333	791960	1407793
HILIC_POS_253_1279a2_142	HILIC	POS	2.142	253.1279				1.13E-01	0.25	1.09	4.53E-01	-0.16	0.76	3.47E-01	0.17	1.12	1.04E-01	0.33	1.17	293683	606735	532435	1034103	610541	1131016	454329	932156
HILIC_POS_207_11263a3_929	HILIC	POS	3.929	207.1126				1.99E-02	0.33	0.88	4.53E-01	0.17	0.85	5.38E-02	0.41	0.89	8.60E-02	0.24	0.82	843089	164515	957852	389871	928390	279390	987314	476729
HILIC_POS_672_40845a1_048	HILIC	POS	1.048	672.4085				5.94E-06	0.55	1.28	4.53E-01	-0.17	0.94	2.17E-03	0.47	1.47	6.26E-04	0.64	1.43	346750	1068907	3270089	5862396	3712711	6409126	2827467	5287726
RP_POS_476_27423a10_389	RP	POS	10.39	476.2742				4.77E-01	0.13	1.00	4.53E-01	-0.16	0.75	8.26E-01	0.05	0.71	3.08E-01	0.21	0.80	497707	155365	522152	204067	537556	193877	506748	214625
HILIC_POS_266_1384a1_438	HILIC	POS	1.438	266.1384				4.88E-01	-0.12	0.54	4.53E-01	0.16	0.62	8.44E-01	-0.04	0.20	2.95E-01	-0.20	0.52	695100	388846	635129	515610	596205	451338	674052	574748
RP_NEG_276_99146a7_339	RP	NEG	7.34	276.9915				4.08E-01	-0.17	0.42	4.54E-01	0.15	0.66	6.79E-01	-0.10	0.27	2.77E-01	-0.25	0.60	9810179	3447790	9229795	3362696	8976182	3214269	9483408	3519009
RP_POS_185_11465a13_109	RP	POS	13.11	185.1147				4.63E-01	-0.14	0.77	4.54E-01	0.16	0.55	7.85E-01	-0.06	0.45	3.19E-01	-0.21	0.73	5343873	548243	5257115	665136	5206958	678981	5307273	653980
HILIC_POS_243_05292a4_123	HILIC	POS	4.123	243.0529				1.29E-02	-0.44	1.02	4.54E-01	-0.16	1.27	1.60E-02	-0.52	1.10	6.50E-02	-0.36	1.01	1162776	447236	908834	604775	954444	553354	863224	654617
HILIC_POS_499_05829a7_642	HILIC	POS	7.642	499.0583				5.01E-02	-0.38	0.58	4.54E-01	-0.15	0.60	3.63E-02	-0.46	0.77	1.63E-01	-0.31	0.52	1037476	46351	1018178	50839	1022009	51726	1014347	50165
HILIC_POS_275_10983a2_143	HILIC	POS	2.143	275.1098				1.29E-01	0.24	1.08	4.54E-01	-0.16	0.76	3.71E-01	0.16	1.10	1.16E-01	0.33	1.17	424419	943200	773671	1553860	890761	1705239	656580	1393705
HILIC_POS_224_12772a5_464	HILIC	POS	5.464	224.1277				1.72E-01	-0.27	0.42	4.54E-01	-0.15	0.61	1.28E-01	-0.35	0.57	3.69E-01	-0.20	0.34	20258308	2631620	19507537	2791806	19717728	2650131	19297347	2938378
RP_NEG_452_27853a10_513	RP	NEG	10.51	452.2785				3.73E-01	0.16	1.01	4.54E-01	-0.16	0.83	7.26E-01	0.08	0.72	2.22E-01	0.24	0.85	10631940	3031300	11238847	4134373	11550088	3665074	10927606	4572139
RP_NEG_197_08165a5_049	RP	NEG	5.05	197.0817				5.98E-01	-0.11	0.22	4.55E-01	-0.15	0.57	4.23E-01	-0.18	0.41	8.85E-01	-0.03	0.25	864147	42465	859570	42380	862759	42178	856381	42767
HILIC_POS_167_01276a7_963	HILIC	POS	7.963	167.0128				1.26E-04	-0.60	1.26	4.55E-01	0.16	0.94	6.39E-03	-0.52	1.34	3.97E-04	-0.67	1.35	35845000	8849410	26923198	15919122	25725776	15859874	28120620	16048269
RP_POS_630_78296a0_5	RP	POS	0.50	630.7830				2.85E-02	-0.31	1.09	4.55E-01	-0.17	1.27	2.10E-02	-0.40	1.12	2.29E-01	-0.23	1.13	1786139	477225	1487620	1048962	1566463	1132948	1408778	962726
HILIC_POS_74_09717a4_078	HILIC	POS	4.078	74.0972				5.50E-01	0.13	0.45	4.55E-01	-0.15	0.70	8.15E-01	0.06	0.15	3.84E-01	0.20	0.40	9779003	3334255	10176539	2972453	10399921	2772694	9953157	3172002
RP_POS_379_24896a5_939	RP	POS	5.94	379.2490				1.90E-07	0.62	1.32	4.55E-01	-0.17	1.19	5.18E-04	0.54	1.40	1.20E-04	0.70	1.42	68439	31069	1076010	1797656	1211043	1933377	940977	1659495
RP_POS_240_15735a6_319	RP	POS	6.32	240.1574				5.23E-04	-0.64	1.02	4.55E-01	-0.15	0.69	1.33E-03	-0.71	1.13	4.00E-03	-0.56	1.05	3295799	387177	2989410	485490	3025875	420683	2952944	544539
RP_NEG_995_61194a10_335	RP	NEG	10.34	995.6119				2.34E-01	0.24	1.01	4.56E-01	-0.15	0.89	4.99E-01	0.16	0.76	1.31E-01	0.31	0.96	3739166	1688229	4157254	1779802	4290813	1423838	4023695	2082383
HILIC_NEG_134_89473a3_102	HILIC	NEG	3.102	134.8947				3.47E-05	-0.75	1.22	4.56E-01	0.15	0.79	1.00E-03	-0.68	1.16	6.53E-05	-0.83	1.36	117444970	37992027	80550312	48977777	76878837	48524911	84221787	49642966
HILIC_NEG_158_93909a2_999	HILIC	NEG	2.999	158.9391				1.36E-01	-0.29	0.91	4.56E-01	0.15	0.83	3.18E-01	-0.21	0.46	1.04E-01	-0.37	0.69	2715904	566386	2537159	627688	2490121	661013	2584196	595458
RP_POS_326_37796a8_98	RP	POS	8.98	326.3780				6.01E-01	-0.08	0.54	4.57E-01	-0.16	0.75	2.88E-01	-0.17	1.06	9.87E-01	0.00	0.24	983509	702436	895582	1123134	979751	1418931	811413	721649
RP_POS_230_09573a0_616	RP	POS	0.62	230.0957				6.43E-03	0.39	0.78	4.57E-01	0.16	0.48	2.82E-03	0.48	1.07	1.27E-01	0.31	0.56	189282	266589	396098	576786	352915	671346	439282	466523
RP_POS_423_27496a6_184	RP	POS	6.18	423.2750				1.58E-07	0.63	1.32	4.57E-01	-0.17	1.19	4.92E-04	0.54	1.39	1.06E-04	0.71	1.43	28584	17785	674595	1144186	760210	1226422	588979	1061119
HILIC_POS_156_0421a3_694	HILIC	POS	3.694	156.0421				4.49E-01	-0.14	0.98	4.57E-01	0.16	0.71	7.83E-01	-0.06	0.97	3.10E-01	-0.21	0.73	20590395	7359201	19359781	9601094	18641504	9870659	20078059	9368055

Supplementary table 1: Metabolomics results (in asceding order according to p-value from progressive ALD vs non-progressive ALD comparison, with molecular features with ID_level of 1-2 first)

								all_ALD_vs_control			Prog_ALD_vs_non-prog_ALD			Prog_ALD_vs_control_ALD			Non-prog_ALD_vs_control			Healthy_control		all_ALD		Non-prog_ALD		Progressive_ALD	
								t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA								
Feature_ID	RP_HILIC	POS_NEG	Average.Rt	Average.Mz	Metabolite.name	curated_MSMS	ID_level	p	d	VIP	p	d	VIP	p	d	VIP	p	d	VIP	Mean	SD	Mean	SD	Mean	SD	Mean	SD
RP_POS_435_34415a11_53	RP	POS	11.53	435.3442				4.21E-02	-0.34	0.95	4.57E-01	0.16	0.80	1.66E-01	-0.26	0.89	4.32E-02	-0.42	0.85	1142587	187275	1053555	275736	1032926	296192	1074184	254978
HILIC_NEG_134_89471a1_69	HILIC	NEG	1.69	134.8947				1.32E-03	-0.63	1.14	4.58E-01	0.15	0.67	9.19E-03	-0.56	0.96	1.55E-03	-0.71	1.29	24936513	7706106	19525402	8407677	18897258	8695960	20153546	8148359
RP_NEG_818_55737a11_651	RP	NEG	11.65	818.5574				7.78E-01	0.05	0.35	4.58E-01	-0.16	0.61	8.42E-01	-0.04	0.32	5.51E-01	0.13	0.43	1873608	2748162	2058727	4400868	2387415	4995102	1730039	3736177
RP_POS_280_26364a9_712	RP	POS	9.71	280.2636				3.68E-01	-0.25	0.87	4.58E-01	-0.11	0.51	2.85E-01	-0.31	0.70	5.01E-01	-0.20	0.56	10703579	20182106	7324251	10106249	8078824	10626118	6569678	9606278
RP_POS_497_39651a13_201	RP	POS	13.20	497.3965				7.04E-01	0.08	0.49	4.58E-01	0.15	0.50	5.03E-01	0.15	0.64	9.81E-01	0.01	0.49	37752118	9799049	38503470	9350003	37805731	9694738	39201209	9035914
RP_NEG_947_612a10_515	RP	NEG	10.52	947.6120				6.11E-01	0.09	0.91	4.59E-01	-0.16	0.78	9.50E-01	0.01	0.65	4.03E-01	0.17	0.73	1245111	356988	1284804	453810	1318626	427119	1250982	480962
HILIC_POS_354_01196a7_39	HILIC	POS	7.39	354.0120				7.33E-01	0.07	0.21	4.59E-01	0.15	0.65	5.23E-01	0.14	0.24	9.69E-01	-0.01	0.31	2644358	107293	2651972	115065	2643401	113042	2660542	117567
HILIC_NEG_134_89474a4_83	HILIC	NEG	4.83	134.8947				2.58E-03	0.52	0.98	4.59E-01	0.16	0.56	2.62E-03	0.60	1.12	3.15E-02	0.44	0.75	30104543	13672817	39797353	19542690	38341817	20397189	41252889	18741897
RP_POS_180_96384a0_25	RP	POS	0.25	180.9638				3.11E-01	0.19	0.57	4.59E-01	-0.15	0.44	5.94E-01	0.11	0.29	2.21E-01	0.27	0.57	738992	105146	761854	125051	771168	129042	752541	121515
RP_NEG_205_83934a1_084	RP	NEG	1.08	205.8393				1.20E-03	0.62	1.08	4.59E-01	-0.15	0.63	1.21E-02	0.54	1.04	1.14E-03	0.69	1.15	1929262	1514888	3021465	1773268	3153473	1715048	2889457	1837437
RP_POS_322_27151a9_943	RP	POS	9.94	322.2715				7.22E-05	0.60	0.97	4.60E-01	-0.16	0.51	2.83E-03	0.52	1.01	6.99E-04	0.68	1.25	384402	307456	718858	599115	763446	653032	674271	542859
RP_POS_261_14615a8_915	RP	POS	8.92	261.1462				9.02E-06	-0.77	1.19	4.60E-01	-0.15	0.56	3.00E-05	-0.84	1.44	5.03E-04	-0.69	1.15	2248874	82889	2159011	118686	2167838	119189	2150185	118724
RP_POS_463_08826a0_694	RP	POS	0.69	463.0883				1.13E-10	-0.88	1.53	4.60E-01	-0.15	1.18	8.99E-08	-0.96	1.75	8.15E-06	-0.80	1.45	587439	86206	394409	228361	411389	233949	377430	223698
RP_POS_194_15178a8_531	RP	POS	8.53	194.1518				2.52E-01	0.26	0.61	4.60E-01	-0.14	0.51	4.47E-01	0.19	0.57	1.67E-01	0.33	0.57	354345	234465	407198	188076	421183	167327	393212	207533
HILIC_POS_583_25488a0_633	HILIC	POS	0.633	583.2549				5.48E-01	0.12	0.66	4.60E-01	0.15	0.97	4.09E-01	0.19	0.31	8.40E-01	0.04	0.09	1128454	581053	1201265	631050	1154346	534730	1248185	717039
RP_POS_312_15924a9_005	RP	POS	9.01	312.1592				2.96E-01	0.18	0.60	4.60E-01	-0.16	0.46	5.61E-01	0.10	0.57	2.52E-01	0.26	0.57	2012784	2829832	2679409	3873140	2967458	4659197	2391360	2903640
RP_POS_157_98714a15_426	RP	POS	15.43	157.9871				1.19E-01	-0.26	1.42	4.60E-01	0.16	0.62	3.14E-01	-0.18	0.68	1.18E-01	-0.34	1.51	1929854	260120	1834238	395793	1804827	455107	1863650	328044
RP_POS_419_75543a13_398	RP	POS	13.40	419.7554				4.21E-01	0.17	0.42	4.60E-01	-0.15	0.56	6.68E-01	0.10	0.38	3.04E-01	0.25	0.70	9768499	2427367	10161466	2232993	10327308	2306011	9995623	2168055
RP_POS_280_05966a3_969	RP	POS	3.97	280.0597				7.94E-01	0.04	0.99	4.61E-01	-0.16	0.54	8.45E-01	-0.04	0.75	4.75E-01	0.12	0.50	2601573	592184	2640239	1046342	2717966	874237	2562512	1198076
HILIC_POS_151_14423a1_508	HILIC	POS	1.508	151.1442				2.98E-01	0.16	0.32	4.61E-01	0.16	0.95	2.53E-01	0.24	0.39	6.33E-01	0.08	0.19	33213452	32178680	41715353	58058530	37406252	46916722	46024454	67611419
HILIC_POS_233_18591a0_55	HILIC	POS	0.55	233.1859				1.45E-01	-0.34	0.77	4.61E-01	-0.14	0.65	1.08E-01	-0.41	0.81	2.74E-01	-0.27	0.55	938808	808504	706365	642108	753980	615877	658750	670140
RP_NEG_225_89645a15_575	RP	NEG	15.58	225.8965				8.13E-01	0.05	0.27	4.61E-01	-0.15	0.59	9.25E-01	-0.02	0.45	5.95E-01	0.12	0.62	2934385	137770	2940937	127811	2950408	124023	2931466	132061
RP_POS_336_05029a4_851	RP	POS	4.85	336.0503				6.32E-01	0.09	0.51	4.62E-01	-0.16	0.55	9.67E-01	0.01	0.45	4.51E-01	0.16	0.52	1673822	731159	1750565	936556	1819929	1010333	1681202	861153
RP_POS_403_73975a6_067	RP	POS	6.07	403.7398				1.44E-07	0.63	1.33	4.62E-01	-0.16	1.20	4.78E-04	0.55	1.41	9.92E-05	0.71	1.43	118152	37932	1684692	2763989	1889382	2954951	1480001	2572536
RP_POS_396_2417a10_142	RP	POS	10.14	396.2417				5.37E-01	-0.18	0.78	4.62E-01	-0.11	0.56	4.32E-01	-0.23	0.52	6.76E-01	-0.13	0.66	1194794	3397901	808448	1541129	922566	1715048	694331	1353020
HILIC_POS_64_01662a5_648	HILIC	POS	5.648	64.0166				7.98E-01	0.05	0.54	4.62E-01	-0.15	0.64	9.17E-01	-0.02	0.23	5.58E-01	0.13	0.33	2697284	617779	2730038	653201	2778363	591285	2681713	712507
RP_POS_740_46301a5_94	RP	POS	5.94	740.4630				2.12E-07	0.62	1.32	4.62E-01	-0.16	1.19	5.30E-04	0.54	1.40	1.32E-04	0.70	1.42	12849	9167	453099	789145	511471	849400	394727	727856
RP_POS_473_34268a10_457	RP	POS	10.46	473.3427				8.32E-01	-0.04	0.71	4.62E-01	0.15	0.79	8.84E-01	0.03	0.56	6.11E-01	-0.12	0.52	26358867	1578366	26289855	1636263	26168836	1738535	26410874	1535239
RP_POS_392_74878a6_067	RP	POS	6.07	392.7488				1.48E-07	0.63	1.33	4.63E-01	-0.16	1.20	4.79E-04	0.55	1.40	1.02E-04	0.71	1.43	19773	13312	507347	861200	571005	921291	443688	800887
HILIC_NEG_351_99756a7_368	HILIC	NEG	7.368	351.9976				9.57E-02	0.35	0.70	4.63E-01	-0.14	0.58	2.42E-01	0.28	0.60	5.95E-02	0.43	0.78	1084401	40248	1098090	37871	1100887	33847	1095294	41667
HILIC_POS_171_18555a5_121	HILIC	POS	5.121	171.1856				9.27E-01	0.02	0.59	4.63E-01	-0.15	0.76	7.95E-01	-0.06	0.20	6.34E-01	0.09	0.18	286906319	47999507	287842267	57079472	292057655	46933743	283626879	65905865
HILIC_NEG_98_93896a5_606	HILIC	NEG	5.606	98.9390				2.33E-01	-0.28	0.81	4.63E-01	0.14	0.73	4.02E-01	-0.22	0.35	1.62E-01	-0.35	0.76	1503638	241294	1447581	180717	1434243	169132	1460919	192393
RP_POS_235_16945a9_111	RP	POS	9.11	235.1695				6.24E-01	-0.09	0.62	4.63E-01	0.15	0.77	9.38E-01	-0.02	0.64	4.51E-01	-0.17	0.60	9590029	366438	9551793	427615	9520242	463121	9583343	391061
RP_POS_326_30518a10_81	RP	POS	10.81	326.3052				1.41E-18	1.18	1.94	4.64E-01	0.14	0.83	1.21E-12	1.25	2.14	1.27E-09	1.11	1.95	523001	197199	1203839	559827	1162558	588885	1245119	531925
RP_POS_280_05978a3_712	RP	POS	3.71	280.0598				2.12E-01	0.22	0.75	4.64E-01	-0.16	0.54	5.22E-01	0.14	0.77	1.20E-01	0.30	0.58	1235242	412503	1351781	568482	1393698	491701	1309864	638423
RP_POS_263_00732a0_549	RP	POS	0.55	263.0073				5.82E-04	0.43	1.19	4.64E-01	-0.17	1.19	3.26E-02	0.34	1.15	4.81E-03	0.51	1.32	918470	90603	1073541	408789	1103674	431157	1043408	387140
RP_POS_440_26535a11_668	RP	POS	11.67	440.2654				7.19E-01	-0.07	0.75	4.64E-01	-0.15	0.48	5.19E-01	-0.15	0.54	9.97E-01	0.00	0.51	1246252	724402	1193232	710918	1245626	715900	1140839	709230
RP_POS_795_54419a10_663	RP	POS	10.66	795.5442				3.10E-01	0.17	0.74	4.64E-01	-0.16	0.44	6.77E-01	0.09	0.43	1.68E-01	0.25	0.71	2388762	204374	2437361	308637	2460115	256973	2414608	354071
RP_POS_820_58289a13_191	RP	POS	13.19	820.5829				1.11E-09	-1.01	1.93	4.64E-01	-0.14	0.56	6.54E-08	-1.09	2.04	4.66E-07	-0.94	1.72	2128772	584102	1183128	908758	1250088	865114	1116167	954443
RP_NEG_453_28665a9_323	RP	NEG	9.32	453.2867				2.50E-01	-0.33	0.66	4.64E-01	0.11	0.49	3.57E-01	-0.27	0.46	1.91E-01	-0.38	0.58	1792878	3562296	1028731	1743963	900266	1638076	1157195	1851461
HILIC_POS_460_27512a0_545	HILIC	POS	0.545	460.2751				3.45E-01	-0.19	0.55	4.65E-01	0.15	0.68	6.14E-01	-0.11	0.31	2.34E-01	-0.26	0.44	970751	139054	943552	145304	932867	139568	954238	151477
RP_POS_132_0808a2_894	RP	POS	2.89	132.0808				7.60E-04	-0.57	1.21	4.65E-01	-0.15	1.03	3.16E-03	-0.65	1.21	5.50E-03	-0.49	1.17	1130002	192156	974690	284441	995618	229558	953763	331472
RP_POS_425_21384a9_946	RP	POS	9.95	425.2138				1.66E-04	-0.69	1.18	4.65E-01	0.15	0.89	2.21E-03	-0.61	1.21	4.05E-04	-0.76	1.16	1067149	53795	1020279	68851	1015216	73177	1025342	64579
RP_NEG_394_90125a15_433	RP	NEG	15.43	394.9013				5.82E-02	-0.41	0.77	4.65E-01	-0.14	0.47	3.91E-02	-0.48	0.83	1.55E-01	-0.34	0.65	1015618	68612	989244	61297	993751	64818	984737	57866
RP_POS_814_55811a11_168	RP	POS	11.17	814.5581				3.25E-02	0.27	0.57	4.65E-01	-0.17	0.61	1.60E-01	0.19	0.56	8.24E-02	0.35	0.63	1203344	721633	1858267	2748513	2060353	3305061	1656181	2063019
HILIC_NEG_134_89471a7_332	HILIC	NEG	7.332	134.8947				8.26E-02	-0.33	0.87	4.66E-01	0.15	0.77	2.14E-01	-0.26	0.70	7.07E-02	-0.41	0.67	7836164	521722	7642986	588084	7599795	637144	7686178	537573
RP_POS_663_45435a13_57	RP	POS	13.57	663.4544	CE(16:0) [M+K]+	495.2669(100), 493.2017(60), 551.3235(50), 607.388(40), 381.1398(35),		3.84E-01	0.16	0.55	4.66E-01	0.15	0.76	2.45E-01	0.24	0.52	7.02E-01	0.08	0.35	61142289	4887120	62065156	5999226	61624739	6470495	62505572	5518404
RP_POS_127_03481a15_448	RP	POS	15.45	127.0348				9.76E-01	0.00	0.18	4.66E-01	0.16	0.59	6.12E-01	0.07	0.46	7.18E-01	-0.08	0.32	22271329	569072	22267247	907194	22200538	1185875	22333955	497408
RP_POS_556_4425a10_461	RP	POS	10.46	556.4425				3.10E-01	-0.20	0.48	4.66E-01	0.15	0.52	5.82E-01	-0.13	0.42	1.94E-01	-0.28	0.59	5177492	402656	5092629	421900	5061659	368802	5123599	470807
RP_POS_377_32785a10_705	RP	POS	10.71	377.3279				1.80E-01	-0.31	1.03	4.66E-01	-0.14	0.49	1.37E-01	-0.38	0.92	3.21E-01	-0.24	0.56	7768763	745848	7571429	597007	7615204	552399	7527654	641134
RP_POS_263_23676a10_977	RP	POS	10.98	263.2368				5.37E-03	0.47	1.39	4.67E-01	-0.15	1.28	4.87E-02	0.39	1.12	6.19E-03	0.55	1.35	931261	457624	1233907	679841	1283722	676781	1184092	686079
RP_POS_804_84253a0_493	RP	POS	0.49	804.8425				8.07E-08	0.64	1.33	4.67E-01	-0.16	1.17	4.38E-04	0.56	1.39	6.10E-05	0.72	1.44	27856	15831	2245001	3824801	2525235	4025600	1964767	3631947
RP_POS_278_24786a9_21	RP	POS	9.21	278.2479				2.45E-01	-0.32	0.94	4.67E-01	-0.11	0.54	1.86E-01	-0.38	0.73	3.57E-01	-0.27	0.62	9142800	17141774	5404557	8996095	6063534	9359395	4745581	8661787
RP_POS_241_15463a4_67	RP	POS	4.67	241.1546				1.06E-11	0.87	1.44	4.67E-01	-0.15	0.52	1.21E-05	0.79	1.48	2.77E-08	0.95	1.62	352772	209291	1007259	792822	1065305	745195	949214	841292
RP_NEG_266_80435a0_521	RP	NEG	0.52	266.8044				2.46E-04	0.46	1.23	4.67E-01	-0.16	1.17	1.74E-02	0.38	1.20	3.10E-03	0.54	1.34	1821411	261620	2247025	1028531	2322319	1099136	2171731	957952
RP_POS_418_31619a10_242	RP	POS	10.24	418.3162				4.60E-08	0.65	1.32	4.67E-01	-0.16	1.17	3.57E-04	0.57	1.34	4.14E-05	0.74	1.46	19246	15254	266016	416079	296439	434911	235593	398420
RP_POS_785_41309a5_862	RP	POS	5.86	785.4131				9.42E-07	0.59	1.27	4.68E-01	-0.16	1.16	1.02E-03	0.50	1.38	2.91E-04	0.67	1.35	41497	58282	466068	806725	525055	874050	407081	737448
HILIC_POS_116_07091a7_152	HILIC	POS	7.152	116.0709				2.48E-03	0.47	0.98	4.68E-01	0.16	0.83	1.16E-02	0.54	0.93	1.47E-02	0.39	0.94	4156254	1157035	5069682	2111765	4915188	1591799	5224175	2535267
RP_POS_159_06534a4_852	RP	POS	4.85	159.0653				5.57E-01	0.10	0.50	4.68E-01	-0.16	0.56	8.96E-01	0.03	0.43	4.00E-01	0.18	0.58	97355935	43035917	103003818	58109051	107251278	62782000	98756359	53327642
RP_POS_388_25415a4_201	RP	POS	4.20	388.2542				9.86E-01	0.00	1.20	4.68E-01	-0.11	1.10	8.30E-01	-0.06	0.93	8.59E-01	0.05	1.01	1900595	6008143	1880970	3102293	2107722	3317780	1654217	2886566
RP_POS_188_07039a2_893	RP	POS	2.89	188.0704	fragment of tryptophan (desethyl atrazine)	146.0602(100), 188.0693(45)		1.02E-03	-0.56	1.20	4.68E-01	-0.15	1.04	3.44E-03	-0.64	1.21	7.16E-03	-0.49	1.16	129950787	22068613	112793151	31569521	115100147	26074177	110486154	36371478
RP_NEG_792_86108a0_482	RP	NEG	0.48	792.8611				6.26E-08	0.65	1.34	4.68E-01	-0.16	1.20	2.87E-04	0.57	1.39	6.91E-05	0.73	1.46	1464144	370472	6965787	9382684	7650981	10053007	6280593	8708906
RP_POS_334_31085a11_149	RP	POS	11.15	334.3109				7.11E-01	-0.08	0.60	4.68E-01	-0.15	0.43	5.10E-01	-0.15	0.38	9.92E-01	0.00	0.36	2207633	1506077	2093529	1515115	2204126	1547980	1982931	1488888
RP_POS_792_76532a0_501	RP	POS	0.50	792.7653				3.93E-03	-0.40	1.14	4.68E-01	-0.16	1.32	5.62E-03	-0.48	1.18	8.26E-02	-0.32	1.18	1193012	189731	1026527	456301	1059820	479323	993234	434348
HILIC_NEG_85_00388a3_061	HILIC	NEG	3.061	85.0039				9.43E-02	-0.39	0.79	4.69E-01	0.13	0.54	1.86E-01	-0.32	0.55	7.39E-02	-0.46	0.98	9448347	3850087	8176463	2998711	7957719	3220479	8395207	2774693
RP_POS_304_09793a7_093	RP	POS	7.09	304.0979				3.48E-01	-0.18	0.53	4.69E-01	0.15	0.55	6.34E-01	-0.10	0.34	2.48E-01	-0.25	0.59	2922297	178860	2886338	211462	2870914	217776	2901762	205993
RP_POS_370_73569a5_94	RP	POS	5.94	370.7357				1.90E-07	0.62	1.32	4.69E-01	-0.16	1.19	5.48E-04	0.54	1.39	1.15E-04	0.70	1.42	26217	17559	601142	1025753	675918	1095614	526365	956049
RP_POS_613_47931a13_873	RP	POS	13.87	613.4793				3.14E-01	0.16	0.66	4.69E-01	0.16	0.43	3.02E-01	0.24	0.47	5.67E-01	0.08	0.41	517395	648886	673761	1035498	598174	569671	749347	1352854
HILIC_NEG_141_92378a4_274	HILIC	NEG	4.274	141.9238				5.28E-01	-0.12	0.63	4.69E-01	-0.15	0.62	3.55E-01	-0.20	0.48	8.32E-01	-0.05	0.15	2842854	787452	2738635	868906	2801928	931829	2675342	805557
RP_NEG_394_89191a14_25	RP	NEG	14.25	394.8919				7.49E-01	0.06	0.24	4.69E-01	0.15	0.64	5.28E-01	0.13	0.37	9.20E-01	-0.02	0.39	2286814	797340	2343349	1052066	2266739	1004738	2419960	1102178
HILIC_NEG_287_70486a1_362	HILIC	NEG	1.362	287.7049				3.74E-11	0.90	1.62	4.70E-01	-0.15	0.42	2.00E-05	0.83	1.45	2.41E-09	0.98	2.16	1337033	189052	1775952	505483	1812743	433598	1739161	570500
RP_POS_261_14444a3_445	RP	POS	3.45	261.1444				3.86E-03	0.44	0.83	4.70E-01	0.16	1.05	1.57E-02	0.52	0.91	2.04E-02	0.37	0.84	979300	398203	1279057	727833	1226084	544114	1332031	876644
RP_POS_599_45172a15_1	RP	POS	15.10	599.4517				4.08E-01	0.18	0.43	4.70E-01	-0.14	0.51	6.45E-01	0.11	0.69	2.97E-01	0.25	0.48	2297570	786359	2427553	703355	2478697	716687	2376408	693206
RP_NEG_826_5979a10_94	RP	NEG	10.94	826.5979				5.07E-08	0.92	1.63	4.70E-01	0.14	0.44	1.18E-06	1.00	1.66	6.05E-06	0.85	1.64	1133810	458084	1772865	683729	1723190	640288	1822541	727673
HILIC_POS_125_02105a4_861	HILIC	POS	4.861	125.0211				1.39E-02	0.38	0.87	4.70E-01	0.16	0.75	1.65E-02	0.46	0.81	1.05E-01	0.31	0.66	1094940	249711	1250885	438249	1219050	435324	1282720	443249
RP_POS_342_18396a5_683	RP	POS	5.68	342.1840				8.70E-01	0.03	0.67	4.70E-01	0.15	0.58	5.89E-01	0.11	0.59	8.57E-01	-0.04	0.47	3323361	1560416	3377011	1749029	3249866	2100598	3504156	1317246
RP_POS_553_45905a13_932	RP	POS	13.93	553.4591				4.09E-01	-0.18	0.39	4.71E-01	-0.14	0.61	2.54E-01	-0.25	0.51	6.76E-01	-0.11	0.48	12919109	2669627	12476017	2460289	12654805	2960008	12297229	1844639
RP_NEG_829_18097a9_373	RP	NEG	9.37	829.1810				3.78E-01	0.15	0.51	4.71E-01	-0.16	0.52	7.19E-01	0.07	0.25	2.56E-01	0.23	0.51	5223433	326360	5289130	465805	5322940	459460	5255320	474280
HILIC_NEG_353_01108a6_639	HILIC	NEG	6.639	353.0111				3.15E-01	-0.20	0.57	4.71E-01	0.15	0.64	5.47E-01	-0.13	0.64	2.38E-01	-0.28	0.57	1850947	252397	1798657	257157	1780005	279213	1817309	234392
HILIC_POS_84_9119a2_83	HILIC	POS	2.83	84.9119				8.13E-06	0.56	1.41	4.71E-01	-0.16	0.64	2.80E-03	0.48	1.17	5.49E-04	0.64	1.86	4731689	700217	6287600	3102178	6512508	3319727	6062693	2884371
RP_NEG_260_98041a0_552	RP	NEG	0.55	260.9804				3.38E-03	0.41	0.76	4.71E-01	-0.16	0.83	8.38E-02	0.33	0.77	3.24E-03	0.49	0.95	3012302	667082	3592027	1537942	3703537	1373942	3480518	1692841
HILIC_NEG_297_73328a0_552	HILIC	NEG	0.552	297.7333				3.71E-01	-0.19	0.37	4.71E-01	-0.14	0.75	2.65E-01	-0.26	0.43	6.10E-01	-0.12	0.27	186839	110346	166948	102353	174366	103178	159529	102020
RP_NEG_327_25543a10_401	RP	NEG	10.40	327.2554	FA 19:1;2O	327.2529(100), 265.2538(60), 309.2448(35)	3	1.28E-01	-0.33	0.57	4.71E-01	0.14	0.45	2.60E-01	-0.26	0.51	1.00E-01	-0.40	0.71	1372103	392429	1251466	353949	1225811	379384	1277120	328392
RP_POS_565_42505a11_156	RP	POS	11.16	565.4251				7.93E-01	-0.06	0.74	4.71E-01	0.14	0.48	9.76E-01	0.01	0.55	6.11E-01	-0.13	0.44	2096937	1806928	2004495	1431724	1900727	1497191	2108262	1370381
RP_POS_384_2355a6_067	RP	POS	6.07	384.2355				1.71E-07	0.62	1.32	4.72E-01	-0.16	1.19	5.31E-04	0.54	1.40	1.07E-04	0.70	1.43	61595	25553	997595	1662867	1118018	1772016	877173	1554687
RP_POS_540_44635a10_878	RP	POS	10.88	540.4464				1.14E-03	-0.74	1.43	4.72E-01	0.13	0.66	4.73E-03	-0.67	1.09	1.09E-03	-0.80	1.41	7614113	1108684	6861564	925390	6794568	963103	6928560	890754

Supplementary table 1: Metabolomics results (in asceding order according to p-value from progressive ALD vs non-progressive ALD comparison, with molecular features with ID_level of 1-2 first)

								all_ALD_vs_control			Prog_ALD_vs_non-prog_ALD			Prog_ALD_vs_control_ALD			Non-prog_ALD_vs_control			Healthy_control		all_ALD		Non-prog_ALD		Progressive_ALD	
								t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA								
Feature_ID	RP_HILIC	POS_NEG	Average.Rt	Average.Mz	Metabolite.name	curated_MSMS	ID_level	p	d	VIP	p	d	VIP	p	d	VIP	p	d	VIP	Mean	SD	Mean	SD	Mean	SD	Mean	SD
RP_POS_605_27509a10_331	RP	POS	10.33	605.2751				2.96E-02	-0.50	1.08	4.72E-01	0.13	0.47	8.06E-02	-0.43	0.87	2.10E-02	-0.57	1.12	640391	309688	505074	250210	486961	242018	523187	259318
RP_POS_263_99258a0_614	RP	POS	0.61	263.9926				2.87E-07	0.66	1.30	4.72E-01	-0.16	1.15	4.17E-04	0.58	1.35	6.84E-05	0.74	1.43	634410	194243	1060895	708340	1112166	749871	1009625	667878
HILIC_POS_146_09219a3_841	HILIC	POS	3.841	146.0922				5.41E-04	0.43	0.69	4.72E-01	0.16	0.69	5.65E-03	0.51	1.02	2.50E-02	0.35	0.70	288702	312206	799003	1326514	703018	1212445	894989	1437485
RP_NEG_127_869a15_551	RP	NEG	15.55	127.8690				3.44E-01	0.19	0.66	4.72E-01	-0.14	0.52	5.98E-01	0.12	0.32	2.36E-01	0.27	0.48	695174	153520	724911	152408	735938	145621	713885	159614
RP_NEG_329_26956a11_611	RP	NEG	11.61	329.2696				8.99E-02	-0.33	0.86	4.72E-01	-0.15	0.96	5.15E-02	-0.40	0.86	2.72E-01	-0.25	0.80	3062551	882284	2742985	1001291	2815439	1130569	2670531	858330
RP_NEG_426_9682a11_253	RP	NEG	11.25	426.9682				7.71E-01	0.07	0.67	4.72E-01	0.13	0.43	6.32E-01	0.14	0.68	9.63E-01	0.01	0.50	23948551	15276997	24790893	9824100	24079268	6065949	25502517	12536598
RP_POS_567_44666a10_881	RP	POS	10.88	567.4467				4.06E-02	-0.40	0.70	4.72E-01	0.15	0.51	1.23E-01	-0.33	0.64	3.62E-02	-0.48	0.73	1585470	272150	1467252	294506	1445957	312917	1488546	276398
RP_POS_745_41852a5_94	RP	POS	5.94	745.4185				2.04E-07	0.62	1.32	4.73E-01	-0.16	1.19	5.38E-04	0.54	1.40	1.26E-04	0.70	1.42	7364	4036	291299	508186	328040	544417	254558	471839
RP_NEG_153_86746a15_592	RP	NEG	15.59	153.8675				9.55E-01	-0.01	0.29	4.73E-01	-0.15	0.43	7.00E-01	-0.08	0.30	7.95E-01	0.06	0.20	818908	42151	818419	42567	821495	46535	815343	38420
RP_POS_1074_18921a10_932	RP	POS	10.93	1074.1892				1.51E-03	-0.76	1.39	4.73E-01	-0.13	1.23	1.38E-03	-0.82	1.33	4.85E-03	-0.70	1.25	399005	218190	257081	162015	268783	152338	245379	171892
RP_POS_432_33209a10_242	RP	POS	10.24	432.3321				3.81E-07	0.61	1.24	4.73E-01	-0.16	1.11	8.11E-04	0.53	1.28	1.56E-04	0.69	1.36	99582	83342	1155792	1936500	1295503	2061391	1016081	1813128
HILIC_NEG_251_86798a7_667	HILIC	NEG	7.667	251.8680				3.35E-01	0.17	0.73	4.73E-01	0.15	0.70	2.48E-01	0.25	0.64	6.32E-01	0.10	0.27	361822	30859	368428	40571	365501	37924	371355	43242
RP_NEG_270_7984a0_521	RP	NEG	0.52	270.7984				4.07E-04	0.45	1.21	4.74E-01	-0.16	1.16	2.05E-02	0.37	1.17	3.87E-03	0.53	1.33	1925498	312882	2365792	1079576	2443655	1154611	2287930	1004617
RP_POS_294_64435a10_514	RP	POS	10.51	294.6444				4.22E-03	-0.58	1.19	4.74E-01	0.14	0.65	2.71E-02	-0.50	1.11	2.96E-03	-0.65	1.13	1964642	425733	1703225	447113	1670986	410701	1735464	482807
HILIC_POS_581_23901a0_633	HILIC	POS	0.633	581.2390				8.69E-01	0.03	0.58	4.74E-01	0.15	0.88	6.55E-01	0.11	0.19	8.48E-01	-0.04	0.08	782004	435521	796811	457368	763826	386484	829796	520624
RP_NEG_350_02948a4_851	RP	NEG	4.85	350.0295				5.87E-01	0.10	0.51	4.74E-01	-0.15	0.56	9.10E-01	0.02	0.42	4.25E-01	0.17	0.55	13342225	5727633	14022135	7262224	14545610	7835477	13498660	6678487
RP_POS_362_33905a12_101	RP	POS	12.10	362.3391				8.10E-01	-0.05	0.59	4.74E-01	-0.15	0.44	5.65E-01	-0.12	0.35	8.99E-01	0.03	0.36	1733474	1158178	1674406	1327800	1770089	1436534	1578724	1216459
HILIC_NEG_171_02756a0_93	HILIC	NEG	0.93	171.0276				1.76E-05	0.67	1.16	4.75E-01	-0.15	1.23	3.38E-03	0.59	0.97	2.77E-05	0.74	1.40	246286	105855	367207	191294	380973	168376	353440	212595
RP_POS_275_9928a4_852	RP	POS	4.85	275.9928				6.03E-01	0.09	0.48	4.75E-01	-0.15	0.54	9.26E-01	0.02	0.43	4.37E-01	0.17	0.56	647019	282577	679162	357866	704912	386960	653413	328113
RP_POS_564_79413a0_5	RP	POS	0.50	564.7941				4.50E-02	-0.34	1.01	4.75E-01	-0.15	1.21	3.65E-02	-0.41	0.99	1.96E-01	-0.26	1.00	494613	197538	401567	294197	422727	301245	380407	288457
RP_POS_357_34729a9_476	RP	POS	9.48	357.3473				3.87E-01	-0.23	0.83	4.75E-01	-0.12	0.55	2.93E-01	-0.29	0.67	5.44E-01	-0.17	0.51	1957290	3090697	1453554	1805111	1583342	1941512	1323765	1667184
RP_NEG_432_85736a0_499	RP	NEG	0.50	432.8574				2.28E-02	-0.32	1.11	4.75E-01	-0.16	1.29	1.93E-02	-0.40	1.17	1.99E-01	-0.25	1.15	1895665	414747	1622410	930326	1689253	998783	1555566	861390
RP_POS_301_03748a0_258	RP	POS	0.26	301.0375				4.33E-01	-0.12	0.48	4.75E-01	0.16	0.52	7.99E-01	-0.04	0.32	3.52E-01	-0.20	0.54	3418144	201483	3377562	372101	3350814	441029	3404311	289442
RP_POS_296_17584a6_887	RP	POS	6.89	296.1758				3.63E-02	-0.30	0.76	4.75E-01	-0.16	0.50	2.61E-03	-0.38	1.07	3.25E-01	-0.22	0.71	2475284	686021	2067856	1492266	2175264	1961481	1960449	792599
RP_NEG_190_92766a15_653	RP	NEG	15.65	190.9277				8.88E-02	0.36	0.69	4.75E-01	-0.14	0.61	2.02E-01	0.29	0.62	6.85E-02	0.43	0.82	12094770	2671444	13019454	2463035	13196372	2554350	12842535	2380821
HILIC_POS_146_08133a4_885	HILIC	POS	4.885	146.0813				5.12E-01	-0.11	0.37	4.75E-01	0.15	1.31	8.83E-01	-0.03	0.24	2.66E-01	-0.19	0.72	4742644	3708508	4182834	5420947	3793163	3783322	4572505	6689518
RP_POS_180_13617a7_649	RP	POS	7.65	180.1362				7.04E-03	-0.51	0.84	4.76E-01	-0.15	0.68	1.09E-02	-0.58	0.93	2.82E-02	-0.43	0.84	8540728	372773	8319269	443161	8351101	374095	8287437	504753
RP_POS_131_96158a15_405	RP	POS	15.41	131.9616				2.07E-01	0.25	0.46	4.76E-01	-0.15	0.44	4.26E-01	0.18	0.36	1.47E-01	0.32	0.70	28631879	8532322	30886596	9160612	31544329	9124436	30228862	9241646
RP_POS_158_15396a7_911	RP	POS	7.91	158.1540				6.32E-01	0.11	0.83	4.76E-01	-0.14	0.45	8.87E-01	0.04	0.65	4.45E-01	0.17	0.62	3060001	632388	3120102	552326	3159758	462638	3080446	631752
HILIC_NEG_127_87013a3_059	HILIC	NEG	3.059	127.8701				3.90E-02	0.34	1.18	4.76E-01	0.15	0.85	2.96E-02	0.42	1.23	1.92E-01	0.26	1.23	476047	66991	508991	103158	501589	108713	516394	97826
HILIC_POS_387_21368a5_921	HILIC	POS	5.921	387.2137				3.79E-01	-0.17	0.99	4.76E-01	0.15	0.82	6.62E-01	-0.09	0.69	2.70E-01	-0.24	0.94	1473286	333440	1411011	382116	1383591	389680	1438431	376325
RP_POS_176_936a0_497	RP	POS	0.50	176.9360				7.12E-07	-0.61	1.31	4.76E-01	0.16	1.18	7.39E-04	-0.53	1.35	2.16E-04	-0.68	1.43	827364	48180	670508	286434	649959	309815	691057	262520
RP_POS_177_00838a15_337	RP	POS	15.34	177.0084				7.37E-01	0.07	0.78	4.76E-01	0.14	0.81	5.34E-01	0.14	0.42	9.95E-01	0.00	1.14	6641843	2540607	6814907	2461514	6638332	2575936	6991481	2354290
HILIC_NEG_176_99812a0_7	HILIC	NEG	0.7	176.9981				2.69E-04	0.59	1.04	4.76E-01	-0.15	0.83	9.84E-03	0.52	0.99	4.00E-04	0.67	1.21	600823	167182	752937	269726	772281	252846	733592	286870
HILIC_NEG_136_89169a1_409	HILIC	NEG	1.409	136.8917				7.39E-01	-0.05	0.86	4.76E-01	0.16	0.79	8.58E-01	0.03	0.14	4.60E-01	-0.13	0.32	4794878	278782	4767340	661385	4719911	622379	4814769	701314
RP_POS_406_74786a13_153	RP	POS	13.15	406.7479				6.89E-02	0.42	0.72	4.76E-01	0.13	0.56	6.57E-02	0.49	0.73	1.24E-01	0.36	0.75	18305811	5993300	20468800	4717584	20130373	3412804	20807227	5751906
RP_POS_419_31503a13_796	RP	POS	13.80	419.3150				1.04E-01	0.37	0.89	4.77E-01	0.14	0.49	7.33E-02	0.43	0.83	2.24E-01	0.30	0.78	5327371	2142371	6022213	1789924	5894035	1855330	6150391	1731261
HILIC_NEG_335_65012a1_364	HILIC	NEG	1.364	335.6501				6.45E-07	0.77	1.30	4.77E-01	-0.15	0.70	5.00E-04	0.70	1.16	1.79E-06	0.85	1.60	267517	71186	363595	129179	372844	113823	354346	143474
RP_POS_820_54364a11_616	RP	POS	11.62	820.5436				6.56E-02	0.25	0.61	4.77E-01	-0.16	0.62	3.08E-01	0.17	0.45	7.57E-02	0.33	0.78	641466	731765	1063202	1865963	1196765	1975427	929638	1759538
RP_NEG_207_96753a13_291	RP	NEG	13.29	207.9675				2.26E-01	-0.25	0.84	4.77E-01	0.14	0.81	4.42E-01	-0.18	0.74	1.51E-01	-0.32	0.62	4237802	794105	4041444	769855	3986338	715529	4096549	824178
RP_POS_426_82114a0_5	RP	POS	0.50	426.8211				1.09E-01	-0.23	1.05	4.77E-01	-0.16	1.25	7.17E-02	-0.31	1.03	4.30E-01	-0.15	1.10	1410826	417150	1223274	895830	1287365	967279	1159183	823037
RP_NEG_718_85681a0_465	RP	NEG	0.47	718.8568				1.23E-09	-0.80	1.42	4.77E-01	0.15	1.14	4.72E-05	-0.72	1.44	7.75E-07	-0.87	1.57	523643	70776	354734	225575	338598	221597	370871	230585
RP_POS_445_3678a11_953	RP	POS	11.95	445.3678				9.30E-01	-0.02	0.85	4.77E-01	-0.14	0.69	7.08E-01	-0.09	0.73	8.28E-01	0.05	0.35	874796	359704	868465	327926	891920	323899	845010	333514
HILIC_POS_509_31198a0_653	HILIC	POS	0.653	509.3120				1.63E-06	0.59	1.31	4.77E-01	-0.16	0.86	1.25E-03	0.51	1.48	2.59E-04	0.67	1.47	77594	298956	875240	1489893	981774	1592099	768706	1388136
RP_POS_203_1209a6_498	RP	POS	6.50	203.1209				6.60E-01	0.09	0.42	4.78E-01	-0.14	0.61	9.28E-01	0.02	0.33	4.91E-01	0.16	0.62	772477	314762	800522	304533	822292	322548	778753	287000
RP_POS_263_23691a9_476	RP	POS	9.48	263.2369				3.41E-01	-0.27	0.88	4.78E-01	-0.11	0.49	2.66E-01	-0.32	0.70	4.69E-01	-0.21	0.57	2581497	4730017	1741486	2440069	1915886	2548818	1567086	2338983
RP_POS_432_28046a4_512	RP	POS	4.51	432.2805				9.11E-01	0.03	1.22	4.78E-01	-0.12	1.10	9.23E-01	-0.03	0.94	7.58E-01	0.09	1.04	1200787	3872448	1281767	2146327	1435171	2276010	1128363	2019705
RP_POS_848_53931a13_163	RP	POS	13.16	848.5393				6.89E-01	-0.08	0.30	4.78E-01	-0.14	0.47	5.06E-01	-0.15	0.47	9.54E-01	-0.01	0.48	10209642	3763924	9906062	3572494	10161337	3598685	9650788	3564039
RP_POS_312_17068a5_873	RP	POS	5.87	312.1707				1.81E-01	0.16	0.63	4.78E-01	-0.16	0.63	1.50E-01	0.08	0.64	2.89E-01	0.25	0.72	539994	701750	1008641	3251566	1241570	4550934	775712	734445
RP_POS_675_67456a11_668	RP	POS	11.67	675.6746	2 M 13-Docosenamide	338.3418(100), 321.3158(20), 303.3019(14)		8.58E-01	0.04	0.69	4.79E-01	-0.15	0.42	8.63E-01	-0.04	0.38	6.32E-01	0.11	0.46	26166921	24082533	27063619	26052133	28921377	27029650	25205861	25172072
RP_POS_469_36386a11_237	RP	POS	11.24	469.3639				4.45E-01	-0.13	0.71	4.79E-01	-0.15	0.64	3.74E-01	-0.21	0.60	7.42E-01	-0.06	0.31	2031387	864769	1881288	1221116	1968457	799624	1794120	1535504
RP_POS_780_55035a11_611	RP	POS	11.61	780.5504				7.59E-01	-0.06	0.54	4.79E-01	0.14	0.72	9.67E-01	0.01	0.35	5.43E-01	-0.13	0.65	964988	254277	949001	258794	930565	240159	967437	277391
RP_POS_277_89148a15_437	RP	POS	15.44	277.8915				7.31E-02	-0.25	0.55	4.79E-01	0.16	0.55	2.81E-01	-0.17	0.49	9.93E-02	-0.33	0.60	3314774	171378	3221545	417314	3191811	474062	3251279	354001
RP_POS_624_63947a15_221	RP	POS	15.22	624.6395				4.61E-02	0.36	0.74	4.79E-01	0.15	0.42	3.17E-02	0.43	0.81	1.88E-01	0.28	0.62	1690176	543996	1933886	717153	1882802	767505	1984969	666877
RP_NEG_268_80139a0_521	RP	NEG	0.52	268.8014				4.74E-04	0.44	1.21	4.79E-01	-0.16	1.16	2.25E-02	0.36	1.17	4.57E-03	0.52	1.33	3018220	451933	3678067	1657005	3796078	1777177	3560056	1536419
RP_POS_250_17767a7_801	RP	POS	7.80	250.1777				9.73E-02	0.29	0.67	4.79E-01	-0.15	0.44	2.58E-01	0.22	0.50	9.26E-02	0.37	0.65	519611	371610	658488	501156	694179	556917	622796	441232
RP_POS_313_27325a10_541	RP	POS	10.54	313.2733				4.65E-02	-0.38	0.88	4.79E-01	0.15	0.80	1.47E-01	-0.30	0.75	4.17E-02	-0.45	0.89	917097	130604	860753	153570	849819	161462	871687	146064
RP_POS_536_3703a10_823	RP	POS	10.82	536.3703				6.58E-01	0.09	0.75	4.79E-01	0.15	0.90	5.04E-01	0.16	0.44	9.44E-01	0.01	0.79	1271907	601560	1327370	651249	1280984	519620	1373755	763223
RP_POS_172_98991a0_249	RP	POS	0.25	172.9899				4.16E-01	-0.17	0.46	4.79E-01	-0.14	0.42	2.74E-01	-0.24	0.57	6.83E-01	-0.10	0.24	1299551	254806	1257436	246789	1275009	278623	1239864	211641
RP_NEG_554_72217a15_49	RP	NEG	15.49	554.7222				1.60E-01	0.30	1.02	4.79E-01	-0.14	0.42	3.30E-01	0.22	0.59	1.16E-01	0.37	0.86	1919414	66072	1938382	63348	1942891	63692	1933874	63321
RP_POS_806_56842a12_799	RP	POS	12.80	806.5684				8.31E-03	-0.70	1.31	4.79E-01	-0.11	0.57	5.69E-03	-0.76	1.38	2.01E-02	-0.65	0.92	42559261	24722840	29744044	14424277	30770610	15632789	28717477	13184493
RP_POS_291_1944a9_075	RP	POS	9.08	291.1944				4.35E-02	-0.46	0.94	4.80E-01	0.13	0.95	1.15E-01	-0.39	0.93	2.92E-02	-0.53	0.86	2182178	74137	2152167	60894	2147835	56168	2156499	65566
RP_NEG_470_19827a11_61	RP	NEG	11.61	470.1983				3.13E-02	-0.41	1.08	4.80E-01	-0.14	0.93	2.08E-02	-0.49	1.04	1.27E-01	-0.34	0.93	2024174	229173	1917894	260677	1936421	281997	1899366	238890
HILIC_POS_296_17023a0_554	HILIC	POS	0.554	296.1702				7.08E-05	0.50	1.00	4.80E-01	-0.16	0.64	7.55E-03	0.42	1.13	1.96E-03	0.58	1.04	468955	33609	531692	140560	541682	152648	521703	128110
RP_POS_144_08049a2_488	RP	POS	2.49	144.0805				5.12E-03	-0.50	1.10	4.80E-01	-0.15	0.92	9.82E-03	-0.57	1.12	2.45E-02	-0.43	0.99	1938832	343688	1719300	455005	1751636	384003	1686965	518356
RP_NEG_125_87193a15_551	RP	NEG	15.55	125.8719				9.66E-01	-0.01	0.23	4.81E-01	0.14	0.48	7.73E-01	0.06	0.32	7.27E-01	-0.08	0.34	1152022	242266	1149890	252537	1131965	267355	1167814	238154
RP_NEG_482_79044a15_487	RP	NEG	15.49	482.7904				4.24E-02	0.44	0.69	4.81E-01	0.14	0.70	3.25E-02	0.51	0.86	1.14E-01	0.37	0.74	2791665	86087	2827312	77951	2821785	78042	2832839	78253
RP_NEG_944_80957a0_486	RP	NEG	0.49	944.8096				3.74E-04	0.45	1.16	4.81E-01	0.16	1.25	3.42E-03	0.53	1.23	2.44E-02	0.37	1.23	1681255	341079	2219919	1344421	2124629	1288234	2315209	1404901
RP_NEG_164_07066a2_198	RP	NEG	2.20	164.0707				8.87E-01	-0.03	0.69	4.82E-01	0.14	0.78	8.78E-01	0.04	0.52	6.51E-01	-0.10	0.70	765120	239601	758290	217286	742895	172702	773686	255109
RP_NEG_190_92766a13_28	RP	NEG	13.28	190.9277				6.26E-01	-0.09	0.72	4.82E-01	0.15	0.51	9.36E-01	-0.02	0.52	4.28E-01	-0.16	0.51	3098190	465230	3049656	552798	3010511	517005	3088801	589055
HILIC_NEG_132_92337a4_215	HILIC	NEG	4.215	132.9234				3.93E-01	-0.16	0.85	4.82E-01	0.15	0.88	6.75E-01	-0.09	0.44	2.93E-01	-0.23	0.37	7854647	1488360	7581694	1771618	7456244	1903519	7707143	1638845
RP_POS_628_85773a0_471	RP	POS	0.47	628.8577				1.52E-09	-0.78	1.41	4.82E-01	0.15	1.15	6.31E-05	-0.70	1.44	1.25E-06	-0.85	1.57	696222	83877	477697	301038	456394	296955	499000	306577
RP_POS_410_75156a13_369	RP	POS	13.37	410.7516				5.09E-01	-0.13	0.50	4.82E-01	-0.15	0.60	3.40E-01	-0.20	0.42	8.14E-01	-0.05	0.27	1004966	357617	954909	409911	983917	445378	925901	373369
HILIC_NEG_165_04167a0_858	HILIC	NEG	0.858	165.0417				1.06E-03	-0.88	1.80	4.82E-01	0.11	0.47	3.49E-03	-0.82	1.32	5.97E-04	-0.93	1.88	469459	401502	204891	229272	188669	172627	221113	275439
RP_POS_797_0882a13_822	RP	POS	13.82	797.0882				2.35E-01	0.20	0.42	4.82E-01	-0.15	0.59	5.51E-01	0.12	0.82	1.59E-01	0.27	0.63	757110	465457	887549	714243	938040	687578	837057	743459
RP_POS_269_08798a1_786	RP	POS	1.79	269.0880	Unknown	137.0454(100)	4	4.23E-09	0.72	1.34	4.82E-01	0.15	0.83	5.57E-05	0.80	1.42	6.62E-06	0.64	1.48	420806	972288	4589482	6311468	4143171	5135645	5035792	7328085
RP_NEG_476_27832a10_336	RP	NEG	10.34	476.2783				6.32E-02	0.36	1.05	4.83E-01	-0.14	0.70	2.15E-01	0.29	0.81	3.37E-02	0.43	1.05	34795843	14013464	40330931	15488624	41424538	12584242	39237324	17996858
RP_POS_360_17526a5_57	RP	POS	5.57	360.1753				7.79E-07	0.59	1.30	4.83E-01	-0.16	1.17	9.97E-04	0.51	1.38	2.58E-04	0.67	1.38	55538	134275	1423897	2585494	1606332	2779095	1241462	2390541
RP_NEG_866_78992a0_495	RP	NEG	0.50	866.7899				2.30E-08	-0.69	1.37	4.83E-01	0.15	1.22	2.40E-04	-0.61	1.41	1.95E-05	-0.76	1.49	1948247	133334	1442695	807800	1385718	831166	1499673	787995
RP_POS_818_52887a11_617	RP	POS	11.62	818.5289				4.53E-02	0.26	0.63	4.83E-01	-0.16	0.60	2.77E-01	0.18	0.45	6.12E-02	0.34	0.79	978793	1182903	1857909	3814683	2126963	3992207	1588856	3648991
RP_POS_303_23178a9_959	RP	POS	9.96	303.2318				3.47E-06	0.55	1.06	4.84E-01	0.16	1.10	7.00E-04	0.63	1.24	1.65E-03	0.47	1.12	146768	120962	1763590	3281949	1532287	2937407	1994894	3608967
RP_POS_820_52399a12_827	RP	POS	12.83	820.5240				2.28E-04	-0.92	1.47	4.84E-01	-0.11	0.63	1.80E-04	-0.98	1.51	8.07E-04	-0.87	1.30	3734327	1832902	2331441	1230161	2418075	1243516	2244806	1223040
RP_POS_329_21463a14_268	RP	POS	14.27	329.2146				3.79E-01	0.14	0.40	4.84E-01	0.15	0.47	3.17E-01	0.21	0.50	7.17E-01	0.06	0.39	2542444	454203	2642724	801581	2586251	635407	2699196	942299
RP_NEG_187_09654a6_033	RP	NEG	6.03	187.0965				1.92E-01	0.20	0.72	4.84E-01	-0.15	0.79	5.20E-01	0.12	0.78	1.38E-01	0.28	0.72	3304337	427545	3446573	776693	3501257	760705	3391888	796266
RP_NEG_201_11285a6_815	RP	NEG	6.82	201.1129				1.07E-01	0.33	0.76	4.84E-01	0.14	0.62	8.63E-02	0.40	0.76	2.46E-01	0.26	0.60	2667750	514843	2840290	530571	2802944	502449	2877636	559871
HILIC_NEG_239_76093a1_358	HILIC	NEG	1.358	239.7609				1.40E-06	0.60	1.15	4.85E-01	0.16	0.44	2.80E-04	0.68	1.20	8.77E-04	0.52	1.38	212805	33273	296772	154604	285897	141187	307647	167682
RP_POS_321_01077a4_851	RP	POS	4.85	321.0108				7.61E-01	0.06	0.49	4.85E-01	-0.15	0.59	9.46E-01	-0.01	0.38	5.60E-01	0.13	0.51	2143389	885551	2200247	1009028	2271183	1073902	2129311	945260
RP_POS_371_22757a4_2	RP	POS	4.20	371.2276				9.55E-01	-0.02	1.20	4.85E-01	-0.11	1.10	8.10E-01	-0.07	0.93	8.99E-01	0.04	0.99	644359	2125314	622026	1062081	696679	1130097	547372	995268

Supplementary table 1: Metabolomics results (in asceding order according to p-value from progressive ALD vs non-progressive ALD comparison, with molecular features with ID_level of 1-2 first)

							all_ALD_vs_control			Prog_ALD_vs_non-prog_ALD			Prog_ALD_vs_control_ALD			Non-prog_ALD_vs_control			Healthy_control		all_ALD		Non-prog_ALD		Progressive_ALD	
							t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA								
Feature_ID	RP_HILIC	POS_NEG	Average.Rt	Average.Mz	Metabolite.name	curated_MSMS	ID_level	p	d	VIP	p	d	VIP	p	d	VIP	p	d	VIP	Mean	SD	Mean	SD	Mean	SD	Mean	SD
RP_NEG_290_85306a15_622	RP	NEG	15.62	290.8531				6.82E-01	-0.08	0.51	4.85E-01	0.14	0.50	9.54E-01	-0.01	0.51	5.12E-01	-0.15	0.57	1905816	76006	1899432	77032	1894017	83521	1904846	70380
RP_POS_130_9626a0_253	RP	POS	0.25	130.9626				2.48E-01	0.25	0.55	4.85E-01	-0.14	0.56	4.41E-01	0.19	0.35	1.78E-01	0.32	0.51	4342712	513266	4461362	452857	4493186	444978	4429538	462894
RP_NEG_201_14943a8_502	RP	NEG	8.50	201.1494				1.61E-02	0.30	1.03	4.85E-01	0.16	0.45	9.12E-02	0.38	0.75	1.29E-02	0.22	0.94	604520	303181	946015	1292506	855034	583791	1036996	1737105
RP_POS_335_68472a5_403	RP	POS	5.40	335.6847				7.77E-07	0.59	1.29	4.86E-01	-0.16	1.16	9.93E-04	0.51	1.38	2.56E-04	0.67	1.38	40647	126918	1222847	2232179	1379530	2397936	1066163	2065608
RP_POS_793_62634a11_129	RP	POS	11.13	793.6263				3.99E-03	0.38	0.97	4.86E-01	-0.16	0.46	2.39E-02	0.30	0.86	2.86E-02	0.46	0.90	906339	1273177	2206954	3823750	2475544	4681557	1938364	2734285
RP_POS_499_8273a4_412	RP	POS	4.41	499.8273				2.60E-01	-0.26	0.48	4.86E-01	-0.13	0.46	1.63E-01	-0.33	0.87	4.61E-01	-0.20	0.48	2225081	2427710	1689179	1918926	1823939	2330290	1554418	1404419
RP_POS_391_77905a13_718	RP	POS	13.72	391.7791				2.51E-03	0.58	1.10	4.86E-01	-0.14	0.41	1.88E-02	0.51	0.94	2.41E-03	0.65	1.13	2628410	848686	3192875	973023	3261146	947166	3124603	1003112
RP_NEG_632_32196a10_336	RP	NEG	10.34	632.3220				8.42E-02	-0.45	1.14	4.86E-01	-0.12	0.45	6.62E-02	-0.50	0.99	1.48E-01	-0.39	1.06	10448740	1904039	9815539	1200813	9899731	1129621	9731347	1273899
HILIC_NEG_297_73337a3_058	HILIC	NEG	3.058	297.7334				2.56E-01	-0.14	0.63	4.86E-01	-0.16	0.92	1.24E-01	-0.22	0.54	7.71E-01	-0.06	0.17	2280977	181177	2142366	1172061	2224541	1347842	2060191	972127
RP_NEG_790_81543a0_494	RP	NEG	0.49	790.8154				2.22E-09	-0.74	1.39	4.86E-01	0.15	1.19	9.23E-05	-0.66	1.43	4.07E-06	-0.81	1.53	2420347	179897	1726601	1020543	1655080	1030131	1798121	1016200
RP_NEG_1044_74609a0_495	RP	NEG	0.50	1044.7461				3.92E-09	-0.73	1.39	4.86E-01	0.15	1.18	1.17E-04	-0.66	1.44	4.55E-06	-0.81	1.52	2127941	162050	1591897	793478	1536309	797398	1647485	793672
RP_POS_971_76349a15_104	RP	POS	15.10	971.7635				2.42E-02	0.44	0.70	4.86E-01	0.14	0.44	2.24E-02	0.51	0.82	8.54E-02	0.37	0.71	2897966	1086367	3422132	1199113	3338142	1155844	3506122	1246883
RP_NEG_341_68329a15_599	RP	NEG	15.60	341.6833				1.33E-01	-0.32	0.89	4.87E-01	-0.14	0.46	1.07E-01	-0.39	0.72	2.67E-01	-0.25	0.78	2057180	98106	2027262	90805	2033616	83890	2020907	97671
RP_POS_406_24872a6_184	RP	POS	6.18	406.2487				1.92E-07	0.62	1.32	4.87E-01	-0.15	1.18	5.50E-04	0.54	1.39	1.17E-04	0.70	1.42	27369	17058	691761	1186039	774664	1261687	608857	1111848
RP_POS_282_2790Sa9_87	RP	POS	9.87	282.2791				2.60E-02	0.44	0.73	4.87E-01	-0.14	0.47	8.02E-02	0.36	0.79	2.80E-02	0.51	0.84	657702	544937	917297	601351	959332	664437	875261	534362
RP_NEG_512_30011a9_952	RP	NEG	9.95	512.3001				5.05E-03	0.44	0.94	4.87E-01	-0.15	0.52	6.70E-02	0.37	0.80	4.66E-03	0.52	0.95	22071746	7173047	27150443	12317365	28011381	11300018	26289506	13316461
RP_POS_414_76196a6_184	RP	POS	6.18	414.7620				1.48E-07	0.63	1.33	4.88E-01	-0.15	1.18	4.73E-04	0.55	1.40	1.04E-04	0.70	1.43	10123	7920	358423	615362	401395	655201	315450	576205
HILIC_POS_584_26245a0_559	HILIC	POS	0.559	584.2625				4.32E-03	-0.57	1.19	4.88E-01	0.14	0.67	3.92E-02	-0.50	0.76	1.38E-03	-0.64	1.53	1080383	604919	709765	636982	665241	423096	754288	797945
RP_POS_174_93758a0_498	RP	POS	0.50	174.9376				7.32E-08	-0.65	1.34	4.88E-01	0.15	1.20	3.00E-04	-0.57	1.39	7.03E-05	-0.73	1.47	11667067	327217	9609689	3502600	9365168	3733091	9854209	3275484
RP_POS_310_91449a15_459	RP	POS	15.46	310.9145				7.03E-01	0.09	0.52	4.88E-01	-0.13	0.68	9.32E-01	0.02	0.48	5.30E-01	0.15	0.43	27334795	6686112	27832726	5377651	28207769	5069327	27457683	5695903
RP_POS_242_24785a10_476	RP	POS	10.48	242.2479				3.45E-04	0.49	0.92	4.88E-01	0.15	0.90	1.19E-02	0.56	0.96	4.19E-04	0.41	1.23	1037218	347806	1446663	927898	1381851	498831	1511475	1217438
HILIC_NEG_195_81093a0_551	HILIC	NEG	0.551	195.8109				6.42E-01	0.10	0.42	4.89E-01	-0.14	0.71	9.07E-01	0.03	0.05	4.89E-01	0.17	0.64	1459577	650395	1521341	650314	1566685	724629	1475996	570232
RP_POS_167_99368a6_185	RP	POS	6.19	167.9937				3.31E-02	0.41	1.01	4.89E-01	-0.14	0.64	9.86E-02	0.34	0.88	3.56E-02	0.48	1.02	2386255	1783360	3204954	2032392	3346544	2259903	3063364	1788144
HILIC_POS_170_09256a6_294	HILIC	POS	6.294	170.0926				7.77E-01	-0.05	0.64	4.89E-01	-0.15	0.74	5.69E-01	-0.12	0.56	8.92E-01	0.03	0.25	25388252	8477029	24844047	11915096	25674018	10423178	24014075	13296161
RP_POS_516_46149a13_614	RP	POS	13.61	516.4615				9.61E-01	0.01	0.19	4.89E-01	0.16	0.59	7.05E-01	0.09	0.23	5.25E-01	-0.07	0.35	790017	90907	791408	234219	775067	120218	807749	309579
HILIC_NEG_234_8201a4_112	HILIC	NEG	4.112	234.8201				2.42E-01	-0.27	0.85	4.89E-01	-0.13	0.51	1.75E-01	-0.34	0.62	4.10E-01	-0.21	0.87	717558	311807	646153	242168	663011	252102	629295	233134
HILIC_POS_368_21854a5_647	HILIC	POS	5.647	368.2185				1.59E-01	-0.27	1.02	4.89E-01	-0.14	0.81	1.17E-01	-0.34	0.78	3.58E-01	-0.20	0.66	727127	134411	686994	150879	697495	151783	676493	150767
RP_POS_464_19113a6_782	RP	POS	6.78	464.1911				4.37E-04	0.53	1.45	4.89E-01	-0.15	0.45	1.46E-02	0.46	1.33	1.25E-03	0.61	1.17	242306	305496	532297	587262	573158	584773	491436	592811
HILIC_NEG_114_98878a7_351	HILIC	NEG	7.351	114.9888				3.87E-03	-0.48	0.89	4.90E-01	0.15	0.82	3.19E-02	-0.41	1.09	6.74E-03	-0.56	0.91	695072	72548	644842	109730	637212	115804	652473	103912
RP_POS_453_24539a3_808	RP	POS	3.81	453.2454				7.06E-06	0.53	1.10	4.90E-01	0.16	1.04	2.93E-04	0.61	1.33	6.79E-03	0.46	1.05	244803	149913	1296572	2204704	1143311	2241242	1449833	2179344
RP_POS_393_19839a10_978	RP	POS	10.98	393.1984				4.78E-03	0.50	1.46	4.90E-01	-0.14	1.36	4.31E-02	0.42	1.24	4.36E-03	0.57	1.40	971186	360237	1205565	491789	1239741	463654	1171389	520856
RP_POS_357_69766a5_569	RP	POS	5.57	357.6977				5.68E-07	0.60	1.30	4.90E-01	-0.15	1.16	8.21E-04	0.52	1.38	2.30E-04	0.67	1.38	66536	139468	2104746	3804003	2368883	4091666	1840610	3514553
HILIC_NEG_312_83664a4_182	HILIC	NEG	4.182	312.8366				3.84E-01	0.13	1.24	4.90E-01	0.15	0.86	2.48E-01	0.20	1.16	7.97E-01	0.05	0.96	725480	60799	740131	128860	731184	136541	749078	121417
HILIC_POS_276_18036a2_383	HILIC	POS	2.383	276.1804				2.91E-05	0.69	1.26	4.90E-01	0.14	1.02	1.41E-04	0.76	1.38	1.29E-03	0.61	1.16	393265	272192	678887	430850	648979	421672	708795	442063
RP_POS_413_13654a8_7	RP	POS	8.70	413.1365				2.48E-01	0.15	0.49	4.91E-01	0.16	0.60	3.03E-01	0.23	0.38	4.66E-01	0.08	0.30	1054298	493705	1244402	1385561	1148072	662354	1340732	1849619
HILIC_NEG_144_92351a1_419	HILIC	NEG	1.419	144.9235				5.01E-02	-0.39	0.71	4.91E-01	-0.14	0.82	6.25E-02	-0.46	0.71	1.03E-01	-0.32	0.67	18726211	3078648	17451827	3296037	17680717	2239054	17222936	4102335
RP_POS_298_2738a9_745	RP	POS	9.75	298.2738				9.97E-01	0.00	0.56	4.91E-01	-0.13	0.58	7.81E-01	-0.07	0.53	8.04E-01	0.06	0.29	3485260	5827809	3481267	4649553	3803883	5338180	3158652	3869019
HILIC_POS_596_32812a0_588	HILIC	POS	0.588	596.3281				5.95E-04	-0.73	1.17	4.91E-01	0.13	0.77	3.96E-03	-0.66	1.13	5.56E-04	-0.79	1.27	779155	340895	528385	323724	505952	316690	550818	332286
RP_POS_395_22656a6_067	RP	POS	6.07	395.2266				1.36E-07	0.63	1.33	4.92E-01	-0.15	1.19	4.70E-04	0.55	1.41	9.62E-05	0.71	1.43	13323	9367	394282	670633	440677	711334	347887	631100
RP_NEG_320_88718a15_46	RP	NEG	15.46	320.8872				3.12E-01	-0.13	0.55	4.92E-01	-0.16	0.42	2.67E-01	-0.21	0.56	7.52E-01	-0.05	0.44	11182162	246392	11078144	927080	11142270	834092	11014019	1016067
HILIC_NEG_174_08821a6_345	HILIC	NEG	6.345	174.0882				1.70E-04	0.62	1.01	4.92E-01	0.14	0.71	7.18E-04	0.69	1.13	3.39E-03	0.55	1.01	441664	117585	551003	184005	538281	171854	563725	196322
RP_POS_264_97281a0_523	RP	POS	0.52	264.9728				8.64E-07	-0.71	1.29	4.92E-01	-0.15	1.18	3.68E-05	-0.78	1.38	3.33E-04	-0.63	1.36	419153	71053	314234	157840	325147	152692	303322	163638
RP_POS_464_3739a11_841	RP	POS	11.84	464.3739				6.52E-01	0.10	0.48	4.92E-01	0.14	0.50	5.01E-01	0.16	0.52	8.96E-01	0.03	0.44	18357124	9283296	19195115	8423452	18612917	7543696	19777312	9260564
RP_POS_425_75281a6_184	RP	POS	6.18	425.7528				1.46E-07	0.63	1.33	4.92E-01	-0.15	1.19	4.74E-04	0.55	1.40	1.03E-04	0.70	1.43	67542	30078	1228897	2050387	1370560	2179138	1087234	1924675
RP_POS_860_53925a11_159	RP	POS	11.16	860.5393				3.54E-01	0.12	0.38	4.93E-01	-0.16	0.52	6.96E-01	0.04	0.27	3.75E-01	0.20	0.47	932070	557140	1142075	2028935	1282470	2681765	1001680	1041672
RP_POS_419_31323a11_165	RP	POS	11.17	419.3132				2.21E-01	0.23	0.65	4.93E-01	-0.14	0.43	4.87E-01	0.16	0.53	1.36E-01	0.30	0.53	5799380	666940	5975495	798658	6030633	692849	5920356	895814
RP_POS_338_16214a5_403	RP	POS	5.40	338.1621		338.1592(100)	4	8.47E-07	0.59	1.29	4.93E-01	-0.15	1.16	1.07E-03	0.51	1.38	2.63E-04	0.66	1.38	31095	89672	1001260	1840656	1128293	1969892	874228	1712240
RP_POS_193_09694a0_709	RP	POS	0.71	193.0969				6.46E-05	0.60	0.97	4.93E-01	0.15	0.48	5.81E-04	0.67	1.10	3.08E-03	0.52	1.03	1435989	707337	2215608	1394392	2119428	1311769	2311788	1479433
RP_NEG_582_88123a0_465	RP	NEG	0.47	582.8812				1.18E-09	-0.77	1.41	4.94E-01	0.15	1.18	6.82E-05	-0.69	1.44	1.54E-06	-0.84	1.56	1061116	108966	730012	464825	697982	459264	762042	472775
RP_POS_475_41324a13_195	RP	POS	13.20	475.4132				4.59E-01	0.14	0.40	4.94E-01	0.14	0.43	3.25E-01	0.21	0.56	7.57E-01	0.07	0.27	9924451	1391759	10146330	1672867	10031058	1694542	10261601	1659967
RP_POS_205_08577a9_46	RP	POS	9.46	205.0858				5.90E-01	0.08	0.34	4.94E-01	0.15	0.78	4.98E-01	0.16	0.57	9.82E-01	0.00	0.14	1019289	61004	1028210	124771	1019599	63874	1036822	164991
HILIC_POS_121_0399a0_701	HILIC	POS	0.701	121.0399				2.17E-01	-0.41	0.80	4.94E-01	0.06	0.69	2.60E-01	-0.38	0.54	1.87E-01	-0.45	0.72	591366	1255151	309201	319851	287182	294038	331220	345325
RP_NEG_688_83386a0_496	RP	NEG	0.50	688.8339				1.36E-08	-0.69	1.37	4.94E-01	0.15	1.21	1.56E-04	-0.62	1.42	2.13E-05	-0.77	1.49	11403035	590494	8562792	4504745	8252876	4702829	8872708	4322843
RP_POS_800_51849a12_25	RP	POS	12.25	800.5185				3.32E-08	0.83	1.48	4.94E-01	0.14	0.49	6.31E-06	0.90	1.53	1.08E-05	0.76	1.41	428963	355654	990850	701284	942618	632062	1039083	767714
RP_POS_590_54895a15_102	RP	POS	15.10	590.5490				7.18E-01	0.07	0.32	4.94E-01	0.14	0.53	5.09E-01	0.14	0.37	9.88E-01	0.00	0.37	11779843	3839532	12065318	3943053	11794142	4384812	12336495	3469291
HILIC_POS_210_04996a3_928	HILIC	POS	3.928	210.0500				4.23E-02	0.30	0.89	4.95E-01	0.15	0.84	7.33E-02	0.38	0.82	1.47E-01	0.23	0.78	1410508	359929	1604840	699282	1556742	544051	1652939	829009
RP_POS_151_00481a15_442	RP	POS	15.44	151.0048				1.78E-01	-0.29	0.82	4.95E-01	-0.13	0.40	9.54E-02	-0.35	0.77	3.90E-01	-0.22	0.61	156481390	39153444	145807813	36380171	148308912	45399960	143306714	24497377
RP_POS_451_36273a10_544	RP	POS	10.54	451.3627				1.20E-01	0.31	0.91	4.95E-01	0.14	0.67	7.48E-02	0.38	0.95	3.05E-01	0.24	0.79	924032	179878	982730	192628	969504	215331	995957	168060
RP_POS_496_80624a0_501	RP	POS	0.50	496.8062				8.20E-02	-0.27	1.06	4.95E-01	-0.15	1.25	5.37E-02	-0.34	1.06	3.37E-01	-0.19	1.07	677761	224905	577736	407201	605684	445888	549787	366878
RP_POS_974_81061a0_489	RP	POS	0.49	974.8106				6.17E-08	0.65	1.34	4.96E-01	-0.15	1.20	2.88E-04	0.57	1.39	6.82E-05	0.72	1.47	699395	209241	3373676	4555731	3685818	4847023	3061534	4270886
RP_POS_404_20126a5_862	RP	POS	5.86	404.2013				7.71E-07	0.59	1.30	4.96E-01	-0.15	1.17	9.15E-04	0.51	1.39	2.75E-04	0.67	1.38	80660	187429	1852335	3344424	2081334	3603339	1623336	3083429
HILIC_POS_114_60739a1_231	HILIC	POS	1.231	114.6074				1.86E-01	-0.34	0.70	4.96E-01	-0.12	0.63	1.46E-01	-0.40	0.62	2.94E-01	-0.28	0.46	1152415	851042	936954	549853	974599	523693	899309	577668
RP_POS_499_82712a3_398	RP	POS	3.40	499.8271				1.23E-01	0.24	0.59	4.96E-01	-0.15	0.53	3.37E-01	0.17	0.60	1.30E-01	0.31	0.70	2059895	1727923	2732568	3057462	2941901	3457573	2523236	2615852
RP_POS_323_00494a4_851	RP	POS	4.85	323.0049				7.11E-01	0.07	0.50	4.97E-01	-0.14	0.58	9.96E-01	0.00	0.40	5.31E-01	0.14	0.53	775517	327613	801042	367043	826163	395792	775922	338011
RP_NEG_724_87354a0_482	RP	NEG	0.48	724.8735				6.26E-08	0.65	1.34	4.97E-01	-0.15	1.21	2.51E-04	0.57	1.40	7.84E-05	0.72	1.46	2772608	520702	10081246	12462209	10933934	13378025	9228558	11546750
HILIC_POS_346_02039a7_803	HILIC	POS	7.803	346.0204				7.02E-01	-0.08	0.91	4.97E-01	0.14	0.62	9.78E-01	-0.01	0.55	5.35E-01	-0.15	1.07	1581375	145876	1569775	156678	1559056	175659	1580494	136038
RP_POS_249_10747a0_608	RP	POS	0.61	249.1075				1.99E-02	-0.37	1.03	4.97E-01	0.15	1.02	1.07E-01	-0.30	0.88	2.68E-02	-0.45	1.13	1064212	302400	890735	499737	856554	529737	924915	470708
RP_POS_445_39969a11_038	RP	POS	11.04	445.3997				3.48E-02	0.34	0.85	4.97E-01	-0.15	0.45	1.30E-01	0.27	0.64	5.07E-02	0.41	0.78	2899098	3075763	4488681	5041968	4833568	5721113	4143794	4288099
RP_POS_419_31677a12_884	RP	POS	12.88	419.3168				1.53E-01	-0.28	0.64	4.97E-01	0.14	0.57	3.38E-01	-0.21	0.58	1.13E-01	-0.35	0.66	7053205	2743014	6231942	2947881	6030378	2925296	6433506	2986148
RP_POS_185_11508a15_208	RP	POS	15.21	185.1151				7.43E-01	-0.07	0.32	4.97E-01	-0.14	0.41	5.56E-01	-0.14	0.23	9.91E-01	0.00	0.59	8622353	5493465	8252266	5613018	8635746	5426710	7868785	5822854
RP_POS_548_50446a11_608	RP	POS	11.61	548.5045				1.22E-01	-0.32	0.81	4.97E-01	0.14	0.47	2.61E-01	-0.25	0.62	9.70E-02	-0.39	0.70	4276298	822037	4015009	805877	3959979	843163	4070040	771379
HILIC_POS_133_0607a6_235	HILIC	POS	6.235	133.0607				7.44E-01	-0.05	1.14	4.98E-01	0.15	0.81	9.28E-01	0.02	0.90	5.04E-01	-0.13	1.00	2405604	600041	2360060	896267	2298860	837300	2421260	956174
RP_NEG_242_94438a15_333	RP	NEG	15.33	242.9444				6.43E-01	-0.09	0.54	4.98E-01	-0.14	0.41	4.37E-01	-0.16	0.53	9.36E-01	-0.02	0.36	5386279	152846	5371339	173547	5383179	195751	5359499	149156
RP_POS_149_96051a0_252	RP	POS	0.25	149.9605				1.96E-01	-0.34	1.17	4.98E-01	0.11	0.41	3.14E-01	-0.28	0.82	1.42E-01	-0.40	0.97	9284930	3514801	8421195	2123386	8276405	1829412	8565985	2391655
RP_POS_478_38898a14_21	RP	POS	14.21	478.3890				1.66E-01	-0.30	0.92	4.98E-01	-0.13	0.61	1.27E-01	-0.37	1.02	3.17E-01	-0.24	0.66	6938590	2268103	6306549	2030216	6444881	1982723	6168217	2087446
HILIC_POS_327_07944a0_852	HILIC	POS	0.852	327.0794				8.12E-01	0.04	0.81	4.99E-01	-0.14	0.93	8.91E-01	-0.03	0.24	5.45E-01	0.11	0.26	453762	145866	461508	196397	474890	164872	448126	224461
RP_POS_290_63864a10_617	RP	POS	10.62	290.6386				2.77E-01	0.25	1.00	4.99E-01	-0.13	0.97	4.54E-01	0.19	0.75	2.01E-01	0.32	0.99	3799708	733859	3955559	569381	3994343	534768	3916776	604945
RP_POS_478_38849a11_966	RP	POS	11.97	478.3885				5.39E-01	-0.14	0.41	4.99E-01	0.13	0.46	7.80E-01	-0.07	0.23	3.85E-01	-0.20	0.53	53664252	4627471	53101264	3998694	52828962	3461589	53373565	4491270
RP_POS_382_18832a5_722	RP	POS	5.72	382.1883				5.10E-07	0.60	1.30	4.99E-01	-0.15	1.16	7.24E-04	0.52	1.39	2.35E-04	0.67	1.38	52414	69038	1794366	3239087	2014880	3494344	1573852	2981243
RP_POS_134_95897a0_252	RP	POS	0.25	134.9590				2.14E-01	0.29	0.63	4.99E-01	-0.13	0.60	3.68E-01	0.22	0.43	1.62E-01	0.35	0.71	6857128	984267	7097916	790991	7151741	804484	7044092	781661
HILIC_POS_227_07893a4_123	HILIC	POS	4.123	227.0789				1.95E-01	-0.21	1.00	5.00E-01	-0.15	1.17	1.57E-01	-0.28	1.04	4.77E-01	-0.14	0.97	442210	164169	390762	266703	408888	258410	372637	276163
RP_POS_355_28162a10_646	RP	POS	10.65	355.2816				3.24E-03	-0.65	1.24	5.00E-01	0.13	1.01	1.44E-02	-0.59	1.08	2.54E-03	-0.71	1.23	14109629	1757398	13033890	1542749	12929042	1474297	13138739	1616396
RP_NEG_171_06586a5_276	RP	NEG	5.28	171.0659				4.65E-02	-0.56	1.08	5.00E-01	-0.10	0.92	3.60E-02	-0.61	0.95	7.81E-02	-0.51	0.84	942264	454791	769983	228563	785511	230542	754455	227831
RP_NEG_287_92508a15_598	RP	NEG	15.60	287.9251				2.55E-02	0.33	0.76	5.00E-01	-0.15	0.43	1.52E-01	0.26	0.59	3.39E-02	0.41	0.81	827217	92748	883076	184090	895582	191433	870570	177494
RP_POS_382_2196a5_862	RP	POS	5.86	382.2196				4.49E-07	0.60	1.29	5.00E-01	-0.15	1.16	6.73E-04	0.53	1.39	2.22E-04	0.68	1.38	18218	21329	1387218	2532748	1559081	2732573	1215355	2330945
RP_NEG_197_04227a3_963	RP	NEG	3.96	197.0423				5.41E-01	0.10	1.09	5.00E-01	-0.15	0.41	8.97E-01	0.03	0.82	3.40E-01	0.17	0.70	2350135	543540	2428552	841672	2485653	731255	2371452	943341
HILIC_POS_280_15424a1_325	HILIC	POS	1.325	280.1542				4.59E-01	-0.14	0.28	5.00E-01	0.14	0.59	7.58E-01	-0.07	0.15	2.80E-01	-0.21	0.45	1983936	1893154	1689290	2101797	1546648	1564792	1831932	2536762
RP_NEG_829_18103a9_654	RP	NEG	9.65	829.1810				6.80E-01	0.08	0.26	5.01E-01	0.14	0.62	4.88E-01	0.15	0.43	9.52E-01	0.01	0.27	9207804	1251669	9314413	1308766	9225706	1404408	9403120	1213373

Supplementary table 1: Metabolomics results (in asceding order according to p-value from progressive ALD vs non-progressive ALD comparison, with molecular features with ID_level of 1-2 first)

							all_ALD_vs_control			Prog_ALD_vs_non-prog_ALD			Prog_ALD_vs_control_ALD			Non-prog_ALD_vs_control			Healthy_control		all_ALD		Non-prog_ALD		Progressive_ALD	
							t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA								
Feature_ID	RP_HILIC	POS_NEG	Average.Rt	Average.Mz	Metabolite.name	curated_MSMS	ID_level	p	d	VIP	p	d	VIP	p	d	VIP	p	d	VIP	Mean	SD	Mean	SD	Mean	SD	Mean	SD
RP_POS_617_52228a9_476	RP	POS	9.48	617.5223			3.20E-01	-0.28	0.88	5.01E-01	-0.10	0.46	2.51E-01	-0.33	0.70	4.38E-01	-0.23	0.58	1482486	4025718	734613	2064929	874556	2204561	594670	1927389
RP_NEG_404_84625a15_462	RP	NEG	15.46	404.8463			8.15E-01	0.04	0.77	5.01E-01	0.15	0.48	5.50E-01	0.11	0.61	8.35E-01	-0.04	0.73	938206	39655	940637	76503	935454	78639	945819	74740
HILIC_POS_168_12306a0_631	HILIC	POS	0.631	168.1231			4.40E-01	0.11	1.11	5.01E-01	-0.15	0.76	8.35E-01	0.03	1.26	3.74E-01	0.18	1.06	829101	114178	856110	283899	875350	336467	836869	221079
RP_POS_323_25562a10_774	RP	POS	10.77	323.2556			3.75E-04	-0.57	1.15	5.01E-01	0.14	1.07	4.94E-03	-0.50	1.15	2.12E-03	-0.64	1.23	4788848	383646	4442189	647428	4398337	724203	4486041	564346
RP_POS_379_71094a5_722	RP	POS	5.72	379.7109			5.64E-07	0.60	1.30	5.01E-01	-0.15	1.17	8.02E-04	0.52	1.39	2.33E-04	0.67	1.39	107752	200253	2778581	4981643	3115867	5351068	2441295	4612363
RP_POS_653_3349a5_399	RP	POS	5.40	653.3349			1.30E-06	0.58	1.27	5.01E-01	-0.15	1.15	1.18E-03	0.50	1.37	3.68E-04	0.65	1.35	49437	125971	1420414	2652805	1599930	2861847	1240899	2441809
RP_POS_368_20035a11_251	RP	POS	11.25	368.2004			3.16E-04	0.70	1.55	5.01E-01	0.13	1.07	7.24E-04	0.76	1.49	2.19E-03	0.63	1.41	6023199	1226313	7010620	1399958	6915882	1255164	7105359	1538184
RP_NEG_258_91592a15_47	RP	NEG	15.47	258.9159			8.35E-01	0.04	0.87	5.02E-01	0.14	0.47	6.02E-01	0.11	0.58	8.80E-01	-0.03	0.66	2077258	403446	2095408	496150	2061881	513618	2128935	480891
RP_POS_697_36084a5_568	RP	POS	5.57	697.3608			1.97E-06	0.57	1.26	5.02E-01	-0.15	1.14	1.30E-03	0.49	1.36	4.93E-04	0.64	1.34	71027	122491	1097384	2021163	1233946	2198835	960821	1838648
RP_POS_328_24808a7_219	RP	POS	7.22	328.2481			1.18E-01	-0.29	0.83	5.03E-01	-0.14	0.45	1.10E-01	-0.36	0.80	2.69E-01	-0.22	0.66	4779753	1925568	4127578	2317241	4284000	2024630	3971156	2588385
RP_POS_360_2066a5_722	RP	POS	5.72	360.2066			5.44E-07	0.60	1.29	5.03E-01	-0.15	1.16	7.85E-04	0.52	1.38	2.34E-04	0.67	1.38	13601	15157	1247217	2301287	1402538	2473212	1091895	2129298
RP_POS_594_3526a10_678	RP	POS	10.68	594.3526			7.48E-07	0.89	1.66	5.03E-01	-0.13	0.73	1.26E-04	0.82	1.47	7.37E-07	0.96	1.80	650943	388976	1118797	514797	1153545	438725	1084049	583521
RP_POS_490_29013a9_797	RP	POS	9.80	490.2901			2.89E-03	0.45	0.95	5.03E-01	-0.15	0.47	5.12E-02	0.38	0.84	4.00E-03	0.52	0.96	682788	240021	874201	461723	905355	437705	843047	486992
HILIC_POS_424_34186a0_613	HILIC	POS	0.613	424.3419			2.44E-03	0.51	1.09	5.03E-01	-0.14	0.67	1.52E-02	0.44	0.91	6.88E-03	0.58	1.21	662679	250188	843506	370729	868520	421162	818491	314691
RP_POS_468_38968a10_535	RP	POS	10.54	468.3897			3.27E-01	0.19	0.43	5.03E-01	0.14	0.54	2.67E-01	0.26	0.45	5.48E-01	0.12	0.43	1909427	684028	2049356	736701	1999662	622242	2099050	839231
HILIC_POS_143_34151a3_5	HILIC	POS	3.5	143.3415			9.29E-02	0.24	0.53	5.03E-01	-0.15	0.57	1.95E-01	0.17	0.48	1.57E-01	0.32	0.51	385977	543904	641808	1163763	720388	1505232	563227	676761
HILIC_POS_626_30249a1_719	HILIC	POS	1.719	626.3025			6.03E-01	-0.09	1.20	5.03E-01	0.15	0.76	9.53E-01	-0.01	1.06	3.70E-01	-0.16	1.41	571205	166384	550836	256891	533512	209981	568160	297705
RP_NEG_426_96704a11_378	RP	NEG	11.38	426.9670			3.71E-01	-0.19	0.50	5.03E-01	-0.13	0.55	2.93E-01	-0.26	0.51	5.74E-01	-0.13	0.40	4253470	2132643	3871366	1915607	4000486	1695947	3742245	2122198
RP_POS_449_284a11_263	RP	POS	11.26	449.2840			2.85E-01	0.19	0.58	5.03E-01	0.14	0.53	2.00E-01	0.26	0.68	5.67E-01	0.12	0.52	235834	371852	323594	479430	291286	497987	355902	462899
RP_POS_261_1445a3_084	RP	POS	3.08	261.1445			1.07E-02	0.40	0.75	5.03E-01	0.15	0.96	3.39E-02	0.47	0.82	3.36E-02	0.33	0.76	1225510	489911	1543157	857581	1485349	587822	1600965	1064681
HILIC_POS_59_06133a3_028	HILIC	POS	3.028	59.0613			5.32E-04	0.46	1.24	5.04E-01	-0.15	0.83	2.50E-02	0.38	1.27	3.20E-03	0.53	1.49	1791188	148550	1974395	443750	2004263	455293	1944526	434437
RP_POS_376_34183a11_265	RP	POS	11.27	376.3418			7.94E-01	0.04	0.31	5.04E-01	0.14	0.59	5.97E-01	0.12	0.52	8.75E-01	-0.03	0.39	225939	258231	241442	378007	215990	305439	266894	440546
RP_POS_551_41003a14_889	RP	POS	14.89	551.4100			6.33E-01	0.07	0.23	5.04E-01	0.15	0.47	5.30E-01	0.14	0.31	9.55E-01	-0.01	0.33	4707952	591524	4788378	1313430	4699914	662497	4876841	1740841
RP_POS_308_29477a9_951	RP	POS	9.95	308.2948			3.84E-01	-0.25	0.90	5.04E-01	-0.10	0.50	3.07E-01	-0.30	0.70	5.06E-01	-0.20	0.56	3679898	7473133	2469454	3711971	2718902	3928541	2220007	3504032
RP_NEG_166_9935a15_459	RP	NEG	15.46	166.9935			9.45E-01	0.02	0.84	5.04E-01	-0.13	0.42	8.44E-01	-0.05	0.45	7.53E-01	0.08	0.67	2105003	123514	2106682	100091	2113408	107244	2099957	92991
RP_POS_299_12872a10_301	RP	POS	10.30	299.1287			1.93E-02	0.53	1.03	5.05E-01	-0.12	0.69	6.31E-02	0.47	0.71	1.17E-02	0.60	1.11	557330	187945	646100	153268	656394	128154	635806	175561
HILIC_NEG_182_82494a1_362	HILIC	NEG	1.362	182.8249			2.74E-11	0.86	1.38	5.05E-01	-0.14	0.84	4.33E-05	0.79	1.26	2.66E-09	0.93	1.98	119612	24852	189901	85831	195663	71636	184139	98411
RP_NEG_296_89056a0_515	RP	NEG	0.52	296.8906			6.15E-04	0.46	1.09	5.05E-01	-0.15	1.03	2.35E-02	0.38	1.06	3.74E-03	0.53	1.24	433942	103939	555429	293155	575093	305305	535765	282195
HILIC_NEG_236_96881a5_607	HILIC	NEG	5.607	236.9688			3.09E-01	-0.20	1.05	5.05E-01	-0.14	0.59	2.42E-01	-0.27	1.07	5.38E-01	-0.13	1.02	234156	68614	219532	74574	224533	68546	214531	80539
RP_POS_401_72394a5_863	RP	POS	5.86	401.7239			4.66E-07	0.60	1.30	5.05E-01	-0.15	1.16	6.70E-04	0.53	1.40	2.30E-04	0.67	1.38	94802	119317	2973467	5331625	3330875	5753820	2616060	4905654
RP_POS_569_36292a12_46	RP	POS	12.46	569.3629			2.15E-01	0.18	0.50	5.05E-01	0.15	0.53	2.48E-01	0.25	0.44	4.50E-01	0.10	0.71	862321	99949	897253	217291	882672	142774	911833	273086
RP_POS_428_2305a6_184	RP	POS	6.18	428.2305			1.38E-07	0.63	1.33	5.06E-01	-0.15	1.18	4.54E-04	0.55	1.40	1.01E-04	0.70	1.43	23768	17660	656499	1114486	731180	1181848	581818	1049457
HILIC_POS_140_14337a0_731	HILIC	POS	0.731	140.1434			7.33E-05	-0.64	1.10	5.06E-01	-0.14	0.91	2.99E-04	-0.71	1.26	2.71E-03	-0.57	1.18	1990524	174312	1815881	284315	1834929	280879	1796832	289286
RP_POS_1067_60181a10_312	RP	POS	10.31	1067.6018			4.90E-03	0.49	1.07	5.06E-01	-0.14	0.54	2.87E-02	0.42	0.95	9.06E-03	0.56	1.06	285212	172715	398278	242153	414501	264914	382054	218531
HILIC_NEG_347_00293a7_428	HILIC	NEG	7.428	347.0029			1.62E-04	-0.59	1.21	5.06E-01	0.14	0.80	7.30E-03	-0.52	1.28	4.49E-04	-0.66	1.30	4001900	138462	3865400	246525	3848903	239385	3881897	254810
HILIC_NEG_100_93346a7_355	HILIC	NEG	7.355	100.9335			8.38E-02	0.35	0.91	5.06E-01	-0.13	0.58	2.12E-01	0.29	0.61	6.08E-02	0.42	1.18	49329297	3916977	50733769	3945615	50997681	3774456	50469856	4130957
RP_POS_261_91946a15_348	RP	POS	15.35	261.9195			9.74E-01	-0.01	0.60	5.06E-01	-0.14	0.41	6.87E-01	-0.08	0.32	7.62E-01	0.07	0.91	2372931	311574	2370646	429580	2399381	477596	2341910	378235
RP_NEG_581_52936a14	RP	NEG	14.00	581.5294			1.44E-01	-0.39	0.74	5.07E-01	0.11	0.50	2.25E-01	-0.34	0.59	1.14E-01	-0.44	0.67	13824138	1730508	13343516	1008008	13276145	1043855	13410886	976729
RP_POS_313_27371a9_607	RP	POS	9.61	313.2737			2.28E-06	0.68	1.21	5.07E-01	0.14	1.06	1.27E-04	0.75	1.28	3.51E-04	0.60	1.25	575499	83643	694461	188001	681900	171632	707022	204036
RP_NEG_319_2287a9_957	RP	NEG	9.96	319.2287			5.60E-06	0.54	1.04	5.07E-01	0.15	1.07	8.05E-04	0.61	1.23	2.45E-03	0.46	1.09	71463	76371	1250998	2453871	1087082	2246521	1414914	2657850
RP_POS_296_21942a8_755	RP	POS	8.76	296.2194			7.11E-01	-0.07	0.77	5.07E-01	-0.14	0.55	5.55E-01	-0.14	0.55	9.94E-01	0.00	0.44	1213887	129404	1203562	157792	1214108	119554	1193017	189169
HILIC_POS_310_17575a1_904	HILIC	POS	1.904	310.1758			4.09E-01	-0.14	0.37	5.07E-01	0.14	0.58	7.75E-01	-0.07	0.10	1.71E-01	-0.21	0.77	757316	572856	648652	830061	593145	430584	704160	1095615
RP_POS_196_00319a15_624	RP	POS	15.62	196.0032			7.53E-01	0.06	0.29	5.07E-01	-0.14	0.43	9.81E-01	-0.01	0.23	5.68E-01	0.13	0.35	88045062	32250189	90150079	34169767	92429726	35955743	87870431	32489272
RP_POS_393_2247a10_241	RP	POS	10.24	393.2247			3.25E-06	0.55	1.08	5.08E-01	-0.15	0.93	2.73E-03	0.48	1.09	4.20E-04	0.63	1.24	52461	56434	1106312	2133823	1248602	2234181	964022	2041186
RP_POS_450_24313a6_292	RP	POS	6.29	450.2431			1.29E-07	0.63	1.33	5.08E-01	-0.15	1.18	4.23E-04	0.56	1.41	1.02E-04	0.70	1.43	12733	11710	443769	757254	494263	804687	393274	711229
RP_POS_257_0426a4_852	RP	POS	4.85	257.0426			3.06E-01	-0.17	0.77	5.08E-01	-0.14	0.92	2.22E-01	-0.25	0.69	6.09E-01	-0.10	0.87	3082601	903150	2870705	1295385	2957075	1308410	2784334	1289624
RP_POS_465_28571a6_222	RP	POS	6.22	465.2857			4.52E-07	0.60	1.30	5.08E-01	-0.15	1.16	5.68E-04	0.53	1.40	2.52E-04	0.68	1.38	30518	60352	783848	1391320	876591	1514081	691105	1265328
RP_POS_404_23285a5_992	RP	POS	5.99	404.2329			4.10E-07	0.60	1.30	5.08E-01	-0.15	1.16	6.36E-04	0.53	1.39	2.15E-04	0.68	1.38	15693	14572	1265352	2303142	1418770	2481818	1111934	2123611
HILIC_POS_550_38513a1_176	HILIC	POS	1.176	550.3851			6.17E-01	-0.12	0.68	5.08E-01	0.12	0.96	8.23E-01	-0.06	0.13	4.66E-01	-0.18	0.45	1536729	767647	1462593	563635	1425049	483173	1500138	636804
RP_NEG_170_87065a15_565	RP	NEG	15.57	170.8707			1.36E-01	-0.32	0.74	5.08E-01	-0.13	0.41	9.48E-02	-0.39	0.85	2.87E-01	-0.26	0.57	1459924	60321	1441740	54890	1445395	58967	1438086	50823
HILIC_NEG_112_98557a0_571	HILIC	NEG	0.571	112.9856			2.69E-02	0.28	0.77	5.09E-01	-0.15	0.56	1.51E-02	0.21	1.08	1.18E-01	0.36	0.73	2812829	765851	3502664	2768542	3687099	3776560	3318228	1074357
RP_POS_548_5022a13_64	RP	POS	13.64	548.5022			2.23E-01	-0.26	0.61	5.10E-01	-0.13	0.42	1.72E-01	-0.33	0.83	3.95E-01	-0.20	0.44	3841838	1151138	3559744	1042093	3628925	1007703	3490563	1081132
RP_POS_663_45312a11_909	RP	POS	11.91	663.4531			7.94E-01	-0.05	0.42	5.10E-01	0.14	0.46	9.29E-01	0.02	0.34	5.87E-01	-0.12	0.60	3470806	599210	3437643	694119	3391592	700310	3483695	691861
RP_POS_412_74606a5_992	RP	POS	5.99	412.7461			4.86E-07	0.60	1.30	5.10E-01	-0.15	1.16	6.47E-04	0.53	1.39	2.43E-04	0.67	1.38	16547	40186	534219	959151	597848	1037362	470590	879964
RP_POS_833_58527a13_877	RP	POS	13.88	833.5853			3.03E-01	-0.23	0.60	5.10E-01	0.13	0.78	5.20E-01	-0.16	0.56	2.02E-01	-0.29	0.54	36522166	10490852	34364354	9234253	33752107	7594037	34976601	10669991
RP_POS_383_29425a11_157	RP	POS	11.16	383.2943			4.77E-01	-0.13	0.70	5.10E-01	0.14	0.69	7.56E-01	-0.07	0.51	3.57E-01	-0.20	0.83	1768686	358501	1714222	421122	1686323	440385	1742120	403458
RP_POS_137_06573a15_299	RP	POS	15.30	137.0657			1.31E-01	0.28	0.60	5.10E-01	-0.14	0.65	3.04E-01	0.22	0.58	1.08E-01	0.35	0.73	3109380	901417	3401851	1057821	3471929	1102767	3331773	1017197
RP_POS_297_18558a11_136	RP	POS	11.14	297.1856			4.73E-02	-0.36	0.81	5.11E-01	0.14	0.59	2.02E-01	-0.29	0.57	2.56E-02	-0.42	0.96	642143	138586	580568	181273	568558	148372	592577	209958
RP_POS_447_76569a6_292	RP	POS	6.29	447.7657			1.46E-07	0.63	1.33	5.11E-01	-0.15	1.18	4.61E-04	0.55	1.40	1.06E-04	0.70	1.43	37596	21661	818853	1379152	910154	1462308	727551	1299069
RP_POS_631_35333a5_401	RP	POS	5.40	631.3533			4.92E-06	0.55	1.27	5.11E-01	-0.15	1.14	2.21E-03	0.48	1.35	6.44E-04	0.62	1.34	51911	138298	576421	1063128	646786	1144059	506055	982126
HILIC_NEG_153_86861a0_55	HILIC	NEG	0.55	153.8686			3.38E-03	-0.48	0.81	5.11E-01	0.14	0.57	5.40E-02	-0.41	0.64	2.19E-03	-0.55	1.47	864522	147372	758126	237944	742377	201074	773875	271023
HILIC_POS_371_23965a6_159	HILIC	POS	6.159	371.2397			5.37E-01	-0.10	0.95	5.11E-01	-0.14	0.79	4.12E-01	-0.17	0.76	8.63E-01	-0.03	0.58	2511925	443682	2448237	663951	2492170	585651	2404304	737382
RP_POS_135_89145a11_667	RP	POS	11.67	135.8915			9.25E-01	-0.02	0.69	5.11E-01	-0.13	0.39	7.07E-01	-0.09	0.38	8.39E-01	0.05	0.45	526610	319519	520461	316665	541400	321813	499522	313276
RP_POS_423_19977a6_582	RP	POS	6.58	423.1998			2.74E-03	-0.50	1.06	5.11E-01	0.14	0.93	3.26E-02	-0.43	0.99	3.59E-03	-0.57	1.19	1318735	53683	1279876	82496	1274425	79998	1285328	85381
RP_POS_423_73691a5_992	RP	POS	5.99	423.7369			3.14E-07	0.61	1.31	5.12E-01	-0.15	1.17	6.21E-04	0.54	1.40	1.70E-04	0.68	1.40	77285	85737	2752049	4872755	3073953	5203792	2430146	4547650
RP_POS_282_20383a7_8	RP	POS	7.80	282.2038			1.34E-01	0.27	0.64	5.12E-01	-0.14	0.42	3.01E-01	0.20	0.49	1.26E-01	0.34	0.60	662756	506934	831172	652945	874310	731177	788034	568293
HILIC_NEG_151_87399a3_022	HILIC	NEG	3.022	151.8740			1.28E-01	-0.31	0.99	5.12E-01	-0.13	0.85	9.48E-02	-0.38	0.63	2.84E-01	-0.25	0.45	1698262	334504	1592841	338180	1615173	347664	1570510	330419
RP_POS_381_29681a11_263	RP	POS	11.26	381.2968			1.17E-01	0.23	0.54	5.12E-01	0.15	0.50	1.33E-01	0.31	0.70	3.40E-01	0.16	0.57	10813376	9189852	14676012	18306126	13467288	15810719	15884735	20593860
RP_POS_772_85352a0_494	RP	POS	0.49	772.8535			1.39E-07	0.63	1.34	5.12E-01	-0.15	1.21	2.90E-04	0.56	1.40	1.32E-04	0.71	1.46	91907	57168	424998	580857	463343	630177	386653	530615
RP_POS_346_70688a5_569	RP	POS	5.57	346.7069			1.98E-06	0.57	1.28	5.12E-01	-0.15	1.15	1.49E-03	0.50	1.37	4.19E-04	0.64	1.36	39117	55634	352285	613547	392787	658039	311784	569386
RP_POS_820_5448a11_69	RP	POS	11.69	820.5448			5.71E-02	0.24	0.61	5.12E-01	-0.15	0.58	2.82E-01	0.17	0.46	9.02E-02	0.32	0.73	458443	554438	881207	1972366	1011367	2160726	751046	1776665
RP_POS_615_54913a11_254	RP	POS	11.25	615.5491			4.47E-02	0.40	1.24	5.12E-01	0.13	1.08	4.81E-02	0.46	1.08	1.11E-01	0.33	1.29	459683	296608	585757	318977	564706	271953	606808	361534
RP_NEG_326_76001a0_521	RP	NEG	0.52	326.7600			2.06E-05	0.52	1.25	5.12E-01	-0.15	1.16	3.63E-03	0.45	1.25	1.40E-03	0.59	1.37	633628	109110	912550	597946	951980	653679	873120	540284
HILIC_POS_254_15956a2_368	HILIC	POS	2.368	254.1596			1.05E-02	0.34	1.05	5.12E-01	-0.15	0.74	9.02E-02	0.27	1.15	3.15E-02	0.41	1.14	405683	336548	699904	963954	763471	1070225	636338	850736
RP_POS_675_37909a5_567	RP	POS	5.57	675.3791			1.90E-06	0.57	1.27	5.13E-01	-0.15	1.14	1.24E-03	0.50	1.37	4.73E-04	0.64	1.35	55898	66003	435816	743315	484757	806484	386875	678973
RP_POS_226_1794a7_715	RP	POS	7.72	226.1794			6.48E-01	-0.10	0.55	5.13E-01	0.13	0.40	8.90E-01	-0.03	0.41	4.63E-01	-0.16	0.43	3502144	625366	3445314	558723	3408520	437561	3482108	660674
RP_POS_301_65186a10_515	RP	POS	10.52	301.6519			5.79E-01	-0.12	0.74	5.13E-01	0.13	0.50	8.23E-01	-0.05	0.54	4.25E-01	-0.18	0.82	5863099	1600603	5684500	1483874	5586861	1384958	5782138	1584657
RP_POS_341_26578a10_433	RP	POS	10.43	341.2658			8.52E-01	0.03	1.20	5.13E-01	-0.14	0.53	8.47E-01	-0.04	0.70	6.36E-01	0.10	1.01	8654524	1345948	8710658	1827418	8830913	2015792	8590404	1629151
RP_NEG_184_95595a15_665	RP	NEG	15.67	184.9560			5.18E-01	-0.12	0.95	5.13E-01	-0.14	0.59	3.82E-01	-0.19	0.54	8.04E-01	-0.05	0.72	1916127	462326	1852084	550145	1888275	541676	1815893	561614
RP_POS_368_72009a5_721	RP	POS	5.72	368.7201			1.10E-06	0.58	1.29	5.13E-01	-0.15	1.15	1.02E-03	0.51	1.38	3.46E-04	0.65	1.37	31151	65499	531151	957170	594119	1032444	468184	881484
RP_POS_355_22006a5_569	RP	POS	5.57	355.2201			7.75E-07	0.59	1.29	5.13E-01	-0.15	1.14	9.05E-04	0.51	1.38	2.86E-04	0.66	1.37	32925	68145	957350	1748717	1072377	1879721	842323	1618047
RP_POS_302_19531a2_424	RP	POS	2.42	302.1953			6.18E-02	-0.39	0.72	5.14E-01	0.13	0.75	1.78E-01	-0.33	0.58	3.78E-02	-0.45	0.82	493805	218684	409622	211717	395694	177871	423550	241928
HILIC_NEG_145_05064a0_658	HILIC	NEG	0.658	145.0506			8.36E-01	-0.04	0.68	5.14E-01	0.14	0.81	8.98E-01	0.03	0.15	6.17E-01	-0.11	0.67	368007	85874	364246	98113	357795	95798	370698	100929
RP_POS_277_13989a7_727	RP	POS	7.73	277.1399			2.04E-02	-0.41	0.70	5.14E-01	-0.14	0.61	2.74E-02	-0.48	0.98	7.83E-02	-0.34	0.76	20202048	1153824	19593392	1555275	19695650	1394097	19491135	1709468
RP_POS_500_27454a10_214	RP	POS	10.21	500.2745			1.21E-01	0.30	1.04	5.14E-01	-0.13	0.80	3.21E-01	0.23	0.77	6.97E-02	0.37	1.01	1667417	758494	1918069	856319	1974378	695905	1861759	995376
RP_POS_338_19336a5_569	RP	POS	5.57	338.1934			5.06E-07	0.60	1.29	5.14E-01	-0.15	1.15	7.80E-04	0.52	1.38	2.21E-04	0.67	1.38	7537	8293	727056	1338061	814986	1431120	639125	1246383
HILIC_NEG_262_98499a4_801	HILIC	NEG	4.801	262.9850			4.17E-01	0.16	0.46	5.14E-01	0.13	0.49	2.84E-01	0.23	0.49	6.83E-01	0.10	0.31	405559	207754	440480	217723	426172	242562	454788	191103
RP_POS_399_24637a5_862	RP	POS	5.86	399.2464			3.91E-07	0.60	1.30	5.15E-01	-0.15	1.16	5.99E-04	0.53	1.40	2.16E-04	0.68	1.38	36851	49560	1438988	2577890	1607986	2779424	1269991	2375537

Supplementary table 1: Metabolomics results (in asceding order according to p-value from progressive ALD vs non-progressive ALD comparison, with molecular features with ID_level of 1-2 first)

								all_ALD_vs_control			Prog_ALD_vs_non-prog_ALD			Prog_ALD_vs_control_ALD			Non-prog_ALD_vs_control			Healthy_control		all_ALD		Non-prog_ALD		Progressive_ALD	
								t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA								
Feature_ID	RP_HILIC	POS_NEG	Average.Rt	Average.Mz	Metabolite.name	curated_MSMS	ID_level	p	d	VIP	p	d	VIP	p	d	VIP	p	d	VIP	Mean	SD	Mean	SD	Mean	SD	Mean	SD
RP_POS_441_29718a13_89	RP	POS	13.89	441.2972				5.44E-01	-0.11	0.51	5.15E-01	-0.14	0.61	3.91E-01	-0.18	0.65	8.41E-01	-0.04	0.46	16155114	6188433	15340922	7646994	15841765	7838478	14840079	7496183
RP_POS_341_18451a10_978	RP	POS	10.98	341.1845				4.80E-03	0.47	1.36	5.15E-01	-0.14	1.21	4.62E-02	0.40	1.13	5.29E-03	0.54	1.36	1638115	730419	2129259	1093349	2200865	1044668	2057653	1146047
RP_POS_780_45776a5_862	RP	POS	5.86	780.4578				5.91E-07	0.59	1.28	5.15E-01	-0.15	1.14	6.49E-04	0.52	1.39	2.93E-04	0.67	1.36	21565	31219	500750	895998	559434	974680	442066	815462
RP_POS_393_21054a5_862	RP	POS	5.86	393.2105				2.89E-07	0.61	1.31	5.15E-01	-0.15	1.17	5.69E-04	0.54	1.40	1.70E-04	0.68	1.40	18354	15835	594667	1046238	663183	1119645	526151	973848
RP_POS_494_22888a11_804	RP	POS	11.80	494.2289				4.81E-03	-0.57	1.28	5.15E-01	0.13	1.33	3.60E-02	-0.51	0.93	2.07E-03	-0.64	1.36	3131408	1157487	2433920	1198432	2355382	882250	2512457	1452872
RP_POS_199_01114a10_445	RP	POS	10.45	199.0111				4.17E-01	-0.20	1.09	5.15E-01	0.12	0.70	6.09E-01	-0.14	0.91	2.98E-01	-0.26	0.50	3290890	1512297	3054611	1069276	2984545	810024	3124677	1282138
RP_POS_494_80829a0_5	RP	POS	0.50	494.8083				1.13E-01	-0.23	1.06	5.15E-01	-0.15	1.24	8.05E-02	-0.30	1.06	4.19E-01	-0.16	1.12	2272249	667349	1974439	1443230	2068942	1559600	1879936	1325805
RP_POS_226_18044a11_042	RP	POS	11.04	226.1804				1.82E-02	0.40	0.77	5.15E-01	-0.14	0.42	7.75E-02	0.33	0.66	2.79E-02	0.47	0.80	356742	363727	559371	540851	594786	598774	523957	479500
RP_POS_276_65277a10_508	RP	POS	10.51	276.6528				5.56E-01	-0.13	0.55	5.16E-01	0.13	0.43	7.87E-01	-0.07	0.49	4.09E-01	-0.19	0.53	552092	215582	526905	186442	514700	168077	539111	204148
RP_POS_650_474a11_821	RP	POS	11.82	650.4740				4.78E-01	0.12	0.70	5.16E-01	0.14	0.61	4.32E-01	0.19	0.51	7.21E-01	0.05	0.31	588026	980578	743926	1328380	656817	568625	831035	1796212
RP_NEG_241_14413a8_771	RP	NEG	8.77	241.1441				4.25E-01	-0.15	0.40	5.16E-01	-0.14	0.90	2.95E-01	-0.21	0.54	7.24E-01	-0.08	0.36	1934062	115908	1913824	146527	1923406	155805	1904242	137534
RP_POS_403_2493a11_61	RP	POS	11.61	403.2493				8.69E-03	-0.54	0.97	5.16E-01	0.13	0.73	2.69E-02	-0.48	0.91	1.11E-02	-0.60	0.96	6804001	817909	6351294	816280	6297910	914716	6404677	709721
HILIC_NEG_113_92627a5_606	HILIC	NEG	5.606	113.9263				6.91E-01	-0.08	0.66	5.16E-01	-0.13	0.64	4.92E-01	-0.14	0.27	9.65E-01	-0.01	0.23	2354692	403032	2321061	447036	2350290	491830	2291833	400151
RP_POS_822_56299a11_684	RP	POS	11.68	822.5630				6.88E-01	0.06	0.35	5.16E-01	-0.14	0.53	9.46E-01	-0.01	0.20	5.38E-01	0.13	0.42	2748001	3752521	3134094	6933489	3587639	8381761	2680550	5143337
HILIC_POS_349_01785a7_45	HILIC	POS	7.45	349.0179				8.40E-01	-0.03	0.95	5.16E-01	-0.14	0.62	5.58E-01	-0.10	0.76	8.66E-01	0.04	0.93	14109634	1010380	14061955	1526658	14161762	1772789	13962147	1243311
RP_POS_394_2597a11_668	RP	POS	11.67	394.2597				6.89E-01	-0.08	0.82	5.16E-01	-0.13	0.43	5.12E-01	-0.15	0.56	9.60E-01	-0.01	0.60	567087	291103	542659	320689	563614	320020	521704	323222
RP_POS_263_23682a9_617	RP	POS	9.62	263.2368				3.82E-01	-0.24	0.85	5.16E-01	-0.10	0.44	3.07E-01	-0.29	0.67	5.08E-01	-0.19	0.56	2271563	4049339	1610535	2142773	1750537	2204047	1470533	2092566
RP_POS_419_31509a14_258	RP	POS	14.26	419.3151				8.21E-03	0.44	0.87	5.17E-01	-0.14	0.53	6.70E-02	0.38	0.65	7.90E-03	0.51	1.03	4202253	1980780	5445829	2960161	5638964	2786279	5252695	3140772
RP_POS_161_13269a8_506	RP	POS	8.51	161.1327				4.15E-01	-0.13	0.66	5.17E-01	0.14	0.70	7.83E-01	-0.06	0.59	2.64E-01	-0.20	0.71	11411112	194639	11371525	339180	11349394	302495	11393657	374074
RP_POS_277_06094a3_314	RP	POS	3.31	277.0609				7.99E-04	-0.53	1.19	5.17E-01	0.14	1.13	1.44E-02	-0.46	1.15	2.04E-03	-0.60	1.27	1444916	355635	1142832	602055	1103579	612132	1182085	595389
RP_POS_791_52747a12_325	RP	POS	12.33	791.5275				1.58E-06	-0.97	1.64	5.18E-01	-0.12	0.47	4.09E-06	-1.03	1.65	2.09E-05	-0.91	1.61	1304874	266342	1010058	279257	1028246	267239	991871	292349
RP_POS_517_83667a15_512	RP	POS	15.51	517.8367				3.46E-02	-0.33	0.88	5.18E-01	0.14	0.60	1.87E-01	-0.25	0.56	3.33E-02	-0.40	1.07	1410028	147510	1329965	267429	1312550	259237	1347380	276900
HILIC_POS_113_52961a1_232	HILIC	POS	1.232	113.5296				1.91E-01	-0.34	0.68	5.18E-01	-0.11	0.63	1.55E-01	-0.39	0.60	2.89E-01	-0.28	0.48	1184281	840354	974328	530341	1008865	485055	939792	574935
RP_POS_556_85919a0_503	RP	POS	0.50	556.8592				1.58E-01	0.20	0.96	5.18E-01	0.15	1.03	1.29E-01	0.27	0.81	4.92E-01	0.13	1.14	789245	124445	841163	292317	822139	298743	860188	287500
HILIC_POS_128_10716a0_538	HILIC	POS	0.538	128.1072				3.53E-03	0.34	0.69	5.18E-01	0.15	0.65	3.89E-02	0.42	0.75	2.52E-02	0.27	0.93	600399	992309	3539173	9687347	2908273	6973409	4170074	11839081
HILIC_NEG_174_95583a8_032	HILIC	NEG	8.032	174.9558				1.27E-03	0.39	0.65	5.18E-01	0.15	0.64	1.00E-02	0.47	0.79	4.19E-02	0.32	0.98	34683799	11855512	56544693	62767594	52460391	58497416	60628995	67111502
HILIC_NEG_176_84979a1_366	HILIC	NEG	1.366	176.8498				7.23E-01	-0.05	0.76	5.18E-01	-0.14	0.74	5.15E-01	-0.13	0.25	9.19E-01	0.02	0.30	566246	66196	560103	127316	568382	122957	551824	132254
HILIC_NEG_341_9996a6_271	HILIC	NEG	6.271	341.9996				1.03E-01	-0.38	0.72	5.18E-01	-0.12	0.61	8.32E-02	-0.44	0.70	1.94E-01	-0.32	0.85	1031110	442372	888536	347714	911142	331972	865929	364731
RP_POS_468_30856a10_733	RP	POS	10.73	468.3086				5.36E-05	-0.85	1.54	5.19E-01	-0.12	0.94	6.99E-05	-0.91	1.50	4.62E-04	-0.79	1.43	408103	183603	244889	177924	256452	178290	233327	178605
RP_POS_293_20706a9_581	RP	POS	9.58	293.2071				9.85E-01	0.00	0.63	5.19E-01	-0.13	0.79	7.65E-01	-0.07	0.43	7.99E-01	0.06	0.76	11699448	1537346	11693451	1458193	11788197	1528263	11598706	1393607
RP_POS_494_35941a10_841	RP	POS	10.84	494.3594				5.24E-04	-0.73	1.25	5.19E-01	-0.12	1.02	4.95E-04	-0.80	1.31	3.59E-03	-0.67	1.15	667814	335088	418248	320250	439048	333848	397447	308020
RP_POS_273_20584a9_88	RP	POS	9.88	273.2058				2.33E-01	0.21	0.52	5.19E-01	-0.14	0.42	4.70E-01	0.14	0.40	1.95E-01	0.28	0.57	1374945	581143	1529901	777077	1580375	840253	1479427	713300
RP_NEG_655_474a10_907	RP	NEG	10.91	655.4740				3.95E-04	0.45	1.36	5.19E-01	0.15	0.57	9.55E-03	0.52	1.05	7.21E-03	0.37	1.39	435553	334235	967116	1335158	880368	1052705	1053865	1574207
RP_POS_509_33554a10_318	RP	POS	10.32	509.3355				8.73E-02	0.27	0.70	5.19E-01	0.14	0.61	9.16E-02	0.34	0.74	2.72E-01	0.20	0.50	477976	1450572	1089979	2441417	931460	2259028	1248498	2624536
RP_NEG_313_23868a11_337	RP	NEG	11.34	313.2387				2.50E-01	-0.23	0.77	5.19E-01	-0.13	0.67	1.67E-01	-0.30	0.65	4.83E-01	-0.16	0.61	2145790	164810	2106291	174100	2117594	193667	2094987	153207
RP_POS_172_16966a8_53	RP	POS	8.53	172.1697				2.65E-01	0.26	0.65	5.19E-01	-0.12	0.47	4.37E-01	0.20	0.61	1.91E-01	0.32	0.54	3025434	1844090	3427872	1438193	3521221	1292836	3334524	1577911
RP_NEG_285_24506a10_947	RP	NEG	10.95	285.2451				3.43E-02	-0.35	0.91	5.19E-01	0.14	0.88	1.31E-01	-0.28	0.85	4.55E-02	-0.42	0.88	771863	111439	715199	174633	703867	191301	726531	157345
RP_POS_283_00754a4_77	RP	POS	4.77	283.0075				6.29E-04	-0.70	1.22	5.19E-01	-0.13	0.51	8.36E-04	-0.76	1.29	3.96E-03	-0.63	1.32	1659658	574296	1233259	589157	1271483	573996	1195036	607324
RP_POS_368_38901a12_71	RP	POS	12.71	368.3890				1.46E-01	-0.29	0.75	5.20E-01	0.13	0.43	3.25E-01	-0.22	0.51	1.08E-01	-0.35	0.86	190002	140323	147250	150675	137483	145278	157017	156745
RP_POS_339_02252a4_855	RP	POS	4.86	339.0225				7.36E-01	0.06	0.51	5.20E-01	-0.13	0.59	9.93E-01	0.00	0.41	5.57E-01	0.13	0.50	477980	202594	492393	229066	507239	242973	477548	215703
RP_NEG_311_16949a10_264	RP	NEG	10.26	311.1695				4.24E-01	-0.16	0.61	5.20E-01	-0.13	0.48	2.95E-01	-0.22	0.57	6.88E-01	-0.09	0.81	12020661	5524202	11102345	5870869	11482810	6440404	10721879	5278579
RP_POS_333_20703a5_403	RP	POS	5.40	333.2070				6.10E-07	0.59	1.30	5.20E-01	-0.14	1.15	7.89E-04	0.52	1.38	2.54E-04	0.67	1.38	25456	41257	477484	845248	532235	907338	422733	783638
RP_POS_371_23257a9_006	RP	POS	9.01	371.2326				3.62E-01	0.16	0.58	5.20E-01	-0.14	0.42	6.09E-01	0.10	0.57	3.10E-01	0.23	0.57	676146	976026	872216	1260336	953886	1487595	790546	991342
RP_POS_740_52185a13_063	RP	POS	13.06	740.5219				1.79E-02	0.47	0.80	5.20E-01	0.13	0.83	1.56E-02	0.54	0.95	6.79E-02	0.41	0.79	2227124	1228821	2846077	1311224	2761199	1336861	2930954	1292984
RP_NEG_163_97694a15_452	RP	NEG	15.45	163.9769				8.52E-01	0.04	0.28	5.20E-01	-0.12	0.49	9.50E-01	-0.02	0.24	6.81E-01	0.10	0.48	2311168	225723	2319342	172013	2330468	171910	2308216	173134
RP_POS_820_50549a12_531	RP	POS	12.53	820.5055				6.16E-01	0.10	0.80	5.21E-01	0.13	0.38	4.75E-01	0.17	0.84	8.63E-01	0.04	0.16	1026120	535501	1081049	534555	1046485	495755	1115613	573688
HILIC_POS_139_05022a0_701	HILIC	POS	0.701	139.0502				2.26E-01	-0.40	0.78	5.21E-01	0.06	0.65	2.70E-01	-0.37	0.53	1.95E-01	-0.43	0.71	1481998	3015196	815956	813386	763369	737861	868543	886912
RP_POS_615_38635a11_897	RP	POS	11.90	615.3864				1.34E-01	0.25	0.69	5.21E-01	0.14	0.56	1.25E-01	0.32	0.62	3.32E-01	0.18	0.46	1020371	2195729	1784724	3220514	1576602	2947829	1992847	3489554
RP_POS_136_65872a11_668	RP	POS	11.67	136.6587				9.17E-01	-0.02	0.68	5.21E-01	-0.13	0.38	7.02E-01	-0.09	0.39	8.47E-01	0.04	0.44	2326330	1250905	2299715	1276585	2382177	1306464	2217253	1253742
RP_POS_338_21585a6_399	RP	POS	6.40	338.2159				5.59E-02	-0.37	0.65	5.21E-01	0.13	0.60	1.62E-01	-0.30	0.55	4.74E-02	-0.43	0.77	790457	49297	770299	55537	766713	55925	773886	55478
HILIC_POS_87_09225a0_798	HILIC	POS	0.798	87.0923				1.39E-03	0.64	1.33	5.21E-01	-0.13	0.89	1.09E-02	0.58	1.04	1.18E-03	0.70	1.56	5816366	2427873	7503271	2583598	7670138	2394606	7336405	2774025
HILIC_POS_130_08646a3_688	HILIC	POS	3.688	130.0865				8.18E-01	-0.04	0.27	5.21E-01	-0.14	0.64	5.16E-01	-0.11	0.45	8.90E-01	0.03	0.31	16286094	19751203	15226110	29910965	17159526	36853654	13292695	21018317
RP_POS_426_21432a5_992	RP	POS	5.99	426.2143				3.00E-07	0.61	1.31	5.21E-01	-0.14	1.16	5.13E-04	0.54	1.41	1.92E-04	0.68	1.39	52030	63845	1738714	3066230	1936713	3303303	1540714	2829061
RP_POS_445_28796a6_292	RP	POS	6.29	445.2880				1.55E-07	0.63	1.32	5.21E-01	-0.14	1.18	4.38E-04	0.55	1.41	1.17E-04	0.70	1.42	15654	16169	438219	747577	486472	795052	389966	701632
RP_POS_526_39819a14_267	RP	POS	14.27	526.3982				2.16E-01	0.19	0.43	5.22E-01	0.14	0.45	2.56E-01	0.26	0.44	3.98E-01	0.12	0.70	2648294	483508	2803332	905555	2744839	527491	2861824	1171138
RP_NEG_197_80806a2_461	RP	NEG	2.46	197.8081				1.93E-01	0.24	0.54	5.22E-01	0.13	0.56	1.39E-01	0.31	0.53	4.20E-01	0.18	0.44	9365583	4244557	10562863	5130320	10232087	5388312	10893639	4890841
HILIC_NEG_257_84482a7_667	HILIC	NEG	7.667	257.8448				2.27E-01	0.22	0.75	5.22E-01	0.13	0.80	1.69E-01	0.29	0.61	4.68E-01	0.15	0.42	791569	53781	805737	66706	801436	68105	810038	65683
HILIC_NEG_167_02104a4_723	HILIC	NEG	4.723	167.0210				1.57E-03	0.54	1.01	5.22E-01	0.13	1.04	5.22E-03	0.61	0.94	8.96E-03	0.48	0.92	13169652	3506493	15783231	4997149	15461173	4150119	16105289	5746081
RP_POS_453_2933a10_657	RP	POS	10.66	453.2933				4.92E-01	0.13	0.52	5.23E-01	0.13	1.13	3.74E-01	0.20	0.47	7.59E-01	0.07	0.30	1235967	502417	1308786	568097	1272227	544051	1345345	594420
HILIC_POS_565_56647a10_709	HILIC	POS	10.709	565.5665				4.71E-01	-0.13	0.39	5.23E-01	-0.14	0.66	3.17E-01	-0.20	0.41	7.77E-01	-0.06	0.26	3008509	109159	2991219	139761	3000205	154694	2982232	123976
RP_NEG_800_54645a12_766	RP	NEG	12.77	800.5465	Unknown	279.2347(100), 253.2187(40), 305.2496(24), 740.5323(23)	4	2.48E-03	0.54	0.97	5.23E-01	-0.13	0.57	1.50E-02	0.47	0.91	5.24E-03	0.60	1.02	10928001	5325781	14630994	7096303	15087177	7784820	14174811	6380799
RP_POS_736_43164a5_721	RP	POS	5.72	736.4316				8.07E-07	0.59	1.28	5.23E-01	-0.14	1.14	7.98E-04	0.52	1.38	3.33E-04	0.66	1.35	28099	53540	848153	1554652	948088	1684592	748218	1423019
RP_POS_448_25909a6_222	RP	POS	6.22	448.2591				3.54E-07	0.61	1.30	5.23E-01	-0.14	1.16	5.43E-04	0.54	1.40	2.14E-04	0.68	1.38	10874	22962	712456	1284466	795022	1386301	629891	1182217
HILIC_NEG_158_93893a2_946	HILIC	NEG	2.946	158.9389				4.06E-01	-0.15	0.94	5.23E-01	-0.14	0.72	2.64E-01	-0.22	0.60	7.17E-01	-0.08	0.53	4871355	950923	4696157	1249787	4776482	1407668	4615833	1077549
HILIC_NEG_164_83592a2_962	HILIC	NEG	2.962	164.8359				8.51E-01	0.04	0.44	5.23E-01	-0.12	0.49	9.31E-01	-0.02	0.15	6.68E-01	0.10	0.39	17467964	9450793	17820237	8235710	18349236	8364825	17291238	8154547
RP_POS_284_12802a8_701	RP	POS	8.70	284.1280				3.84E-01	0.15	0.47	5.24E-01	-0.14	0.46	6.34E-01	0.09	0.38	3.31E-01	0.22	0.56	638743	998691	831635	1314615	916094	1569563	747175	1006783
RP_POS_458_2742a11_862	RP	POS	11.86	458.2742				9.54E-02	0.30	0.83	5.24E-01	-0.13	0.53	2.78E-01	0.23	0.64	7.24E-02	0.36	0.69	4592043	2063303	5362449	2729928	5537730	2612316	5187168	2858357
RP_POS_308_29486a10_059	RP	POS	10.06	308.2949				4.47E-01	-0.19	0.80	5.24E-01	-0.11	0.49	3.50E-01	-0.25	0.61	6.15E-01	-0.13	0.44	9481289	16460729	7095853	10937401	7797754	11408807	6393951	10513254
RP_POS_415_22379a5_991	RP	POS	5.99	415.2238				6.64E-07	0.59	1.30	5.24E-01	-0.14	1.16	7.61E-04	0.52	1.40	2.74E-04	0.67	1.38	28515	61925	478078	840845	532031	905605	424124	776150
RP_NEG_313_23868a10_16	RP	NEG	10.16	313.2387	FA 18:1;2O	313.2389(100), 251.2392(60), 295.2254(37)	3	3.01E-01	-0.23	0.51	5.24E-01	0.12	0.38	4.73E-01	-0.17	0.34	2.37E-01	-0.29	0.65	1941430	446964	1849874	374439	1825854	395688	1873895	354293
RP_POS_142_94946a15_381	RP	POS	15.38	142.9495				7.91E-01	-0.04	0.27	5.24E-01	0.14	0.44	7.05E-01	0.04	0.27	6.40E-01	-0.11	0.43	15036932	365362	15006070	962980	14944207	1319719	15067933	352304
RP_POS_421_2594a5_992	RP	POS	5.99	421.2594				4.16E-07	0.60	1.31	5.25E-01	-0.14	1.16	6.23E-04	0.53	1.40	2.18E-04	0.67	1.39	44589	101340	1337015	2378705	1489267	2556375	1184763	2202179
RP_POS_381_21259a10_705	RP	POS	10.71	381.2126				4.42E-03	0.53	1.39	5.25E-01	0.13	1.22	1.07E-02	0.59	1.36	1.44E-02	0.46	1.27	899741	158494	1000701	196336	988129	149909	1013274	234707
RP_POS_171_11656a7_342	RP	POS	7.34	171.1166				6.69E-03	-0.53	0.87	5.25E-01	0.13	0.57	3.15E-02	-0.47	0.84	6.92E-03	-0.60	1.00	1023397	82356	975194	90098	969430	90669	980958	90068
RP_POS_663_46381a10_658	RP	POS	10.66	663.4638				6.71E-01	0.09	0.24	5.25E-01	0.12	0.38	5.19E-01	0.16	0.48	8.97E-01	0.03	0.26	12024864	937961	12104025	825661	12051209	823089	12156841	833172
RP_POS_371_19769a5_722	RP	POS	5.72	371.1977				5.95E-07	0.60	1.29	5.25E-01	-0.14	1.15	7.23E-04	0.52	1.39	2.66E-04	0.67	1.37	21556	56243	588570	1058574	656277	1140439	520862	976766
RP_POS_187_97154a15_578	RP	POS	15.58	187.9715				2.90E-01	-0.18	0.58	5.25E-01	0.14	0.81	5.79E-01	-0.11	0.69	2.21E-01	-0.25	0.50	1962458	66434	1946222	97107	1940012	98394	1952432	96393
RP_POS_343_28375a10_16	RP	POS	10.16	343.2838				2.91E-01	-0.23	0.47	5.25E-01	0.12	0.39	4.81E-01	-0.17	0.39	2.21E-01	-0.29	0.67	657937	169266	622107	151861	612400	152201	631814	152437
RP_POS_216_15952a6_464	RP	POS	6.46	216.1595				6.67E-01	-0.11	0.65	5.26E-01	-0.11	0.42	5.56E-01	-0.17	0.61	8.33E-01	-0.05	0.46	674484	838664	605958	542195	640616	421591	571299	643242
RP_POS_648_48578a11_246	RP	POS	11.25	648.4858				5.70E-10	0.90	1.40	5.26E-01	0.13	0.84	5.48E-06	0.96	1.44	3.34E-08	0.83	1.72	261561	155822	558357	340756	536575	251325	580139	412875
HILIC_POS_353_00952a7_45	HILIC	POS	7.45	353.0095				9.05E-01	-0.02	0.99	5.26E-01	-0.14	0.55	6.11E-01	-0.09	0.83	8.20E-01	0.05	0.94	592478	46858	591156	73062	595823	85454	586488	58636
RP_POS_835_66479a11_612	RP	POS	11.61	835.6648				4.29E-01	-0.17	0.37	5.26E-01	0.13	0.41	6.33E-01	-0.11	0.44	3.48E-01	-0.23	0.49	602026	627679	502178	579080	465195	657568	539162	492263
HILIC_POS_372_31027a0_627	HILIC	POS	0.627	372.3103				1.02E-03	0.57	1.02	5.26E-01	-0.13	0.85	7.28E-03	0.50	1.08	3.33E-03	0.63	0.98	1253724	642623	1751722	910953	1809897	1021762	1693547	791013
RP_NEG_463_20804a10_905	RP	NEG	10.91	463.2080				2.05E-03	0.47	1.57	5.26E-01	0.14	0.86	7.40E-03	0.54	1.32	2.02E-02	0.41	1.36	856911	299233	1097723	545912	1062890	487781	1132556	601428
HILIC_NEG_92_92761a3_016	HILIC	NEG	3.016	92.9276				7.13E-01	0.07	0.69	5.26E-01	-0.13	0.84	9.79E-01	0.01	0.21	5.37E-01	0.14	0.43	1081133	313740	1105390	349094	1127661	356691	1083120	343482
RP_POS_766_75732a0_499	RP	POS	0.50	766.7573				2.83E-02	-0.31	1.11	5.27E-01	-0.14	1.26	2.74E-02	-0.38	1.13	2.02E-01	-0.24	1.15	2287596	580913	1919536	1300641	2002446	1385958	1836626	1217763
RP_POS_776_79108a0_498	RP	POS	0.50	776.7911				7.89E-10	-0.75	1.42	5.27E-01	0.14	1.19	3.62E-05	-0.68	1.49	5.10E-06	-0.82	1.54	2468516	130401	1782353	991850	1719187	1027755	1845520	960827
RP_POS_349_18442a5_569	RP	POS	5.57	349.1844				4.92E-07	0.60	1.30	5.27E-01	-0.14	1.16	8.02E-04	0.53	1.39	2.09E-04	0.67	1.39	32407	21902	529538	922830	588305	980757	470772	866993

Supplementary table 1: Metabolomics results (in asceding order according to p-value from progressive ALD vs non-progressive ALD comparison, with molecular features with ID_level of 1-2 first)

							all_ALD_vs_control			Prog_ALD_vs_non-prog_ALD			Prog_ALD_vs_control_ALD			Non-prog_ALD_vs_control			Healthy_control		all_ALD		Non-prog_ALD		Progressive_ALD	
							t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA								
Feature_ID	RP_HILIC	POS_NEG	Average.Rt	Average.Mz	Metabolite.name	curated_MSMS	ID_level	p	d	VIP	p	d	VIP	p	d	VIP	p	d	VIP	Mean	SD	Mean	SD	Mean	SD	Mean	SD
RP_NEG_167_02026a0_709	RP	NEG	0.71	167.0203				3.70E-02	0.37	0.84	5.27E-01	-0.13	0.45	1.52E-01	0.30	0.85	3.07E-02	0.43	0.80	117860014	20001848	127334562	27120022	129061538	25879092	125607586	28463788
RP_NEG_369_17401a11_379	RP	NEG	11.38	369.1740				2.27E-01	-0.23	0.89	5.27E-01	-0.13	1.02	1.55E-01	-0.30	0.81	4.65E-01	-0.16	0.91	1076763	291126	1001737	335702	1023112	366168	980362	304435
RP_POS_182_02362a10_568	RP	POS	10.57	182.0236				9.84E-01	0.00	0.21	5.27E-01	-0.13	0.43	7.81E-01	-0.07	0.37	7.95E-01	0.06	0.81	1911944	616246	1909443	580796	1946410	524178	1872475	635595
RP_POS_741_38696a5_722	RP	POS	5.72	741.3870				3.79E-06	0.55	1.27	5.27E-01	-0.14	1.14	1.82E-03	0.48	1.37	6.48E-04	0.62	1.34	60949	137220	748624	1387840	836948	1498722	660299	1276486
RP_POS_377_2334a5_721	RP	POS	5.72	377.2334				5.80E-07	0.60	1.30	5.27E-01	-0.14	1.15	7.39E-04	0.52	1.39	2.58E-04	0.67	1.38	43445	108847	1340555	2421111	1494617	2601827	1186493	2241706
HILIC_POS_186_18518a0_973	HILIC	POS	0.973	186.1852				2.32E-01	-0.20	0.53	5.27E-01	0.14	0.84	5.51E-01	-0.13	0.40	1.31E-01	-0.27	0.57	481222	255446	409672	386694	385060	310478	434284	452198
RP_POS_295_88986a0_254	RP	POS	0.25	295.8899				9.12E-01	-0.02	0.30	5.28E-01	-0.13	0.63	7.05E-01	-0.09	0.26	8.52E-01	0.04	0.14	3475569	393688	3466648	402929	3492262	395880	3441034	412258
RP_POS_195_12234a2_646	RP	POS	2.65	195.1223				1.21E-01	0.23	0.93	5.28E-01	-0.14	0.86	3.36E-01	0.17	0.99	1.34E-01	0.30	0.91	2199735	278534	2312228	525188	2345617	585282	2278838	460916
RP_NEG_544_26617a10_344	RP	NEG	10.34	544.2662				7.14E-06	0.75	1.26	5.28E-01	0.13	0.58	9.11E-05	0.81	1.37	2.25E-04	0.68	1.23	1214318	288346	1539667	447561	1511233	405985	1568101	488095
RP_POS_656_79065a0_504	RP	POS	0.50	656.7907				7.41E-04	-0.53	1.15	5.28E-01	-0.14	1.22	1.05E-03	-0.60	1.25	2.00E-02	-0.46	1.14	769168	207174	590597	357047	613276	385282	567917	328747
RP_POS_906_82343a0_489	RP	POS	0.49	906.8234				6.51E-08	0.65	1.35	5.28E-01	-0.14	1.20	2.45E-04	0.58	1.41	8.33E-05	0.72	1.47	1685175	341025	5835279	7082695	6285054	7571012	5385504	6604530
RP_POS_428_81912a0_501	RP	POS	0.50	428.8191				2.73E-01	-0.18	0.99	5.29E-01	-0.14	1.10	1.96E-01	-0.25	0.90	5.75E-01	-0.11	1.04	436335	182031	389355	278045	406996	290409	371714	266877
RP_NEG_453_78607a15_515	RP	NEG	15.52	453.7861				8.75E-01	-0.04	0.40	5.29E-01	0.12	0.53	9.19E-01	0.03	0.23	6.87E-01	-0.10	0.55	3634703	116610	3631082	97929	3624869	90924	3637295	105025
RP_NEG_376_98389a9_269	RP	NEG	9.27	376.9839				2.97E-01	0.21	0.62	5.29E-01	0.13	0.70	2.52E-01	0.27	0.59	4.96E-01	0.14	0.63	2854097	1219467	3119828	1312782	3036545	1105472	3203112	1498579
RP_POS_411_18686a11_253	RP	POS	11.25	411.1869				2.65E-06	0.81	1.66	5.29E-01	0.13	0.83	3.77E-05	0.87	1.61	6.38E-05	0.75	1.69	1070627	397748	1530579	569696	1494444	504241	1566713	631511
RP_POS_294_91995a0_256	RP	POS	0.26	294.9200				7.88E-01	0.06	0.34	5.29E-01	-0.12	0.46	9.98E-01	0.00	0.34	6.21E-01	0.12	0.61	722014	202603	732696	166581	743257	164589	722136	169550
HILIC_POS_650_39532a1_037	HILIC	POS	1.037	650.3953				1.18E-05	0.55	1.25	5.29E-01	-0.14	0.82	2.89E-03	0.48	1.41	7.54E-04	0.62	1.39	373359	1231835	2969876	5252597	3302868	5604696	2636884	4909552
HILIC_POS_174_12364a1_87	HILIC	POS	1.87	174.1236				1.31E-01	0.19	0.94	5.29E-01	0.14	0.55	1.33E-01	0.27	0.75	4.66E-01	0.12	0.51	466149	256281	612000	846728	558350	828059	665650	870041
RP_POS_261_09985a15_341	RP	POS	15.34	261.0999				4.17E-02	-0.34	0.65	5.29E-01	-0.13	0.55	5.00E-02	-0.41	0.69	1.45E-01	-0.28	0.68	7042701	845607	6639728	1245232	6718622	1143327	6560834	1346459
HILIC_POS_182_07881a4_596	HILIC	POS	4.596	182.0788				4.42E-01	0.14	0.34	5.29E-01	0.13	0.83	3.17E-01	0.20	0.41	7.40E-01	0.07	0.31	494473	1168544	693183	1530906	596227	1596872	790138	1471731
RP_POS_200_1644a10_779	RP	POS	10.78	200.1644				3.09E-02	0.39	0.79	5.29E-01	-0.13	0.40	1.61E-01	0.33	0.61	1.23E-02	0.46	0.95	320535	169545	401727	213485	415257	149892	388197	263135
RP_POS_438_3783a10_656	RP	POS	10.66	438.3783				1.40E-01	-0.29	0.51	5.29E-01	0.13	0.46	2.84E-01	-0.23	0.59	1.23E-01	-0.36	0.61	5904709	475258	5757903	505783	5725876	549888	5789930	460850
HILIC_NEG_136_89172a2_172	HILIC	NEG	2.172	136.8917				4.09E-01	0.15	0.68	5.30E-01	-0.13	0.78	6.85E-01	0.09	0.19	2.96E-01	0.22	0.44	12829942	2684322	13306313	3212688	13509400	3093948	13103227	3346145
RP_NEG_341_27017a11_868	RP	NEG	11.87	341.2702				1.57E-01	-0.27	0.67	5.30E-01	0.13	0.92	3.35E-01	-0.21	0.53	1.26E-01	-0.34	0.72	2711646	224983	2643918	254330	2627846	260494	2659990	249607
RP_POS_402_25949a10_449	RP	POS	10.45	402.2595				8.62E-01	-0.03	0.65	5.30E-01	-0.14	0.49	5.66E-01	-0.10	0.32	8.72E-01	0.04	0.69	1270884	166049	1264368	231739	1279023	289539	1249713	155662
RP_POS_207_01419a0_523	RP	POS	0.52	207.0142				6.73E-07	-0.71	1.29	5.31E-01	-0.13	1.17	3.61E-05	-0.78	1.39	2.80E-04	-0.64	1.37	1891396	324661	1401376	735080	1447786	714751	1354966	759242
RP_POS_692_40546a5_567	RP	POS	5.57	692.4055				1.43E-06	0.57	1.27	5.31E-01	-0.14	1.13	1.13E-03	0.50	1.37	4.10E-04	0.65	1.35	52062	160154	1252645	2326326	1399435	2506445	1105856	2146576
RP_POS_277_17917a8_349	RP	POS	8.35	277.1792				6.11E-01	0.09	0.65	5.31E-01	0.13	0.87	4.46E-01	0.16	0.69	9.02E-01	0.03	0.57	1136641	121161	1150103	153342	1140431	156779	1159776	150788
RP_POS_537_39355a14_268	RP	POS	14.27	537.3936				2.43E-01	0.24	0.46	5.31E-01	0.13	0.39	2.05E-01	0.30	0.57	4.23E-01	0.17	0.48	1153377848	128353274	#########	132381118	1176040838	116871264	1192737596	146989934
RP_NEG_372_90237a15_34	RP	NEG	15.34	372.9024				5.14E-01	-0.11	0.77	5.31E-01	-0.13	0.50	3.67E-01	-0.18	0.83	8.19E-01	-0.05	0.30	2764766	77678	2753439	104537	2760029	109211	2746848	100316
RP_POS_962_73065a0_496	RP	POS	0.50	962.7307				1.10E-01	-0.26	1.02	5.31E-01	-0.14	1.13	9.72E-02	-0.33	0.99	3.23E-01	-0.19	1.04	673028	126357	624439	201812	637161	200427	611718	204415
HILIC_POS_182_10345a1_386	HILIC	POS	1.386	182.1035				3.58E-18	1.11	1.87	5.31E-01	-0.13	0.61	8.33E-09	1.05	1.81	1.64E-11	1.17	2.31	1813495	1093728	6843739	4531189	7129291	4301974	6558187	4775875
RP_POS_784_57294a13_72	RP	POS	13.72	784.5729				9.31E-07	0.87	1.40	5.32E-01	-0.12	0.60	8.25E-05	0.81	1.32	2.94E-06	0.93	1.58	13818388	3990833	18599603	5412855	18940538	5162573	18258667	5683885
RP_POS_560_87079a0_471	RP	POS	0.47	560.8708				2.63E-09	-0.76	1.39	5.32E-01	0.14	1.16	7.84E-05	-0.69	1.43	2.72E-06	-0.82	1.54	802060	88333	555017	352299	532832	349338	577201	357380
HILIC_POS_628_38232a1_029	HILIC	POS	1.029	628.3823				6.20E-06	0.55	1.27	5.32E-01	-0.14	0.83	2.09E-03	0.48	1.46	7.01E-04	0.62	1.40	362289	1037887	3214985	5737159	3576249	6180481	2853722	5295001
RP_POS_690_59918a11_258	RP	POS	11.26	690.5992				4.05E-03	0.38	0.72	5.32E-01	0.14	0.40	1.61E-02	0.45	0.89	6.01E-02	0.31	0.67	186522	169960	361918	518706	329259	482857	394577	555224
RP_POS_448_22775a6_11	RP	POS	6.11	448.2278		448.2265(100)	4	3.39E-07	0.61	1.31	5.32E-01	-0.14	1.16	5.93E-04	0.54	1.41	1.92E-04	0.68	1.39	39362	49251	1388932	2466225	1544032	2637152	1233833	2298912
RP_POS_323_25565a10_653	RP	POS	10.65	323.2557				8.27E-03	-0.49	0.98	5.32E-01	0.13	0.82	4.58E-02	-0.42	0.91	8.48E-03	-0.55	1.01	6373859	892273	5849896	1098397	5780823	1077722	5918968	1125323
HILIC_NEG_200_8586a5_573	HILIC	NEG	5.573	200.8586				3.78E-01	-0.16	0.46	5.32E-01	-0.13	0.79	3.09E-01	-0.22	0.45	6.38E-01	-0.09	0.51	3098301	292756	3041409	378129	3065179	334217	3017638	419555
RP_NEG_277_89676a15_584	RP	NEG	15.58	277.8968				6.56E-01	0.09	0.68	5.33E-01	-0.12	0.39	8.90E-01	0.03	0.42	5.20E-01	0.16	0.36	1106688	45111	1110751	43439	1113481	48293	1108021	38276
RP_POS_390_28519a10_242	RP	POS	10.24	390.2852				2.22E-06	0.56	1.09	5.33E-01	-0.14	0.96	1.86E-03	0.49	1.14	4.19E-04	0.63	1.21	22414	20299	309190	569623	344976	602110	273403	538900
HILIC_POS_315_08008a7_811	HILIC	POS	7.811	315.0801				2.70E-01	-0.19	0.57	5.33E-01	-0.13	0.86	2.15E-01	-0.26	0.59	5.27E-01	-0.13	0.50	1660724	743522	1476688	1005814	1539864	970128	1413513	1046267
RP_NEG_443_27267a6_111	RP	POS	6.11	443.2727				2.38E-07	0.62	1.31	5.33E-01	-0.14	1.15	4.28E-04	0.55	1.41	1.81E-04	0.69	1.39	26155	30967	1083101	1903297	1202638	2052876	963565	1753725
HILIC_POS_145_13342a1_695	HILIC	POS	1.695	145.1334				9.56E-02	-0.35	1.09	5.33E-01	0.12	0.79	2.14E-01	-0.29	1.11	7.65E-02	-0.41	1.00	666749	398478	530275	386948	505980	388195	554570	388089
RP_POS_467_76337a6_222	RP	POS	6.22	467.7634				2.40E-07	0.62	1.31	5.33E-01	-0.14	1.16	4.79E-04	0.55	1.41	1.66E-04	0.69	1.40	35554	39604	1634019	2879898	1814811	3084751	1453228	2678524
RP_POS_648_37976a5_399	RP	POS	5.40	648.3798				7.58E-07	0.59	1.28	5.34E-01	-0.14	1.14	8.52E-04	0.52	1.38	2.98E-04	0.66	1.36	42955	111170	1581382	2907517	1763586	3121616	1399179	2695848
RP_POS_296_25818a9_691	RP	POS	9.69	296.2582				2.07E-01	-0.38	0.90	5.34E-01	-0.08	0.41	1.76E-01	-0.43	0.82	2.65E-01	-0.34	0.69	2576098	4512832	1522688	1828244	1637268	1619020	1408109	2026116
RP_POS_424_2717a10_458	RP	POS	10.46	424.2717				1.52E-01	-0.26	0.99	5.34E-01	0.13	0.39	2.99E-01	-0.19	0.56	1.58E-01	-0.33	1.13	1239014	158673	1188878	202283	1176200	240392	1201555	156701
HILIC_POS_287_09995a1_904	HILIC	POS	1.904	287.1000				3.46E-01	-0.17	0.38	5.34E-01	0.13	0.57	6.82E-01	-0.10	0.15	1.53E-01	-0.23	0.82	1157257	895907	968111	1211687	892085	643147	1044137	1594020
RP_NEG_656_88599a0_484	RP	NEG	0.48	656.8860				7.49E-08	0.64	1.34	5.34E-01	-0.14	1.21	2.34E-04	0.58	1.41	9.83E-05	0.71	1.45	4840282	791438	13295353	14497392	14203149	15590954	12387556	13411874
HILIC_NEG_173_92604a4_284	HILIC	NEG	4.284	173.9260				9.15E-01	0.02	0.65	5.34E-01	-0.12	0.63	8.67E-01	-0.04	0.12	7.20E-01	0.08	0.53	1223530	358802	1231255	334961	1252226	341608	1210283	330293
RP_POS_432_76474a13_872	RP	POS	13.87	432.7647				5.18E-01	-0.12	0.59	5.34E-01	0.13	0.86	8.08E-01	-0.06	0.54	3.47E-01	-0.19	0.47	8220679	1722767	7982522	2042353	7854652	1680529	8110391	2360083
RP_NEG_214_14482a6_461	RP	NEG	6.46	214.1448				7.50E-01	-0.08	0.64	5.34E-01	-0.11	0.42	6.25E-01	-0.13	0.60	9.27E-01	-0.02	0.46	949037	1094815	882413	753805	929618	578193	835209	899547
RP_POS_295_22446a10_282	RP	POS	10.28	295.2245				9.74E-01	-0.01	0.92	5.34E-01	0.13	1.09	7.96E-01	0.06	0.85	7.58E-01	-0.07	0.74	1611456	325334	1609300	343228	1587824	354848	1630776	333403
RP_NEG_900_78381a0_495	RP	NEG	0.50	900.7838				6.92E-08	-0.69	1.34	5.35E-01	0.14	1.16	3.16E-04	-0.62	1.38	1.98E-05	-0.76	1.45	1680511	132467	1364468	499592	1333235	502608	1395701	499671
RP_POS_221_98215a0_74	RP	POS	0.74	221.9822				4.02E-07	0.77	1.26	5.35E-01	-0.13	0.66	8.76E-05	0.71	1.36	1.72E-05	0.84	1.38	419915	314599	861748	595659	898977	624768	824519	568943
HILIC_NEG_134_89481a3_667	HILIC	NEG	3.667	134.8948				1.16E-01	0.32	0.67	5.35E-01	0.12	0.72	8.63E-02	0.39	0.69	2.60E-01	0.26	0.42	15969885	7625871	18441918	7593986	17967326	7990907	18916510	7224950
HILIC_POS_224_12819a7_69	HILIC	POS	7.69	224.1282				2.13E-01	-0.27	0.73	5.35E-01	0.12	0.45	3.76E-01	-0.21	0.51	1.70E-01	-0.33	0.82	8129550	2819328	7420793	2599253	7258385	2690558	7583201	2521345
HILIC_POS_199_18045a4_245	HILIC	POS	4.245	199.1805				1.22E-02	0.48	1.10	5.35E-01	0.13	0.80	1.07E-02	0.54	0.96	5.74E-02	0.42	0.71	7658052	1430630	8437894	1642123	8335295	1720384	8540492	1570657
RP_POS_467_3013a6_393	RP	POS	6.39	467.3013				1.33E-07	0.63	1.33	5.35E-01	-0.14	1.17	4.52E-04	0.56	1.40	9.84E-05	0.70	1.43	8540	6488	257398	437666	284742	460515	230055	416427
HILIC_NEG_103_03991a0_656	HILIC	NEG	0.656	103.0399				6.81E-02	0.29	1.01	5.35E-01	0.13	1.01	9.71E-02	0.36	0.56	1.79E-01	0.23	0.69	318726	127283	375316	207790	362331	162461	388300	245960
RP_POS_548_50305a13_015	RP	POS	13.02	548.5031				1.65E-01	-0.33	0.80	5.35E-01	0.11	0.47	2.87E-01	-0.28	0.81	1.22E-01	-0.39	0.65	1639275	467379	1513057	340493	1491794	314284	1534320	366797
RP_POS_442_33694a12_243	RP	POS	12.24	442.3369				1.06E-01	-0.30	0.63	5.36E-01	0.13	0.47	2.45E-01	-0.24	0.46	9.85E-02	-0.37	0.71	3348164	211379	3274218	251618	3258522	271646	3289913	231563
RP_POS_277_17874a9_207	RP	POS	9.21	277.1787				5.37E-03	-0.53	0.82	5.36E-01	0.13	0.45	2.78E-02	-0.47	0.87	6.49E-03	-0.59	0.91	1462641	94168	1405010	110028	1398148	112463	1411873	108237
RP_NEG_353_30853a11_037	RP	NEG	11.04	353.3085				9.69E-03	-0.48	0.97	5.36E-01	-0.13	0.95	6.08E-03	-0.54	1.09	6.58E-02	-0.41	0.91	706956	133913	629778	166614	640163	189908	619393	140719
RP_NEG_174_95599a15_344	RP	NEG	15.34	174.9560				5.11E-01	-0.15	0.49	5.36E-01	0.12	0.57	7.08E-01	-0.09	0.44	4.17E-01	-0.21	0.48	40859881	2587557	40523705	2207932	40386110	2518587	40661301	1862121
RP_POS_429_22702a9_327	RP	POS	9.33	429.2270				2.66E-05	0.54	1.15	5.36E-01	0.14	0.50	5.27E-04	0.61	1.19	5.86E-03	0.48	1.21	264847	223139	630586	740971	584424	740887	676748	745666
HILIC_NEG_131_03481a0_81	HILIC	NEG	0.81	131.0348				6.81E-01	-0.08	0.76	5.36E-01	0.13	0.78	9.49E-01	-0.01	0.03	5.20E-01	-0.14	0.73	656535	163789	642251	189399	630454	198964	654049	180569
HILIC_NEG_202_92863a2_946	HILIC	NEG	2.946	202.9286				3.56E-01	-0.17	0.99	5.36E-01	-0.13	0.75	2.57E-01	-0.23	0.72	6.28E-01	-0.10	0.49	8907884	1785752	8549484	2205546	8686845	2312064	8412123	2108079
RP_POS_281_91193a15_635	RP	POS	15.64	281.9119				4.59E-01	0.18	0.76	5.36E-01	0.11	1.27	3.59E-01	0.23	0.78	6.41E-01	0.12	0.61	5418304	1415126	5621335	1059243	5555375	1074639	5687296	1050315
RP_POS_256_22693a11_018	RP	POS	11.02	256.2269				9.48E-03	0.41	0.84	5.36E-01	-0.13	0.40	4.91E-02	0.34	0.71	2.19E-02	0.48	0.82	351764	471809	658132	799994	707945	901011	608318	690041
RP_POS_130_06549a5_353	RP	POS	5.35	130.0655	Fragment of 3-indoleacetic acid	130.0655(100), 103.0546(1)		5.00E-01	-0.14	0.41	5.36E-01	0.12	0.56	7.38E-01	-0.08	0.42	3.59E-01	-0.20	0.66	2948812	1284983	2773957	1204254	2698974	1031129	2848941	1362113
HILIC_NEG_477_52896a1_365	HILIC	NEG	1.365	477.5290				5.43E-01	-0.09	0.33	5.36E-01	-0.14	0.44	4.32E-01	-0.16	0.35	8.90E-01	-0.02	0.38	195210	68128	184460	128578	192465	110894	176454	144823
RP_POS_765_45886a10_893	RP	POS	10.89	765.4589				6.26E-03	0.38	1.09	5.37E-01	-0.14	0.94	3.57E-02	0.31	1.06	3.08E-02	0.45	1.07	1231379	562438	1710348	1406174	1797887	1672757	1622808	1086852
RP_POS_323_21442a9_889	RP	POS	9.89	323.2144				8.40E-01	0.04	0.53	5.37E-01	0.12	0.45	6.59E-01	0.10	0.30	9.42E-01	-0.02	0.55	1653258	293894	1665109	265574	1648589	269419	1681629	263353
RP_POS_852_53381a11_254	RP	POS	11.25	852.5338				1.47E-02	0.30	0.60	5.37E-01	-0.14	0.51	4.38E-02	0.23	0.72	7.96E-02	0.37	0.66	475013	286524	834137	1358857	918658	1718370	749617	873668
RP_NEG_410_1748a11_262	RP	NEG	11.26	410.1748				1.30E-06	0.89	1.74	5.37E-01	0.12	1.06	9.87E-06	0.95	1.69	2.59E-05	0.83	1.68	572448	128595	721079	161069	711074	147462	731083	174546
RP_POS_734_8103a0_497	RP	POS	0.50	734.8103				1.31E-08	-0.68	1.37	5.37E-01	0.14	1.19	1.42E-04	-0.62	1.43	2.81E-05	-0.75	1.49	11629346	314934	8596331	4871218	8293848	5096077	8898814	4667446
RP_POS_166_98494a10_441	RP	POS	10.44	166.9849				1.20E-01	-0.31	0.57	5.38E-01	-0.12	1.04	7.77E-02	-0.37	0.83	2.90E-01	-0.25	0.41	12422318	4958054	10811350	5190931	11133585	5885023	10489115	4426740
RP_POS_198_14888a6_462	RP	POS	6.46	198.1489				6.90E-01	-0.10	0.63	5.38E-01	-0.11	0.40	5.76E-01	-0.16	0.60	8.57E-01	-0.05	0.43	1239230	1099589	1155697	728923	1200955	582422	1110439	854461
HILIC_POS_171_18561a5_784	HILIC	POS	5.784	171.1856				6.07E-01	-0.11	0.72	5.38E-01	-0.12	0.84	4.81E-01	-0.17	0.47	8.27E-01	-0.05	0.22	74955656	16139278	73297213	14609877	74202851	13512695	72391575	15715798
RP_POS_551_2757a10_311	RP	POS	10.31	551.2757				1.25E-02	0.44	1.19	5.38E-01	0.13	0.53	1.47E-02	0.51	1.08	6.35E-02	0.38	1.00	269862	131419	344643	176334	333714	174755	355572	178995
RP_NEG_316_94928a12_881	RP	NEG	12.88	316.9493				7.86E-01	-0.05	0.36	5.38E-01	0.13	0.42	9.70E-01	0.01	0.29	5.89E-01	-0.12	0.33	3648149	937707	3595699	980736	3534925	895233	3656473	1065052
HILIC_POS_343_29504a0_891	HILIC	POS	0.891	343.2950				6.25E-01	0.07	0.15	5.38E-01	0.14	0.49	5.13E-01	0.14	0.38	9.73E-01	0.01	0.22	182727	352219	227869	677409	185865	490150	269872	826609
RP_POS_445_75043a6_111	RP	POS	6.11	445.7504				3.17E-07	0.61	1.31	5.38E-01	-0.14	1.16	5.59E-04	0.54	1.41	1.89E-04	0.68	1.40	69159	107627	2216110	3910617	2458325	4181568	1973895	3645917
HILIC_POS_202_18036a1_345	HILIC	POS	1.345	202.1804				9.97E-02	-0.36	0.59	5.39E-01	-0.12	0.46	6.86E-02	-0.42	0.75	2.22E-01	-0.30	0.47	17118349	9713392	13897331	8546580	14426413	9526911	13368250	7499697
RP_POS_426_24576a6_11	RP	POS	6.11	426.2458				3.57E-07	0.61	1.31	5.39E-01	-0.14	1.15	5.50E-04	0.54	1.40	2.13E-04	0.68	1.38	21051	56894	1008470	1807095	1120314	1942092	896626	1673493
RP_POS_285_00549a4_771	RP	POS	4.77	285.0055				5.98E-04	-0.70	1.23	5.39E-01	-0.12	0.53	8.44E-04	-0.76	1.29	3.58E-03	-0.64	1.34	1626548	563591	1206370	576860	1242064	559680	1170676	597062

Supplementary table 1: Metabolomics results (in asceding order according to p-value from progressive ALD vs non-progressive ALD comparison, with molecular features with ID_level of 1-2 first)

							all_ALD_vs_control			Prog_ALD_vs_non-prog_ALD			Prog_ALD_vs_control_ALD			Non-prog_ALD_vs_control			Healthy_control		all_ALD		Non-prog_ALD		Progressive_ALD	
							t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA								
Feature_ID	RP_HILIC	POS_NEG	Average.Rt	Average.Mz	Metabolite.name	curated_MSMS	ID_level	p	d	VIP	p	d	VIP	p	d	VIP	p	d	VIP	Mean	SD	Mean	SD	Mean	SD	Mean	SD
RP_POS_284_67712a10_505	RP	POS	10.51	284.6771				1.45E-01	-0.33	0.87	5.39E-01	0.12	0.81	2.77E-01	-0.27	0.61	1.05E-01	-0.39	0.90	1554806	677320	1359456	551964	1325301	500287	1393611	602394
RP_POS_218_91927a0_515	RP	POS	0.52	218.9193				4.87E-06	0.56	1.27	5.39E-01	-0.14	1.15	1.84E-03	0.49	1.29	6.11E-04	0.63	1.40	508953	128256	861417	699501	904688	751339	818147	648272
RP_POS_159_02777a0_709	RP	POS	0.71	159.0278				1.40E-14	0.95	1.56	5.39E-01	0.13	0.90	3.54E-07	1.01	1.68	2.22E-09	0.88	1.78	56392	49287	888420	919639	831560	749749	945279	1067713
HILIC_NEG_259_8161a2_946	HILIC	NEG	2.946	259.8161				2.17E-06	0.59	1.30	5.39E-01	-0.14	0.82	1.43E-03	0.53	1.42	2.38E-04	0.66	1.45	1241931	80231	1423339	336377	1444123	350367	1402554	323990
RP_POS_617_51111a11_379	RP	POS	11.38	617.5111				2.67E-01	-0.36	0.79	5.39E-01	-0.07	0.38	2.33E-01	-0.40	0.63	3.19E-01	-0.33	0.74	2633919	5453216	1531374	1612531	1630992	1652442	1431755	1582011
HILIC_POS_199_18042a4_123	HILIC	POS	4.123	199.1804				7.90E-03	-0.52	1.23	5.39E-01	-0.12	1.04	8.11E-03	-0.58	1.06	3.65E-02	-0.46	1.06	6667328	891981	6154833	989941	6215989	999307	6093678	986772
RP_POS_617_52216a9_616	RP	POS	9.62	617.5222				3.32E-01	-0.27	0.88	5.40E-01	-0.09	0.41	2.70E-01	-0.32	0.69	4.41E-01	-0.23	0.59	1647425	4520409	831319	2272552	971677	2414019	690961	2136981
RP_POS_703_57404a12_661	RP	POS	12.66	703.5740				1.20E-06	-1.17	1.97	5.40E-01	-0.10	0.56	8.76E-07	-1.22	1.97	7.16E-06	-1.12	1.75	1607127	608513	947797	445683	975302	484079	920291	406748
RP_POS_390_73294a5_862	RP	POS	5.86	390.7329				4.27E-07	0.60	1.30	5.40E-01	-0.14	1.15	6.13E-04	0.53	1.40	2.32E-04	0.67	1.38	16273	25182	585821	1050814	650629	1128419	521013	974193
HILIC_POS_635_41479a1_24	HILIC	POS	1.24	635.4148				1.90E-04	0.71	1.17	5.40E-01	-0.12	0.72	3.75E-03	0.65	1.05	1.34E-04	0.77	1.49	3638293	1619796	5001383	1884100	5117594	1594639	4885173	2145153
HILIC_NEG_142_92892a5_425	HILIC	NEG	5.425	142.9289				8.81E-02	-0.33	0.54	5.40E-01	-0.13	0.49	5.86E-02	-0.39	0.73	2.49E-01	-0.26	0.41	3057233	539292	2859877	621546	2898190	694235	2821563	543660
HILIC_NEG_315_04199a5_882	HILIC	NEG	5.882	315.0420				9.79E-01	0.01	0.60	5.40E-01	0.12	0.64	7.79E-01	0.07	0.19	8.11E-01	-0.06	0.52	4646198	1129348	4652139	1061482	4586726	1031663	4717553	1097005
RP_POS_553_36963a14_24	RP	POS	14.24	553.3696				1.88E-01	-0.24	0.68	5.41E-01	-0.13	0.62	1.62E-01	-0.31	0.82	3.85E-01	-0.18	0.59	165747176	48042245	151966956	59389763	155623246	55633551	148310665	63276346
HILIC_POS_184_16968a0_777	HILIC	POS	0.777	184.1697				9.18E-01	0.01	0.22	5.41E-01	-0.14	0.37	5.76E-01	-0.06	0.20	7.12E-01	0.08	0.21	1783827	243126	1792554	729104	1837531	976852	1747577	340095
RP_POS_335_16562a10_979	RP	POS	10.98	335.1656				5.49E-02	0.36	1.45	5.41E-01	-0.13	1.33	1.70E-01	0.30	1.27	4.35E-02	0.43	1.29	2592129	648385	2861072	756920	2907658	721729	2814486	795127
RP_POS_424_36359a10_45	RP	POS	10.45	424.3636				3.28E-02	-0.45	0.86	5.41E-01	-0.12	1.19	3.25E-02	-0.51	0.80	8.00E-02	-0.40	0.88	3369059	278132	3246902	259992	3262892	238231	3230912	281595
RP_POS_506_36023a10_795	RP	POS	10.80	506.3602				1.32E-01	-0.37	0.89	5.41E-01	-0.11	1.00	1.00E-01	-0.43	0.88	2.28E-01	-0.32	0.74	1953814	890992	1693872	612359	1731523	647686	1656222	578991
RP_POS_336_32626a11_37	RP	POS	11.37	336.3263				8.82E-01	-0.03	0.62	5.41E-01	-0.12	0.36	6.86E-01	-0.09	0.35	8.91E-01	0.03	0.38	8229848	5460619	8065167	5450028	8400204	5534572	7730129	5399186
RP_POS_357_34729a9_619	RP	POS	9.62	357.3473				5.14E-01	-0.17	0.75	5.42E-01	-0.10	0.44	4.13E-01	-0.22	0.61	6.71E-01	-0.12	0.45	1464877	2287346	1182685	1417001	1269747	1491679	1095624	1347659
HILIC_POS_351_01309a7_45	HILIC	POS	7.45	351.0131				4.91E-01	-0.11	1.01	5.42E-01	-0.13	0.63	3.01E-01	-0.17	0.97	8.50E-01	-0.04	0.96	4816100	320042	4761001	561729	4795515	651784	4726486	458547
HILIC_NEG_129_9364a0_596	HILIC	NEG	0.596	129.9364				3.92E-01	-0.15	0.85	5.42E-01	-0.13	0.71	2.89E-01	-0.21	0.38	6.86E-01	-0.08	0.65	759871	133407	734122	183900	745415	188761	722829	180103
HILIC_POS_118_0865a4_057	HILIC	POS	4.057	118.0865				3.03E-01	0.14	0.53	5.42E-01	0.14	0.97	3.23E-01	0.21	0.32	5.76E-01	0.08	0.19	9188401	3603219	10285605	8468114	9765040	5701543	10806170	10574532
RP_POS_238_14136a6_464	RP	POS	6.46	238.1414		238.1423(100)	4	6.22E-01	-0.13	0.65	5.42E-01	-0.10	0.39	5.24E-01	-0.18	0.61	7.74E-01	-0.08	0.46	626108	794916	552237	490505	582346	393897	522127	573668
RP_POS_485_11307a10_133	RP	POS	10.13	485.1131				8.58E-01	0.04	0.59	5.43E-01	-0.12	0.54	9.42E-01	-0.02	0.53	6.74E-01	0.10	0.49	1514348	288230	1524470	241695	1539284	210734	1509655	270496
RP_POS_834_58771a13_869	RP	POS	13.87	834.5877				2.31E-01	-0.26	0.65	5.43E-01	-0.12	0.83	4.18E-01	-0.21	0.60	1.55E-01	-0.32	0.59	9947147	2776863	9283961	2408965	9136295	1932119	9431627	2819056
RP_POS_304_26056a11_252	RP	POS	11.25	304.2606				3.57E-11	1.00	1.52	5.43E-01	-0.12	0.42	1.09E-06	0.94	1.51	3.09E-09	1.06	1.76	10981931	4178411	19101752	8095723	19597651	7479935	18605854	8715947
RP_POS_627_46881a10_458	RP	POS	10.46	627.4688				4.72E-01	-0.13	0.63	5.43E-01	-0.13	0.88	3.51E-01	-0.20	0.91	7.47E-01	-0.07	0.14	964824	133213	944134	162352	954074	166126	934194	159546
RP_POS_328_8989a15_377	RP	POS	15.38	328.8989				3.09E-01	0.23	0.61	5.43E-01	-0.12	0.59	4.87E-01	0.17	0.48	2.34E-01	0.29	0.53	1771652	115245	1794725	94158	1800489	88952	1788960	99660
RP_POS_499_8262a3_786	RP	POS	3.79	499.8262				1.18E-01	0.26	0.62	5.43E-01	-0.13	0.42	3.72E-01	0.19	0.69	6.96E-02	0.32	0.89	1668517	1552783	2246962	2415909	2394887	2005739	2099037	2779335
RP_POS_540_36578a9_53	RP	POS	9.53	540.3658				7.14E-05	-0.76	1.36	5.44E-01	0.12	0.84	3.71E-03	-0.70	1.29	1.27E-05	-0.82	1.73	1398332	559869	891434	659185	851062	383367	931806	853007
RP_POS_343_33157a9_476	RP	POS	9.48	343.3316				4.51E-01	-0.20	0.90	5.44E-01	-0.10	0.44	3.57E-01	-0.25	0.66	6.03E-01	-0.15	0.53	1442446	1742953	1194074	1068019	1259389	1174115	1128759	957788
RP_NEG_702_32214a10_63	RP	NEG	10.63	702.3221				1.61E-02	-0.48	1.13	5.44E-01	0.12	0.43	6.02E-02	-0.42	0.90	1.46E-02	-0.54	1.23	2319722	339550	2146036	359054	2124082	352491	2167990	367746
RP_POS_236_11311a4_851	RP	POS	4.85	236.1131				6.25E-01	0.09	0.52	5.44E-01	-0.13	0.54	9.02E-01	0.03	0.43	4.83E-01	0.15	0.55	66501938	19729879	68603452	24739091	70115511	26555631	67091392	22949247
RP_POS_344_66132a5_682	RP	POS	5.68	344.6613				8.89E-01	0.03	0.68	5.44E-01	0.13	0.52	6.48E-01	0.09	0.62	8.83E-01	-0.04	0.46	9879189	4601675	10014170	5076679	9703740	6143822	10324599	3758737
RP_POS_332_15396a10_73	RP	POS	10.73	332.1540				2.88E-03	0.48	1.39	5.44E-01	-0.13	1.26	2.96E-02	0.42	1.20	5.42E-03	0.55	1.38	498233	250298	682152	404182	706833	410288	657471	400601
RP_POS_295_1879a9_88	RP	POS	9.88	295.1879	Unknown	295.1868(100)	4	1.76E-01	0.24	0.52	5.44E-01	-0.13	0.39	3.74E-01	0.17	0.43	1.60E-01	0.30	0.56	3957647	1889536	4530188	2532136	4684763	2754115	4375612	2306590
HILIC_POS_312_21677a0_819	HILIC	POS	0.819	312.2168				4.60E-01	-0.13	0.29	5.45E-01	0.13	0.68	7.89E-01	-0.06	0.26	2.67E-01	-0.19	0.69	2573286	1249999	2362799	1779207	2254204	1271856	2471393	2180385
RP_POS_371_0199a0_666	RP	POS	0.67	371.0199				6.04E-08	-0.66	1.35	5.45E-01	0.13	1.19	3.71E-04	-0.59	1.40	4.13E-05	-0.72	1.48	1489861	74927	1139019	587996	1103164	602491	1174874	576990
RP_NEG_305_86047a15_522	RP	NEG	15.52	305.8605				1.45E-01	0.41	0.70	5.45E-01	-0.09	0.63	2.15E-01	0.36	0.56	1.15E-01	0.46	0.73	1240571	103841	1269026	53359	1272278	50171	1265774	56690
RP_POS_482_4054a10_709	RP	POS	10.71	482.4054				9.66E-01	-0.01	0.54	5.45E-01	0.12	0.44	8.19E-01	0.05	0.42	7.65E-01	-0.07	0.38	10666799	1100052	10657379	1075857	10591831	1107599	10722928	1050246
RP_NEG_325_18567a11_611	RP	NEG	11.61	325.1857				8.45E-02	-0.33	0.83	5.46E-01	0.12	0.56	2.06E-01	-0.26	0.69	7.89E-02	-0.39	0.85	3107807	546122	2904939	636693	2866221	673581	2943658	601879
RP_POS_428_26151a6_293	RP	POS	6.29	428.2615				1.44E-07	0.63	1.33	5.46E-01	-0.13	1.17	4.63E-04	0.56	1.40	1.05E-04	0.69	1.43	12651	9811	446717	765938	493279	804934	400156	730037
RP_POS_227_12578a7_012	RP	POS	7.01	227.1258				5.67E-02	-0.36	0.75	5.46E-01	0.12	0.75	1.56E-01	-0.30	0.66	5.29E-02	-0.43	0.77	1256773	115972	1209234	133369	1201130	137748	1217338	129727
HILIC_POS_161_20473a4_817	HILIC	POS	4.817	161.2047				2.30E-02	0.40	0.90	5.46E-01	-0.13	0.53	9.69E-02	0.34	0.58	2.54E-02	0.46	1.23	1165276	848816	1605266	1153505	1675344	1174955	1535187	1139193
RP_NEG_374_13452a11_162	RP	NEG	11.16	374.1345				3.67E-03	0.52	1.31	5.46E-01	-0.13	1.31	2.70E-02	0.46	1.24	4.73E-03	0.58	1.34	2280482	249041	2445668	327904	2465586	324899	2425750	332966
RP_POS_472_25647a6_394	RP	POS	6.39	472.2565				1.32E-07	0.63	1.33	5.46E-01	-0.13	1.17	4.06E-04	0.56	1.41	1.08E-04	0.70	1.43	10090	9709	279848	474169	308649	501151	251047	448793
RP_NEG_267_07404a1_789	RP	NEG	1.79	267.0740				2.30E-09	0.73	1.36	5.46E-01	0.13	0.77	4.70E-05	0.80	1.43	4.44E-06	0.67	1.51	261595	1049863	4888310	6870853	4470916	5684297	5305705	7919212
RP_POS_376_3187a10_453	RP	POS	10.45	376.3187				8.71E-01	-0.03	0.76	5.46E-01	-0.12	0.48	6.69E-01	-0.09	0.79	9.05E-01	0.03	0.57	696173	207760	689275	210374	702050	227824	676500	192824
RP_POS_207_39899a10_591	RP	POS	10.59	207.3990				1.09E-03	0.57	1.02	5.46E-01	-0.13	0.45	1.29E-02	0.51	0.88	1.65E-03	0.64	1.30	1114629	485755	1484936	667415	1525460	652354	1444411	686337
RP_POS_492_8812a0_471	RP	POS	0.47	492.8812				4.39E-09	-0.74	1.38	5.47E-01	0.13	1.15	9.98E-05	-0.67	1.43	4.75E-06	-0.80	1.53	1016655	103457	709413	450716	682073	449610	736754	454709
HILIC_NEG_132_92363a5_428	HILIC	NEG	5.428	132.9236				4.75E-02	-0.46	1.00	5.47E-01	-0.11	0.39	3.99E-02	-0.51	0.97	1.02E-01	-0.40	0.83	5324126	619174	5079315	494098	5109247	487039	5049383	504196
HILIC_NEG_115_92069a4_16	HILIC	NEG	4.16	115.9207				4.64E-01	0.12	0.66	5.48E-01	-0.13	0.61	7.70E-01	0.06	0.38	3.47E-01	0.19	0.51	41602743	8486526	43039966	12489476	43795814	12493834	42284118	12565652
RP_NEG_852_57843a13_375	RP	NEG	13.38	852.5784	Unknown	301.2182(100), 283.2661(85), 792.5403(60)	4	1.42E-02	0.51	1.07	5.48E-01	-0.12	0.41	4.35E-02	0.46	0.85	1.46E-02	0.57	1.00	11748149	4150887	13872194	4008337	14114759	4192455	13629630	3842482
RP_POS_621_44519a15_102	RP	POS	15.10	621.4452				3.91E-01	0.18	0.57	5.48E-01	0.12	0.52	2.88E-01	0.24	0.43	6.14E-01	0.12	0.73	7951055	2169081	8328253	2074000	8202775	2239635	8453731	1908572
HILIC_POS_512_33557a1_847	HILIC	POS	1.847	512.3356				8.35E-02	-0.30	0.93	5.48E-01	-0.13	0.74	1.01E-01	-0.36	0.55	1.99E-01	-0.23	0.48	2823726	738238	2531307	1036077	2593971	848231	2468643	1200546
RP_POS_531_31696a10_323	RP	POS	10.32	531.3170				4.55E-02	-0.44	0.87	5.48E-01	-0.12	0.54	4.05E-02	-0.50	0.87	1.05E-01	-0.38	0.63	644118	346414	503466	306621	522004	295474	484928	319288
HILIC_NEG_191_81656a3_005	HILIC	NEG	3.005	191.8166				1.81E-01	-0.27	0.48	5.48E-01	-0.12	0.50	1.19E-01	-0.33	0.63	3.85E-01	-0.21	0.56	550726	85216	526900	90503	532373	103511	521427	75981
HILIC_POS_86_90928a2_83	HILIC	POS	2.83	86.9093				5.54E-05	0.50	1.38	5.48E-01	-0.13	0.65	5.51E-03	0.44	1.13	2.03E-03	0.57	1.68	1748844	284205	2284172	1179647	2355469	1277011	2212875	1081851
RP_NEG_722_82727a0_495	RP	NEG	0.50	722.8273				2.90E-08	-0.69	1.36	5.48E-01	0.13	1.19	2.33E-04	-0.62	1.40	2.18E-05	-0.75	1.49	2108931	169838	1544540	900599	1490122	916792	1598958	890032
RP_POS_811_54382a13_387	RP	POS	13.39	811.5438				4.86E-01	-0.15	0.52	5.49E-01	-0.12	0.45	3.89E-01	-0.21	0.55	7.00E-01	-0.09	0.50	1261113	572121	1180660	541153	1213351	498897	1147969	583601
RP_NEG_319_88931a15_356	RP	NEG	15.36	319.8893				6.11E-01	-0.10	0.70	5.49E-01	-0.12	0.41	4.61E-01	-0.16	0.57	8.56E-01	-0.04	0.49	2340206	83086	2331517	85352	2336671	89764	2326362	81282
RP_NEG_226_97752a15_725	RP	NEG	15.73	226.9775				3.57E-01	-0.13	0.59	5.49E-01	0.14	0.39	5.68E-01	-0.06	0.39	3.96E-01	-0.20	0.63	7940261	229828	7877028	550317	7843743	745616	7910314	231674
RP_POS_207_96658a0_917	RP	POS	0.92	207.9666				6.23E-13	0.94	1.46	5.49E-01	0.13	0.87	2.49E-07	1.00	1.61	3.60E-08	0.88	1.57	1352257	302400	2257534	998327	2197292	878977	2317776	1110696
RP_POS_153_07024a15_462	RP	POS	15.46	153.0702				9.19E-01	0.02	0.47	5.50E-01	0.12	0.70	7.22E-01	0.08	0.28	8.83E-01	-0.04	0.60	7177170	678890	7190963	608119	7154324	685406	7227602	524065
RP_POS_169_09721a2_321	RP	POS	2.32	169.0972				1.15E-07	0.71	1.33	5.50E-01	0.13	0.39	9.65E-05	0.77	1.34	3.17E-05	0.64	1.39	516433	208737	914172	604620	877762	511657	950581	688543
HILIC_POS_186_11261a4_033	HILIC	POS	4.033	186.1126				1.95E-02	0.44	0.89	5.50E-01	-0.12	0.69	6.08E-02	0.38	0.71	2.68E-02	0.50	0.82	5636863	2699278	7019060	3231854	7213585	3607038	6824535	2831072
RP_NEG_365_2326a10_804	RP	NEG	10.80	365.2326				9.66E-01	-0.01	0.78	5.50E-01	0.13	0.80	7.93E-01	0.06	0.66	7.40E-01	-0.07	0.75	737641	108223	736657	133379	728631	135670	744683	131928
RP_NEG_207_83691a3_108	RP	NEG	3.11	207.8369				3.65E-02	0.38	0.92	5.51E-01	-0.13	0.42	1.21E-01	0.31	1.06	4.04E-02	0.44	0.70	1819660	1220973	2391923	1591671	2487557	1675705	2296290	1513896
RP_NEG_360_23993a7_233	RP	NEG	7.23	360.2399				4.92E-01	-0.11	0.78	5.51E-01	-0.13	1.04	3.04E-01	-0.18	0.58	8.23E-01	-0.05	0.71	607477	420254	539847	638606	578234	756550	501460	498580
RP_NEG_210_84201a0_523	RP	NEG	0.52	210.8420				7.32E-03	0.37	1.15	5.51E-01	-0.13	1.11	7.57E-02	0.30	1.07	2.02E-02	0.43	1.27	1197474	174323	1344821	443982	1371475	469235	1318167	420275
RP_POS_198_18532a8_862	RP	POS	8.86	198.1853				2.54E-01	0.17	0.67	5.51E-01	0.13	0.60	2.27E-01	0.24	0.44	5.48E-01	0.11	0.50	612076	280394	695361	529610	663598	492231	727124	567756
HILIC_POS_105_04266a5_463	HILIC	POS	5.463	105.0427				9.98E-01	0.00	0.35	5.51E-01	0.12	0.66	7.95E-01	0.06	0.44	7.91E-01	-0.06	0.11	1855478	248738	1855366	246774	1840571	246805	1870161	248352
RP_POS_325_21078a10_979	RP	POS	10.98	325.2108				1.16E-02	0.45	1.45	5.52E-01	-0.12	1.41	6.65E-02	0.39	1.22	1.12E-02	0.51	1.39	7604494	2742510	9177553	3645771	9396105	3466957	8959001	3838916
RP_POS_221_98225a1_709	RP	POS	1.71	221.9823				2.17E-12	0.92	1.48	5.52E-01	0.12	0.48	1.54E-06	0.98	1.49	3.55E-09	0.86	1.73	1187991	363418	2221846	1166737	2151874	901483	2291818	1388404
RP_POS_249_88596a0_246	RP	POS	0.25	249.8860				8.88E-01	-0.03	0.73	5.52E-01	-0.12	0.46	6.88E-01	-0.09	0.34	8.76E-01	0.03	1.20	697306	76428	695051	84443	700112	83606	689989	85817
RP_POS_561_37604a10_896	RP	POS	10.90	561.3760				7.39E-01	-0.06	0.53	5.52E-01	0.12	0.39	9.88E-01	0.00	0.62	5.44E-01	-0.13	0.44	2448631	865139	2388397	952154	2331327	825861	2445468	1069114
RP_NEG_665_43024a11_253	RP	NEG	11.25	665.4302				4.52E-06	0.85	1.68	5.52E-01	0.12	1.04	2.68E-05	0.90	1.64	8.02E-05	0.79	1.61	992290	272832	1288498	343052	1267940	318330	1309056	368204
RP_POS_649_42542a10_902	RP	POS	10.90	649.4254				4.96E-01	0.12	0.41	5.52E-01	-0.13	0.40	7.81E-01	0.06	0.40	3.82E-01	0.18	0.64	1240513	456373	1309785	612658	1346425	631683	1273145	597157
RP_POS_372_12274a7_727	RP	POS	7.73	372.1227				2.29E-01	-0.21	0.43	5.53E-01	-0.13	0.46	2.46E-01	-0.28	0.62	3.78E-01	-0.15	0.48	891991	57634	876510	76863	881109	48125	871912	97864
RP_NEG_1061_68005a10_502	RP	NEG	10.50	1061.6801				1.01E-03	0.66	1.44	5.53E-01	0.12	0.88	2.51E-03	0.72	1.30	3.30E-03	0.60	1.38	3174651	1091945	3954307	1145372	3885894	908848	4022719	1347209
HILIC_NEG_234_82008a6_89	HILIC	NEG	6.89	234.8201				5.05E-01	0.14	0.76	5.53E-01	-0.12	0.40	7.32E-01	0.08	0.46	3.80E-01	0.20	0.74	1034830	473161	1098496	445740	1125109	414156	1071884	477966
HILIC_NEG_134_89476a0_824	HILIC	NEG	0.824	134.8948				9.58E-01	0.01	0.53	5.54E-01	-0.11	0.86	8.51E-01	-0.05	0.20	7.76E-01	0.07	0.11	19809288	3471933	19844956	2954259	20020928	2947987	19668985	2979863
RP_POS_896_54144a12_957	RP	POS	12.96	896.5414				1.08E-05	-1.05	1.65	5.54E-01	-0.10	0.61	1.00E-05	-1.10	1.74	5.31E-05	-1.00	1.51	6030919	1888653	4222735	1418286	4307184	1463889	4138287	1380797
RP_POS_177_10202a0_71	RP	POS	0.71	177.1020				1.57E-06	0.84	1.46	5.54E-01	0.12	0.48	2.97E-05	0.90	1.39	2.74E-05	0.78	1.64	2262403	4376048	7416711	6109719	7052884	5240371	7780538	6905615
HILIC_NEG_116_92861a7_66	HILIC	NEG	7.66	116.9286				2.86E-01	0.19	0.33	5.54E-01	-0.12	0.42	5.13E-01	0.13	0.26	2.41E-01	0.26	0.47	15046410	2776462	15694721	3496529	15902869	3778448	15486572	3214941
RP_POS_756_55267a11_642	RP	POS	11.64	756.5527				6.61E-01	0.07	0.41	5.54E-01	-0.13	0.51	9.59E-01	0.01	0.20	5.18E-01	0.14	0.48	414220	652551	480763	973942	538742	1082729	422783	858675
HILIC_NEG_397_88855a5_427	HILIC	NEG	5.427	397.8886				9.24E-01	-0.02	0.55	5.54E-01	-0.12	0.57	7.36E-01	-0.08	0.18	8.66E-01	0.04	0.79	540769	52642	539760	50065	542739	49167	536781	51271
HILIC_POS_118_12292a1_142	HILIC	POS	1.142	118.1229				1.46E-02	-0.53	1.14	5.55E-01	0.11	0.77	4.11E-02	-0.48	1.07	1.41E-02	-0.59	1.04	2799169	1436055	2078430	1279496	2002365	1323485	2154496	1242664

Supplementary table 1: Metabolomics results (in asceding order according to p-value from progressive ALD vs non-progressive ALD comparison, with molecular features with ID_level of 1-2 first)

								all_ALD_vs_control			Prog_ALD_vs_non-prog_ALD			Prog_ALD_vs_control_ALD			Non-prog_ALD_vs_control			Healthy_control		all_ALD		Non-prog_ALD		Progressive_ALD	
								t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA								
Feature_ID	RP_HILIC	POS_NEG	Average.Rt	Average.Mz	Metabolite.name	curated_MSMS	ID_level	p	d	VIP	p	d	VIP	p	d	VIP	p	d	VIP	Mean	SD	Mean	SD	Mean	SD	Mean	SD
RP_NEG_1087_6958a10_619	RP	NEG	10.62	1087.6958				1.72E-03	0.66	1.42	5.55E-01	-0.11	0.86	1.18E-02	0.60	1.18	1.09E-03	0.72	1.45	15206392	6827963	19754223	6553637	20143851	5458158	19364594	7528317
HILIC_NEG_200_85867a6_161	HILIC	NEG	6.161	200.8587				5.03E-01	-0.10	0.81	5.55E-01	-0.13	0.73	4.29E-01	-0.17	0.69	8.24E-01	-0.04	0.64	3945014	354665	3883340	669959	3923176	533011	3843505	787091
RP_POS_513_84283a11_328	RP	POS	11.33	513.8428				3.00E-01	0.15	0.37	5.55E-01	-0.13	0.41	5.37E-01	0.08	0.40	3.29E-01	0.22	0.44	125704	132904	164391	287425	181489	365203	147293	181499
RP_POS_309_2034a9_825	RP	POS	9.83	309.2034				1.54E-02	-0.52	0.84	5.55E-01	0.11	0.78	4.94E-02	-0.46	0.80	1.32E-02	-0.58	0.90	1677871	132365	1611537	122514	1604261	118945	1618814	126766
RP_POS_406_24927a13_155	RP	POS	13.16	406.2493				7.02E-01	0.08	0.44	5.55E-01	-0.12	0.55	9.17E-01	0.02	0.31	5.48E-01	0.14	0.69	1976085	780307	2035752	702396	2077454	677207	1994050	731185
HILIC_POS_330_33643a3_028	HILIC	POS	3.028	330.3364				2.10E-08	0.70	1.33	5.55E-01	-0.13	0.78	7.65E-05	0.64	1.38	3.76E-05	0.76	1.41	1102221	70847	1311655	325951	1331004	349756	1292305	302594
RP_NEG_650_86877a0_465	RP	NEG	0.47	650.8688				6.96E-10	-0.80	1.43	5.56E-01	0.13	1.15	2.89E-05	-0.74	1.47	1.05E-06	-0.86	1.57	774924	96909	526014	331938	506326	328654	545701	337356
RP_POS_140_06854a0_46	RP	POS	0.46	140.0685				1.56E-06	0.58	1.31	5.56E-01	-0.13	1.18	1.04E-03	0.52	1.36	3.90E-04	0.65	1.41	751748	39749	895975	275252	912299	295113	879650	255809
RP_POS_698_77014a0_5	RP	POS	0.50	698.7701				2.98E-02	-0.31	1.09	5.56E-01	-0.13	1.24	2.74E-02	-0.38	1.10	2.00E-01	-0.25	1.14	1884815	507056	1574321	1090073	1638878	1184836	1509764	994195
RP_POS_169_0972a1_766	RP	POS	1.77	169.0972				2.38E-07	0.68	1.30	5.57E-01	0.13	0.38	2.94E-04	0.74	1.27	1.72E-05	0.61	1.38	979255	397926	1773162	1273906	1697710	981786	1848613	1517652
RP_POS_805_55762a13_207	RP	POS	13.21	805.5576				6.33E-02	0.39	0.84	5.57E-01	0.12	0.67	6.09E-02	0.44	0.79	1.40E-01	0.33	0.81	8216729	1443937	8770406	1412812	8686777	1297431	8854035	1528140
RP_POS_497_39621a12_891	RP	POS	12.89	497.3962				4.39E-01	0.15	0.62	5.57E-01	-0.12	0.44	7.01E-01	0.09	0.66	3.10E-01	0.21	0.56	3088501	726615	3207020	816412	3255268	708172	3158771	916734
RP_POS_254_24792a10_421	RP	POS	10.42	254.2479				1.25E-05	0.70	1.15	5.57E-01	-0.12	0.73	1.78E-03	0.64	1.09	2.03E-05	0.77	1.40	11613463	4160029	16271308	6858163	16676485	5945087	15866131	7703868
HILIC_POS_173_12859a4_008	HILIC	POS	4.008	173.1286				3.87E-01	0.15	0.87	5.58E-01	-0.13	0.96	6.88E-01	0.09	0.53	2.70E-01	0.21	0.57	2375820	759047	2525080	1069608	2588236	963023	2461924	1172995
RP_POS_790_53485a13_852	RP	POS	13.85	790.5349				3.76E-01	0.19	0.52	5.58E-01	0.12	0.60	3.13E-01	0.25	0.59	5.59E-01	0.13	0.44	921805	666865	1040366	610432	1004331	538279	1076402	678576
HILIC_POS_90_09186a1_814	HILIC	POS	1.814	90.0919				1.94E-05	-0.63	1.33	5.58E-01	0.13	0.81	1.92E-03	-0.56	1.42	2.34E-04	-0.69	1.43	1970592	408760	1472059	850960	1421851	863934	1522267	843515
HILIC_NEG_68_99498a0_572	HILIC	NEG	0.572	68.9950				1.17E-01	0.19	0.49	5.58E-01	-0.14	0.52	5.60E-02	0.12	0.65	2.64E-01	0.25	0.58	256951	56689	322276	400657	345979	552486	298573	133942
RP_POS_443_33432a10_709	RP	POS	10.71	443.3343				9.59E-02	-0.38	0.65	5.58E-01	0.11	0.39	1.96E-01	-0.32	0.52	7.30E-02	-0.43	0.70	81138979	9329636	78040223	7757519	77582568	7298971	78497878	8239171
RP_POS_497_39526a11_257	RP	POS	11.26	497.3953				4.51E-02	0.35	1.34	5.58E-01	0.12	1.30	6.32E-02	0.41	1.23	1.19E-01	0.29	1.12	3460326	987811	3909986	1345797	3830680	1108349	3989293	1555001
RP_POS_344_85773a0_5	RP	POS	0.50	344.8577				1.33E-02	-0.36	1.11	5.59E-01	-0.13	1.23	1.60E-02	-0.42	1.15	1.26E-01	-0.29	1.13	892871	168461	773823	368045	795487	392298	752158	344708
RP_POS_497_25983a6_08	RP	POS	6.08	497.2598				9.08E-01	0.02	0.49	5.59E-01	0.12	0.56	7.15E-01	0.08	0.51	8.43E-01	-0.04	0.44	3992866	239921	3998835	288161	3981882	248517	4015787	324685
RP_NEG_316_77795a15_615	RP	NEG	15.62	316.7780				2.15E-01	-0.27	0.77	5.59E-01	-0.11	0.64	1.74E-01	-0.33	0.59	3.64E-01	-0.21	0.72	1494821	74031	1476434	65366	1480277	63989	1472592	67140
HILIC_NEG_173_92599a7_355	HILIC	NEG	7.355	173.9260				9.70E-01	-0.01	0.18	5.59E-01	-0.11	0.76	7.88E-01	-0.07	0.15	8.36E-01	0.05	0.08	2143285	282663	2141205	248504	2155809	240000	2126600	258328
RP_POS_553_45697a11_256	RP	POS	11.26	553.4570				2.63E-02	0.41	1.13	5.59E-01	0.12	1.14	3.31E-02	0.47	1.12	8.30E-02	0.35	0.96	18551932	4900896	20953882	6040895	20598875	5499826	21308889	6574517
RP_POS_199_13043a11_65	RP	POS	11.65	199.1304				5.44E-01	0.11	0.56	5.60E-01	0.12	0.36	4.79E-01	0.17	0.48	7.75E-01	0.05	0.50	4919353	1505190	5117495	1869575	5007500	1089336	5227490	2418804
RP_POS_434_75906a6_111	RP	POS	6.11	434.7591				1.26E-06	0.58	1.30	5.60E-01	-0.13	1.15	1.10E-03	0.51	1.39	3.60E-04	0.65	1.38	28295	65070	412491	737427	455814	785472	369168	691302
RP_POS_181_0493a7_494	RP	POS	7.49	181.0493	fragment of Diethyl-phthalate	149.0228(100), 163.0386(45), 84.9603(70)	3	7.22E-01	0.07	0.43	5.60E-01	0.12	1.03	5.55E-01	0.13	0.45	9.87E-01	0.00	0.44	1304624	110737	1313187	138169	1305076	134015	1321298	143097
HILIC_POS_138_05505a4_254	HILIC	POS	4.254	138.0551				7.03E-01	-0.07	0.31	5.60E-01	-0.12	0.88	5.32E-01	-0.13	0.26	9.55E-01	-0.01	0.18	51938899	63714489	46815563	72224917	51052654	75804338	42578472	68966651
RP_NEG_299_25934a10_219	RP	NEG	10.22	299.2593				3.80E-01	0.16	0.79	5.60E-01	0.12	0.69	3.06E-01	0.22	0.69	6.32E-01	0.10	0.73	15168146	2069509	15565370	2613663	15412113	2486231	15718627	2751836
HILIC_NEG_200_85867a4_112	HILIC	NEG	4.112	200.8587				6.95E-02	-0.38	0.67	5.61E-01	0.12	0.75	1.71E-01	-0.32	0.55	5.44E-02	-0.43	0.79	3558995	1309972	3067811	1287088	2992410	1223548	3143211	1355849
RP_NEG_379_15878a10_978	RP	NEG	10.98	379.1588				1.34E-02	0.42	1.37	5.61E-01	-0.12	1.24	7.71E-02	0.35	1.12	1.61E-02	0.48	1.32	4906409	2539076	6393134	3792508	6615245	3753966	6171023	3855752
RP_POS_517_37115a10_546	RP	POS	10.55	517.3712				5.28E-01	0.14	0.37	5.61E-01	-0.11	0.38	7.43E-01	0.08	0.30	4.09E-01	0.19	0.89	7360722	1349076	7531241	1229827	7603264	1189298	7459219	1277028
RP_POS_702_86194a0_491	RP	POS	0.49	702.8619				7.64E-08	0.64	1.35	5.61E-01	-0.13	1.20	2.36E-04	0.58	1.41	1.00E-04	0.71	1.46	6308905	1056056	17136482	18574252	18224240	19864592	16048723	17321368
RP_POS_353_03723a4_852	RP	POS	4.85	353.0372				6.79E-01	0.08	0.50	5.61E-01	-0.12	0.59	9.24E-01	0.02	0.37	5.32E-01	0.14	0.52	1041733	423963	1078451	467143	1105804	490559	1051098	445784
RP_POS_216_92223a0_516	RP	POS	0.52	216.9222				9.29E-06	0.54	1.26	5.61E-01	-0.13	1.15	2.82E-03	0.48	1.27	8.13E-04	0.61	1.39	1667280	388166	2724190	2172857	2851373	2307586	2597007	2044751
RP_POS_437_23682a6_111	RP	POS	6.11	437.2368				2.63E-07	0.61	1.32	5.61E-01	-0.13	1.16	5.18E-04	0.55	1.41	1.71E-04	0.68	1.40	7558	6840	372166	659437	410763	700678	333569	620160
HILIC_NEG_117_91911a7_351	HILIC	NEG	7.351	117.9191				3.09E-01	-0.17	0.60	5.61E-01	-0.12	0.59	2.65E-01	-0.24	0.47	5.59E-01	-0.11	0.21	2466663	277909	2402132	394287	2425187	359623	2379078	428584
RP_POS_431_38412a11_038	RP	POS	11.04	431.3841				4.51E-02	0.33	0.90	5.61E-01	-0.13	0.43	1.47E-01	0.26	0.68	6.34E-02	0.39	0.76	1037789	999942	1523238	1603584	1616995	1780484	1429480	1416820
RP_POS_224_86421a0_519	RP	POS	0.52	224.8642				2.17E-05	-0.72	1.29	5.62E-01	0.12	1.06	6.28E-04	-0.66	1.25	1.38E-04	-0.78	1.34	348547	69398	275947	103820	269878	108505	282016	99642
RP_POS_575_33826a15_435	RP	POS	15.44	575.3383				8.30E-01	-0.04	0.76	5.62E-01	-0.12	0.37	6.48E-01	-0.10	0.36	9.35E-01	0.02	0.67	632521	228879	622229	250387	636858	245340	607599	256980
RP_POS_173_96153a0_251	RP	POS	0.25	173.9615				8.81E-01	0.03	0.22	5.62E-01	-0.11	0.47	9.17E-01	-0.03	0.32	7.00E-01	0.09	0.63	2095788	355059	2106427	325382	2125402	307729	2087451	344202
HILIC_NEG_157_86234a3_023	HILIC	NEG	3.023	157.8623				2.74E-01	-0.22	0.98	5.62E-01	-0.12	0.83	2.16E-01	-0.27	0.47	4.83E-01	-0.16	0.26	3745986	700625	3585681	758662	3629919	764903	3541444	757504
RP_NEG_321_92273a6_867	RP	NEG	6.87	321.9227				1.89E-01	-0.24	0.54	5.63E-01	0.12	0.95	3.59E-01	-0.18	0.36	1.82E-01	-0.30	0.51	1675872	184518	1622957	229531	1609577	260316	1636336	195741
RP_POS_325_32242a10_585	RP	POS	10.59	325.3224				1.67E-01	0.30	0.63	5.63E-01	-0.11	0.40	3.16E-01	0.25	0.43	1.23E-01	0.36	0.84	2275185	855043	2512438	756777	2556532	685350	2468344	826704
RP_POS_237_14659a7_809	RP	POS	7.81	237.1466				7.79E-01	0.06	0.59	5.63E-01	0.11	0.73	6.31E-01	0.12	0.52	9.87E-01	0.00	0.40	2255941	255695	2270241	230239	2256848	210386	2283634	249946
RP_POS_770_84924a0_49	RP	POS	0.49	770.8492				8.04E-08	0.64	1.35	5.64E-01	-0.13	1.20	2.48E-04	0.58	1.41	1.01E-04	0.71	1.46	4458927	822041	12700429	14163835	13524025	15117619	11876834	13243712
HILIC_NEG_194_92735a7_667	HILIC	NEG	7.667	194.9274				3.87E-01	0.17	0.72	5.64E-01	0.12	0.79	3.01E-01	0.23	0.45	6.23E-01	0.11	0.49	6859004	525390	6954675	585753	6920631	588522	6988719	586935
RP_POS_419_70483a7_55	RP	POS	7.55	419.7048				5.92E-01	-0.11	0.90	5.64E-01	0.12	0.81	8.30E-01	-0.05	0.77	4.65E-01	-0.17	0.84	4055644	261397	4026531	278444	4010354	288522	4042707	269936
HILIC_NEG_134_89476a1_408	HILIC	NEG	1.408	134.8948				8.95E-01	-0.02	0.73	5.64E-01	0.13	0.86	8.38E-01	0.04	0.23	6.03E-01	-0.08	0.19	15687884	1006878	15654052	1837554	15547241	1431419	15760863	2179422
RP_POS_532_43884a14_268	RP	POS	14.27	532.4388				3.06E-01	0.18	0.36	5.64E-01	0.12	0.37	2.96E-01	0.24	0.47	4.97E-01	0.12	0.45	27064279	27892354	27696769	36543701	27482960	29585194	27909243	44889831
RP_POS_172_97864a15_38	RP	POS	15.38	172.9786				9.18E-01	-0.02	0.42	5.64E-01	0.12	0.39	8.55E-01	0.04	0.32	7.30E-01	-0.08	0.45	85174751	11391055	84930867	12297078	84217229	13373295	85644506	11208835
RP_POS_680_38324a11_426	RP	POS	11.43	680.3832				9.35E-01	-0.02	0.23	5.65E-01	0.12	0.74	8.48E-01	0.04	0.54	7.38E-01	-0.08	0.26	968570	162928	965811	172198	955823	174340	975799	171205
HILIC_POS_137_04587a2_457	HILIC	POS	2.457	137.0459				1.03E-09	0.74	1.25	5.65E-01	0.13	0.63	5.17E-05	0.80	1.26	1.87E-06	0.67	1.72	14241	17329	10443340	15455827	9546692	12458282	11339989	18049675
RP_POS_184_17029a2_197	RP	POS	2.20	184.1703				2.65E-02	0.29	0.50	5.65E-01	-0.13	0.34	3.22E-02	0.22	0.79	1.12E-01	0.36	0.64	810627	47081	848387	146264	856884	193726	839890	74471
RP_POS_838_83618a0_49	RP	POS	0.49	838.8362				7.21E-08	0.65	1.35	5.65E-01	-0.13	1.20	2.29E-04	0.58	1.41	9.78E-05	0.71	1.46	3706745	701748	11051508	12573514	11779673	13436109	10323343	11738901
RP_POS_524_27405a10_326	RP	POS	10.33	524.2741				1.51E-08	1.10	1.82	5.66E-01	0.10	0.45	1.88E-07	1.16	1.77	1.83E-07	1.05	1.84	3275951	1068304	4748244	1208978	4678291	1051323	4818198	1355662
RP_POS_265_17914a8_529	RP	POS	8.53	265.1791	1S,2R,9R,10S,12S)-12-hydroxy-7,15-diazatetracyclo[7.7.1.0^{2,7}.0^{10,15}]heptadecan-6-one	265.1796(100), 57.0705(45)	3	4.64E-01	0.14	0.54	5.66E-01	0.12	0.51	3.76E-01	0.20	0.56	7.14E-01	0.07	0.45	984148	49602	992006	60761	988491	55713	995521	65803
RP_POS_634_87494a0_493	RP	POS	0.49	634.8749				1.11E-07	0.64	1.34	5.66E-01	-0.13	1.20	2.78E-04	0.57	1.40	1.23E-04	0.70	1.45	6369906	1037929	15663044	16160683	16597890	17299621	14728197	15053400
RP_POS_185_11479a13_013	RP	POS	13.01	185.1148				3.45E-01	0.20	0.74	5.66E-01	0.11	0.40	2.74E-01	0.25	0.78	5.44E-01	0.14	0.41	6961375	1553001	7259318	1500142	7172569	1491641	7346067	1518694
RP_POS_636_55511a14_987	RP	POS	14.99	636.5551				2.44E-02	-0.32	0.81	5.66E-01	0.13	0.36	2.56E-01	-0.26	0.56	1.65E-03	-0.39	1.07	1696044	912849	1105203	2025915	987837	1021008	1222569	2687351
HILIC_POS_440_18939a0_947	HILIC	POS	0.947	440.1894				7.07E-01	-0.09	0.51	5.66E-01	-0.11	0.38	5.46E-01	-0.14	0.55	8.99E-01	-0.03	0.38	1091552	694945	1040733	538530	1071859	658653	1009608	387488
RP_POS_223_09395a11_629	RP	POS	11.63	223.0940				3.21E-01	-0.20	0.38	5.66E-01	0.12	0.42	5.75E-01	-0.14	0.38	1.87E-01	-0.26	0.72	8703874	1770887	8340180	1839208	8233883	1125936	8446478	2354489
RP_NEG_397_00366a4_57	RP	NEG	4.57	397.0037				1.03E-02	-0.56	0.90	5.67E-01	-0.11	0.40	1.20E-02	-0.62	0.94	2.64E-02	-0.51	0.84	1917037	1535440	1105745	1360258	1184225	1215946	1027264	1499089
RP_POS_570_35291a10_753	RP	POS	10.75	570.3529				1.33E-01	0.30	1.03	5.67E-01	-0.12	0.81	3.04E-01	0.25	0.75	8.68E-02	0.36	1.00	1744363	825079	2002284	852789	2051478	700645	1953091	986660
RP_POS_562_79602a0_5	RP	POS	0.50	562.7960				2.83E-02	-0.32	1.09	5.67E-01	-0.13	1.23	2.66E-02	-0.39	1.10	1.82E-01	-0.26	1.12	1669684	482712	1381970	972894	1438032	1054771	1325908	890733
RP_POS_285_13071a8_608	RP	POS	8.61	285.1307				4.41E-02	0.39	0.84	5.67E-01	-0.12	0.38	1.34E-01	0.34	0.61	3.62E-02	0.45	0.96	686983	274590	804672	301661	822048	286221	787297	318305
RP_NEG_197_80769a0_702	RP	NEG	0.70	197.8077				8.71E-02	0.26	0.60	5.67E-01	-0.13	0.56	2.99E-01	0.20	0.36	8.28E-02	0.32	0.88	12736704	7004521	15837829	12988373	16585528	12778246	15090129	13282093
HILIC_NEG_136_89166a4_83	HILIC	NEG	4.83	136.8917				3.88E-02	0.42	0.80	5.68E-01	0.11	0.52	3.44E-02	0.48	0.89	1.07E-01	0.37	0.59	10231134	4697818	12257703	4745125	11984586	4812022	12530820	4710005
RP_NEG_588_8985a0_49	RP	NEG	0.49	588.8985				1.46E-07	0.63	1.34	5.68E-01	-0.13	1.20	2.93E-04	0.57	1.40	1.50E-04	0.69	1.44	9671097	1425574	21219558	20283232	22387044	21824667	20052071	18764790
RP_POS_844_54449a11_619	RP	POS	11.62	844.5445				6.90E-01	0.06	0.64	5.68E-01	-0.13	0.59	9.99E-01	0.00	0.38	5.43E-01	0.13	0.63	934572	883483	1021185	1498137	1107415	1665062	934956	1321752
HILIC_POS_134_11755a1_649	HILIC	POS	1.649	134.1176				1.99E-04	-0.67	1.30	5.68E-01	0.12	0.81	3.03E-03	-0.61	1.31	4.45E-04	-0.72	1.35	1522440	469013	1115106	621951	1079340	621016	1150872	627111
RP_POS_170_1176a4_742	RP	POS	4.74	170.1176				9.76E-01	0.00	0.49	5.68E-01	0.13	0.54	8.05E-01	0.06	0.55	6.44E-01	-0.07	0.57	1968681	1836273	1955641	2987549	1783692	1625072	2127590	3915590
RP_POS_181_03862a15_342	RP	POS	15.34	181.0386				8.48E-01	0.04	0.69	5.68E-01	-0.11	0.40	9.39E-01	-0.02	0.28	6.78E-01	0.10	1.02	18904576	6757305	19166422	6545889	19542477	6763263	18790366	6367218
RP_POS_443_33426a10_657	RP	POS	10.66	443.3343				5.84E-01	-0.11	0.72	5.68E-01	0.11	0.67	8.02E-01	-0.06	0.37	4.64E-01	-0.17	0.68	56606156	4033035	56158072	3889488	55934704	4022390	56381441	3779357
RP_POS_229_1192a7_341	RP	POS	7.34	229.1192				1.51E-02	-0.48	0.78	5.69E-01	-0.11	0.38	1.62E-02	-0.54	0.88	5.22E-02	-0.42	0.71	2352458	196791	2250409	211269	2262538	207542	2238281	216347
RP_NEG_514_8938a0_465	RP	NEG	0.47	514.8938				6.48E-10	-0.77	1.42	5.69E-01	0.12	1.17	3.77E-05	-0.71	1.47	2.10E-06	-0.83	1.55	1423254	132382	975633	624269	939799	624224	1011467	628570
RP_POS_266_04352a3_97	RP	POS	3.97	266.0435				4.96E-01	0.11	0.83	5.69E-01	-0.12	0.35	8.16E-01	0.05	0.59	3.22E-01	0.17	0.42	1351729	335159	1405448	514705	1434998	416302	1375898	600132
HILIC_POS_374_15552a0_552	HILIC	POS	0.552	374.1555				6.45E-04	0.51	0.93	5.69E-01	0.12	0.92	4.86E-03	0.57	1.09	7.40E-03	0.45	1.03	23386514	8167724	30946165	15908362	30033137	13717466	31859194	17928933
HILIC_NEG_180_84201a1_366	HILIC	NEG	1.366	180.8420				8.76E-01	-0.03	0.89	5.69E-01	-0.12	0.81	6.80E-01	-0.09	0.14	8.61E-01	0.03	0.19	11986967	2331203	11905017	3222172	12089789	2940764	11720244	3501272
RP_POS_470_24081a6_222	RP	POS	6.22	470.2408				2.59E-07	0.61	1.31	5.69E-01	-0.13	1.16	4.79E-04	0.55	1.41	1.81E-04	0.68	1.40	30663	39546	1035930	1816398	1140058	1935555	931803	1702185
HILIC_POS_138_09137a0_752	HILIC	POS	0.752	138.0914				1.26E-07	-1.04	1.55	5.69E-01	-0.11	0.75	2.29E-07	-1.09	1.81	5.32E-06	-0.99	1.55	653445	86150	545090	95434	550558	101818	539623	89294
RP_POS_441_29675a11_254	RP	POS	11.25	441.2968				6.23E-06	0.85	1.63	5.70E-01	0.11	1.18	3.30E-05	0.91	1.74	8.11E-05	0.80	1.49	12368503	2810771	15336349	3379491	15143148	3107128	15529550	3653023
RP_NEG_319_98462a3_961	RP	NEG	3.96	319.9846				6.88E-01	0.07	1.01	5.70E-01	-0.12	0.41	9.71E-01	0.01	0.85	4.76E-01	0.13	0.50	1776171	448885	1816919	628365	1852833	507878	1781004	732919
RP_POS_355_36877a11_247	RP	POS	11.25	355.3688				1.08E-11	0.99	1.52	5.71E-01	0.12	0.90	5.36E-07	1.04	1.59	2.28E-09	0.93	1.77	506875	238373	1010732	515548	981281	398875	1040182	613297
RP_NEG_344_85251a15_438	RP	NEG	15.44	344.8525				3.27E-01	0.27	0.80	5.71E-01	0.09	0.66	2.49E-01	0.31	0.69	4.55E-01	0.22	0.44	1149606	141453	1175623	78296	1171149	98415	1180097	51570

Supplementary table 1: Metabolomics results (in asceding order according to p-value from progressive ALD vs non-progressive ALD comparison, with molecular features with ID_level of 1-2 first)

								all_ALD_vs_control			Prog_ALD_vs_non-prog_ALD			Prog_ALD_vs_control_ALD			Non-prog_ALD_vs_control			Healthy_control		all_ALD		Non-prog_ALD		Progressive_ALD	
								t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA								
Feature_ID	RP_HILIC	POS_NEG	Average.Rt	Average.Mz	Metabolite.name	curated_MSMS	ID_level	p	d	VIP	p	d	VIP	p	d	VIP	p	d	VIP	Mean	SD	Mean	SD	Mean	SD	Mean	SD
RP_POS_198_18518a11_128	RP	POS	11.13	198.1852				4.42E-02	0.34	0.72	5.71E-01	-0.12	0.39	1.43E-01	0.28	0.60	5.48E-02	0.40	0.71	363434	304069	505993	443349	531298	476006	480687	411388
HILIC_NEG_153_86867a3_022	HILIC	NEG	3.022	153.8687				6.32E-01	-0.09	0.95	5.71E-01	-0.12	0.84	4.90E-01	-0.15	0.26	8.82E-01	-0.03	0.32	37369172	6825190	36675570	7865375	37123848	7883898	36227293	7900938
RP_POS_511_78964a6_421	RP	POS	6.42	511.7896				2.44E-07	0.62	1.31	5.72E-01	-0.13	1.15	4.23E-04	0.55	1.42	1.90E-04	0.68	1.39	21964	30249	670328	1168394	736887	1251807	603770	1087238
HILIC_POS_171_18555a6_962	HILIC	POS	6.962	171.1856				7.46E-01	0.05	1.10	5.72E-01	-0.13	0.75	9.35E-01	-0.02	1.08	5.40E-01	0.11	1.07	6222887	1146858	6322859	2323186	6455146	2252066	6190572	2407700
RP_POS_173_98438a0_253	RP	POS	0.25	173.9844				7.97E-01	0.05	0.69	5.72E-01	0.11	0.38	6.29E-01	0.11	0.34	9.81E-01	-0.01	0.45	873158	90690	877955	93082	872656	93423	883254	93382
RP_NEG_524_27899a10_307	RP	NEG	10.31	524.2790				1.90E-02	0.37	1.12	5.72E-01	-0.12	0.36	9.89E-02	0.31	0.84	2.96E-02	0.43	1.01	18489676	5965638	22026643	10402387	22618638	10863424	21434647	9994922
RP_POS_498_25931a10_052	RP	POS	10.05	498.2593				1.66E-02	0.40	0.93	5.72E-01	0.12	0.92	3.60E-02	0.46	0.98	5.07E-02	0.34	0.96	342112	241276	478563	358610	458165	282273	498961	423437
RP_NEG_690_83386a0_495	RP	NEG	0.50	690.8339				1.27E-07	-0.64	1.34	5.73E-01	0.13	1.19	3.97E-04	-0.58	1.38	7.73E-05	-0.71	1.45	1708447	107479	1285926	723924	1244811	752014	1327041	699894
RP_POS_265_17734a9_625	RP	POS	9.63	265.1773				8.93E-03	0.40	1.37	5.73E-01	0.12	1.46	9.22E-03	0.46	1.32	9.02E-02	0.34	1.12	1805381	630777	2236007	1167320	2169735	1277595	2302279	1054452
HILIC_POS_332_09671a2_458	HILIC	POS	2.458	332.0967				1.72E-05	0.52	1.04	5.73E-01	0.13	0.61	2.66E-03	0.58	0.97	1.35E-03	0.45	1.41	315173	60942	519873	442331	494757	367618	544989	508798
HILIC_NEG_243_75554a1_358	HILIC	NEG	1.358	243.7555				3.97E-07	0.63	1.16	5.73E-01	0.12	0.37	1.69E-04	0.69	1.21	4.18E-04	0.57	1.48	257098	32987	349144	161302	339989	150697	358300	172298
RP_POS_468_724a6_453	RP	POS	6.45	468.7240				9.92E-01	0.00	0.61	5.73E-01	0.12	0.44	7.36E-01	0.06	0.56	8.08E-01	-0.06	0.44	498018	242670	498526	300607	481452	372988	515600	207023
HILIC_POS_160_06046a7_687	HILIC	POS	7.687	160.0605				8.10E-01	-0.05	0.47	5.73E-01	0.12	0.49	9.53E-01	0.01	0.22	6.47E-01	-0.10	0.20	1046809	66400	1043455	74847	1039210	82326	1047700	67113
HILIC_POS_141_13869a3_025	HILIC	POS	3.025	141.1387				9.01E-03	0.35	1.02	5.74E-01	0.13	0.73	1.98E-02	0.42	0.99	9.96E-02	0.29	1.07	3949093	263984	4175033	712586	4134680	713381	4215385	716718
RP_POS_645_49579a11_466	RP	POS	11.47	645.4958				1.46E-04	-0.89	1.54	5.74E-01	-0.10	0.44	1.28E-04	-0.94	1.51	7.07E-04	-0.84	1.34	626217	321420	367774	251011	381988	266874	353560	235933
RP_POS_469_77896a6_393	RP	POS	6.39	469.7790				1.54E-07	0.63	1.32	5.74E-01	-0.13	1.16	5.01E-04	0.56	1.40	1.04E-04	0.69	1.43	20544	14363	494587	838685	542071	872953	447103	809007
RP_POS_199_1304a14_168	RP	POS	14.17	199.1304				7.29E-02	0.34	0.68	5.74E-01	0.12	0.37	6.76E-02	0.40	0.78	1.83E-01	0.29	0.86	28200890	14074557	33609745	16065183	32700715	15796919	34518775	16438319
HILIC_POS_356_27933a0_654	HILIC	POS	0.654	356.2793				7.38E-02	-0.37	0.75	5.74E-01	-0.11	0.71	7.79E-02	-0.42	0.65	1.46E-01	-0.31	0.80	2472368	1173895	2037996	1165782	2103970	988477	1972021	1326598
RP_POS_531_38605a10_661	RP	POS	10.66	531.3861				8.13E-01	0.05	0.32	5.75E-01	0.11	0.42	6.43E-01	0.11	0.28	9.89E-01	0.00	0.29	31384161	2322532	31493148	2061102	31376620	2297349	31609677	1810373
RP_NEG_218_98579a6_853	RP	NEG	6.85	218.9858				3.35E-01	-0.14	0.44	5.75E-01	-0.13	0.38	3.30E-01	-0.20	0.35	6.16E-01	-0.08	0.45	3153723	170561	3108714	353388	3128698	278798	3088730	416859
HILIC_POS_87_09232a3_031	HILIC	POS	3.031	87.0923				3.80E-03	0.45	1.30	5.75E-01	-0.12	0.79	3.29E-02	0.39	1.38	9.40E-03	0.51	1.45	2876984	569890	3297044	993723	3353195	1044885	3240893	947051
RP_POS_199_13075a13_943	RP	POS	13.94	199.1308				2.39E-01	0.24	0.57	5.75E-01	-0.11	0.50	4.20E-01	0.18	0.34	1.93E-01	0.30	0.70	22453238	9939232	24872537	10189187	25447754	10274161	24297320	10174683
HILIC_POS_157_09726a4_871	HILIC	POS	4.871	157.0973				5.30E-01	0.12	0.49	5.76E-01	0.12	0.57	3.81E-01	0.18	0.34	7.87E-01	0.06	0.14	2162162	909538	2282952	1032711	2224738	1174610	2341167	876426
RP_NEG_499_08923a8_858	RP	NEG	8.86	499.0892				7.02E-01	-0.07	0.52	5.76E-01	-0.12	0.34	5.60E-01	-0.13	0.65	9.59E-01	-0.01	0.28	983604	56683	978870	71502	982899	64027	974841	78720
RP_NEG_311_16937a10_556	RP	NEG	10.56	311.1694				2.25E-01	0.23	0.49	5.76E-01	0.12	0.41	1.95E-01	0.28	0.50	4.19E-01	0.17	0.56	6991018	4902196	8275774	5897764	7943604	5574798	8607944	6242881
RP_POS_294_24265a9_231	RP	POS	9.23	294.2427	Unknown	294.2417(25), 71.0859(100), 99.0803(85), 179.1436(85), 236.8788(80), 250.8921(60)	4	5.48E-01	-0.12	0.84	5.76E-01	0.11	0.80	7.97E-01	-0.06	0.55	3.91E-01	-0.18	0.97	1099273	974143	977602	1043338	918817	837888	1036387	1220744
RP_NEG_173_08138a5_102	RP	NEG	5.10	173.0814				5.22E-01	0.13	0.68	5.77E-01	0.11	0.61	4.18E-01	0.19	0.52	7.44E-01	0.07	0.55	1598085	285502	1635670	293196	1619187	283726	1652153	304348
RP_POS_163_03891a7_494	RP	POS	7.49	163.0389	Unknown	163.0379(100), 105.9346(55), 123.9451(40), 55.935(20)	4	3.42E-01	0.19	0.59	5.77E-01	0.11	0.99	2.76E-01	0.25	0.72	5.44E-01	0.14	0.54	1209459	116562	1232298	119444	1225584	117122	1239012	122537
RP_POS_375_28922a9_305	RP	POS	9.31	375.2892				2.29E-01	0.21	0.91	5.77E-01	-0.12	0.34	4.47E-01	0.15	0.58	2.03E-01	0.27	0.92	290903	224673	352112	310353	369549	329769	334675	291952
RP_NEG_394_97269a10_108	RP	NEG	10.11	394.9727				9.63E-02	0.28	0.77	5.77E-01	-0.12	0.39	2.38E-01	0.22	0.56	1.06E-01	0.34	0.86	1111679	697062	1378922	1000033	1435111	1093977	1322732	904054
RP_NEG_652_79449a0_499	RP	NEG	0.50	652.7945				2.05E-02	-0.33	1.12	5.77E-01	-0.12	1.24	2.05E-02	-0.39	1.16	1.71E-01	-0.26	1.15	1704524	408295	1424283	950133	1477658	1042141	1370909	855603
RP_POS_366_37207a12_166	RP	POS	12.17	366.3721				6.49E-01	-0.09	0.61	5.77E-01	-0.11	0.34	5.08E-01	-0.15	0.37	8.72E-01	-0.04	0.42	5340150	3224378	5040471	3206482	5220573	3320617	4860368	3111301
RP_NEG_297_24426a10_289	RP	NEG	10.29	297.2443				8.48E-01	0.04	0.56	5.77E-01	0.12	0.61	6.67E-01	0.09	0.58	9.24E-01	-0.02	0.49	1903439	319949	1916348	358622	1896207	354495	1936489	365171
RP_POS_515_31146a10_501	RP	POS	10.50	515.3115				5.55E-02	-0.42	0.78	5.77E-01	-0.11	1.16	4.54E-02	-0.47	1.03	1.28E-01	-0.37	0.68	1039505	363171	898682	319805	916638	332509	880725	308897
HILIC_POS_446_0531a3_076	HILIC	POS	3.076	446.0531				1.65E-02	0.32	1.20	5.77E-01	-0.13	0.93	1.18E-01	0.25	1.28	4.37E-02	0.38	1.34	1208941	72984	1270928	220202	1283289	238438	1258567	201998
RP_POS_487_36093a10_659	RP	POS	10.66	487.3609				2.61E-01	0.24	0.63	5.78E-01	0.11	0.42	1.98E-01	0.29	0.78	4.49E-01	0.18	0.49	45198061	3372786	45969470	3245835	45787545	3489638	46151396	3006789
RP_POS_199_01112a15_468	RP	POS	15.47	199.0111				7.23E-01	0.07	0.39	5.78E-01	0.12	0.35	5.57E-01	0.13	0.34	9.64E-01	0.01	0.27	8592059	3005462	8816778	3417260	8625514	3576901	9008041	3274870
HILIC_POS_387_21371a5_649	HILIC	POS	5.649	387.2137				1.74E-01	-0.26	1.06	5.79E-01	-0.11	0.78	1.49E-01	-0.32	0.79	3.40E-01	-0.21	0.80	1664000	331141	1568655	369893	1589323	361283	1547986	380837
RP_POS_153_00526a15_348	RP	POS	15.35	153.0053				4.74E-01	-0.15	0.31	5.79E-01	-0.11	0.39	6.79E-01	-0.10	0.35	3.72E-01	-0.21	0.47	7499742	2759101	7103625	2531540	6962297	2446301	7244954	2631165
RP_POS_280_88818a0_249	RP	POS	0.25	280.8882				9.44E-01	0.01	0.40	5.79E-01	-0.11	0.36	8.48E-01	-0.04	0.30	7.56E-01	0.07	0.17	806290	84436	807502	87949	812411	90348	802594	86117
RP_POS_263_23636a10_59	RP	POS	10.59	263.2364				1.60E-04	0.63	1.08	5.80E-01	-0.12	0.36	4.17E-03	0.57	0.99	4.02E-04	0.69	1.33	13996563	6486763	19981819	9831847	20530290	9518367	19433347	10202449
RP_POS_146_97417a15_439	RP	POS	15.44	146.9742				8.60E-01	-0.03	0.40	5.80E-01	-0.12	0.45	6.85E-01	-0.09	0.35	9.08E-01	0.02	0.39	6665600	1761642	6599928	2029981	6713062	1879003	6486795	2183797
HILIC_POS_184_09442a4_861	HILIC	POS	4.861	184.0944				8.92E-03	0.41	0.88	5.80E-01	-0.12	0.67	1.74E-02	0.47	0.79	6.04E-02	0.35	0.76	41411166	7916968	46705970	14046150	45923304	13513161	47488635	14654672
RP_POS_228_06311a4_896	RP	POS	4.90	228.0631				2.14E-02	0.33	0.69	5.80E-01	-0.12	0.44	1.26E-01	0.27	0.61	3.68E-02	0.39	0.74	1065592	361592	1299666	773219	1342732	803102	1256601	747782
RP_POS_666_82306a0_497	RP	POS	0.50	666.8231				1.10E-08	-0.69	1.38	5.80E-01	0.12	1.19	1.05E-04	-0.63	1.45	3.02E-05	-0.75	1.49	11571250	432372	8509257	4870118	8238142	5108459	8780372	4655510
RP_POS_375_21887a11_608	RP	POS	11.61	375.2189				9.56E-02	-0.32	0.82	5.81E-01	0.11	0.76	1.80E-01	-0.26	0.69	1.15E-01	-0.37	0.90	1875975	158683	1819070	185076	1808765	222332	1829374	139847
RP_POS_348_99115a8_122	RP	POS	8.12	348.9912				8.05E-01	-0.05	0.54	5.81E-01	-0.11	0.34	6.48E-01	-0.11	0.57	9.92E-01	0.00	0.61	1734422	523344	1708368	490625	1735651	485980	1681085	498641
HILIC_POS_144_86832a3_498	HILIC	POS	3.498	144.8683				9.72E-02	0.24	0.51	5.81E-01	-0.12	0.54	1.84E-01	0.18	0.50	1.73E-01	0.30	0.50	385521	531363	629370	1115112	691390	1423887	567351	690668
HILIC_POS_371_23972a5_785	HILIC	POS	5.785	371.2397				5.56E-01	-0.11	0.92	5.81E-01	-0.12	0.88	4.46E-01	-0.17	0.72	8.00E-01	-0.05	0.55	8030481	1712581	7814928	2021646	7927224	1914884	7702632	2136585
RP_POS_407_24023a10_377	RP	POS	10.38	407.2402				5.13E-08	0.65	1.29	5.81E-01	-0.12	1.09	5.99E-04	0.59	1.28	2.31E-05	0.71	1.48	111028	105758	1945281	3106033	2117759	3031737	1772804	3199942
RP_POS_478_38864a13_012	RP	POS	13.01	478.3886				3.68E-02	-0.47	1.03	5.81E-01	0.10	0.35	9.29E-02	-0.42	0.98	2.76E-02	-0.52	0.90	4772160	1032742	4338228	858968	4290524	769667	4385932	945346
RP_NEG_397_33371a11_345	RP	NEG	11.35	397.3337				6.06E-02	-0.34	0.84	5.81E-01	0.12	0.67	1.78E-01	-0.28	0.82	5.92E-02	-0.39	0.70	1642422	227166	1547160	296656	1530689	299321	1563630	296073
RP_POS_419_35181a15_099	RP	POS	15.10	419.3518				9.82E-01	0.00	0.57	5.82E-01	0.11	0.48	8.02E-01	0.06	0.38	8.39E-01	-0.05	0.56	28669739	4207242	28688491	3742512	28480814	3928275	28896168	3574811
RP_NEG_934_77313a0_494	RP	NEG	0.49	934.7731				2.45E-09	-0.74	1.40	5.82E-01	0.12	1.17	5.80E-05	-0.68	1.46	7.13E-06	-0.80	1.53	1540347	118628	1106741	637303	1071386	650517	1142097	628392
RP_POS_422_88062a0_513	RP	POS	0.51	422.8806				1.87E-06	0.58	1.28	5.82E-01	-0.12	1.12	1.48E-03	0.52	1.26	3.25E-04	0.64	1.40	115228	41854	257569	273045	272716	284603	242422	262986
RP_NEG_402_16299a11_611	RP	NEG	11.61	402.1630				3.92E-02	-0.39	0.78	5.82E-01	0.11	0.57	1.03E-01	-0.33	0.73	4.87E-02	-0.44	0.75	3403792	338328	3251320	407363	3228720	451013	3273920	361690
RP_POS_536_36597a11_821	RP	POS	11.82	536.3660				3.35E-01	-0.17	0.46	5.82E-01	-0.12	0.73	5.99E-01	-0.11	0.28	2.69E-01	-0.22	0.72	677630	53041	665973	75212	661804	75686	670143	75268
RP_POS_540_3656a10_589	RP	POS	10.59	540.3656				3.69E-01	0.16	1.03	5.82E-01	-0.12	0.54	6.44E-01	0.10	0.74	2.58E-01	0.22	1.40	989355	362492	1061384	471750	1087538	406988	1035230	531603
RP_NEG_328_75708a0_521	RP	NEG	0.52	328.7571				1.10E-05	0.54	1.27	5.83E-01	-0.12	1.16	2.48E-03	0.48	1.29	1.05E-03	0.60	1.38	500560	86870	727362	469032	753315	504273	701409	434518
RP_POS_363_25272a11_149	RP	POS	11.15	363.2527				9.22E-01	-0.02	0.60	5.83E-01	-0.12	0.73	6.99E-01	-0.08	0.51	8.45E-01	0.04	0.66	2236029	77547	2234337	105482	2240172	113919	2228501	97125
HILIC_NEG_99_9257a5_424	HILIC	NEG	5.424	99.9257				2.27E-01	-0.26	0.83	5.83E-01	0.11	0.42	3.77E-01	-0.21	0.35	1.84E-01	-0.32	0.85	4156026	821422	3957174	725630	3917040	724383	3997308	731987
RP_POS_272_94431a0_469	RP	POS	0.47	272.9443				4.50E-04	-0.60	1.10	5.83E-01	-0.11	0.99	1.28E-03	-0.66	1.18	5.55E-03	-0.55	1.15	570335	100573	486240	144475	494230	140775	478249	149077
HILIC_NEG_283_70966a1_362	HILIC	NEG	1.362	283.7097				1.88E-11	0.90	1.62	5.83E-01	-0.12	0.31	1.55E-05	0.84	1.47	3.24E-09	0.95	2.16	627668	82836	836957	243727	850433	208018	823481	276363
RP_NEG_308_99936a7_015	RP	NEG	7.02	308.9994				1.14E-01	0.35	0.54	5.83E-01	-0.11	0.39	2.17E-01	0.29	0.49	9.66E-02	0.40	0.66	4805170	2425411	5577887	2150962	5696664	2183214	5459110	2133654
RP_POS_381_29709a11_171	RP	POS	11.17	381.2971				4.63E-01	0.12	0.42	5.84E-01	0.12	0.46	3.91E-01	0.18	0.53	7.51E-01	0.06	0.45	1036952	775469	1175915	1291326	1104652	1152464	1247178	1424971
HILIC_POS_302_19629a1_251	HILIC	POS	1.251	302.1963				8.87E-03	-0.59	1.00	5.84E-01	0.10	0.44	2.19E-02	-0.54	0.93	1.04E-02	-0.64	1.00	1452643	693892	1080874	588218	1048419	645756	1113329	529066
RP_POS_497_3959a11_161	RP	POS	11.16	497.3959				3.01E-01	-0.19	0.57	5.84E-01	0.11	0.51	4.99E-01	-0.14	0.45	2.68E-01	-0.25	0.52	3571222	521585	3455237	621217	3420960	693668	3489514	544172
RP_POS_666_33282a5_684	RP	POS	5.68	666.3328				8.38E-01	0.04	0.66	5.85E-01	0.11	0.50	6.19E-01	0.10	0.61	9.42E-01	-0.02	0.45	2438446	1194261	2490083	1352871	2415591	1651402	2564574	979500
RP_POS_407_75516a13_72	RP	POS	13.72	407.7552				5.08E-09	1.07	1.70	5.85E-01	0.10	0.44	1.60E-07	1.12	1.74	1.45E-07	1.02	1.77	13386265	3016294	17809433	3871477	17596421	3450120	18022444	4276287
HILIC_POS_188_12817a0_549	HILIC	POS	0.549	188.1282				4.17E-01	-0.19	0.59	5.85E-01	-0.10	0.60	3.51E-01	-0.24	0.57	5.77E-01	-0.13	0.37	1612557	1155986	1428765	929530	1479897	843065	1377633	1014687
HILIC_NEG_84_9902a4_234	HILIC	NEG	4.234	84.9902				2.39E-01	-0.23	0.82	5.85E-01	0.11	0.77	4.33E-01	-0.17	0.31	1.99E-01	-0.28	0.74	1506168	397468	1406552	454494	1381567	464681	1431537	447373
RP_POS_406_32831a11_061	RP	POS	11.06	406.3283				9.79E-01	0.00	0.86	5.85E-01	0.12	0.82	7.79E-01	0.06	0.62	7.35E-01	-0.06	0.82	3564864	309584	3562905	512428	3534751	494570	3591059	533203
RP_NEG_402_14639a11_253	RP	NEG	11.25	402.1464				8.49E-07	0.94	1.85	5.86E-01	0.10	1.20	6.62E-06	0.99	1.78	1.18E-05	0.88	1.77	428739	279842	755270	332513	737010	301545	773531	363011
HILIC_NEG_197_80797a4_081	HILIC	NEG	4.081	197.8080				5.27E-01	0.10	0.33	5.86E-01	0.12	0.87	3.85E-01	0.16	0.30	8.29E-01	0.04	0.61	413887	415662	476204	648870	440584	700059	511823	598319
HILIC_POS_74_09716a4_186	HILIC	POS	4.186	74.0972				9.88E-02	0.31	0.53	5.86E-01	0.11	0.60	1.06E-01	0.37	0.58	2.11E-01	0.25	0.55	7419324	3175911	8556680	3811610	8347489	3347452	8765870	4249530
RP_POS_397_23096a11_609	RP	POS	11.61	397.2310				4.95E-01	-0.13	0.54	5.86E-01	0.11	0.59	7.19E-01	-0.08	0.42	4.10E-01	-0.19	0.64	2029740	359664	1977930	404732	1955730	444044	2000129	364387
RP_NEG_207_96751a15_449	RP	NEG	15.45	207.9675				7.40E-01	-0.07	0.37	5.86E-01	-0.11	0.46	5.81E-01	-0.12	0.32	9.52E-01	-0.01	0.36	8831198	297610	8811128	290492	8827058	313653	8795199	267578
RP_NEG_620_84607a0_497	RP	NEG	0.50	620.8461				5.63E-08	-0.66	1.35	5.86E-01	0.12	1.20	2.02E-04	-0.60	1.42	6.43E-05	-0.72	1.46	13433106	827876	10139333	5464075	9839835	5753371	10438831	5199732
RP_POS_247_2415a10_848	RP	POS	10.85	247.2415				1.50E-08	0.88	1.37	5.86E-01	-0.11	0.55	2.85E-05	0.82	1.35	2.23E-07	0.93	1.65	2631168	814379	3904857	1473745	3985623	1349034	3824090	1598426
RP_POS_302_24524a11_252	RP	POS	11.25	302.2452				1.41E-08	0.91	1.41	5.86E-01	-0.11	0.59	1.75E-05	0.86	1.38	1.25E-07	0.97	1.65	1751283	870280	3070767	1446009	3149990	1311492	2991543	1578524
RP_NEG_287_70569a15_59	RP	NEG	15.59	287.7057				4.11E-01	-0.15	0.60	5.86E-01	-0.11	0.36	2.93E-01	-0.21	0.53	6.74E-01	-0.09	0.19	2436119	84759	2421020	103745	2426703	116965	2415336	89438
HILIC_POS_371_23972a5_921	HILIC	POS	5.921	371.2397				8.03E-01	-0.05	0.83	5.87E-01	0.11	0.78	9.68E-01	0.01	0.47	6.26E-01	-0.10	0.72	7339882	1823071	7243586	2091572	7129092	2018566	7358079	2176526
RP_NEG_520_91077a0_492	RP	NEG	0.49	520.9108				1.99E-07	0.62	1.34	5.87E-01	-0.12	1.21	3.07E-04	0.56	1.41	1.90E-04	0.68	1.44	13551579	1769262	25704305	21571129	26882881	23277859	24525729	19885421
RP_NEG_395_22052a10_907	RP	NEG	10.91	395.2205				1.74E-03	0.45	1.52	5.87E-01	0.12	0.72	1.02E-02	0.51	1.22	1.86E-02	0.39	1.37	3651303	1409692	4928005	3104852	4758354	2738189	5097657	3452613
HILIC_POS_176_12822a4_238	HILIC	POS	4.238	176.1282				2.17E-02	0.39	0.61	5.88E-01	0.12	1.10	3.15E-02	0.45	0.75	8.54E-02	0.33	0.59	5040916	7287771	8960489	10658023	8378603	10025429	9542375	11327175
RP_POS_842_56537a13_287	RP	POS	13.29	842.5654				1.26E-08	-1.37	2.59	5.88E-01	-0.08	0.55	1.13E-08	-1.41	2.41	4.75E-08	-1.33	2.23	1011145	503429	333407	364333	353278	366794	313536	364477
HILIC_POS_175_1189a6_962	HILIC	POS	6.962	175.1189				5.51E-02	0.25	1.10	5.88E-01	-0.12	0.80	2.69E-01	0.19	1.03	7.65E-02	0.31	1.18	26703129	8000501	32128600	24208206	33448651	24529786	30808549	24057595

Supplementary table 1: Metabolomics results (in asceding order according to p-value from progressive ALD vs non-progressive ALD comparison, with molecular features with ID_level of 1-2 first)

							all_ALD_vs_control			Prog_ALD_vs_non-prog_ALD			Prog_ALD_vs_control_ALD			Non-prog_ALD_vs_control			Healthy_control		all_ALD		Non-prog_ALD		Progressive_ALD	
							t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA								
Feature_ID	RP_HILIC	POS_NEG	Average.Rt	Average.Mz	Metabolite.name	curated_MSMS	ID_level	p	d	VIP	p	d	VIP	p	d	VIP	p	d	VIP	Mean	SD	Mean	SD	Mean	SD	Mean	SD
RP_NEG_873_56793a13_746	RP	NEG	13.75	873.5679				8.04E-01	0.05	0.48	5.88E-01	0.11	0.38	6.48E-01	0.11	0.43	9.87E-01	0.00	0.53	3945867	1545194	4023969	1537510	3940145	1502817	4107793	1582188
RP_POS_609_41461a13_499	RP	POS	13.50	609.4146				8.08E-01	0.04	0.25	5.88E-01	0.12	0.36	6.62E-01	0.10	0.26	9.01E-01	-0.02	0.19	13563357	2259044	13694512	3624942	13496714	2531100	13892310	4479092
RP_POS_198_05247a5_353	RP	POS	5.35	198.0525				5.98E-01	-0.11	0.38	5.88E-01	0.11	0.51	8.14E-01	-0.06	0.40	4.57E-01	-0.17	0.63	2507312	1225451	2377166	1155161	2314183	992295	2440148	1305098
RP_NEG_787_10187a9_549	RP	NEG	9.55	787.1019				3.27E-01	-0.21	0.53	5.88E-01	0.11	0.39	4.97E-01	-0.16	0.37	2.73E-01	-0.26	0.61	4528675	544336	4421214	501369	4393883	529817	4448544	475017
HILIC_POS_394_31534a7_72	HILIC	POS	7.72	394.3153				1.41E-01	0.26	0.66	5.89E-01	0.11	0.60	1.37E-01	0.32	0.59	3.02E-01	0.21	0.56	4053552	757978	4301863	992094	4247855	922686	4355870	1063620
RP_POS_223_09409a10_573	RP	POS	10.57	223.0941				4.94E-03	-0.55	1.28	5.89E-01	-0.11	0.56	9.13E-03	-0.60	1.18	1.62E-02	-0.49	1.01	8508296	1662367	7492250	1856459	7593164	1595150	7391336	2097124
RP_POS_326_90259a15_377	RP	POS	15.38	326.9026				9.77E-01	-0.01	0.23	5.89E-01	0.09	0.36	9.01E-01	0.04	0.13	8.57E-01	-0.05	0.37	1593448	143739	1592685	78183	1588437	76731	1596933	80159
RP_POS_539_41333a10_453	RP	POS	10.45	539.4133				8.18E-01	-0.04	0.38	5.90E-01	-0.12	0.63	5.82E-01	-0.10	0.39	9.39E-01	0.02	0.59	1881371	184152	1871873	250628	1885492	303861	1858255	184934
RP_POS_840_84283a0_494	RP	POS	0.49	840.8428				4.44E-08	0.66	1.34	5.90E-01	-0.12	1.17	1.55E-04	0.60	1.40	8.22E-05	0.72	1.44	65057	49991	419899	593851	452123	635140	387676	554069
RP_POS_513_84259a14_974	RP	POS	14.97	513.8426				5.44E-01	-0.13	0.35	5.90E-01	0.11	0.39	7.52E-01	-0.07	0.67	4.30E-01	-0.18	0.32	220253	206511	194951	194662	184390	187828	205512	202616
RP_POS_621_43829a11_254	RP	POS	11.25	621.4383				3.62E-01	0.17	0.97	5.91E-01	0.11	0.75	3.16E-01	0.23	0.87	5.64E-01	0.12	1.02	748760	304954	807754	349203	788831	305796	826677	390042
RP_POS_491_79153a6_487	RP	POS	6.49	491.7915				9.68E-08	0.64	1.33	5.91E-01	-0.12	1.17	3.58E-04	0.58	1.41	9.10E-05	0.70	1.43	10032	6432	282997	474152	308681	495125	257313	455777
RP_POS_235_99771a1_711	RP	POS	1.71	235.9977				1.96E-11	0.87	1.42	5.91E-01	0.11	0.40	5.41E-06	0.93	1.41	1.54E-08	0.82	1.67	1484441	554547	3037901	1871667	2936504	1442789	3139299	2230503
RP_POS_830_56561a13_37	RP	POS	13.37	830.5656				2.24E-02	0.46	1.05	5.91E-01	-0.11	0.39	7.03E-02	0.41	0.77	2.14E-02	0.52	1.02	17187292	6402812	20270952	6629987	20629735	6539858	19912170	6765950
RP_POS_329_26761a9_889	RP	POS	9.89	329.2676				7.88E-01	-0.06	0.51	5.91E-01	0.11	0.35	9.88E-01	0.00	0.18	6.42E-01	-0.11	0.58	779023	146179	771100	137744	763647	143680	778553	132577
HILIC_POS_606_36926a1_017	HILIC	POS	1.017	606.3693				5.46E-06	0.55	1.23	5.91E-01	-0.12	0.77	1.66E-03	0.49	1.42	8.82E-04	0.61	1.36	316899	938227	3478405	6405940	3824959	6928480	3131852	5887331
RP_POS_312_15933a9_128	RP	POS	9.13	312.1593				1.65E-01	0.24	0.55	5.92E-01	-0.12	0.38	3.12E-01	0.18	0.66	1.89E-01	0.29	0.59	681543	1073363	1025518	1553701	1109520	1845904	941516	1206432
RP_POS_170_02113a3_945	RP	POS	3.95	170.0211				1.38E-02	-0.63	1.14	5.92E-01	0.09	0.71	3.31E-02	-0.59	0.85	9.72E-03	-0.68	1.35	2442502	1900681	1521818	1213244	1456275	989874	1587361	1409023
RP_POS_764_83142a0_472	RP	POS	0.47	764.8314				3.72E-09	-0.78	1.40	5.92E-01	0.11	1.12	4.09E-05	-0.72	1.46	2.71E-06	-0.84	1.54	501624	71076	344103	214903	332515	214675	355691	216678
HILIC_NEG_199_80495a0_552	HILIC	NEG	0.552	199.8050				5.19E-01	0.13	0.43	5.92E-01	-0.11	0.68	7.23E-01	0.08	0.14	4.35E-01	0.19	0.62	832676	377707	882626	383672	903314	425935	861937	339292
RP_POS_457_2706a15_421	RP	POS	15.42	457.2706				3.48E-02	0.40	1.02	5.92E-01	0.11	0.39	4.07E-02	0.46	0.84	9.65E-02	0.35	1.16	2922001	1099370	3424782	1281955	3355668	1193913	3493896	1373018
RP_POS_559_51898a10_589	RP	POS	10.59	559.5190				8.96E-04	0.56	0.91	5.92E-01	-0.11	0.45	1.54E-02	0.50	0.86	1.24E-03	0.61	1.15	4407983	3760631	7427097	5685866	7733561	5214479	7120632	6159176
RP_NEG_326_98917a7_73	RP	NEG	7.73	326.9892				1.96E-01	-0.22	0.55	5.93E-01	-0.12	0.36	1.53E-01	-0.28	0.69	4.39E-01	-0.16	0.43	7004525	1493678	6557326	2190101	6675361	2337356	6439292	2049221
RP_NEG_297_24445a10_802	RP	NEG	10.80	297.2445				5.12E-01	-0.12	0.79	5.93E-01	0.11	0.83	7.64E-01	-0.06	0.66	4.09E-01	-0.18	0.81	5475935	695266	5376496	876832	5329285	898587	5423707	861019
RP_POS_796_54559a11_628	RP	POS	11.63	796.5456				4.18E-01	0.13	0.45	5.93E-01	-0.12	0.53	7.15E-01	0.07	0.33	3.55E-01	0.18	0.58	5896671	8297575	7599254	14923870	8401840	15947977	6796667	13940465
RP_POS_132_95819a0_253	RP	POS	0.25	132.9582				4.59E-01	0.16	0.46	5.94E-01	-0.11	0.56	6.56E-01	0.10	0.29	3.72E-01	0.21	0.37	74694239	7577325	75825763	7139470	76209483	7238250	75442043	7091654
RP_POS_199_98743a11_166	RP	POS	11.17	199.9874				4.51E-11	0.97	1.61	5.94E-01	-0.11	0.85	4.06E-06	0.91	1.53	1.46E-09	1.02	1.87	316953	117161	551010	244211	564126	208964	537894	276546
RP_POS_456_77225a6_222	RP	POS	6.22	456.7723				2.30E-07	0.62	1.31	5.94E-01	-0.12	1.14	3.64E-04	0.56	1.42	2.06E-04	0.68	1.38	8860	7204	294888	514459	322513	552901	267263	476950
RP_POS_299_63199a10_302	RP	POS	10.30	299.6320				4.59E-02	0.46	0.82	5.94E-01	-0.10	0.75	1.09E-01	0.41	0.63	3.41E-02	0.51	0.84	500182	178355	571450	145260	579243	127224	563656	162238
RP_POS_214_18015a10_278	RP	POS	10.28	214.1802				1.31E-01	0.28	0.68	5.94E-01	-0.11	0.47	3.37E-01	0.22	0.53	8.21E-02	0.33	0.70	445125	317039	550377	398811	571765	316528	528990	469279
HILIC_NEG_157_96739a0_7	HILIC	NEG	0.7	157.9674				2.84E-06	0.82	1.43	5.95E-01	-0.11	0.87	1.84E-05	0.87	1.67	1.19E-04	0.76	1.36	63277	44443	114118	62094	110793	61621	117443	63010
RP_NEG_500_27875a10_323	RP	NEG	10.32	500.2788				3.83E-08	0.94	1.66	5.96E-01	-0.11	0.54	2.98E-05	0.89	1.45	5.17E-08	0.99	1.84	20599978	5827792	28778251	8550104	29235431	6959608	28321071	9941720
RP_POS_810_7843a0_496	RP	POS	0.50	810.7843				4.62E-09	-0.72	1.39	5.96E-01	0.12	1.18	7.83E-05	-0.66	1.46	1.23E-05	-0.78	1.51	1971551	124236	1456548	780603	1414835	800462	1498261	766046
RP_NEG_270_9043a15_623	RP	NEG	15.62	270.9043				3.28E-01	-0.21	0.96	5.96E-01	-0.10	0.38	2.69E-01	-0.26	0.58	4.98E-01	-0.16	0.65	904391	42924	895994	38297	898039	38208	893948	38663
RP_POS_497_39651a11_607	RP	POS	11.61	497.3965				1.30E-01	-0.30	0.70	5.97E-01	0.11	0.37	2.51E-01	-0.24	0.54	1.27E-01	-0.35	0.61	7740263	1363592	7304255	1496259	7224544	1636212	7383967	1353925
RP_POS_826_75793a0_498	RP	POS	0.50	826.7579				5.88E-02	-0.29	1.08	5.97E-01	-0.12	1.17	5.50E-02	-0.35	1.02	2.44E-01	-0.23	1.09	896914	177065	809677	332182	827349	355234	792005	310022
RP_POS_406_164a4_143	RP	POS	4.14	406.1640				7.35E-05	0.69	1.09	5.97E-01	0.11	0.46	5.64E-05	0.74	1.49	3.58E-03	0.64	1.01	5305838	2072826	7272405	2910258	7117587	3390390	7427222	2359745
RP_POS_487_2988a6_325	RP	POS	6.33	487.2988				2.42E-06	0.57	1.29	5.98E-01	-0.12	1.14	1.25E-03	0.51	1.38	5.63E-04	0.63	1.36	57341	109910	525307	918953	574154	983400	476460	856876
RP_POS_721_50757a10_864	RP	POS	10.86	721.5076				2.15E-01	-0.22	0.54	5.98E-01	0.11	0.65	4.73E-01	-0.16	0.47	1.37E-01	-0.27	0.64	5168901	494071	5031472	667066	4996022	527169	5066921	786488
RP_POS_172_77734a10_583	RP	POS	10.58	172.7773				2.32E-03	0.56	0.90	5.98E-01	-0.11	0.43	1.64E-02	0.51	0.86	3.31E-03	0.61	1.11	585977	280816	778766	350967	797394	345865	760139	358523
RP_POS_548_50397a13_291	RP	POS	13.29	548.5040				6.11E-04	0.65	1.13	5.99E-01	-0.11	0.46	2.86E-03	0.60	1.13	1.80E-03	0.71	1.25	2101259	1075004	2924319	1251944	2990711	1406304	2857926	1086291
RP_POS_355_65216a5_683	RP	POS	5.68	355.6522				8.50E-01	0.04	0.68	5.99E-01	0.11	0.48	6.41E-01	0.09	0.62	9.39E-01	-0.02	0.46	2434725	1149779	2480649	1302901	2411549	1574742	2549750	969634
RP_POS_293_03442a5_353	RP	POS	5.35	293.0344				6.78E-01	-0.09	0.35	5.99E-01	0.10	0.52	8.77E-01	-0.04	0.38	5.33E-01	-0.14	0.60	564355	323881	537586	289007	522269	247528	552902	327117
RP_POS_501_94785a6_786	RP	POS	6.79	501.9479				1.37E-07	0.63	1.33	5.99E-01	-0.12	1.17	3.59E-04	0.57	1.45	1.28E-04	0.69	1.41	10848	14432	1058558	1845199	1156308	1947257	960808	1751483
HILIC_POS_147_14914a5_424	HILIC	POS	5.424	147.1491				1.05E-02	0.48	0.99	5.99E-01	0.11	0.54	1.73E-02	0.53	0.92	3.59E-02	0.42	0.96	57882396	20403124	69423765	24811771	68109252	22199938	70738279	27339496
RP_POS_412_84506a0_499	RP	POS	0.50	412.8451				6.53E-03	-0.37	1.15	5.99E-01	-0.12	1.23	1.06E-02	-0.43	1.19	9.75E-02	-0.31	1.20	1722720	305323	1453623	809498	1496499	871772	1410747	748470
RP_POS_752_04541a12_764	RP	POS	12.76	752.0454				3.66E-02	0.41	0.70	5.99E-01	0.11	0.33	3.81E-02	0.46	0.81	1.01E-01	0.36	0.66	902369	442004	1099291	485164	1073613	473508	1124969	500017
RP_POS_130_06499a4_897	RP	POS	4.90	130.0650				1.26E-01	0.23	0.60	5.99E-01	-0.12	0.43	3.45E-01	0.18	0.48	1.28E-01	0.29	0.59	1222512	311207	1345301	574685	1375696	586497	1314906	566922
RP_POS_765_53284a10_863	RP	POS	10.86	765.5328				1.66E-03	-0.62	0.98	6.00E-01	0.10	0.37	1.14E-02	-0.57	0.89	1.67E-03	-0.67	1.07	3068932	439432	2767860	476149	2742686	439802	2793035	513170
RP_POS_564_43835a11_638	RP	POS	11.64	564.4384				6.58E-05	-1.05	1.75	6.00E-01	-0.08	0.63	5.62E-05	-1.09	1.66	1.79E-04	-1.01	1.56	875530	509682	449718	303324	465738	316058	433698	292357
RP_POS_446_28693a10_457	RP	POS	10.46	446.2869				1.75E-01	-0.30	0.60	6.00E-01	0.10	0.36	2.81E-01	-0.25	0.46	1.60E-01	-0.35	0.62	937401	217670	878380	187981	868457	208312	888304	166734
RP_POS_776_55725a14_095	RP	POS	14.10	776.5573				1.64E-02	-0.51	1.17	6.00E-01	-0.10	0.32	2.11E-02	-0.57	1.05	3.70E-02	-0.46	0.91	2019683	1008365	1520115	930759	1569244	795095	1470986	1055084
RP_POS_441_29727a10_854	RP	POS	10.85	441.2973				5.65E-01	-0.11	0.78	6.01E-01	0.11	0.77	8.01E-01	-0.06	0.60	4.43E-01	-0.16	0.79	3420967	1500264	3238608	1705530	3148677	1644589	3328538	1776472
RP_POS_362_30292a11_128	RP	POS	11.13	362.3029				1.43E-02	0.39	0.88	6.01E-01	-0.11	0.40	5.66E-02	0.34	0.75	3.25E-02	0.45	0.84	295128	359714	513087	596385	544536	673934	481639	512253
HILIC_POS_490_29001a1_416	HILIC	POS	1.416	490.2900				5.38E-06	0.67	1.03	6.01E-01	-0.11	0.33	1.02E-03	0.61	1.05	7.15E-05	0.73	1.32	321566	126337	485626	260117	499318	254135	471935	267836
RP_POS_283_26297a10_648	RP	POS	10.65	283.2630				8.29E-04	-0.57	1.04	6.01E-01	0.11	0.71	7.32E-03	-0.52	1.06	2.56E-03	-0.63	1.05	5979848	656402	5458669	944858	5408935	1003372	5508403	889903
HILIC_NEG_134_89473a4_671	HILIC	NEG	4.671	134.8947				4.19E-01	0.17	0.53	6.01E-01	0.10	0.74	3.66E-01	0.22	0.78	5.93E-01	0.12	0.25	23673825	8660682	25099334	8434405	24655579	7059201	25543089	9669333
RP_POS_489_77646a6_325	RP	POS	6.33	489.7765				2.85E-07	0.61	1.31	6.02E-01	-0.12	1.15	5.10E-04	0.55	1.41	1.87E-04	0.67	1.40	39205	73037	1090821	1905621	1190967	2013727	990675	1805914
RP_POS_982_79895a0_494	RP	POS	0.49	982.7990				5.46E-08	0.65	1.33	6.02E-01	-0.12	1.13	2.33E-04	0.59	1.40	7.67E-05	0.71	1.44	55565	37662	725054	1136396	784758	1193756	665350	1084813
RP_POS_198_86171a0_521	RP	POS	0.52	198.8617				1.95E-05	0.53	1.24	6.02E-01	-0.12	1.13	3.08E-03	0.47	1.24	1.42E-03	0.59	1.35	342690	64578	491839	315315	508402	339049	475275	292167
RP_NEG_157_08632a7_16	RP	NEG	7.16	157.0863				2.71E-02	-0.57	0.96	6.02E-01	-0.09	0.33	2.18E-02	-0.62	0.97	5.30E-02	-0.53	0.84	2856616	2092604	1954909	1313225	2023872	1405712	1885946	1224166
RP_POS_301_21347a10_73	RP	POS	10.73	301.2135				3.71E-03	0.46	1.31	6.02E-01	-0.11	1.08	2.29E-02	0.41	1.14	1.18E-02	0.52	1.29	5945185	2807265	7976949	4670920	8222148	5161415	7731751	4161411
RP_POS_342_85999a0_499	RP	POS	0.50	342.8600				6.03E-03	-0.37	1.17	6.02E-01	-0.12	1.25	1.13E-02	-0.42	1.22	9.52E-02	-0.31	1.21	4156491	770815	3436117	2190842	3551039	2336896	3321196	2051705
RP_POS_553_45856a12_131	RP	POS	12.13	553.4586				4.89E-01	0.13	0.64	6.03E-01	-0.11	0.34	7.11E-01	0.08	0.55	3.97E-01	0.19	0.53	12034239	5153059	12781988	5689688	13080313	5814754	12483663	5604708
RP_POS_321_3158a11_668	RP	POS	11.67	321.3158				9.41E-01	-0.01	0.68	6.03E-01	-0.11	0.31	7.63E-01	-0.07	0.38	8.66E-01	0.04	0.44	1373520	807212	1361240	835492	1405038	845917	1317441	831173
RP_POS_514_26715a6_421	RP	POS	6.42	514.2672				1.09E-06	0.58	1.29	6.03E-01	-0.12	1.14	8.82E-04	0.52	1.39	4.15E-04	0.64	1.37	50445	37192	447562	762216	487438	814610	407686	712018
RP_POS_270_2063a7_55	RP	POS	7.55	270.2063				7.03E-06	0.53	1.16	6.04E-01	-0.12	1.01	3.05E-03	0.47	1.20	8.39E-04	0.59	1.24	36433	20858	394955	754902	434409	790458	355500	723453
RP_POS_615_33655a14_265	RP	POS	14.27	615.3366				4.22E-01	0.18	0.79	6.04E-01	-0.10	0.31	5.97E-01	0.13	0.38	3.42E-01	0.23	0.91	11815813	2872649	12271432	2424792	12398020	2359035	12144843	2506287
RP_NEG_720_78223a0_499	RP	NEG	0.50	720.7822				1.23E-02	-0.34	1.14	6.05E-01	-0.12	1.25	1.64E-02	-0.40	1.17	1.33E-01	-0.28	1.18	2087241	446425	1732664	1151844	1792739	1249173	1672590	1054878
RP_NEG_383_19125a11_612	RP	NEG	11.61	383.1913				8.66E-02	-0.29	0.85	6.05E-01	-0.11	0.81	8.90E-02	-0.34	0.74	2.43E-01	-0.23	0.75	23305066	1662934	22633578	2517047	22764806	2492957	22502350	2559369
RP_POS_704_86676a0_495	RP	POS	0.50	704.8668				8.03E-08	0.65	1.34	6.05E-01	-0.11	1.19	1.77E-04	0.59	1.41	1.25E-04	0.70	1.45	145209	62366	532930	662321	567439	713700	498420	611958
RP_POS_211_16925a11_038	RP	POS	11.04	211.1693				1.32E-02	0.39	0.79	6.05E-01	-0.11	0.35	5.59E-02	0.34	0.70	3.03E-02	0.45	0.77	484715	536579	815379	900663	862308	1007338	768449	787222
HILIC_POS_265_11816a1_903	HILIC	POS	1.903	265.1182				2.54E-01	-0.21	0.36	6.05E-01	0.11	0.61	5.29E-01	-0.15	0.24	1.28E-01	-0.26	0.81	7112752	5311000	5786036	6681329	5437458	3814962	6134615	8682709
RP_POS_496_26852a9_952	RP	POS	9.95	496.2685				2.60E-04	0.49	0.96	6.05E-01	-0.11	0.34	1.10E-02	0.44	0.96	2.67E-03	0.55	0.97	197551	113030	334567	305000	350455	316357	318680	295553
RP_POS_354_28528a9_039	RP	POS	9.04	354.2853				5.45E-02	-0.38	0.93	6.05E-01	0.10	0.96	1.26E-01	-0.33	1.03	5.71E-02	-0.44	0.79	1058843	55443	1036409	58590	1033358	62335	1039460	55054
RP_NEG_159_10202a7_085	RP	NEG	7.09	159.1020				2.07E-02	-0.73	1.53	6.05E-01	0.06	0.31	2.75E-02	-0.70	1.24	1.84E-02	-0.76	1.17	1601622	1361355	1006437	466521	982163	505391	1030711	427904
HILIC_POS_143_08165a5_339	HILIC	POS	5.339	143.0817				9.09E-01	-0.03	0.37	6.06E-01	-0.09	0.55	7.68E-01	-0.07	0.14	9.53E-01	0.02	0.51	2065161	3580388	1987687	2354765	2110194	2922693	1865181	1621801
HILIC_POS_508_33984a1_286	HILIC	POS	1.286	508.3398				1.03E-05	0.71	1.15	6.06E-01	0.11	0.64	2.19E-04	0.77	1.25	2.26E-04	0.66	1.35	1581778	470294	2113629	773961	2073430	680850	2153828	862208
RP_POS_793_62677a11_038	RP	POS	11.04	793.6268				1.15E-03	0.42	0.96	6.06E-01	-0.12	0.35	7.89E-03	0.37	0.95	1.88E-02	0.48	0.86	915496	1240069	2413733	3935900	2618248	4735204	2209218	2965003
RP_POS_478_29263a10_337	RP	POS	10.34	478.2926				1.48E-02	0.45	1.10	6.06E-01	-0.11	0.61	8.18E-02	0.39	0.91	9.69E-03	0.50	1.15	57548987	20008618	68396081	24968439	69692494	20352992	67099668	29015420
RP_POS_440_27701a9_247	RP	POS	9.25	440.2770				4.87E-01	0.11	0.58	6.06E-01	0.11	0.73	4.63E-01	0.17	0.46	7.24E-01	0.05	0.32	532320	604313	635360	1018219	582455	654327	688265	1288736
RP_POS_244_19102a7_716	RP	POS	7.72	244.1910				7.77E-01	-0.06	0.45	6.07E-01	0.10	0.33	9.59E-01	-0.01	0.35	6.25E-01	-0.11	0.36	4214896	790111	4170589	678864	4135377	578992	4205802	770296
RP_NEG_293_17679a8_346	RP	NEG	8.35	293.1768				1.32E-01	0.24	0.73	6.07E-01	-0.11	0.47	3.21E-01	0.18	0.58	1.47E-01	0.29	0.79	2008795	234632	2097012	406080	2118069	438593	2075956	374029
HILIC_POS_116_07094a4_87	HILIC	POS	4.87	116.0709				5.07E-01	0.13	0.45	6.07E-01	0.11	0.52	3.68E-01	0.18	0.37	7.53E-01	0.07	0.14	379179022	187232457	405424864	212704227	394392676	248136515	416457052	172015664
RP_POS_120_94345a0_251	RP	POS	0.25	120.9435				6.40E-01	0.10	0.38	6.07E-01	0.10	0.45	5.21E-01	0.15	0.47	8.25E-01	0.05	0.35	1166894	277492	1192565	237163	1180270	247085	1204861	228651
RP_NEG_369_30145a10_991	RP	NEG	10.99	369.3015	FA 22:1;2O	369.2983(100), 307.2993(60), 351.2933(25)	3	5.20E-02	-0.39	0.77	6.07E-01	0.10	0.46	1.23E-01	-0.34	0.71	5.22E-02	-0.44	0.84	1645342	338486	1507626	349554	1489519	363424	1525733	337822
RP_POS_553_45874a13_104	RP	POS	13.10	553.4587				8.31E-01	-0.04	0.53	6.07E-01	0.10	0.38	9.78E-01	0.01	0.54	6.73E-01	-0.10	0.38	2868308	634297	2840989	604238	2809695	570737	2872284	640249
RP_POS_130_08649a0_611	RP	POS	0.61	130.0865				4.20E-01	-0.14	0.92	6.07E-01	-0.11	0.68	2.97E-01	-0.20	0.82	6.98E-01	-0.09	0.74	1094333	941865	923531	1290964	990328	1479660	856733	1081059

Supplementary table 1: Metabolomics results (in asceding order according to p-value from progressive ALD vs non-progressive ALD comparison, with molecular features with ID_level of 1-2 first)

								all_ALD_vs_control			Prog_ALD_vs_non-prog_ALD			Prog_ALD_vs_control_ALD			Non-prog_ALD_vs_control			Healthy_control		all_ALD		Non-prog_ALD		Progressive_ALD	
								t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA								
Feature_ID	RP_HILIC	POS_NEG	Average.Rt	Average.Mz	Metabolite.name	curated_MSMS	ID_level	p	d	VIP	p	d	VIP	p	d	VIP	p	d	VIP	Mean	SD	Mean	SD	Mean	SD	Mean	SD
RP_POS_569_36511a14_948	RP	POS	14.95	569.3651				2.79E-02	0.30	0.71	6.08E-01	0.12	0.32	9.81E-02	0.36	0.63	5.86E-02	0.24	0.65	17373309	1891997	18678974	4822613	18429279	3090985	18928668	6108062
RP_NEG_151_02534a0_71	RP	NEG	0.71	151.0253				4.62E-03	0.33	1.04	6.08E-01	0.12	0.59	2.90E-02	0.39	1.11	7.58E-02	0.27	0.94	244908	82217	2663192	8343172	2231871	7745452	3094514	8959125
RP_POS_199_08235a0_708	RP	POS	0.71	199.0824				1.35E-03	-0.73	1.33	6.08E-01	-0.09	0.34	1.58E-03	-0.77	1.41	4.55E-03	-0.68	1.21	760859	528806	407677	442547	430543	433346	384811	454793
RP_POS_566_88757a0_494	RP	POS	0.49	566.8876				1.23E-07	0.63	1.34	6.08E-01	-0.11	1.20	2.66E-04	0.58	1.41	1.41E-04	0.69	1.45	9134206	1328967	19764425	18540474	20722223	19795459	18806627	17343047
HILIC_POS_173_12871a4_25	HILIC	POS	4.25	173.1287				3.63E-01	0.15	0.96	6.08E-01	0.11	0.85	3.27E-01	0.21	0.52	6.01E-01	0.10	0.45	798350	249526	850867	368005	831862	326896	869872	407456
RP_POS_304_26038a10_973	RP	POS	10.97	304.2604				5.93E-03	0.34	0.66	6.08E-01	-0.12	0.44	6.19E-02	0.28	0.65	3.39E-02	0.40	0.70	19136723	9121301	31463683	40961585	33578745	45519135	29348621	36177667
RP_POS_509_31195a6_42	RP	POS	6.42	509.3120				4.47E-07	0.60	1.30	6.08E-01	-0.11	1.14	5.31E-04	0.54	1.40	2.75E-04	0.66	1.38	27760	24577	326936	552178	355439	590532	298432	515400
HILIC_NEG_134_89481a1_329	HILIC	NEG	1.329	134.8948				4.42E-06	-0.82	1.24	6.08E-01	0.10	0.60	2.63E-04	-0.77	1.23	9.80E-06	-0.87	1.53	15716542	1978632	13531160	2648338	13394448	2422745	13667872	2874490
RP_POS_278_24765a9_3	RP	POS	9.30	278.2477				7.01E-01	0.03	0.70	6.08E-01	-0.09	0.33	5.98E-01	-0.14	0.48	8.46E-01	-0.05	0.38	9543874	9451729	8852638	6292559	9177328	5980811	8527949	6634412
RP_POS_302_245a10_586	RP	POS	10.59	302.2450				1.10E-03	0.60	0.99	6.09E-01	-0.10	0.45	1.04E-02	0.55	0.92	1.51E-03	0.65	1.20	112029017	47252342	147012075	59287858	150068412	56354523	143955738	62505520
HILIC_POS_199_18039a0_854	HILIC	POS	0.854	199.1804				7.14E-01	-0.07	0.44	6.09E-01	0.11	0.51	9.49E-01	-0.01	0.14	5.53E-01	-0.12	0.31	4716494	1438295	4602679	1752145	4512366	1621915	4692992	1885582
RP_POS_195_13745a7_726	RP	POS	7.73	195.1375				3.39E-01	-0.23	0.44	6.09E-01	-0.09	0.59	3.02E-01	-0.28	0.61	4.52E-01	-0.19	0.54	1549831	144770	1523160	102661	1528451	82928	1517868	119831
RP_NEG_500_84528a0_499	RP	NEG	0.50	500.8453				2.77E-03	-0.41	1.18	6.09E-01	-0.11	1.26	6.09E-03	-0.47	1.24	5.80E-02	-0.35	1.21	3767178	724400	3081625	1845072	3176677	1966899	2986574	1729429
RP_POS_601_26544a5_446	RP	POS	5.45	601.2654				6.18E-01	0.08	0.64	6.09E-01	0.11	0.91	5.29E-01	0.13	0.45	9.10E-01	0.02	0.68	779186	412866	832824	787053	792268	635652	873380	918769
HILIC_POS_258_1098a6_241	HILIC	POS	6.241	258.1098				1.02E-09	0.83	1.33	6.09E-01	-0.11	0.72	3.26E-05	0.78	1.29	2.53E-07	0.88	1.59	4251236	1575594	7605977	4254829	7825015	3960056	7386938	4560334
RP_POS_233_11482a7_367	RP	POS	7.37	233.1148				3.23E-01	0.18	0.43	6.09E-01	0.11	0.59	2.86E-01	0.24	0.39	5.21E-01	0.13	0.51	764970	881609	952786	1057436	898354	963130	1007218	1151301
RP_NEG_229_14487a8_023	RP	NEG	8.02	229.1449				2.63E-01	0.23	0.62	6.09E-01	0.10	0.40	2.19E-01	0.29	0.54	4.27E-01	0.18	0.59	2841291	528378	2961691	507886	2935552	507865	2987831	511703
HILIC_NEG_141_92368a2_928	HILIC	NEG	2.928	141.9237				3.10E-03	0.47	1.10	6.09E-01	0.11	0.83	9.26E-03	0.53	0.92	2.27E-02	0.42	0.90	1541555	320527	1778534	534903	1751006	495663	1806061	575198
HILIC_NEG_134_89468a7_915	HILIC	NEG	7.915	134.8947				6.93E-01	0.08	0.54	6.10E-01	-0.10	0.70	8.97E-01	0.03	0.05	5.68E-01	0.13	0.65	19458662	6119782	19952342	6134226	20267667	6388465	19637017	5916925
RP_POS_352_16562a4_669	RP	POS	4.67	352.1656				4.10E-10	0.77	1.46	6.10E-01	-0.11	1.08	1.24E-05	0.71	1.50	7.15E-06	0.82	1.54	1283192	319195	2909930	2301021	3028085	2438348	2791775	2173343
HILIC_NEG_183_93419a5_882	HILIC	NEG	5.882	183.9342				7.60E-01	-0.06	0.68	6.10E-01	0.10	0.73	9.73E-01	-0.01	0.31	5.80E-01	-0.11	0.46	862116	166468	851530	178550	842358	140216	860701	211137
RP_NEG_431_1955a11_616	RP	NEG	11.62	431.1955				9.33E-01	-0.02	0.32	6.10E-01	0.10	0.40	9.03E-01	0.03	0.32	7.68E-01	-0.07	0.54	1196036	581355	1186339	499403	1160697	428512	1211982	564741
RP_POS_476_27493a10_521	RP	POS	10.52	476.2749				5.69E-01	-0.10	0.90	6.10E-01	0.11	0.45	8.22E-01	-0.05	0.75	4.50E-01	-0.16	0.55	1498270	350908	1453913	464183	1430090	459905	1477736	471866
HILIC_POS_262_16467a3_481	HILIC	POS	3.481	262.1647				2.06E-04	0.47	0.89	6.10E-01	0.11	0.71	1.68E-02	0.53	0.86	7.35E-05	0.41	1.26	714073	287749	1169961	1078827	1114512	571712	1225409	1420689
RP_POS_163_97687a15_549	RP	POS	15.55	163.9769				8.61E-01	-0.03	0.22	6.11E-01	-0.10	0.46	6.88E-01	-0.09	0.21	9.38E-01	0.02	0.49	96538501	1990901	96466084	2144931	96576034	2282280	96356134	2015410
RP_POS_796_58258a13_312	RP	POS	13.31	796.5826				9.59E-07	-1.01	1.81	6.11E-01	0.09	0.61	3.85E-05	-0.96	1.68	5.40E-07	-1.06	1.85	7222814	2049384	4908546	2074045	4802222	1582827	5014871	2482479
RP_NEG_568_33716a10_59	RP	NEG	10.59	568.3372				3.20E-07	0.77	1.44	6.11E-01	0.11	0.71	2.25E-04	0.82	1.34	6.16E-07	0.71	1.72	839151	564307	1653708	1108897	1596839	684512	1710576	1417478
RP_NEG_355_28546a10_81	RP	NEG	10.81	355.2855	FA 21:1;2O	355.2854(100), 293.2865(55), 337.2757(30)	3	1.59E-01	-0.30	0.55	6.11E-01	0.10	0.38	2.77E-01	-0.25	0.56	1.45E-01	-0.35	0.62	1566142	394419	1452985	374932	1433782	399174	1472189	352030
RP_POS_273_20596a9_812	RP	POS	9.81	273.2060				1.03E-02	-0.57	0.99	6.11E-01	-0.10	0.47	1.01E-02	-0.61	1.08	2.99E-02	-0.52	0.78	1016898	40468	995535	35556	997355	36115	993715	35260
RP_NEG_221_94637a13_292	RP	NEG	13.29	221.9464				1.73E-01	-0.31	0.65	6.11E-01	0.10	0.74	3.01E-01	-0.26	0.55	1.34E-01	-0.36	0.64	12654162	1989084	12117018	1636456	12033272	1458127	12200763	1808365
RP_NEG_442_16678a11_165	RP	NEG	11.17	442.1668				3.98E-02	0.36	1.07	6.11E-01	-0.11	1.11	1.21E-01	0.31	0.97	5.01E-02	0.42	1.16	1007507	92593	1050741	125737	1057175	133302	1044308	118695
RP_POS_508_33963a10_584	RP	POS	10.58	508.3396				8.80E-01	-0.03	0.79	6.12E-01	-0.10	1.10	7.18E-01	-0.08	0.55	9.23E-01	0.02	0.48	1809066	789199	1784611	819519	1826524	807020	1742699	837892
RP_POS_391_31787a11_229	RP	POS	11.23	391.3179				8.41E-01	0.04	1.01	6.12E-01	0.11	1.03	6.62E-01	0.09	0.88	9.38E-01	-0.02	0.95	1563997	428814	1582598	529043	1555541	556098	1609655	504725
RP_NEG_502_85986a15_342	RP	NEG	15.34	502.8599				5.07E-01	-0.12	0.74	6.12E-01	-0.11	0.43	3.97E-01	-0.18	0.66	7.45E-01	-0.07	0.44	1031735	36961	1026484	43794	1028722	46186	1024247	41613
RP_POS_470_27228a6_325	RP	POS	6.33	470.2723				1.47E-07	0.63	1.32	6.12E-01	-0.11	1.14	2.97E-04	0.57	1.42	1.62E-04	0.68	1.39	7536	10822	465866	809507	507170	864604	424562	756937
RP_NEG_353_89877a15_487	RP	NEG	15.49	353.8988				4.41E-01	0.18	0.49	6.13E-01	0.09	0.62	3.50E-01	0.23	0.60	6.11E-01	0.13	0.41	1946614	235603	1982021	184486	1972631	206663	1991411	160859
HILIC_POS_171_14915a0_543	HILIC	POS	0.543	171.1492				3.45E-01	-0.18	0.73	6.13E-01	-0.10	0.66	2.86E-01	-0.23	0.55	5.54E-01	-0.13	0.53	4269476	1000956	4068895	1142501	4127020	1139283	4010770	1154295
HILIC_POS_368_22012a5_92	HILIC	POS	5.92	368.2201				1.54E-01	-0.28	1.20	6.13E-01	0.10	0.78	3.11E-01	-0.23	0.82	1.29E-01	-0.33	1.29	617004	158501	569253	175307	560336	169755	578171	181969
RP_POS_332_24313a6_463	RP	POS	6.46	332.2431				6.22E-01	0.09	0.73	6.14E-01	-0.11	0.80	8.63E-01	0.04	0.51	4.75E-01	0.14	0.86	1037636	490553	1089740	593170	1119905	530206	1059574	654145
RP_POS_567_29852a6_22	RP	POS	6.22	567.2985				5.26E-06	0.54	1.23	6.14E-01	-0.11	1.09	1.65E-03	0.49	1.35	9.80E-04	0.60	1.28	46216	186094	937381	1826959	1030110	1973521	844653	1682660
HILIC_POS_231_08374a2_368	HILIC	POS	2.368	231.0837				8.69E-03	0.35	1.06	6.15E-01	-0.11	0.70	7.50E-02	0.29	1.16	3.07E-02	0.40	1.16	461785	446948	868370	1305475	934577	1405462	802163	1207908
RP_POS_174_9756a15_38	RP	POS	15.38	174.9756				6.45E-01	-0.08	0.30	6.15E-01	0.11	0.32	8.79E-01	-0.03	0.17	5.30E-01	-0.14	0.47	49702075	4943309	49207367	6163208	48894972	6607913	49519762	5734266
RP_POS_798_56329a11_694	RP	POS	11.69	798.5633				1.62E-01	0.19	0.57	6.15E-01	-0.11	0.51	4.37E-01	0.13	0.38	1.78E-01	0.25	0.67	1281868	1703193	2035095	4430951	2259664	4611815	1810527	4277333
RP_POS_211_1329a8_837	RP	POS	8.84	211.1329				2.13E-01	-0.29	0.87	6.15E-01	-0.09	0.37	1.98E-01	-0.33	0.56	3.13E-01	-0.24	0.75	773618	796014	578596	637569	610896	530192	546296	733520
RP_NEG_266_82684a0_771	RP	NEG	0.77	266.8268				4.54E-10	0.93	1.44	6.15E-01	-0.10	0.46	8.28E-06	0.88	1.38	1.40E-08	0.98	1.80	660192	962941	2426317	1928139	2523948	1698858	2328686	2145307
RP_POS_774_56384a11_642	RP	POS	11.64	774.5638				8.01E-01	0.04	0.36	6.15E-01	-0.11	0.49	9.47E-01	-0.01	0.24	6.50E-01	0.10	0.41	7535358	11004340	8181012	16502700	9015839	18388064	7346184	14515265
RP_POS_301_23709a10_082	RP	POS	10.08	301.2371				3.43E-05	-0.95	1.48	6.16E-01	-0.09	0.88	4.65E-05	-0.99	1.53	1.49E-04	-0.91	1.39	922090	91971	839695	75060	843491	73670	835899	76982
RP_POS_174_14874a0_71	RP	POS	0.71	174.1487				3.53E-01	-0.19	0.66	6.16E-01	0.10	0.43	5.53E-01	-0.14	0.59	2.85E-01	-0.24	0.45	1921334	254309	1872501	264460	1859128	255397	1885874	275160
RP_POS_294_11258a8_874	RP	POS	8.87	294.1126				5.37E-01	-0.13	0.54	6.16E-01	-0.10	0.37	4.45E-01	-0.18	0.47	7.38E-01	-0.07	0.27	619737	108317	606021	109757	611569	105615	600473	114551
HILIC_POS_138_05255a4_873	HILIC	POS	4.873	138.0526				9.16E-01	0.02	0.37	6.16E-01	0.10	0.50	7.16E-01	0.07	0.20	9.05E-01	-0.03	0.10	817489	500864	828317	514307	802295	645119	854339	341850
RP_POS_141_50729a11_249	RP	POS	11.25	141.5073				3.94E-15	1.18	1.80	6.16E-01	0.10	0.61	3.26E-10	1.23	1.90	5.65E-11	1.14	1.93	757130	376026	1666912	730218	1630023	664651	1703800	795474
RP_POS_356_90875a0_47	RP	POS	0.47	356.9088				2.26E-09	-0.74	1.40	6.16E-01	0.11	1.16	6.42E-05	-0.68	1.45	5.80E-06	-0.79	1.53	1686251	137793	1178315	744981	1140688	747752	1215941	747862
HILIC_POS_64_01668a4_872	HILIC	POS	4.872	64.0167				9.97E-01	0.00	0.72	6.17E-01	0.11	0.71	8.11E-01	0.05	0.12	7.98E-01	-0.05	0.35	7487108	1533147	7488458	1860259	7394709	1664844	7582207	2049905
RP_NEG_370_6756a15_577	RP	NEG	15.58	370.6756				2.10E-01	-0.25	0.82	6.17E-01	-0.10	0.35	1.74E-01	-0.30	0.80	3.75E-01	-0.20	0.55	1509347	58205	1494247	60024	1497271	61994	1491223	58457
RP_NEG_506_32407a10_62	RP	NEG	10.62	506.3241				6.83E-03	0.60	1.34	6.17E-01	-0.09	1.00	2.62E-02	0.56	1.11	4.77E-03	0.65	1.35	3105040	921605	3617746	790445	3657548	651341	3577944	913718
RP_POS_431_1785a12_339	RP	POS	12.34	431.1785				2.34E-01	0.19	0.50	6.18E-01	0.11	0.34	2.56E-01	0.25	0.52	4.17E-01	0.14	0.48	8778741	1207309	9124040	1936563	9026610	1528701	9221470	2284904
HILIC_NEG_178_84396a1_366	HILIC	NEG	1.366	178.8440				8.70E-01	-0.03	0.89	6.18E-01	-0.11	0.80	7.02E-01	-0.08	0.13	8.96E-01	0.03	0.18	12442341	2419229	12353282	3351196	12521767	3058330	12184797	3644025
RP_POS_533_80267a6_511	RP	POS	6.51	533.8027				2.11E-07	0.62	1.32	6.18E-01	-0.11	1.16	3.79E-04	0.56	1.42	1.78E-04	0.68	1.40	25923	38142	401344	670503	435031	712014	367658	631699
HILIC_POS_212_14926a0_619	HILIC	POS	0.619	212.1493				7.34E-01	-0.06	1.03	6.18E-01	-0.10	0.89	5.83E-01	-0.12	0.49	9.56E-01	-0.01	0.22	1278313	652719	1231077	763460	1269418	797152	1192735	734294
RP_POS_567_58173a11_166	RP	POS	11.17	567.5817				2.80E-07	0.64	1.08	6.18E-01	0.11	0.90	9.81E-04	0.69	1.12	2.36E-06	0.58	1.38	515508	444276	1753503	2134529	1646221	1434842	1860785	2668923
RP_POS_490_29028a9_952	RP	POS	9.95	490.2903	LPC 14:0 [M+Na+]	104.1076(100), 431.2133(60), 490.2904(30), 86.097(17), 285.2434(12)		4.49E-04	0.50	1.00	6.18E-01	-0.11	0.39	1.62E-02	0.45	0.94	1.77E-03	0.56	1.01	6905894	2576494	9540075	5691611	9825850	5492603	9254300	5925760
HILIC_POS_201_15968a0_528	HILIC	POS	0.528	201.1597				3.37E-02	0.36	0.58	6.19E-01	-0.11	0.39	1.10E-01	0.31	0.57	4.70E-02	0.42	0.69	237988	347356	409567	502302	434726	535702	384408	470633
RP_POS_248_16789a6_845	RP	POS	6.85	248.1679				2.24E-03	0.59	1.39	6.19E-01	0.10	0.90	5.06E-03	0.64	1.25	8.18E-03	0.54	1.24	514786	270607	696526	307377	681146	267661	711905	344621
RP_POS_792_08875a14_251	RP	POS	14.25	792.0888				1.51E-01	0.18	0.54	6.20E-01	0.11	0.44	2.42E-01	0.24	0.51	3.41E-01	0.13	0.50	908739	688418	1312869	2518580	1186971	1861226	1438768	3052775
RP_POS_128_95074a0_813	RP	POS	0.81	128.9507				8.40E-03	0.47	0.85	6.20E-01	0.10	0.34	1.42E-02	0.52	0.94	3.71E-02	0.42	0.89	4320639	2556042	5857353	3415780	5686757	3243644	6027949	3604526
RP_NEG_798_80322a0_497	RP	NEG	0.50	798.8032				5.92E-08	-0.68	1.36	6.20E-01	0.11	1.19	1.62E-04	-0.63	1.43	4.97E-05	-0.73	1.45	2157117	200027	1614403	871073	1570902	909385	1657905	837961
HILIC_NEG_225_06168a4_984	HILIC	NEG	4.984	225.0617				1.29E-01	-0.26	0.74	6.20E-01	0.11	0.49	3.23E-01	-0.21	0.47	1.01E-01	-0.32	1.09	9524290	3958605	8162660	5440183	7891302	4900988	8434018	5968687
HILIC_POS_113_55412a0_505	HILIC	POS	0.505	113.5541				6.41E-01	-0.08	0.84	6.20E-01	-0.11	0.50	4.86E-01	-0.14	0.67	8.87E-01	-0.03	0.87	291542	217114	269345	278389	283231	311740	255459	242914
RP_POS_286_22876a10_857	RP	POS	10.86	286.2288				7.95E-04	-0.85	1.34	6.20E-01	0.08	0.47	2.79E-03	-0.81	1.15	5.40E-04	-0.89	1.37	794495	603962	380835	397956	360982	314879	400687	469058
RP_POS_336_32669a10_453	RP	POS	10.45	336.3267				9.55E-01	-0.01	0.67	6.21E-01	-0.10	0.45	7.91E-01	-0.06	0.63	8.76E-01	0.04	0.58	1061209	347481	1057304	323734	1073438	339853	1041170	309378
RP_NEG_512_26947a8_188	RP	NEG	8.19	512.2695				2.62E-01	-0.31	0.99	6.21E-01	0.08	0.38	3.49E-01	-0.27	0.68	2.22E-01	-0.35	0.91	1024342	1654092	675719	899842	630917	872643	720521	932928
RP_POS_593_56909a11_262	RP	POS	11.26	593.5691				3.88E-02	-0.46	0.88	6.21E-01	0.09	0.35	8.97E-02	-0.41	0.72	3.35E-02	-0.51	0.96	361349	199907	277895	170484	269408	162872	286382	179020
RP_POS_261_01031a0_548	RP	POS	0.55	261.0103				2.20E-04	0.46	1.22	6.21E-01	-0.11	1.17	1.34E-02	0.40	1.21	4.06E-03	0.51	1.33	2802336	277694	3304525	1224306	3365469	1282680	3243580	1172857
RP_NEG_170_83275a15_349	RP	NEG	15.35	170.8328				7.30E-01	-0.08	0.34	6.21E-01	0.09	0.45	8.86E-01	-0.04	0.24	6.16E-01	-0.13	0.37	1084362	152308	1074211	113172	1068579	113170	1079842	114040
RP_POS_276_22971a10_422	RP	POS	10.42	276.2297				4.55E-05	0.66	1.11	6.21E-01	-0.10	0.67	3.37E-03	0.61	1.04	7.60E-05	0.71	1.35	4099628	1483438	5636274	2436308	5757432	2108757	5515117	2741443
RP_POS_577_13269a9_666	RP	POS	9.67	577.1327				2.26E-02	-0.43	0.71	6.22E-01	0.10	0.38	8.92E-02	-0.38	0.63	1.89E-02	-0.48	0.84	2997883	109638	2943426	128758	2937026	115019	2949826	142066
RP_NEG_350_01294a6_867	RP	NEG	6.87	350.0129				7.33E-01	-0.07	0.36	6.22E-01	-0.10	0.30	5.92E-01	-0.12	0.28	9.39E-01	-0.02	0.18	1320051	114818	1311913	122430	1317992	126121	1305835	119591
RP_NEG_264_83023a0_771	RP	NEG	0.77	264.8302				8.12E-10	0.93	1.44	6.22E-01	-0.10	0.45	9.97E-06	0.88	1.37	1.87E-08	0.98	1.80	1558664	2232963	5534600	4357910	5750833	3828845	5318367	4859513
RP_NEG_306_00504a3_953	RP	NEG	3.95	306.0050				5.31E-01	-0.11	0.77	6.22E-01	-0.11	0.35	4.44E-01	-0.16	0.67	7.85E-01	-0.05	0.32	944337	233915	910606	341582	927552	321375	893660	363138
RP_POS_696_37738a10_562	RP	POS	10.56	696.3774				1.33E-03	-0.60	0.95	6.22E-01	0.10	0.60	1.49E-02	-0.55	0.83	1.05E-03	-0.65	1.16	1335942	161801	1219235	197424	1209438	165125	1229032	226463
RP_POS_219_03145a15_441	RP	POS	15.44	219.0315				8.00E-01	0.05	0.37	6.23E-01	0.10	0.63	6.53E-01	0.10	0.38	9.90E-01	0.00	0.52	5594468	1489991	5671019	1457602	5598768	1524355	5743269	1399377
RP_POS_195_13803a8_816	RP	POS	8.82	195.1380				2.35E-01	0.18	0.79	6.23E-01	0.11	0.62	2.67E-01	0.23	0.67	4.39E-01	0.13	0.61	1436885	754358	1671174	1435466	1600053	1146407	1742295	1684817
RP_POS_333_14929a10_73	RP	POS	10.73	333.1493				1.48E-03	0.51	1.40	6.23E-01	-0.11	1.19	1.35E-02	0.46	1.23	5.12E-03	0.56	1.36	634515	291850	865918	480087	889688	509427	842148	452772
RP_POS_362_26541a12_326	RP	POS	12.33	362.2654				1.57E-04	-0.73	1.27	6.23E-01	0.10	0.50	2.34E-03	-0.68	1.11	1.58E-04	-0.78	1.46	752577	171426	607063	194398	597443	170236	616683	217216
RP_POS_798_54126a13_716	RP	POS	13.72	798.5413	Unknown	184.0732(100), 798.5428(25), 162.955(57), 86.097(55), 739.4587(33)	4	2.50E-05	0.71	1.20	6.23E-01	0.10	0.39	1.25E-04	0.76	1.29	8.28E-04	0.66	1.19	7743364	2320690	10151280	3473461	9979512	3505237	10323049	3468312
RP_NEG_201_88861a15_537	RP	NEG	15.54	201.8886				8.07E-01	-0.06	0.51	6.24E-01	-0.09	0.33	7.08E-01	-0.10	0.40	9.45E-01	-0.02	0.26	1969501	266916	1957086	180170	1965995	127638	1948177	221656

Supplementary table 1: Metabolomics results (in asceding order according to p-value from progressive ALD vs non-progressive ALD comparison, with molecular features with ID_level of 1-2 first)

							all_ALD_vs_control			Prog_ALD_vs_non-prog_ALD			Prog_ALD_vs_control_ALD			Non-prog_ALD_vs_control			Healthy_control		all_ALD		Non-prog_ALD		Progressive_ALD	
							t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA								
Feature_ID	RP_HILIC	POS_NEG	Average.Rt	Average.Mz	Metabolite.name	curated_MSMS	ID_level	p	d	VIP	p	d	VIP	p	d	VIP	p	d	VIP	Mean	SD	Mean	SD	Mean	SD	Mean	SD
RP_NEG_484_80441a15_5	RP	NEG	15.50	484.8044				9.72E-01	-0.01	0.64	6.24E-01	-0.10	0.49	8.01E-01	-0.06	0.51	8.49E-01	0.04	0.48	1099428	370043	1096729	383327	1115656	380276	1077801	389277
RP_POS_253_14134a8_027	RP	POS	8.03	253.1413				8.56E-03	0.51	0.96	6.24E-01	-0.10	0.36	3.65E-02	0.46	0.80	9.64E-03	0.56	1.05	2144950	363855	2352659	411053	2372945	400354	2332373	424563
RP_NEG_788_76935a0_499	RP	NEG	0.50	788.7694				5.49E-03	-0.38	1.16	6.24E-01	-0.11	1.24	9.10E-03	-0.44	1.22	8.23E-02	-0.33	1.19	2388550	513419	1947847	1267546	2010401	1373741	1885294	1162319
RP_POS_510_7592Ba4_629	RP	POS	4.63	510.7593				1.48E-05	0.51	1.06	6.24E-01	0.11	1.08	1.72E-03	0.57	1.20	2.98E-03	0.46	1.15	84618	57821	495286	896356	451058	826341	539515	967715
RP_POS_450_3567Sa11_568	RP	POS	11.57	450.3568				1.01E-01	-0.33	0.63	6.24E-01	0.10	0.37	2.01E-01	-0.28	0.58	1.01E-01	-0.38	0.69	2123119	147579	2072406	156438	2064689	167226	2080124	146147
RP_NEG_213_91505a13_287	RP	NEG	13.29	213.9151				2.96E-01	0.20	0.40	6.24E-01	-0.10	0.32	4.96E-01	0.15	0.30	2.51E-01	0.25	0.53	625624	196693	669710	231768	681138	234269	658282	231042
RP_POS_242_21132a11_127	RP	POS	11.13	242.2113				2.13E-02	0.39	0.76	6.25E-01	-0.10	0.34	7.34E-02	0.34	0.68	3.73E-02	0.44	0.76	1361093	2153225	2528669	3194520	2686110	3509729	2371228	2872177
RP_POS_256_2269Ba11_1	RP	POS	11.10	256.2270				1.50E-02	0.39	0.82	6.25E-01	-0.11	0.34	5.95E-02	0.34	0.69	3.18E-02	0.45	0.78	398645	534350	715969	861541	758408	953153	673530	766472
RP_POS_548_2744Ba10_212	RP	POS	10.21	548.2745				5.78E-03	0.38	1.33	6.25E-01	0.11	0.39	3.48E-02	0.44	1.19	2.50E-02	0.33	1.02	824306	263547	1046816	640474	1015256	490489	1078376	765620
RP_NEG_957_20636a9_484	RP	NEG	9.48	957.2064				2.60E-01	0.21	0.94	6.25E-01	0.10	0.29	2.30E-01	0.26	0.80	4.47E-01	0.16	0.54	1668139	260827	1731333	310674	1716034	300344	1746632	322991
RP_NEG_627_11353a9_125	RP	NEG	9.13	627.1135				7.16E-01	0.08	0.59	6.25E-01	-0.10	0.62	9.13E-01	0.03	0.30	5.74E-01	0.12	0.49	1812835	162470	1824845	159424	1832694	142861	1816996	175543
RP_POS_486_86682a0_466	RP	POS	0.47	486.8668				2.97E-07	-0.69	1.32	6.25E-01	0.11	1.12	2.97E-04	-0.63	1.36	4.05E-05	-0.74	1.44	337408	55318	237549	156564	229846	158391	245253	155936
RP_POS_485_2866Sa6_728	RP	POS	6.73	485.2867				1.59E-07	0.63	1.33	6.26E-01	-0.11	1.17	4.32E-04	0.57	1.43	1.25E-04	0.68	1.42	24078	33852	899441	1550383	975569	1614078	823312	1496448
RP_POS_424_89758a0_47	RP	POS	0.47	424.8976				2.28E-09	-0.75	1.40	6.26E-01	0.11	1.15	5.02E-05	-0.70	1.46	5.31E-06	-0.80	1.53	1653698	163096	1151094	723568	1115597	728532	1186592	724194
RP_POS_948_80518a0_494	RP	POS	0.49	948.8052				1.71E-08	0.68	1.38	6.26E-01	-0.11	1.20	1.27E-04	0.62	1.46	4.35E-05	0.73	1.49	70432	46347	857640	1280182	920433	1338130	794847	1229853
RP_POS_312_2168a6_293	RP	POS	6.29	312.2168				3.67E-01	-0.16	0.45	6.26E-01	0.10	0.39	6.52E-01	-0.11	0.68	2.10E-01	-0.21	0.83	939302	453126	848114	604708	818432	366517	877797	776320
RP_POS_255_23178a9_753	RP	POS	9.75	255.2318				1.80E-04	0.61	1.27	6.27E-01	-0.10	1.02	3.10E-03	0.56	1.20	9.31E-04	0.66	1.35	1253455	368681	1597427	587810	1626206	612438	1568648	566852
RP_POS_453_24554a3_475	RP	POS	3.48	453.2455				2.28E-05	0.50	1.09	6.27E-01	0.11	1.00	9.09E-04	0.56	1.28	8.15E-03	0.45	1.06	254136	165198	1483183	2751395	1348657	2799752	1617708	2723839
RP_POS_430_91287a0_495	RP	POS	0.50	430.9129				1.68E-07	0.63	1.34	6.27E-01	-0.11	1.20	2.90E-04	0.57	1.41	1.73E-04	0.68	1.44	21498991	2596943	39770270	32216641	41344683	34414891	38195857	30125775
HILIC_NEG_303_78622a1_363	HILIC	NEG	1.363	303.7862				2.98E-09	0.75	1.18	6.28E-01	0.11	0.77	5.43E-05	0.80	1.24	2.14E-06	0.69	1.46	163678	88374	424409	376730	405998	307952	442820	437288
RP_POS_561_39844a10_464	RP	POS	10.46	561.3984				1.61E-01	-0.37	0.70	6.28E-01	0.08	0.44	2.20E-01	-0.33	0.56	1.48E-01	-0.41	0.65	15907580	1726297	15447872	1017980	15398184	1155636	15497559	867860
RP_NEG_256_90634a15_545	RP	NEG	15.55	256.9063				3.79E-01	-0.18	0.41	6.28E-01	-0.10	0.36	3.15E-01	-0.23	0.50	5.74E-01	-0.13	0.39	1510604	46267	1502167	48608	1504538	49147	1499795	48444
RP_POS_211_16916a11_127	RP	POS	11.13	211.1692				1.41E-02	0.39	0.79	6.28E-01	-0.10	0.33	5.73E-02	0.34	0.70	3.28E-02	0.44	0.77	371415	419186	627606	706327	662061	787100	593152	621311
HILIC_NEG_144_92345a5_743	HILIC	NEG	5.743	144.9235				4.45E-02	-0.39	1.28	6.28E-01	0.10	0.66	1.29E-01	-0.34	0.60	4.10E-02	-0.44	1.15	41128479	7529319	37874724	8596747	37455551	8190706	38293897	9048210
RP_NEG_681_29761a10_563	RP	NEG	10.56	681.2976				7.74E-03	-0.54	1.01	6.29E-01	0.10	0.31	2.87E-02	-0.49	0.87	8.87E-03	-0.59	1.12	1246851	107795	1185697	112058	1180240	111327	1191154	113647
RP_POS_397_31015a11_71	RP	POS	11.71	397.3102				4.86E-01	-0.14	0.37	6.29E-01	-0.10	0.41	4.04E-01	-0.19	0.38	6.75E-01	-0.10	0.32	2774262	1376737	2579384	1338147	2644527	1333666	2514241	1352958
RP_NEG_590_34747a10_589	RP	NEG	10.59	590.3475				3.11E-08	0.85	1.54	6.29E-01	0.10	0.70	4.88E-05	0.90	1.45	8.92E-08	0.80	1.82	1792455	1166710	3594154	2179141	3487967	1401597	3700341	2758032
RP_NEG_578_30469a10_302	RP	NEG	10.30	578.3047				4.75E-04	0.72	1.27	6.29E-01	-0.09	0.79	3.61E-03	0.68	1.12	4.52E-04	0.77	1.32	789780	221260	957110	219862	967812	196530	946408	242501
RP_POS_242_21133a11_038	RP	POS	11.04	242.2113				2.81E-02	0.38	0.74	6.29E-01	-0.10	0.35	8.44E-02	0.33	0.66	4.59E-02	0.43	0.73	1324592	2018991	2351788	2879123	2491913	3194594	2211664	2549974
HILIC_POS_132_10211a4_005	HILIC	POS	4.005	132.1021				4.12E-01	0.14	0.87	6.29E-01	-0.10	0.96	6.76E-01	0.09	0.48	3.11E-01	0.19	0.56	182530633	58623901	193420833	81701969	197396466	72325048	189445200	90683423
RP_POS_217_12216a8_264	RP	POS	8.26	217.1222				1.05E-01	-0.36	0.69	6.29E-01	-0.09	0.52	8.19E-02	-0.41	0.90	2.08E-01	-0.31	0.63	1234006	86657	1205767	75194	1209425	83348	1202109	66705
RP_POS_405_74149a12_757	RP	POS	12.76	405.7415				2.15E-03	0.56	0.98	6.29E-01	0.10	0.37	3.63E-03	0.61	1.05	1.43E-02	0.51	0.92	1540944	1138920	2333006	1446411	2262662	1454405	2403349	1449659
RP_POS_488_8714a0_512	RP	POS	0.51	488.8714				2.88E-06	0.56	1.26	6.30E-01	-0.11	1.11	1.53E-03	0.51	1.26	5.65E-04	0.62	1.38	219161	67090	505346	566951	532863	597080	477830	539793
RP_POS_321_23898a11_254	RP	POS	11.25	321.2390				9.80E-08	0.92	1.54	6.30E-01	-0.10	0.91	1.25E-05	0.87	1.55	9.44E-07	0.97	1.67	1508722	507697	2190010	726005	2225240	710106	2154780	747088
HILIC_POS_191_00827a0_849	HILIC	POS	0.849	191.0083				3.42E-01	0.15	0.83	6.30E-01	-0.11	0.95	6.43E-01	0.10	0.39	2.23E-01	0.21	0.45	575057	135741	605944	217033	616481	167210	595408	258809
RP_POS_403_32703a11_61	RP	POS	11.61	403.3270				5.31E-03	-0.53	1.13	6.30E-01	0.10	0.75	2.03E-02	-0.48	1.06	9.46E-03	-0.58	1.05	1606066	124966	1529210	147905	1522033	159448	1536387	136636
RP_POS_763_3775a13_569	RP	POS	13.57	763.3775				6.60E-01	0.09	0.45	6.30E-01	0.10	0.37	5.40E-01	0.14	0.53	8.52E-01	0.04	0.26	981877	214055	1000941	205773	990960	214500	1010923	198332
RP_POS_393_33304a11_265	RP	POS	11.27	393.3330				9.07E-01	-0.02	0.94	6.30E-01	0.11	0.90	8.64E-01	0.03	0.83	7.08E-01	-0.07	0.88	447202	118106	443880	192861	434532	186642	453229	200341
HILIC_POS_70_06599a4_871	HILIC	POS	4.871	70.0660				5.82E-01	0.10	0.43	6.30E-01	0.10	0.49	4.31E-01	0.15	0.33	8.17E-01	0.05	0.11	19307025	9509762	20420468	11013443	19886561	13045514	20954375	8619751
HILIC_NEG_279_01562a4_159	HILIC	NEG	4.159	279.0156				1.69E-01	0.21	0.94	6.30E-01	0.11	0.83	2.00E-01	0.26	0.67	3.66E-01	0.15	0.55	199893	51015	218345	97852	213603	85447	223087	109537
RP_POS_322_24326a10_427	RP	POS	10.43	322.2433				3.12E-02	0.34	0.78	6.31E-01	-0.10	0.71	1.51E-01	0.29	0.89	3.12E-02	0.40	0.73	1785371	217782	1901497	364789	1919163	334525	1883831	395366
RP_POS_724_7782a0_502	RP	POS	0.50	724.7782				7.97E-04	-0.47	1.17	6.31E-01	-0.11	1.25	2.57E-03	-0.52	1.24	2.62E-02	-0.42	1.22	1137539	225857	907272	537108	933255	569506	881289	507093
RP_POS_553_45837a12_602	RP	POS	12.60	553.4584				3.97E-01	-0.20	0.73	6.31E-01	-0.09	0.43	3.37E-01	-0.25	0.57	5.35E-01	-0.16	0.41	15115686	5666196	14186342	4210746	14389932	4184055	13982751	4269860
RP_NEG_207_93056a15_702	RP	NEG	15.70	207.9306				8.69E-01	-0.04	0.65	6.32E-01	-0.10	0.38	7.19E-01	-0.08	0.27	9.58E-01	0.01	0.66	11008952	5404686	10829942	5028717	11072644	5323661	10587241	4757151
HILIC_NEG_214_96556a0_999	HILIC	NEG	0.999	214.9656				1.28E-01	0.22	0.73	6.32E-01	-0.11	1.11	3.46E-01	0.17	0.31	1.44E-01	0.28	0.67	1776343	378521	1934206	781711	1971925	807393	1896486	761465
RP_NEG_446_37741a12_334	RP	NEG	12.33	446.3774				8.20E-01	-0.05	0.64	6.32E-01	-0.09	0.40	6.94E-01	-0.10	0.55	9.95E-01	0.00	0.31	549091	202819	539837	186606	548839	166134	530835	206369
RP_POS_409_1734a10_977	RP	POS	10.98	409.1734				5.82E-03	0.47	1.35	6.32E-01	-0.10	1.16	4.28E-02	0.42	1.15	6.97E-03	0.52	1.32	515528	211229	651890	302006	666457	280208	637323	324541
RP_POS_171_09929a4_112	RP	POS	4.11	171.0993				9.63E-01	0.01	0.29	6.32E-01	0.10	0.66	8.06E-01	0.06	0.54	8.56E-01	-0.04	0.49	1971471	1454229	1985259	1488383	1913499	1333326	2057019	1639363
HILIC_POS_307_04355a2_456	HILIC	POS	2.456	307.0436				1.83E-05	0.53	1.03	6.33E-01	0.11	0.63	3.04E-03	0.58	0.96	7.58E-04	0.48	1.45	925607	317231	1638696	1496239	1566623	1212675	1710770	1744125
RP_POS_545_64026a6_946	RP	POS	6.95	545.6403				2.37E-07	0.62	1.30	6.33E-01	-0.11	1.12	3.54E-04	0.56	1.39	2.20E-04	0.67	1.38	17502	30230	983296	1738945	1067011	1859347	899580	1624222
RP_POS_331_65222a5_615	RP	POS	5.62	331.6522				1.78E-01	-0.27	0.99	6.33E-01	-0.10	0.76	1.77E-01	-0.32	0.89	3.01E-01	-0.22	0.92	671879	201326	615236	214355	625552	187821	604919	239458
RP_POS_337_14667a10_731	RP	POS	10.73	337.1467				2.76E-03	0.49	1.37	6.33E-01	-0.10	1.14	2.03E-02	0.44	1.20	7.83E-03	0.54	1.34	2037062	930970	2722419	1494283	2794326	1580349	2650513	1415372
RP_NEG_411_34738a11_534	RP	NEG	11.53	411.3474				4.47E-02	-0.33	0.83	6.33E-01	0.10	0.69	1.42E-01	-0.28	0.81	5.88E-02	-0.39	0.73	1356704	194322	1264382	294914	1250199	308667	1278564	282910
RP_POS_834_09357a14_024	RP	POS	14.02	834.0936				1.37E-05	0.67	1.12	6.33E-01	0.10	0.76	8.41E-04	0.72	1.12	1.00E-04	0.62	1.41	845334	535275	1473359	993489	1425556	744833	1521162	1197808
RP_POS_516_62372a6_84	RP	POS	6.84	516.6237				2.22E-07	0.62	1.32	6.34E-01	-0.11	1.16	3.76E-04	0.56	1.43	1.96E-04	0.67	1.39	17390	30622	1012804	1787295	1098590	1898668	927017	1683472
RP_POS_175_14812a11_038	RP	POS	11.04	175.1481				8.23E-03	0.42	0.82	6.34E-01	-0.10	0.34	3.69E-02	0.37	0.75	2.31E-02	0.47	0.80	269883	366110	510847	613186	540282	686195	481412	535757
RP_POS_398_76251a13_154	RP	POS	13.15	398.7625				2.13E-01	-0.27	0.44	6.34E-01	0.09	0.30	3.68E-01	-0.22	0.50	1.67E-01	-0.31	0.62	6157125	2044605	5641056	1908949	5549468	1706188	5732644	2105789
RP_NEG_265_14896a13_621	RP	NEG	13.62	265.1490				8.79E-01	0.03	0.58	6.34E-01	-0.10	0.51	9.28E-01	-0.02	0.37	6.79E-01	0.08	0.64	346940	210169	353789	250104	365792	184459	341786	303416
RP_NEG_452_92313a0_494	RP	NEG	0.49	452.9231				3.70E-07	0.61	1.33	6.34E-01	-0.11	1.20	3.58E-04	0.56	1.40	2.87E-04	0.66	1.42	22255410	2429329	35288296	23630810	36421507	25514222	34155086	21786012
RP_POS_619_43866a11_253	RP	POS	11.25	619.4387				1.77E-02	0.48	1.02	6.34E-01	0.09	0.56	1.40E-02	0.53	1.08	6.36E-02	0.44	0.79	2745870	505055	2997673	511159	2973181	573892	3022166	444210
HILIC_NEG_115_92065a5_425	HILIC	NEG	5.425	115.9207				9.49E-01	0.01	0.14	6.34E-01	-0.09	0.51	8.91E-01	-0.03	0.22	8.02E-01	0.06	0.13	92181680	15912576	92385342	14048629	93058166	14551808	91712517	13640997
RP_POS_199_01102a11_21	RP	POS	11.21	199.0110				2.55E-01	-0.25	0.47	6.35E-01	-0.09	0.29	2.10E-01	-0.30	0.53	4.00E-01	-0.21	0.55	3740312	862914	3544612	746801	3580364	786347	3508860	711235
RP_POS_158_11772a3_361	RP	POS	3.36	158.1177	Unknown	112.1118(100), 158.0968(17), 95.0867(14)	4	1.99E-01	-0.20	0.65	6.35E-01	0.11	0.48	5.41E-01	-0.14	0.71	5.59E-02	-0.25	1.05	1074535	639027	862038	1194087	804786	564695	919290	1598504
RP_POS_422_18185a7_55	RP	POS	7.55	422.1819				9.57E-01	0.01	0.85	6.35E-01	0.10	0.69	7.99E-01	0.06	0.67	8.76E-01	-0.04	0.88	6459456	443877	6464269	426497	6443861	434538	6484677	421709
RP_POS_189_13455a0_543	RP	POS	0.54	189.1346				5.29E-01	-0.11	0.60	6.35E-01	-0.10	0.56	4.62E-01	-0.16	0.55	7.72E-01	-0.05	0.32	386827	138646	366548	207230	376462	182261	356633	230966
RP_POS_265_1767a8_795	RP	POS	8.80	265.1767	Unknown	265.1756(100)	4	8.17E-01	0.05	0.59	6.35E-01	-0.10	0.59	6.89E-01	0.10	0.44	9.97E-01	0.00	0.58	3816970	587522	3844665	587862	3816547	521606	3872784	651559
RP_NEG_336_85922a15_49	RP	NEG	15.49	336.8592				2.48E-01	0.23	0.56	6.35E-01	-0.10	0.43	4.07E-01	0.18	0.40	2.17E-01	0.28	0.62	14188123	278649	14254852	288689	14268647	296617	14241056	282866
RP_POS_307_26004a11_609	RP	POS	11.61	307.2600				9.23E-01	-0.02	0.57	6.35E-01	0.10	0.60	8.67E-01	0.03	0.46	7.57E-01	-0.07	0.78	1246923	233076	1241957	301542	1227557	331724	1256356	270641
RP_POS_492_25397a6_325	RP	POS	6.33	492.2540				2.80E-07	0.61	1.31	6.36E-01	-0.11	1.14	4.52E-04	0.56	1.42	2.09E-04	0.67	1.39	17561	29042	689099	1217118	747106	1287018	631092	1153128
RP_POS_473_34482a10_543	RP	POS	10.54	473.3448				6.80E-01	0.09	0.34	6.36E-01	-0.09	0.36	8.58E-01	0.04	0.26	5.80E-01	0.13	0.47	11332899	1604567	11465932	1501372	11537448	1655693	11394417	1342564
RP_POS_149_0229a11_911	RP	POS	11.91	149.0229				8.22E-02	-0.38	0.67	6.36E-01	-0.09	0.61	5.64E-02	-0.43	1.19	1.87E-01	-0.33	0.55	4062985	1227873	3631517	1092645	3683578	1303656	3579457	840869
RP_POS_158_11748a0_708	RP	POS	0.71	158.1175				2.98E-01	0.17	0.43	6.36E-01	-0.10	0.31	5.05E-01	0.12	0.48	3.00E-01	0.22	0.75	703716	737528	886762	1164117	942187	1328203	831338	983667
HILIC_NEG_185_96262a0_655	HILIC	NEG	0.655	185.9626				3.08E-02	0.37	0.91	6.37E-01	0.10	1.08	5.37E-02	0.42	0.66	8.70E-02	0.31	0.71	298363	99823	348861	146794	341874	126169	355849	165887
HILIC_NEG_115_92071a7_955	HILIC	NEG	7.955	115.9207				9.77E-01	-0.01	0.44	6.37E-01	0.10	0.40	8.54E-01	0.04	0.30	8.10E-01	-0.05	0.55	45580926	26897351	45419439	27388454	44116263	26832366	46722616	28144658
RP_POS_342_26382a7_82	RP	POS	7.82	342.2638				3.04E-01	0.20	0.64	6.37E-01	0.10	0.48	2.77E-01	0.25	0.50	4.73E-01	0.15	0.71	2845241	1272322	3119675	1396197	3053316	1273006	3186033	1519534
RP_POS_738_50677a12_693	RP	POS	12.69	738.5068				5.05E-04	0.59	0.97	6.37E-01	-0.10	0.73	5.01E-03	0.54	0.96	2.01E-03	0.64	1.06	362578	316903	628345	471578	650738	499956	605952	445344
RP_POS_617_51056a11_257	RP	POS	11.26	617.5106				3.23E-01	-0.33	1.03	6.37E-01	-0.04	0.47	2.95E-01	-0.36	0.77	3.61E-01	-0.31	0.76	3803917	10228973	1971626	2464551	2088695	2876204	1854556	1992853
RP_POS_499_82703a4_778	RP	POS	4.78	499.8270				3.43E-01	-0.22	0.57	6.38E-01	-0.09	0.76	3.06E-01	-0.27	0.61	4.62E-01	-0.18	0.63	2013119	1747877	1691012	1321361	1753575	1165364	1628449	1470226
HILIC_POS_110_06044a1_505	HILIC	POS	1.505	110.0604				6.93E-01	0.07	0.27	6.39E-01	0.10	0.89	5.96E-01	0.12	0.28	9.23E-01	0.02	0.12	730884	1472822	862618	2068274	764721	1651134	960514	2428377
RP_POS_470_61133a6_669	RP	POS	6.67	470.6113				2.40E-07	0.62	1.32	6.39E-01	-0.10	1.13	3.92E-04	0.56	1.40	2.02E-04	0.67	1.40	23304	55931	840053	1469450	909558	1558768	770548	1386730
RP_POS_399_30771a13_003	RP	POS	13.00	399.3077				3.24E-01	-0.22	0.46	6.39E-01	0.09	0.34	4.74E-01	-0.17	0.42	2.77E-01	-0.26	0.44	4436218	1845879	4073113	1620883	3996463	1645636	4149763	1608736
RP_POS_499_9624a6_788	RP	POS	6.79	499.9624				2.13E-07	0.62	1.31	6.39E-01	-0.10	1.14	3.75E-04	0.57	1.41	1.91E-04	0.67	1.39	19991	26359	970398	1703887	1050964	1806264	889832	1609309
RP_POS_332_29169a11_249	RP	POS	11.25	332.2917				2.57E-15	1.19	1.81	6.39E-01	0.09	0.61	3.40E-10	1.23	1.90	3.42E-11	1.14	1.95	101588884	49080475	221789828	96083065	217247999	86799635	226331658	105242782
RP_POS_460_27957a10_706	RP	POS	10.71	460.2796				2.59E-01	0.20	0.76	6.39E-01	-0.10	0.92	4.58E-01	0.15	0.94	2.44E-01	0.25	0.65	518767	166491	561301	230149	572167	244969	550435	216257
HILIC_POS_134_11755a1_716	HILIC	POS	1.716	134.1176				3.71E-05	-0.62	1.33	6.39E-01	0.10	0.82	2.00E-03	-0.57	1.44	4.02E-04	-0.67	1.42	1256086	304656	910068	595363	881973	604746	938162	590610
RP_POS_126_02209a0_531	RP	POS	0.53	126.0221				4.20E-06	0.56	1.16	6.39E-01	0.10	1.12	6.05E-04	0.62	1.28	1.59E-03	0.51	1.18	280830	63309	453852	340430	437791	324494	469913	358227
RP_NEG_976_75726a0_495	RP	NEG	0.50	976.7573				6.63E-08	-0.66	1.35	6.40E-01	0.10	1.19	2.74E-04	-0.61	1.41	5.17E-05	-0.71	1.46	2892014	205753	2148663	1233843	2090462	1260599	2206865	1216464
HILIC_NEG_114_94934a2_945	HILIC	NEG	2.945	114.9493				2.16E-02	-0.44	1.00	6.40E-01	-0.10	0.73	2.62E-02	-0.49	0.92	6.54E-02	-0.39	0.67	1213133	266405	1081059	302283	1095316	295315	1066802	311431

Supplementary table 1: Metabolomics results (in asceding order according to p-value from progressive ALD vs non-progressive ALD comparison, with molecular features with ID_level of 1-2 first)

							all_ALD_vs_control			Prog_ALD_vs_non-prog_ALD			Prog_ALD_vs_control_ALD			Non-prog_ALD_vs_control			Healthy_control		all_ALD		Non-prog_ALD		Progressive_ALD	
							t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA								
Feature_ID	RP_HILIC	POS_NEG	Average.Rt	Average.Mz	Metabolite.name	curated_MSMS	ID_level	p	d	VIP	p	d	VIP	p	d	VIP	p	d	VIP	Mean	SD	Mean	SD	Mean	SD	Mean	SD
RP_NEG_353_00983a1_093	RP	NEG	1.09	353.0098				1.23E-02	-0.60	1.07	6.40E-01	0.08	0.87	2.70E-02	-0.56	0.96	1.24E-02	-0.64	1.03	2700540	2159689	1617127	1613178	1541068	1655540	1693185	1582776
RP_NEG_446_90628a0_464	RP	NEG	0.46	446.9063				6.99E-10	-0.77	1.42	6.40E-01	0.10	1.17	2.81E-05	-0.72	1.49	3.68E-06	-0.82	1.54	1713518	149001	1178233	753085	1142742	761462	1213724	750635
RP_POS_254_82314a0_521	RP	POS	0.52	254.8231				5.02E-06	0.56	1.25	6.40E-01	-0.10	1.12	1.80E-03	0.51	1.25	6.70E-04	0.61	1.37	710570	120622	1048332	672519	1080013	707183	1016650	641591
HILIC_NEG_97_93105a2_956	HILIC	NEG	2.956	97.9311				8.88E-01	0.03	0.56	6.40E-01	-0.10	0.43	9.23E-01	-0.02	0.25	7.34E-01	0.08	0.29	231357	96239	234193	106882	239226	110017	229160	104524
RP_POS_266_69232a10_731	RP	POS	10.73	266.6923				3.09E-06	0.72	1.22	6.40E-01	-0.10	0.81	1.12E-03	0.68	1.16	5.46E-06	0.77	1.47	392681	134259	560721	242246	572127	199008	549316	280524
HILIC_POS_314_23267a0_776	HILIC	POS	0.776	314.2327				1.61E-01	-0.23	0.62	6.41E-01	-0.10	0.78	1.05E-01	-0.28	0.60	4.04E-01	-0.18	0.61	20141733	11475282	16377158	17215408	17186746	20350087	15567569	13539767
RP_POS_617_27515a7_187	RP	POS	7.19	617.2752				1.49E-01	-0.26	0.76	6.41E-01	0.10	0.68	2.87E-01	-0.21	0.64	1.57E-01	-0.31	0.89	1407363	80937	1381586	103219	1376735	112773	1386438	93594
HILIC_POS_491_47672a1_308	HILIC	POS	1.308	491.4767				3.35E-01	0.18	0.41	6.41E-01	-0.10	0.43	5.54E-01	0.13	0.24	2.80E-01	0.22	0.50	292062	227136	339877	285656	353296	278529	326458	294818
RP_POS_192_13849a2_004	RP	POS	2.00	192.1385	Unknown	192.1387(100), 133.0653	4	1.84E-01	0.24	0.49	6.41E-01	-0.10	0.38	3.84E-01	0.19	0.39	1.47E-01	0.29	0.63	21233534	7679721	23485443	9869579	23948938	8935978	23021948	10794210
RP_NEG_241_18117a9_624	RP	NEG	9.62	241.1812				1.39E-02	0.39	1.42	6.41E-01	0.10	1.48	1.57E-02	0.44	1.31	9.18E-02	0.34	1.16	1774422	1160521	2481357	1932110	2390682	2101098	2572033	1763771
HILIC_NEG_305_78415a1_363	HILIC	NEG	1.363	305.7842				4.32E-09	0.75	1.14	6.41E-01	0.10	0.74	8.32E-05	0.80	1.21	9.64E-07	0.69	1.52	78857	46212	205294	182988	196704	142389	213885	217319
HILIC_NEG_100_93341a7_676	HILIC	NEG	7.676	100.9334				6.61E-01	-0.09	0.65	6.41E-01	-0.10	1.11	5.37E-01	-0.13	0.29	8.69E-01	-0.04	0.84	33808830	4097458	33431116	4562506	33645189	4766171	33217043	4387237
HILIC_POS_387_21344a2_224	HILIC	POS	2.224	387.2134				7.85E-01	0.05	0.73	6.41E-01	-0.10	0.72	9.89E-01	0.00	0.20	6.39E-01	0.10	0.34	2148433	555232	2180591	646245	2210904	629810	2150278	667272
RP_POS_239_16177a9_162	RP	POS	9.16	239.1618				2.09E-03	0.49	1.46	6.42E-01	0.10	1.37	2.64E-03	0.54	1.42	3.30E-02	0.44	1.17	1112629	459292	1470358	784858	1433573	873991	1507143	691341
HILIC_POS_244_15462a1_49	HILIC	POS	1.49	244.1546				2.14E-03	0.43	0.82	6.42E-01	-0.10	1.04	5.46E-02	0.38	0.67	2.66E-03	0.49	1.04	913590	360149	1242296	831253	1281258	705826	1203333	945925
RP_POS_228_19574a11_127	RP	POS	11.13	228.1957				1.58E-02	0.40	0.77	6.42E-01	-0.10	0.33	6.18E-02	0.35	0.69	3.15E-02	0.45	0.77	14227900	20313494	26080169	31988950	27579294	34849107	24581045	29127696
RP_POS_591_38672a10_704	RP	POS	10.70	591.3867				4.38E-01	0.13	0.35	6.42E-01	0.10	0.53	4.17E-01	0.18	0.45	6.48E-01	0.08	0.49	4070225	872720	4226846	1290261	4166356	1003469	4287336	1532678
HILIC_NEG_259_81641a3_027	HILIC	NEG	3.027	259.8164				1.12E-07	-0.74	1.29	6.42E-01	0.10	0.74	1.13E-04	-0.69	1.40	1.36E-05	-0.79	1.51	3668473	150385	3415807	360289	3398927	361658	3432687	361784
HILIC_NEG_315_04202a5_743	HILIC	NEG	5.743	315.0420				4.01E-01	-0.18	0.67	6.42E-01	-0.09	0.90	3.47E-01	-0.23	0.40	5.60E-01	-0.14	0.40	5096951	1065107	4918036	959465	4962988	913971	4873083	1010181
RP_POS_374_28027a11_369	RP	POS	11.37	374.2803				8.03E-01	-0.05	0.64	6.42E-01	-0.09	0.29	6.69E-01	-0.10	0.40	9.89E-01	0.00	0.37	318436	253384	305473	259235	317617	254357	293330	266043
RP_POS_427_28256a11_608	RP	POS	11.61	427.2826				1.86E-01	-0.26	0.71	6.42E-01	0.09	0.37	3.17E-01	-0.22	0.56	1.79E-01	-0.31	0.61	2129315	301133	2046317	318641	2031393	343854	2061241	294018
RP_POS_739_51318a12_325	RP	POS	12.33	739.5132				5.41E-06	-1.00	1.69	6.42E-01	0.08	0.57	3.60E-05	-0.96	1.54	8.04E-06	-1.05	1.69	782107	218344	561053	192745	552031	190474	570074	196501
RP_NEG_235_92618a15_681	RP	NEG	15.68	235.9262				8.03E-01	-0.05	0.27	6.42E-01	0.10	0.30	9.87E-01	0.00	0.40	6.28E-01	-0.09	0.46	23564748	5897808	23243127	7439154	22894875	6368966	23591379	8426162
HILIC_NEG_221_84235a2_947	HILIC	NEG	2.947	221.8424				1.69E-04	0.61	1.20	6.42E-01	-0.10	0.70	4.67E-03	0.56	1.02	5.13E-04	0.66	1.21	459937	41369	498904	66765	502029	63885	495780	70035
HILIC_POS_175_0343a0_852	HILIC	POS	0.852	175.0343				4.57E-01	0.13	0.77	6.42E-01	-0.10	0.93	7.07E-01	0.09	0.22	3.36E-01	0.18	0.37	2310159	671979	2419524	854252	2459511	693085	2379537	995367
HILIC_POS_163_02809a4_818	HILIC	POS	4.818	163.0281				5.98E-03	0.47	1.14	6.42E-01	0.10	0.35	1.16E-02	0.52	0.91	3.36E-02	0.42	1.45	1098466	818089	1630069	1201500	1573864	1170728	1686275	1240812
HILIC_POS_105_04279a4_324	HILIC	POS	4.324	105.0428				5.68E-01	0.11	0.86	6.43E-01	0.10	0.78	4.61E-01	0.15	0.27	7.93E-01	0.06	0.19	55054853	11728059	56496980	14225894	55831923	14807569	57162037	13737375
RP_NEG_332_92242a0_497	RP	NEG	0.50	332.9224				2.22E-07	-0.63	1.33	6.43E-01	0.10	1.20	3.07E-04	-0.58	1.40	1.71E-04	-0.68	1.43	24224868	1275741	19405347	8434331	19011065	8963880	19799630	7940985
RP_NEG_615_14105a8_509	RP	NEG	8.51	615.1411				3.31E-01	-0.21	0.48	6.43E-01	0.09	0.95	4.93E-01	-0.16	0.38	2.84E-01	-0.25	0.50	916186	63176	903758	59776	900965	60617	906551	59405
HILIC_NEG_115_92072a0_677	HILIC	NEG	0.677	115.9207				1.58E-02	0.58	1.13	6.43E-01	0.08	0.61	1.59E-02	0.62	1.08	3.32E-02	0.54	0.95	14896241	3587257	16625474	2669640	16500759	2601582	16750190	2756706
RP_NEG_178_97713a15_515	RP	NEG	15.52	178.9771				2.33E-02	-0.31	0.86	6.43E-01	0.10	0.53	6.15E-02	-0.26	0.83	8.39E-02	-0.37	0.90	1357390	52471	1320671	130137	1314593	159367	1326750	93507
RP_NEG_637_14539a9_125	RP	NEG	9.13	637.1454				5.07E-01	0.15	0.72	6.43E-01	-0.09	0.64	6.72E-01	0.10	0.39	4.32E-01	0.19	0.71	16633073	1370287	16813812	1197437	16869629	1236663	16757995	1166739
HILIC_POS_371_23959a2_224	HILIC	POS	2.224	371.2396				4.66E-01	0.14	0.67	6.44E-01	-0.10	0.80	6.73E-01	0.10	0.20	3.80E-01	0.19	0.38	16118929	4770413	16847000	5215023	17090025	4994833	16603975	5466175
HILIC_POS_286_20126a0_914	HILIC	POS	0.914	286.2013				7.95E-01	0.04	0.35	6.44E-01	0.10	0.75	6.59E-01	0.09	0.31	9.79E-01	-0.01	0.60	2844890	1681264	2944259	2374302	2833728	2141185	3054791	2603855
HILIC_NEG_214_85135a7_668	HILIC	NEG	7.668	214.8514				3.78E-01	-0.18	0.47	6.45E-01	0.09	0.42	5.63E-01	-0.13	0.22	3.19E-01	-0.22	0.38	325393	18743	321982	19350	321084	19278	322881	19575
RP_POS_612_323a10_619	RP	POS	10.62	612.3230				1.50E-03	0.60	1.34	6.45E-01	-0.09	0.75	1.32E-02	0.56	1.11	1.41E-03	0.65	1.41	2497434	534497	2874649	627443	2903757	545773	2845540	704135
RP_POS_498_90024a0_495	RP	POS	0.50	498.9002				1.87E-07	0.63	1.34	6.45E-01	-0.10	1.20	2.97E-04	0.57	1.41	1.88E-04	0.68	1.44	12585656	1653792	23696776	19665018	24608471	20972319	22785081	18432216
RP_POS_352_24579a10_713	RP	POS	10.71	352.2458				4.65E-03	0.57	1.42	6.45E-01	0.09	1.30	4.56E-03	0.62	1.37	2.15E-02	0.53	1.28	2438963	759720	2898124	782619	2861845	846936	2934402	719372
RP_POS_364_83392a15_454	RP	POS	15.45	364.8339				5.09E-01	-0.12	0.61	6.45E-01	-0.10	0.37	3.79E-01	-0.17	0.71	7.49E-01	-0.07	0.89	2342040	126991	2323904	154919	2331087	181110	2316722	124834
HILIC_NEG_100_93347a2_175	HILIC	NEG	2.175	100.9335				5.98E-01	0.10	0.67	6.46E-01	0.10	0.62	5.09E-01	0.15	0.25	8.08E-01	0.05	0.23	22387901	3911007	22832182	4722815	22613434	4360713	23050930	5094281
RP_POS_635_49567a11_61	RP	POS	11.61	635.4957				5.07E-01	-0.13	0.66	6.46E-01	0.10	0.68	6.96E-01	-0.08	0.58	4.55E-01	-0.17	0.69	418505	124448	400876	145741	394127	168748	407625	119773
RP_POS_441_2981a11_831	RP	POS	11.83	441.2981				8.08E-01	-0.05	0.71	6.46E-01	0.09	0.95	9.99E-01	0.00	0.86	6.58E-01	-0.09	0.41	306171074	74419220	302387454	82090488	298587802	76527451	306187107	87916490
RP_POS_880_81769a0_495	RP	POS	0.50	880.8177				2.97E-08	0.67	1.37	6.46E-01	-0.10	1.20	1.55E-04	0.61	1.44	6.10E-05	0.72	1.47	144068	91467	1186491	1726697	1266409	1806920	1106573	1657051
RP_POS_209_11487a7_603	RP	POS	7.60	209.1149	Unknown	209.1136(100)	4	3.30E-01	-0.23	0.78	6.46E-01	-0.08	1.35	2.76E-01	-0.27	1.09	4.63E-01	-0.19	0.41	1789156	232625	1745208	173289	1753228	183919	1737188	163442
RP_NEG_1085_23169a9_788	RP	NEG	9.79	1085.2317				4.37E-01	-0.17	0.54	6.46E-01	0.09	0.68	6.01E-01	-0.12	0.27	3.81E-01	-0.21	0.76	3572312	332298	3520324	309718	3505992	331267	3534657	289224
RP_POS_503_26837a15_341	RP	POS	15.34	503.2684				2.49E-01	-0.22	0.94	6.46E-01	-0.10	0.37	2.06E-01	-0.27	0.53	4.38E-01	-0.17	0.80	1116871	335859	1034408	386359	1052265	409577	1016551	364950
RP_POS_375_21933a11_164	RP	POS	11.16	375.2193				5.48E-01	-0.10	0.55	6.47E-01	-0.10	0.61	4.22E-01	-0.15	0.48	8.05E-01	-0.05	0.62	3105787	188818	3079864	271066	3092384	301150	3067344	239670
RP_POS_362_9256a0_495	RP	POS	0.50	362.9256				2.01E-07	0.62	1.34	6.47E-01	-0.10	1.20	3.07E-04	0.57	1.40	1.93E-04	0.68	1.44	24186674	2652053	41048777	29899711	42429396	31877786	39668159	28038312
RP_NEG_161_00838a0_617	RP	NEG	0.62	161.0084				2.02E-03	-0.61	1.02	6.47E-01	-0.09	0.56	2.92E-03	-0.65	1.10	1.02E-02	-0.56	0.92	659379	421566	375926	459448	397139	463823	354712	458740
RP_POS_421_32843a11_612	RP	POS	11.61	421.3284				7.23E-03	-0.64	1.03	6.47E-01	-0.08	0.57	4.92E-03	-0.68	1.25	2.34E-02	-0.59	0.86	1944137	466495	1690960	354981	1707357	422933	1674564	274178
RP_POS_196_00262a3_885	RP	POS	3.89	196.0026				9.65E-01	0.01	0.45	6.47E-01	0.09	0.42	8.10E-01	0.06	0.16	8.68E-01	-0.04	0.53	12954072	5736628	13005046	5766109	12738954	5650305	13271138	5924872
RP_POS_413_26593a11_578	RP	POS	11.58	413.2659				2.30E-02	-0.43	0.69	6.47E-01	-0.09	0.43	3.27E-02	-0.48	0.77	6.17E-02	-0.39	0.74	10723974	945355	10257537	1097113	10308151	999940	10206923	1194475
RP_NEG_283_85654a15_723	RP	NEG	15.72	283.8565				2.25E-01	-0.25	0.48	6.47E-01	-0.09	0.87	1.80E-01	-0.30	0.64	3.86E-01	-0.21	0.39	525587	239146	466195	234084	476985	256904	455405	210883
RP_POS_133_03459a0_45	RP	POS	0.45	133.0346				8.73E-06	-0.64	1.30	6.47E-01	-0.10	1.15	1.11E-04	-0.69	1.39	1.70E-03	-0.59	1.32	1333642	231007	1028598	512660	1052218	537616	1004978	490750
RP_NEG_129_0546a3_713	RP	NEG	3.71	129.0546				1.62E-01	0.23	0.87	6.47E-01	0.10	0.72	1.96E-01	0.28	0.65	3.03E-01	0.18	0.43	25745544	6857317	28012748	10532066	27527394	8597686	28498102	12235671
HILIC_POS_185_02325a7_963	HILIC	POS	7.963	185.0233				7.94E-04	-0.52	1.21	6.47E-01	0.10	0.82	1.14E-02	-0.47	1.30	3.18E-03	-0.57	1.27	3968033	1057545	3049474	1878013	2962977	1925162	3135972	1845081
HILIC_POS_560_31213a1_255	HILIC	POS	1.255	560.3121				6.47E-07	0.86	1.53	6.48E-01	-0.09	0.66	1.04E-04	0.82	1.38	1.50E-06	0.91	1.88	770362	230512	1054825	327176	1069882	285184	1039768	366715
RP_POS_613_56274a11_25	RP	POS	11.25	613.5627				3.86E-07	0.68	1.19	6.48E-01	-0.10	0.69	2.78E-04	0.73	1.20	2.90E-05	0.63	1.30	122202	167782	420217	471253	398544	384267	441889	547788
RP_POS_120_32705a0_496	RP	POS	0.50	120.3271				3.71E-07	0.61	1.33	6.48E-01	-0.10	1.20	4.59E-04	0.56	1.39	2.41E-04	0.66	1.43	196464	32946	386171	344544	402009	365253	370333	325457
RP_POS_196_00294a10_58	RP	POS	10.58	196.0029				4.09E-01	-0.18	0.49	6.49E-01	0.09	0.46	5.72E-01	-0.13	0.32	3.47E-01	-0.22	0.54	2685209	1038762	2513971	927876	2471408	924539	2556535	938620
RP_POS_295_22516a9_676	RP	POS	9.68	295.2252				6.03E-03	0.49	1.07	6.49E-01	0.10	0.63	1.22E-02	0.54	1.03	2.57E-02	0.44	1.17	7180572	931393	7764200	1237242	7707443	1150762	7820957	1327384
RP_POS_350_1748a10_13	RP	POS	10.13	350.1748				1.45E-01	0.22	0.99	6.49E-01	0.10	0.76	2.24E-01	0.27	0.80	2.49E-01	0.17	1.00	1113885	384766	1262781	752194	1228249	504273	1297313	941496
RP_POS_375_28937a9_926	RP	POS	9.93	375.2894				2.71E-02	0.34	1.25	6.49E-01	0.10	0.35	2.46E-02	0.39	0.96	1.57E-01	0.29	1.18	681729	645728	1050421	1181777	996264	1328450	1104579	1025150
RP_POS_435_36612a10_881	RP	POS	10.88	435.3661				5.66E-01	0.09	0.44	6.49E-01	-0.10	0.30	8.55E-01	0.04	0.26	3.82E-01	0.14	0.72	3911055	226882	3943268	389604	3961126	285855	3925410	473620
RP_POS_278_24503a10_731	RP	POS	10.73	278.2450				1.17E-06	0.78	1.24	6.49E-01	-0.09	0.71	4.14E-04	0.73	1.21	2.50E-06	0.83	1.49	54972853	15651035	74816924	26066867	76010452	21811754	73623396	29902680
HILIC_POS_86_09712a4_005	HILIC	POS	4.005	86.0971				4.35E-01	0.14	0.88	6.50E-01	-0.10	0.95	6.86E-01	0.09	0.46	3.37E-01	0.18	0.55	26868440	8319300	28330771	11431987	28854033	10146236	27807509	12670552
RP_NEG_208_84506a0_522	RP	NEG	0.52	208.8451				7.39E-04	0.45	1.19	6.50E-01	-0.10	1.09	1.89E-02	0.40	1.16	6.39E-03	0.50	1.31	852571	118524	992285	345572	1008093	360749	976478	332607
RP_NEG_411_09113a0_708	RP	NEG	0.71	411.0911				8.66E-01	-0.03	0.43	6.50E-01	-0.10	0.62	7.15E-01	-0.08	0.79	9.38E-01	0.02	0.73	1071880	213558	1064170	256753	1075908	250887	1052431	264507
RP_NEG_957_20624a9_894	RP	NEG	9.89	957.2062				5.97E-01	-0.11	0.41	6.50E-01	0.09	0.52	7.84E-01	-0.06	0.28	4.98E-01	-0.15	0.41	3944714	275351	3915063	272151	3902621	268735	3927505	277686
RP_POS_188_12819a4_741	RP	POS	4.74	188.1282				8.36E-01	-0.03	0.48	6.50E-01	0.10	0.49	9.50E-01	0.01	0.51	5.87E-01	-0.08	0.68	1258792	1126796	1204303	1697472	1126590	968642	1282015	2207043
RP_POS_583_44031a10_461	RP	POS	10.46	583.4403				1.62E-01	-0.29	0.62	6.50E-01	0.09	0.69	2.93E-01	-0.24	0.60	1.44E-01	-0.33	0.57	1367848	163154	1320741	164941	1313212	163541	1328269	167644
RP_POS_373_20407a11_254	RP	POS	11.25	373.2041				2.61E-04	0.69	1.52	6.51E-01	0.09	1.10	8.81E-04	0.73	1.47	1.58E-03	0.64	1.39	7164229	1409404	8329603	1684405	8252758	1543361	8406447	1827108
RP_POS_136_07356a3_319	RP	POS	3.32	136.0736				4.87E-05	-0.63	1.26	6.51E-01	0.10	1.12	1.56E-03	-0.58	1.27	5.06E-04	-0.68	1.31	24384568	4819241	19220905	8643208	18826656	8998457	19615154	8345372
RP_NEG_411_65292a15_581	RP	NEG	15.58	411.6529				1.60E-01	-0.28	0.73	6.51E-01	-0.09	0.30	1.33E-01	-0.32	0.64	3.12E-01	-0.23	0.59	751933	37749	740815	40654	742667	43761	738963	37646
RP_POS_644_83203a0_472	RP	POS	0.47	644.8320				1.08E-07	-0.67	1.34	6.51E-01	0.10	1.17	2.95E-04	-0.62	1.38	4.80E-05	-0.72	1.46	640626	65571	470323	278707	457634	282394	483011	277245
HILIC_POS_323_21759a4_834	HILIC	POS	4.834	323.2176				2.44E-05	0.59	0.99	6.52E-01	0.10	0.42	3.28E-03	0.64	0.93	6.11E-05	0.54	1.32	412440	193546	667245	469062	645887	305864	688604	591647
HILIC_POS_267_14359a0_537	HILIC	POS	0.537	267.1436				7.93E-02	-0.34	0.81	6.52E-01	0.09	0.81	1.88E-01	-0.29	0.58	7.42E-02	-0.38	0.64	557021	60794	534171	69435	531014	67249	537329	72098
RP_POS_408_30804a11_129	RP	POS	11.13	408.3080				1.95E-02	0.38	0.82	6.52E-01	-0.10	0.35	6.78E-02	0.33	0.70	3.98E-02	0.43	0.79	11852717	13519131	19498316	21449375	20473592	23759444	18523040	19054878
RP_NEG_583_17444a0_621	RP	NEG	0.62	583.1744				6.93E-02	-0.31	0.89	6.52E-01	-0.10	0.92	6.84E-02	-0.36	0.89	2.03E-01	-0.26	0.93	2563952	942653	2169996	1339106	2230862	1405636	2109129	1280481
RP_POS_288_92184a0_469	RP	POS	0.47	288.9218				5.35E-09	-0.72	1.39	6.52E-01	0.10	1.16	7.94E-05	-0.68	1.45	1.05E-05	-0.77	1.52	3663335	323503	2575691	1630754	2501608	1643703	2649775	1630960
HILIC_NEG_117_91909a5_424	HILIC	NEG	5.424	117.9191				1.78E-01	0.27	0.64	6.52E-01	-0.09	0.62	3.02E-01	0.23	0.51	1.69E-01	0.32	0.68	2048147	461056	2176301	466964	2197506	494361	2155096	441870
RP_POS_1017_68683a10_502	RP	POS	10.50	1017.6868				2.11E-03	0.60	1.39	6.52E-01	-0.09	0.86	1.74E-02	0.56	1.12	1.44E-03	0.65	1.43	15999210	7488085	21033924	8325188	21411994	6611993	20655855	9799072
RP_NEG_425_36435a11_739	RP	NEG	11.74	425.3644				2.31E-02	-0.38	0.89	6.52E-01	0.10	0.69	9.04E-02	-0.33	0.86	3.41E-02	-0.43	0.79	980242	169759	888698	256900	877041	263666	900356	252082
RP_POS_306_27698a11_164	RP	POS	11.16	306.2770				1.07E-11	1.11	1.76	6.52E-01	-0.09	0.55	8.98E-08	1.07	1.71	3.10E-10	1.15	1.94	41281320	13479695	66642426	21814208	67631939	19679622	65652912	23919553
RP_POS_914_81097a0_494	RP	POS	0.49	914.8110				2.29E-08	0.67	1.36	6.53E-01	-0.10	1.18	1.36E-04	0.62	1.43	5.39E-05	0.72	1.47	99972	65687	972660	1433000	1037567	1497169	907753	1377960
RP_POS_788_53479a13_155	RP	POS	13.16	788.5348				3.94E-02	-0.47	0.81	6.53E-01	-0.08	0.27	3.88E-02	-0.51	0.91	7.89E-02	-0.43	0.71	1622652	555763	1392809	456210	1413466	447503	1372151	468373
HILIC_NEG_136_89166a5_496	HILIC	NEG	5.496	136.8917				3.01E-01	-0.22	0.58	6.53E-01	-0.09	0.42	2.48E-01	-0.27	0.68	4.64E-01	-0.18	0.35	4107743	1887973	3714437	1745339	3793470	1878622	3635404	1616359
RP_POS_185_11488a11_219	RP	POS	11.22	185.1149				9.06E-03	-0.75	1.63	6.53E-01	-0.06	0.38	9.25E-03	-0.78	1.20	1.28E-02	-0.72	1.47	3017490	935430	2544831	444042	2564917	359549	2524744	517950

Supplementary table 1: Metabolomics results (in asceding order according to p-value from progressive ALD vs non-progressive ALD comparison, with molecular features with ID_level of 1-2 first)

								all_ALD_vs_control			Prog_ALD_vs_non-prog_ALD			Prog_ALD_vs_control_ALD			Non-prog_ALD_vs_control			Healthy_control		all_ALD		Non-prog_ALD		Progressive_ALD	
								t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA								
Feature_ID	RP_HILIC	POS_NEG	Average.Rt	Average.Mz	Metabolite.name	curated_MSMS	ID_level	p	d	VIP	p	d	VIP	p	d	VIP	p	d	VIP	Mean	SD	Mean	SD	Mean	SD	Mean	SD
HILIC_NEG_193_8157a2_95	HILIC	NEG	2.95	193.8157				8.12E-07	0.61	1.31	6.54E-01	-0.10	0.78	7.47E-04	0.56	1.42	2.28E-04	0.66	1.51	880220	90448	1143640	479567	1165316	497526	1121964	464943
RP_NEG_530_27368a13_287	RP	NEG	13.29	530.2737				7.42E-01	-0.06	0.59	6.54E-01	-0.09	0.48	6.22E-01	-0.11	0.72	9.36E-01	-0.02	0.38	307355	69577	302541	77469	306042	74507	299039	80926
RP_POS_228_1958a11_038	RP	POS	11.04	228.1958				1.31E-02	0.40	0.80	6.54E-01	-0.10	0.33	5.09E-02	0.35	0.71	3.11E-02	0.45	0.77	18800639	24406067	33659706	39768792	35456924	44152619	31862489	35204328
RP_NEG_882_7652a0_499	RP	NEG	0.50	882.7652				6.50E-03	-0.40	1.14	6.54E-01	-0.10	1.23	1.38E-02	-0.45	1.16	6.10E-02	-0.35	1.19	885652	201229	734517	412372	753148	423602	715886	404259
RP_POS_756_55237a12_762	RP	POS	12.76	756.5524				4.45E-02	0.36	0.73	6.54E-01	0.09	0.30	4.84E-02	0.40	0.78	1.38E-01	0.31	0.62	47889311	24946535	59194930	33279157	57692118	34154797	60697742	32656506
RP_NEG_289_8981a3_705	RP	NEG	3.71	289.8981				1.44E-01	0.24	0.80	6.54E-01	0.10	0.59	1.83E-01	0.29	0.62	2.61E-01	0.19	0.42	1071673	402658	1213682	646844	1184474	534667	1242889	746822
HILIC_POS_124_087a6_286	HILIC	POS	6.286	124.0870				3.29E-01	0.18	0.43	6.54E-01	-0.09	0.49	5.54E-01	0.13	0.29	2.67E-01	0.22	0.46	1317829	746618	1478387	962247	1521818	889855	1434955	1036843
RP_POS_636_87848a0_495	RP	POS	0.50	636.8785				1.14E-07	0.65	1.34	6.54E-01	-0.10	1.19	3.06E-04	0.60	1.40	9.09E-05	0.70	1.45	106467	72084	392745	488587	414793	505897	370697	474744
RP_POS_318_60794a7_093	RP	POS	7.09	318.6079				5.57E-01	-0.12	0.57	6.54E-01	0.09	0.48	7.39E-01	-0.08	0.33	4.73E-01	-0.17	0.66	3566913	233389	3538878	233430	3528349	240508	3549407	228081
HILIC_NEG_301_78824a1_363	HILIC	NEG	1.363	301.7882				4.36E-10	0.79	1.21	6.54E-01	0.10	0.72	2.89E-05	0.84	1.29	3.54E-07	0.74	1.58	81901	45613	223539	192812	214844	154539	232233	225997
HILIC_POS_406_16391a0_889	HILIC	POS	0.889	406.1639				1.24E-03	0.44	0.81	6.54E-01	0.10	0.63	2.20E-02	0.49	0.83	3.52E-03	0.39	1.16	4868349	1430069	6367339	3766775	6197409	2561841	6537270	4695189
RP_NEG_498_78397a15_518	RP	NEG	15.52	498.7840				2.06E-01	-0.21	0.61	6.55E-01	0.10	0.42	3.22E-01	-0.16	0.42	2.61E-01	-0.26	0.63	1576603	43912	1563407	68503	1560317	85723	1566497	45967
RP_POS_848_79364a0_474	RP	POS	0.47	848.7936				2.17E-08	-0.72	1.37	6.55E-01	0.10	1.16	9.62E-05	-0.67	1.43	1.62E-05	-0.77	1.50	412738	50216	294745	176656	286786	179308	302705	175416
HILIC_POS_76_03998a5_922	HILIC	POS	5.922	76.0400				5.21E-01	-0.12	1.04	6.55E-01	0.09	0.82	7.56E-01	-0.07	0.76	4.12E-01	-0.16	1.16	858655	287535	817964	372270	801199	336568	834730	407612
RP_POS_356_29224a11_155	RP	POS	11.16	356.2922				6.48E-01	-0.09	0.57	6.55E-01	-0.09	0.30	5.46E-01	-0.14	0.35	8.29E-01	-0.05	0.31	1667789	1237837	1552972	1214314	1607631	1208140	1498312	1230249
RP_POS_406_29245a10_818	RP	POS	10.82	406.2925				3.52E-04	0.53	1.12	6.55E-01	0.10	0.40	1.89E-03	0.58	1.17	9.15E-03	0.48	1.00	159920	188604	345841	377257	328864	379327	362817	378249
RP_POS_340_3577a12_1	RP	POS	12.10	340.3577				8.30E-01	-0.04	0.59	6.55E-01	-0.09	0.27	6.80E-01	-0.09	0.31	9.82E-01	0.01	0.38	4352368	2832729	4223994	3211938	4368482	3422113	4079506	3014990
RP_POS_352_8967a0_514	RP	POS	0.51	352.8967				2.88E-06	0.56	1.26	6.55E-01	-0.10	1.14	1.60E-03	0.51	1.26	5.28E-04	0.61	1.40	385225	99100	784037	788284	819464	820733	748611	761119
RP_POS_390_77277a13_152	RP	POS	13.15	390.7728				3.83E-01	0.18	0.85	6.56E-01	-0.09	0.85	5.61E-01	0.14	0.88	3.13E-01	0.23	0.60	3017047	1055490	3204167	1015638	3249736	937534	3158597	1095850
RP_POS_343_33142a9_618	RP	POS	9.62	343.3314				6.64E-01	-0.11	0.85	6.56E-01	-0.08	0.28	5.75E-01	-0.15	0.64	7.93E-01	-0.07	0.56	1218716	1426185	1100824	939697	1142932	967419	1058716	919001
HILIC_NEG_315_04166a7_071	HILIC	NEG	7.071	315.0417				7.04E-01	-0.07	0.62	6.57E-01	0.09	0.64	9.02E-01	-0.03	0.17	5.75E-01	-0.12	0.37	1765193	371170	1735588	411569	1717154	385582	1754022	439168
RP_POS_161_96875a0_25	RP	POS	0.25	161.9688				1.68E-02	-0.49	0.98	6.57E-01	-0.09	0.32	1.91E-02	-0.53	1.03	4.77E-02	-0.45	0.83	918743	146846	844956	147835	851575	147361	838337	149506
RP_POS_243_19542a11_038	RP	POS	11.04	243.1954				1.17E-02	0.40	0.81	6.57E-01	-0.10	0.33	4.66E-02	0.35	0.72	3.06E-02	0.45	0.77	1248629	1624708	2270395	2740219	2392981	3061383	2147810	2401689
RP_POS_267_17059a9_425	RP	POS	9.43	267.1706				3.57E-01	-0.20	0.60	6.57E-01	-0.09	0.41	2.63E-01	-0.25	0.63	5.40E-01	-0.16	0.32	777092	105162	757786	92463	761922	114458	753650	64326
HILIC_POS_189_07312a5_648	HILIC	POS	5.648	189.0731				2.73E-01	-0.21	1.00	6.57E-01	-0.09	0.76	2.47E-01	-0.26	0.61	4.41E-01	-0.17	0.85	5096605	985944	4868476	1103698	4917791	1071836	4819160	1143400
RP_POS_316_11163a0_551	RP	POS	0.55	316.1116				9.34E-01	-0.01	1.04	6.57E-01	-0.10	0.85	7.59E-01	-0.06	0.97	8.50E-01	0.04	1.05	820399	203718	816333	334389	831273	316876	801393	353621
HILIC_NEG_206_10359a4_741	HILIC	NEG	4.741	206.1036				4.32E-04	0.56	1.00	6.57E-01	-0.09	0.37	1.76E-02	0.51	0.78	2.93E-04	0.60	1.24	983014	224661	1185309	386057	1202562	297753	1168056	460280
RP_POS_647_26917a11_805	RP	POS	11.81	647.2692				4.41E-03	-0.57	1.25	6.58E-01	0.09	1.36	2.85E-02	-0.52	0.93	2.78E-03	-0.61	1.32	1106870	417729	850323	449357	830253	344187	870393	537286
RP_POS_530_32397a10_684	RP	POS	10.68	530.3240				4.18E-15	1.04	1.84	6.58E-01	0.09	0.30	2.18E-07	1.09	1.74	1.53E-12	1.00	2.13	817850	388562	2034673	1182134	1981897	839530	2087449	1453585
HILIC_POS_319_16495a1_44	HILIC	POS	1.44	319.1650				5.51E-03	0.41	0.71	6.58E-01	-0.10	0.44	6.97E-02	0.36	0.65	6.98E-03	0.46	0.88	937915	575240	1375068	1160451	1426844	1020017	1323293	1294167
RP_POS_383_35159a11_227	RP	POS	11.23	383.3516				6.52E-02	-0.35	0.95	6.58E-01	-0.09	0.96	1.43E-01	-0.31	0.89	7.48E-02	-0.40	0.90	574227	142962	517726	162891	510461	174193	524991	152177
HILIC_NEG_207_83672a2_943	HILIC	NEG	2.943	207.8367				3.83E-03	0.47	1.08	6.58E-01	-0.09	0.80	2.66E-02	0.42	0.83	9.41E-03	0.52	1.00	432072	86608	493470	138493	499643	143245	487298	134741
HILIC_NEG_136_89162a2_952	HILIC	NEG	2.952	136.8916				3.89E-03	0.43	1.11	6.58E-01	-0.10	0.81	3.52E-02	0.39	0.91	1.16E-02	0.48	1.10	51911865	8092531	58176821	15661951	58874319	16117077	57479324	15324701
RP_POS_1083_92676a15_101	RP	POS	15.10	1083.9268				6.30E-01	-0.10	0.21	6.58E-01	-0.09	0.27	5.31E-01	-0.14	0.31	8.15E-01	-0.05	0.29	7407742	1021631	7306568	1042025	7352960	1038748	7260177	1053757
RP_POS_780_8056a0_472	RP	POS	0.47	780.8056				3.60E-08	-0.68	1.35	6.58E-01	0.10	1.16	1.79E-04	-0.63	1.41	3.37E-05	-0.73	1.47	510273	45011	369581	225109	359560	229086	379602	222927
RP_POS_459_35532a9_778	RP	POS	9.78	459.3553				4.11E-02	-0.38	0.64	6.59E-01	0.09	0.32	1.39E-01	-0.33	0.57	3.29E-02	-0.43	0.90	795777	58630	769549	71269	766378	61143	772721	80643
RP_POS_688_31476a5_683	RP	POS	5.68	688.3148				6.91E-01	0.07	0.64	6.59E-01	0.09	0.47	5.15E-01	0.12	0.65	9.09E-01	0.03	0.45	951069	481278	992324	585504	966281	724700	1018367	407494
HILIC_NEG_473_53348a1_365	HILIC	NEG	1.365	473.5335				3.84E-01	-0.14	0.44	6.59E-01	-0.10	0.37	3.70E-01	-0.18	0.39	6.22E-01	-0.09	0.47	224698	78938	207439	139808	213652	123408	201225	155509
RP_POS_371_2092a11_254	RP	POS	11.25	371.2092				2.22E-04	0.70	1.50	6.59E-01	0.09	1.04	7.87E-04	0.74	1.45	1.34E-03	0.65	1.40	19857360	3855359	23081083	4587961	22877195	4196359	23284972	4983381
HILIC_NEG_183_9342a5_607	HILIC	NEG	5.607	183.9342				1.45E-01	-0.26	1.01	6.59E-01	0.09	0.71	3.27E-01	-0.21	0.41	1.25E-01	-0.30	1.09	1001381	123662	960777	167848	953319	155432	968234	180688
RP_POS_338_26651a9_152	RP	POS	9.15	338.2665				8.07E-02	0.31	0.55	6.59E-01	0.09	0.43	1.25E-01	0.36	0.66	1.37E-01	0.26	0.61	985827	1469854	1561057	1943265	1474721	1371548	1647394	2394424
RP_POS_381_98285a0_627	RP	POS	0.63	381.9829				3.66E-10	-0.77	1.43	6.60E-01	0.10	1.17	9.29E-06	-0.72	1.54	7.53E-06	-0.82	1.52	1756713	93317	1336415	588934	1310303	624240	1362527	556506
RP_POS_598_83228a0_497	RP	POS	0.50	598.8323				3.21E-08	-0.67	1.37	6.60E-01	0.10	1.20	1.27E-04	-0.62	1.45	6.70E-05	-0.72	1.46	13043307	645209	9684501	5514469	9440411	5809520	9928591	5250449
RP_POS_168_98062a15_4	RP	POS	15.40	168.9806				9.29E-01	0.02	0.51	6.61E-01	0.09	0.35	7.92E-01	0.06	0.64	9.25E-01	-0.02	0.38	42250512	20555838	42612191	17888748	41821020	19044880	43403363	16809535
RP_POS_350_89117a0_465	RP	POS	0.47	350.8912				1.90E-06	-0.63	1.29	6.61E-01	0.10	1.14	8.27E-04	-0.58	1.32	1.64E-04	-0.68	1.40	580556	93139	416847	283802	404300	288409	429394	281478
RP_POS_800_57819a11_745	RP	POS	11.75	800.5782				5.22E-01	0.09	0.42	6.61E-01	-0.10	0.42	7.98E-01	0.05	0.22	4.56E-01	0.14	0.47	1443999	1973788	1782840	3961564	1957982	4181854	1607699	3762680
RP_POS_244_19063a11_127	RP	POS	11.13	244.1906				1.78E-02	0.39	0.76	6.61E-01	-0.09	0.31	6.60E-02	0.34	0.69	3.45E-02	0.44	0.76	3273657	4497028	5833289	6991408	6142076	7568391	5524502	6425106
RP_POS_256_22693a11_476	RP	POS	11.48	256.2269				8.19E-03	0.42	0.82	6.61E-01	-0.10	0.32	3.63E-02	0.37	0.74	2.45E-02	0.46	0.80	243683	340600	470764	585881	496638	653523	444891	514840
RP_POS_687_54352a12_091	RP	POS	12.09	687.5435				3.33E-08	-1.15	1.98	6.61E-01	-0.08	0.36	5.01E-08	-1.19	2.06	7.65E-07	-1.11	1.76	779781	281665	409577	280815	421969	305108	397185	256747
RP_POS_219_09738a0_706	RP	POS	0.71	219.0974				2.92E-01	0.18	0.70	6.61E-01	-0.09	0.68	5.19E-01	0.13	0.69	2.47E-01	0.23	0.71	303680	168766	344018	236037	354429	224101	333607	249241
RP_POS_245_03481a3_316	RP	POS	3.32	245.0348				1.41E-05	-0.66	1.27	6.61E-01	0.09	1.09	7.24E-04	-0.61	1.31	2.79E-04	-0.70	1.30	3495153	748113	2606705	1429404	2543662	1497991	2669748	1369672
RP_POS_298_27408a9_153	RP	POS	9.15	298.2741				2.23E-01	0.22	0.46	6.62E-01	0.09	0.44	2.63E-01	0.27	0.58	3.19E-01	0.18	0.47	360896	640259	530974	794640	495935	511634	566014	1005742
RP_POS_485_6207a6_73	RP	POS	6.73	485.6207				7.86E-07	0.59	1.32	6.62E-01	-0.10	1.14	8.63E-04	0.54	1.38	2.82E-04	0.64	1.40	44625	109565	647138	1130084	696906	1173296	597371	1094790
RP_POS_286_20114a5_285	RP	POS	5.29	286.2011				3.14E-01	-0.20	0.56	6.62E-01	-0.09	0.54	3.06E-01	-0.24	0.53	4.60E-01	-0.15	0.63	2077422	1218104	1818804	1356243	1878547	1121829	1759061	1565422
HILIC_NEG_146_08212a4_741	HILIC	NEG	4.741	146.0821				5.44E-05	0.63	1.19	6.62E-01	-0.09	0.50	5.70E-03	0.59	0.90	4.59E-05	0.68	1.40	412391	115911	534303	202597	543225	157965	525380	240443
RP_POS_632_82983a0_496	RP	POS	0.50	632.8298				1.14E-09	-0.74	1.41	6.62E-01	0.10	1.17	2.82E-05	-0.69	1.50	1.04E-05	-0.79	1.51	2402902	116072	1712157	1014178	1667512	1052894	1756801	982574
HILIC_POS_352_24512a5_648	HILIC	POS	5.648	352.2451				9.78E-01	-0.01	0.83	6.62E-01	-0.09	0.75	8.09E-01	-0.05	0.36	8.43E-01	0.04	0.46	946317	177564	945230	224987	955132	220915	935327	230798
HILIC_NEG_144_92352a4_796	HILIC	NEG	4.796	144.9235				2.71E-01	-0.23	0.76	6.62E-01	-0.09	0.51	2.36E-01	-0.27	0.51	4.25E-01	-0.18	0.54	61419338	19732658	56979822	19385465	57832484	19718957	56127161	19207831
RP_POS_898_55426a13_362	RP	POS	13.36	898.5543				6.76E-03	0.58	1.07	6.63E-01	0.08	0.32	7.36E-03	0.62	1.08	2.20E-02	0.54	0.99	700320	494743	980003	462632	959671	477745	1000335	450933
RP_NEG_271_19229a9_269	RP	NEG	9.27	271.1923	Unknown	271.1903(100), 253.1806(55), 209.191(45)	4	8.22E-01	-0.05	0.46	6.63E-01	-0.09	0.33	6.96E-01	-0.09	0.28	9.83E-01	-0.01	0.41	2574871	438604	2555082	402822	2572785	415921	2537380	392700
HILIC_NEG_98_93899a5_43	HILIC	NEG	5.43	98.9390				9.74E-01	-0.01	0.33	6.63E-01	-0.09	0.98	8.17E-01	-0.05	0.35	8.62E-01	0.04	0.33	2537595	361715	2535176	395159	2552519	399153	2517834	394399
RP_POS_407_07483a8_977	RP	POS	8.98	407.0748				1.78E-01	-0.30	0.75	6.63E-01	0.08	0.47	2.85E-01	-0.25	0.69	1.63E-01	-0.34	0.76	1752155	158671	1709310	139683	1703180	144610	1715440	135766
RP_POS_210_11011a4_742	RP	POS	4.74	210.1101				9.68E-01	-0.01	0.51	6.63E-01	0.10	0.50	8.61E-01	0.04	0.56	7.20E-01	-0.05	0.54	1682986	1665953	1667281	2596907	1553180	1462592	1781383	3385224
RP_POS_239_06834a0_494	RP	POS	0.49	239.0683				1.39E-04	-0.48	1.23	6.63E-01	0.10	1.17	6.92E-03	-0.43	1.27	3.91E-03	-0.53	1.31	1875740	209932	1532017	792154	1497268	850715	1566766	735964
HILIC_POS_210_88203a2_992	HILIC	POS	2.992	210.8820				3.08E-05	-0.58	1.34	6.63E-01	0.10	0.79	2.19E-03	-0.53	1.40	8.46E-04	-0.62	1.43	944911	166356	724091	417091	705800	437276	742382	399484
RP_POS_259_19016a11_128	RP	POS	11.13	259.1902				1.03E-02	0.41	0.87	6.63E-01	-0.09	0.28	4.71E-02	0.36	0.73	2.64E-02	0.45	0.80	585880	347525	809931	595622	836045	649980	783816	541208
RP_POS_226_95065a0_495	RP	POS	0.50	226.9507				2.62E-07	0.62	1.33	6.64E-01	-0.10	1.20	3.18E-04	0.57	1.40	2.37E-04	0.67	1.43	109842252	9429737	164844432	98459454	169157261	105286768	160531604	91995145
HILIC_NEG_144_92349a8_036	HILIC	NEG	8.036	144.9235				3.35E-02	-0.40	0.83	6.64E-01	-0.09	1.27	4.87E-02	-0.44	0.69	8.18E-02	-0.35	0.68	35256866	12104407	29612319	14702590	30256327	13113102	28968310	16246353
RP_POS_321_15692a10_13	RP	POS	10.13	321.1569				3.97E-01	0.13	0.95	6.64E-01	0.10	0.75	4.31E-01	0.18	0.73	5.83E-01	0.08	0.94	955648	334427	1030479	651405	1001942	422327	1059015	822979
RP_POS_227_17459a3_318	RP	POS	3.32	227.1746				5.55E-05	-0.71	1.29	6.64E-01	0.09	1.11	8.24E-04	-0.67	1.29	2.51E-04	-0.76	1.32	49982486	15772854	34911987	21336106	33978276	21952636	35845698	20881855
RP_POS_316_28476a9_152	RP	POS	9.15	316.2848				2.14E-01	0.23	0.47	6.64E-01	0.09	0.44	2.55E-01	0.27	0.59	3.05E-01	0.18	0.48	933714	1636469	1378525	2041526	1289120	1310440	1467929	2585952
HILIC_POS_330_33633a0_692	HILIC	POS	0.692	330.3363				5.45E-02	-0.42	0.72	6.64E-01	-0.08	0.47	4.36E-02	-0.46	0.85	1.26E-01	-0.38	0.57	3297863	924268	2937025	825001	2973101	928468	2900949	714446
RP_POS_277_1795a9_095	RP	POS	9.10	277.1795				1.99E-02	0.43	0.71	6.64E-01	0.09	0.51	2.86E-02	0.48	0.80	6.10E-02	0.39	0.84	3448858	115111	3507994	141178	3501822	134346	3514166	148805
RP_NEG_267_07391a0_711	RP	NEG	0.71	267.0739				5.62E-09	0.74	1.37	6.64E-01	0.09	0.66	4.80E-05	0.79	1.42	6.07E-06	0.69	1.50	799629	2373825	7132080	9214887	6729208	7935741	7534953	10404518
RP_POS_348_26596a11_248	RP	POS	11.25	348.2660				6.35E-14	1.06	1.61	6.65E-01	0.09	0.65	7.48E-08	1.10	1.65	7.15E-11	1.01	1.90	4175735	1759101	8577319	4147503	8396231	3288242	8758406	4886222
RP_POS_617_56555a11_608	RP	POS	11.61	617.5656				2.08E-01	-0.23	0.97	6.65E-01	-0.09	0.58	1.34E-01	-0.27	0.83	4.35E-01	-0.18	0.76	1402363	468416	1272259	599308	1298419	732309	1246098	433584
RP_NEG_459_59665a15_583	RP	NEG	15.58	459.5967				5.75E-01	-0.12	0.64	6.65E-01	-0.09	0.33	4.84E-01	-0.16	0.39	7.50E-01	-0.07	0.73	698514	41684	693791	39591	695517	41101	692064	38361
RP_NEG_249_7896a15_551	RP	NEG	15.55	249.7896				1.31E-02	-0.58	1.15	6.66E-01	-0.08	0.39	1.53E-02	-0.62	1.03	2.66E-02	-0.54	1.03	1215132	89042	1170621	69802	1173658	64091	1167585	75615
RP_POS_252_23283a10_08	RP	POS	10.08	252.2328	(2E,4E)-N-(2-methylpropyl)dodeca-2,4-dienamide	252.1301(100), 95.0861(45), 81.0702(40), 109.1017(30), 69.0704(30), 55.0551(15)	3	4.26E-04	0.63	1.00	6.66E-01	-0.09	0.45	7.02E-03	0.59	0.95	4.97E-04	0.67	1.22	1248598	580173	1722923	767184	1756298	665907	1689547	862234
RP_POS_465_37708a10_659	RP	POS	10.66	465.3771				4.33E-01	-0.16	0.84	6.66E-01	0.09	0.28	5.93E-01	-0.12	0.69	3.91E-01	-0.20	0.88	5397273	428887	5328328	433114	5309489	479371	5347166	385335
HILIC_NEG_80_97431a2_985	HILIC	NEG	2.985	80.9743				7.13E-01	0.07	0.96	6.66E-01	-0.09	0.84	9.18E-01	0.02	0.22	5.98E-01	0.11	0.52	5863000	1085204	5949520	1349548	6008163	1382642	5890876	1327030
RP_POS_599_11755a9_666	RP	POS	9.67	599.1176				4.00E-02	-0.38	0.75	6.66E-01	-0.09	1.10	4.59E-02	-0.42	1.00	1.16E-01	-0.33	0.77	2880866	130407	2821606	163664	2828717	164725	2814494	163954
RP_POS_513_36938a13_2	RP	POS	13.20	513.3694				6.90E-01	0.08	0.50	6.67E-01	-0.09	0.55	8.63E-01	0.04	0.50	5.82E-01	0.13	0.32	7862057	1971409	8021099	1887661	8103010	1843494	7939188	1946043
RP_POS_276_87073a0_499	RP	POS	0.50	276.8707				3.05E-03	-0.40	1.16	6.67E-01	-0.10	1.24	7.83E-03	-0.45	1.21	5.73E-02	-0.35	1.21	3428712	670989	2779659	1791738	2857284	1912291	2702034	1678395
RP_POS_321_23972a10_173	RP	POS	10.17	321.2397		321.2402(100)	4	9.86E-01	0.00	0.93	6.67E-01	0.09	0.84	8.09E-01	0.05	0.70	8.48E-01	-0.04	0.88	37229135	5522419	37249625	6891094	36951319	7572012	37547931	6198911
HILIC_POS_304_21143a1_562	HILIC	POS	1.562	304.2114				2.30E-02	0.38	0.81	6.67E-01	-0.09	0.87	9.85E-02	0.34	0.61	2.88E-02	0.43	0.74	4419639	2170281	5586736	3255516	5727627	3143951	5445845	3389414

Supplementary table 1: Metabolomics results (in asceding order according to p-value from progressive ALD vs non-progressive ALD comparison, with molecular features with ID_level of 1-2 first)

							all_ALD_vs_control			Prog_ALD_vs_non-prog_ALD			Prog_ALD_vs_control_ALD			Non-prog_ALD_vs_control			Healthy_control		all_ALD		Non-prog_ALD		Progressive_ALD	
							t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA								
Feature_ID	RP_HILIC	POS_NEG	Average.Rt	Average.Mz	Metabolite.name	curated_MSMS	ID_level	p	d	VIP	p	d	VIP	p	d	VIP	p	d	VIP	Mean	SD	Mean	SD	Mean	SD	Mean	SD
RP_POS_233_9818a0_706	RP	POS	0.71	233.9818				1.22E-01	0.22	0.72	6.68E-01	0.10	0.79	1.96E-01	0.27	0.82	2.68E-01	0.17	0.52	1027757	279315	1155657	656760	1127240	525142	1184074	770745
RP_POS_431_28098a12_126	RP	POS	12.13	431.2810				1.05E-01	-0.29	0.83	6.68E-01	0.09	0.72	2.13E-01	-0.25	0.75	1.23E-01	-0.34	0.78	1065701	183900	999748	235649	989565	257847	1009932	213301
RP_POS_418_87854a0_465	RP	POS	0.47	418.8785				3.79E-07	-0.66	1.31	6.68E-01	0.09	1.14	3.74E-04	-0.62	1.36	6.80E-05	-0.71	1.43	447902	67000	317347	213184	308136	215881	326558	212237
HILIC_POS_518_3172a0_985	HILIC	POS	0.985	518.3172				6.82E-05	0.49	1.15	6.68E-01	-0.10	0.77	7.13E-03	0.44	1.29	2.41E-03	0.54	1.29	162332	616730	1497924	3047010	1629355	3166908	1366492	2948466
RP_NEG_459_14697a11_611	RP	NEG	11.61	459.1470				6.71E-01	-0.09	0.55	6.69E-01	0.09	0.61	8.38E-01	-0.05	0.41	5.80E-01	-0.13	0.53	578950	70568	572900	67248	570002	71666	575798	63117
RP_NEG_924_74475a0_498	RP	NEG	0.50	924.7448				1.42E-02	-0.35	1.14	6.69E-01	-0.09	1.24	2.24E-02	-0.40	1.16	1.09E-01	-0.31	1.17	1941405	352022	1694762	770471	1727960	818801	1661565	725728
RP_POS_818_58881a11_999	RP	POS	12.00	818.5888				4.72E-01	0.10	0.36	6.69E-01	-0.10	0.35	7.10E-01	0.05	0.19	4.97E-01	0.15	0.40	879076	848788	1080299	2350211	1181589	2947789	979009	1565027
RP_POS_193_15875a11_038	RP	POS	11.04	193.1588				1.51E-02	0.39	0.79	6.69E-01	-0.09	0.32	5.32E-02	0.35	0.71	3.54E-02	0.44	0.75	492334	604441	850269	970494	892041	1082954	808496	852401
HILIC_NEG_257_83884a1_362	HILIC	NEG	1.362	257.8388				5.23E-15	1.03	1.62	6.69E-01	0.09	0.67	6.21E-08	1.07	1.68	2.90E-10	0.99	2.01	94874	35967	210744	114301	205824	96196	215664	130741
RP_NEG_258_98245a0_553	RP	NEG	0.55	258.9825				7.68E-04	0.48	0.84	6.70E-01	-0.09	0.80	2.99E-02	0.43	0.86	1.25E-03	0.53	1.03	2382398	622595	2998342	1402562	3058642	1196677	2938042	1592185
RP_NEG_262_99207a8_627	RP	NEG	8.63	262.9921				8.66E-02	-0.35	0.79	6.70E-01	-0.09	0.36	8.55E-02	-0.39	0.73	1.72E-01	-0.31	0.63	4728174	288731	4625797	288290	4638184	285931	4613410	292999
RP_POS_156_07649a0_514	RP	POS	0.51	156.0765				1.95E-02	0.34	0.89	6.71E-01	-0.09	0.89	7.62E-02	0.30	0.87	5.22E-02	0.39	0.99	1867713	279860	2046735	570597	2071187	639499	2022284	497621
RP_POS_250_1774a11_129	RP	POS	11.13	250.1774				1.45E-02	0.39	0.83	6.71E-01	-0.09	0.32	5.34E-02	0.35	0.72	3.48E-02	0.44	0.80	1422751	1803388	2511149	2976974	2638669	3308612	2383629	2631638
RP_POS_791_58746a14_267	RP	POS	14.27	791.5875				2.94E-01	0.15	0.35	6.71E-01	0.09	0.34	3.70E-01	0.20	0.36	4.23E-01	0.11	0.53	1147642	460226	1278756	939184	1238506	552199	1319007	1214046
RP_POS_603_52252a15_221	RP	POS	15.22	603.5225				8.17E-01	0.05	0.31	6.71E-01	0.08	0.82	6.89E-01	0.09	0.50	9.79E-01	0.01	0.58	1700305	561997	1726631	535780	1703711	568378	1749551	505820
RP_NEG_480_30984a10_932	RP	NEG	10.93	480.3098				1.14E-01	0.29	1.09	6.71E-01	0.09	0.93	1.41E-01	0.34	0.82	2.00E-01	0.25	0.92	8343076	2752910	9287041	3315081	9145331	2712418	9428751	3847806
HILIC_NEG_115_92072a0_547	HILIC	NEG	0.547	115.9207				2.26E-04	-0.57	1.04	6.71E-01	0.09	0.67	4.70E-03	-0.52	0.94	1.50E-03	-0.61	1.03	8867036	754102	8133382	1374855	8074638	1417820	8192127	1342301
RP_NEG_666_45483a11_612	RP	NEG	11.61	666.4548				8.18E-02	-0.33	0.87	6.71E-01	0.09	0.75	1.70E-01	-0.28	0.78	9.43E-02	-0.37	0.73	6699177	579358	6481469	681219	6452361	732563	6510577	631832
RP_NEG_150_88582a0_524	RP	NEG	0.52	150.8858				5.58E-02	0.29	0.84	6.72E-01	-0.09	0.82	1.82E-01	0.24	0.87	8.16E-02	0.34	1.00	1808800	529101	2072507	990826	2114819	1032607	2030196	955812
RP_POS_478_38892a12_018	RP	POS	12.02	478.3889				9.94E-01	0.00	0.45	6.72E-01	0.09	0.45	8.55E-01	0.04	0.65	8.48E-01	-0.04	0.42	43388616	15947151	43362931	15890136	42684656	16495159	44041207	15398593
HILIC_NEG_115_92072a5_607	HILIC	NEG	5.607	115.9207				5.58E-01	-0.11	0.72	6.72E-01	0.09	0.75	7.75E-01	-0.06	0.17	4.67E-01	-0.15	0.49	50522328	6873398	49635397	8893444	49255973	8736442	50014820	9120397
RP_POS_384_18402a10_585	RP	POS	10.59	384.1840				2.03E-03	0.56	0.99	6.72E-01	-0.09	0.41	1.43E-02	0.52	0.89	3.30E-03	0.60	1.20	582918	279865	779287	358866	794596	347704	763978	372588
RP_POS_352_35684a11_904	RP	POS	11.90	352.3568				9.23E-01	-0.02	0.67	6.72E-01	-0.08	0.28	7.85E-01	-0.06	0.32	9.26E-01	0.02	0.49	215722	183686	212149	174992	219613	182555	204684	168610
RP_POS_722_52521a11_912	RP	POS	11.91	722.5252				9.11E-01	0.02	0.73	6.72E-01	0.09	0.68	7.65E-01	0.07	0.88	9.18E-01	-0.02	0.49	6884225	841441	6904071	952423	6863450	953986	6944692	958787
RP_POS_259_18988a9_303	RP	POS	9.30	259.1899				4.65E-03	-0.44	1.01	6.72E-01	0.09	1.01	3.38E-02	-0.39	1.10	1.28E-02	-0.49	1.04	1167571	123518	1077684	220218	1068302	228350	1087066	213679
RP_POS_375_21915a15_44	RP	POS	15.44	375.2192				6.69E-01	0.08	0.37	6.72E-01	0.09	0.34	5.54E-01	0.12	0.40	8.73E-01	0.03	0.87	1083990	231713	1105293	280479	1093345	293979	1117241	268752
RP_NEG_426_96716a10_998	RP	NEG	11.00	426.9672				8.53E-01	0.04	0.37	6.72E-01	0.08	0.45	7.52E-01	0.08	0.42	9.85E-01	0.00	0.22	1472347	2400739	1558558	1809918	1481447	1539099	1635669	2058518
HILIC_POS_498_90005a4_324	HILIC	POS	4.324	498.9001				1.22E-01	0.24	1.05	6.73E-01	-0.09	0.91	3.19E-01	0.19	0.65	1.31E-01	0.28	1.04	13690295	2046823	14504670	3766495	14665025	3727058	14344315	3836541
HILIC_POS_430_38919a0_517	HILIC	POS	0.517	430.3892				3.75E-01	0.14	0.64	6.73E-01	-0.09	0.80	5.95E-01	0.09	0.52	3.67E-01	0.19	0.44	84541	99602	106221	167524	113350	186735	99093	147403
RP_POS_196_8647a0_521	RP	POS	0.52	196.8647				8.59E-06	0.54	1.25	6.73E-01	-0.09	1.12	2.19E-03	0.50	1.24	9.46E-04	0.59	1.36	333643	57957	487898	315080	501295	330894	474501	301198
RP_POS_221_17502a11_039	RP	POS	11.04	221.1750				7.53E-03	0.41	0.90	6.73E-01	-0.09	0.34	3.60E-02	0.36	0.80	2.58E-02	0.45	0.81	214318	233153	377643	434138	396102	484050	359183	381836
HILIC_NEG_214_91925a2_911	HILIC	NEG	2.911	214.9193				1.50E-06	-0.62	1.36	6.73E-01	-0.09	0.81	4.29E-04	-0.58	1.49	3.28E-04	-0.67	1.47	1228457	141019	955967	479089	935605	513819	976330	445961
RP_POS_313_14249a9_475	RP	POS	9.48	313.1425				9.51E-02	-0.40	0.73	6.73E-01	0.08	0.42	1.48E-01	-0.36	0.68	9.27E-02	-0.44	0.65	774189	60701	754360	44396	752474	47895	756246	41000
RP_POS_846_82361a0_493	RP	POS	0.49	846.8236				4.17E-08	0.66	1.37	6.73E-01	-0.09	1.20	1.71E-04	0.61	1.44	7.72E-05	0.70	1.47	207948	106592	1302099	1834109	1379997	1917618	1224200	1762645
RP_NEG_499_27466a11_821	RP	POS	11.82	499.2747				5.63E-01	0.11	0.51	6.73E-01	-0.09	0.49	7.64E-01	0.07	0.42	4.63E-01	0.16	0.47	828302	64381	836144	72258	839213	66698	833075	77982
RP_POS_666_43732a10_903	RP	POS	10.90	666.4373				1.01E-06	0.78	1.55	6.73E-01	-0.09	0.52	8.37E-06	0.83	1.57	2.01E-04	0.74	1.46	268963	165790	481629	279665	469751	299259	493507	261108
RP_POS_266_17258a11_038	RP	POS	11.04	266.1726				7.87E-03	0.43	0.85	6.73E-01	-0.09	0.32	3.50E-02	0.38	0.79	2.16E-02	0.47	0.83	563685	415195	835311	676759	864042	742801	806580	609847
RP_POS_168_98027a15_484	RP	POS	15.48	168.9803				3.30E-01	0.19	0.74	6.74E-01	0.09	0.41	2.82E-01	0.23	0.40	5.14E-01	0.15	1.05	20507439	3096451	21141968	3423780	20997012	3581163	21286924	3288794
RP_POS_708_80408a0_498	RP	POS	0.50	708.8041				7.67E-09	-0.70	1.39	6.74E-01	0.09	1.20	6.52E-05	-0.66	1.48	2.93E-05	-0.75	1.48	2755230	145438	2027142	1133255	1979197	1182492	2075088	1091679
RP_POS_419_3143a11_253	RP	POS	11.25	419.3143				2.18E-04	0.69	1.23	6.75E-01	-0.08	1.00	2.83E-03	0.65	1.21	3.44E-04	0.73	1.32	6057999	1051659	6943957	1280568	6998119	1182190	6889795	1381887
RP_NEG_893_1936a9_433	RP	NEG	9.43	893.1936				8.30E-02	-0.31	0.72	6.75E-01	0.09	0.70	1.85E-01	-0.26	0.59	1.01E-01	-0.35	0.78	3305518	278467	3197084	371204	3181385	398235	3212784	345403
RP_NEG_378_91846a0_463	RP	NEG	0.46	378.9185				1.92E-09	-0.75	1.41	6.75E-01	0.09	1.18	4.00E-05	-0.70	1.48	7.55E-06	-0.79	1.52	2736057	238555	1897745	1217557	1846269	1236095	1949222	1209052
RP_POS_408_30829a11_038	RP	POS	11.04	408.3083				1.11E-02	0.42	0.83	6.75E-01	-0.09	0.34	4.36E-02	0.37	0.76	2.66E-02	0.46	0.80	14658051	16155458	24595437	25446372	25671238	27934846	23519636	22924503
RP_POS_132_95834a15_441	RP	POS	15.44	132.9583				1.44E-01	-0.41	0.75	6.75E-01	-0.07	0.29	1.23E-01	-0.44	0.85	2.01E-01	-0.37	0.54	22580187	61974127	208754489	32570816	210130940	36016910	207378039	29022093
RP_NEG_182_89629a15_534	RP	NEG	15.53	182.8963				1.52E-01	-0.26	0.78	6.75E-01	-0.09	0.36	1.38E-01	-0.30	0.93	3.15E-01	-0.22	0.71	1502828	336119	1396794	427706	1414865	450001	1378724	407958
RP_NEG_137_02351a5_647	RP	NEG	5.65	137.0235				7.80E-02	0.20	0.92	6.75E-01	-0.10	0.37	3.08E-01	0.16	0.86	1.51E-01	0.25	0.63	1192298	590242	3454774	12665000	3989608	13538845	2919940	11840351
HILIC_NEG_279_01553a3_869	HILIC	NEG	3.869	279.0155				2.30E-01	0.22	0.89	6.75E-01	-0.09	0.92	4.35E-01	0.17	0.45	1.85E-01	0.26	0.61	297730	105769	325635	134926	331332	118761	319939	150369
RP_NEG_227_90472a1_469	RP	NEG	1.47	227.9047				2.83E-10	0.88	1.48	6.75E-01	-0.09	0.59	1.06E-06	0.93	1.63	1.18E-06	0.84	1.50	1924792	1476796	4976075	3590225	4824564	3396126	5127587	3802890
RP_POS_420_88394a0_512	RP	POS	0.51	420.8839				1.69E-06	0.58	1.27	6.75E-01	-0.09	1.14	1.05E-03	0.53	1.29	4.74E-04	0.62	1.39	322461	92946	723793	774733	756479	813297	691107	740971
RP_POS_810_60004a13_653	RP	POS	13.65	810.6000				3.89E-06	1.01	1.73	6.76E-01	0.07	0.36	1.69E-05	1.05	1.53	1.05E-05	0.97	1.78	15455077	6669710	22349722	6003746	22096587	4779300	22602857	7060670
RP_NEG_381_17526a11_254	RP	NEG	11.25	381.1753				2.02E-06	0.93	1.79	6.76E-01	0.08	1.07	1.28E-05	0.97	1.74	1.86E-05	0.89	1.72	16529704	6050189	23225172	6829963	22937501	6293321	23512843	7380652
RP_NEG_517_24243a10_209	RP	NEG	10.21	517.2424				6.97E-02	0.30	0.69	6.76E-01	-0.09	0.26	1.69E-01	0.25	0.57	1.00E-01	0.34	0.64	717608	515236	940224	798166	973816	879635	906631	714897
RP_POS_247_99725a0_727	RP	POS	0.73	247.9973				1.47E-09	0.82	1.38	6.76E-01	-0.09	0.82	1.50E-05	0.78	1.42	1.25E-06	0.87	1.54	358312	255063	892291	683099	921029	676225	863553	695561
RP_POS_413_32361a10_881	RP	POS	10.88	413.3236				4.74E-06	-0.71	1.26	6.76E-01	-0.09	0.98	2.58E-04	-0.67	1.38	1.23E-04	-0.75	1.28	40685384	1476126	38877770	2660948	38765916	2803790	38989625	2533579
HILIC_POS_192_06172a7_377	HILIC	POS	7.377	192.0617				3.36E-04	-0.59	1.19	6.77E-01	-0.09	0.83	1.06E-03	-0.64	1.24	5.66E-03	-0.55	1.26	4772073	592020	4250650	919393	4289261	945270	4212038	900689
RP_NEG_920_56598a13_215	RP	NEG	13.22	920.5660				1.52E-04	0.69	1.14	6.77E-01	0.08	0.53	1.52E-03	0.73	1.14	4.22E-04	0.64	1.30	1558087	303222	1825056	393296	1808529	287857	1841583	478645
RP_NEG_164_92662a0_444	RP	NEG	0.44	164.9266				1.10E-08	-0.70	1.38	6.77E-01	0.09	1.20	1.20E-04	-0.65	1.45	2.26E-05	-0.74	1.49	1336791	76910	962897	588769	938176	596970	987618	585451
RP_NEG_383_31604a11_164	RP	NEG	11.16	383.3160				5.29E-02	0.31	0.91	6.77E-01	-0.09	0.65	6.05E-02	0.36	0.98	1.78E-01	0.27	0.83	1430109	256710	1550556	413087	1533225	430374	1567887	398660
RP_NEG_397_20599a9_913	RP	NEG	9.91	397.2060				8.98E-01	-0.02	0.90	6.77E-01	-0.09	0.75	7.62E-01	-0.07	0.55	9.32E-01	0.02	0.48	23343468	14361885	22956416	16057323	23629685	15215329	22283147	16985462
RP_POS_478_38867a11_211	RP	POS	11.21	478.3887				2.11E-07	-0.97	1.61	6.77E-01	0.08	0.69	8.79E-06	-0.93	1.59	9.17E-07	-1.01	1.62	1965748	190717	1727289	232186	1717556	224489	1737022	241521
RP_POS_519_23914a6_08	RP	POS	6.08	519.2391				7.18E-01	0.07	0.55	6.77E-01	0.09	0.54	6.25E-01	0.11	0.58	9.10E-01	0.02	0.37	18437571	1111152	18524700	1377211	18466957	1183657	18582443	1557010
RP_POS_192_97971a15_442	RP	POS	15.44	192.9797				8.60E-02	-0.35	0.80	6.78E-01	0.08	0.52	1.69E-01	-0.31	0.58	8.89E-02	-0.39	0.74	18912704	6072505	16739305	6259835	16477229	6482235	17001381	6083686
RP_POS_250_17754a11_039	RP	POS	11.04	250.1775				9.90E-03	0.41	0.84	6.78E-01	-0.09	0.32	4.14E-02	0.37	0.76	2.59E-02	0.46	0.81	853444	978431	1476375	1609168	1543728	1768253	1409022	1447658
RP_POS_256_82013a0_521	RP	POS	0.52	256.8201				2.27E-06	0.57	1.26	6.78E-01	-0.09	1.11	1.11E-03	0.53	1.26	5.47E-04	0.62	1.38	890546	129514	1344872	881709	1381773	928652	1307971	839948
HILIC_POS_114_63306a0_505	HILIC	POS	0.505	114.6331				7.05E-01	-0.07	0.85	6.78E-01	-0.09	0.48	5.64E-01	-0.11	0.64	9.15E-01	-0.02	0.89	282542	212482	264886	274369	276370	309721	253401	236424
HILIC_POS_640_31641a1_343	HILIC	POS	1.343	640.3164				3.73E-02	-0.41	1.32	6.78E-01	-0.08	0.50	3.84E-02	-0.45	1.23	1.02E-01	-0.36	1.43	385091	137070	324117	151762	330458	158003	317777	146584
RP_POS_429_2699a10_614	RP	POS	10.61	429.2699				8.02E-02	0.33	0.83	6.78E-01	-0.09	0.46	9.27E-02	0.37	0.69	1.66E-01	0.29	0.83	837914	497019	1025428	581644	1001136	542659	1049720	622769
RP_POS_395_81531a15_502	RP	POS	15.50	395.8153				1.36E-01	-0.24	0.43	6.79E-01	-0.09	0.49	1.50E-01	-0.29	0.54	3.03E-01	-0.20	0.42	1603000	123231	1558969	195010	1567106	189980	1550832	201510
RP_POS_516_28906a6_842	RP	POS	6.84	516.2891				1.95E-07	0.62	1.33	6.79E-01	-0.09	1.15	4.04E-04	0.57	1.43	1.65E-04	0.67	1.41	20990	48717	1347997	2370018	1446883	2470149	1249111	2286266
RP_POS_379_24234a12_325	RP	POS	12.33	379.2423				1.29E-04	-0.78	1.33	6.79E-01	0.08	0.62	1.48E-03	-0.74	1.19	1.20E-04	-0.82	1.50	3071418	652614	2520189	673097	2492126	570199	2548252	767224
RP_POS_296_89896a0_257	RP	POS	0.26	296.8990				2.88E-01	0.21	0.61	6.80E-01	-0.08	0.29	4.65E-01	0.17	0.35	2.37E-01	0.25	0.54	1869069	355958	1947738	375289	1963353	337749	1932124	412294
RP_NEG_1012_79669a0_489	RP	NEG	0.49	1012.7967				1.22E-05	0.54	1.23	6.80E-01	0.09	1.21	9.75E-04	0.59	1.33	2.58E-03	0.50	1.29	814481	260165	1395122	1187357	1345728	1145786	1444515	1237173
RP_NEG_158_97772a0_449	RP	NEG	0.45	158.9777				6.64E-07	-0.67	1.31	6.80E-01	-0.09	1.18	4.06E-05	-0.72	1.44	5.75E-04	-0.63	1.35	3369289	448709	2602605	1231816	2653847	1280351	2551363	1192079
RP_POS_451_30252a11_047	RP	POS	11.05	451.3025				7.57E-05	0.47	0.89	6.80E-01	0.09	0.80	6.86E-03	0.51	1.00	3.11E-03	0.42	1.24	27642	28671	253260	544273	230630	460327	275890	620941
RP_POS_940_52722a13_071	RP	POS	13.07	940.5272				6.58E-01	-0.09	0.59	6.80E-01	0.08	0.31	8.27E-01	-0.05	0.41	5.66E-01	-0.13	0.68	738746	447035	698442	442063	680080	453319	716804	434328
RP_POS_337_05789a0_616	RP	POS	0.62	337.0579				3.99E-05	-0.58	0.96	6.80E-01	-0.09	0.44	2.41E-04	-0.63	1.20	5.19E-03	-0.54	1.08	2060199	251604	1747864	581200	1771999	632244	1723730	530622
RP_POS_178_99969a15_442	RP	POS	15.44	178.9997				6.06E-01	-0.10	0.44	6.80E-01	0.09	0.43	7.90E-01	-0.06	0.49	5.23E-01	-0.14	0.40	4648426	1271435	4510841	1409002	4452349	1466307	4569333	1361634
RP_NEG_509_11502a8_859	RP	NEG	8.86	509.1150				6.32E-01	-0.09	0.58	6.80E-01	-0.09	0.45	5.39E-01	-0.13	0.44	8.25E-01	-0.05	0.26	9786508	520251	9733329	610075	9758653	605171	9708005	620030
RP_POS_182_99545a15_45	RP	POS	15.45	182.9955				6.04E-01	0.09	0.57	6.80E-01	0.09	0.33	5.44E-01	0.13	0.46	8.05E-01	0.05	0.18	7937083	1471219	8108192	2012486	8024636	1684802	8191748	2308689
HILIC_NEG_257_81924a2_946	HILIC	NEG	2.946	257.8192				6.97E-04	0.51	1.14	6.80E-01	-0.09	0.80	1.10E-02	0.46	0.95	3.87E-03	0.55	1.15	3582915	695911	4225400	1366108	4282097	1412857	4168703	1329609
HILIC_POS_236_0713a4_324	HILIC	POS	4.324	236.0713				7.67E-01	-0.05	0.84	6.80E-01	0.09	0.69	9.64E-01	-0.01	0.34	6.47E-01	-0.10	0.44	1405531	348271	1382781	452970	1363982	467644	1401579	441746
HILIC_POS_291_06946a2_456	HILIC	POS	2.456	291.0695				2.49E-09	0.73	1.25	6.80E-01	0.09	0.62	5.23E-05	0.77	1.30	6.57E-06	0.68	1.64	655687	645206	3839903	4766542	3642109	4140156	4037697	5355630
RP_POS_441_29742a11_934	RP	POS	11.93	441.2974				9.40E-01	-0.01	0.39	6.80E-01	-0.09	0.36	7.83E-01	-0.06	0.28	8.93E-01	0.03	0.45	144239553	37678800	143627130	45734757	145524099	48048772	141730161	43703486
RP_NEG_417_22507a11_255	RP	NEG	11.26	417.2251				4.71E-04	0.68	1.51	6.80E-01	0.08	0.96	1.24E-03	0.72	1.42	2.40E-03	0.64	1.38	2272908	529472	2684408	597688	2659617	560829	2709199	637157
RP_NEG_131_07033a4_556	RP	NEG	4.56	131.0703				1.06E-04	0.53	0.91	6.81E-01	0.09	0.40	3.22E-04	0.57	1.15	1.40E-02	0.48	0.76	1151013	361072	1614856	967582	1574733	1096537	1654978	828165
RP_NEG_530_86743a0_466	RP	NEG	0.47	530.8674				4.89E-08	-0.68	1.36	6.81E-01	0.09	1.23	1.96E-04	-0.63	1.41	4.13E-05	-0.72	1.46	895985	84690	638560	415757	621325	422646	655795	412310
RP_NEG_156_92947a15_399	RP	NEG	15.40	156.9295				5.77E-01	0.15	0.46	6.81E-01	0.07	0.26	4.88E-01	0.19	0.32	6.94E-01	0.12	0.42	905915	126999	919156	70876	916214	93017	922099	38464
HILIC_NEG_202_9292a4_277	HILIC	NEG	4.277	202.9292				4.98E-01	0.12	0.93	6.81E-01	-0.09	0.78	6.97E-01	0.08	0.15	4.34E-01	0.17	0.34	12268307	2297215	12605736	2830203	12722946	2911442	12488527	2771107

Supplementary table 1: Metabolomics results (in asceding order according to p-value from progressive ALD vs non-progressive ALD comparison, with molecular features with ID_level of 1-2 first)

								all_ALD_vs_control			Prog_ALD_vs_non-prog_ALD			Prog_ALD_vs_control_ALD			Non-prog_ALD_vs_control			Healthy_control		all_ALD		Non-prog_ALD		Progressive_ALD	
								t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA								
Feature_ID	RP_HILIC	POS_NEG	Average.Rt	Average.Mz	Metabolite.name	curated_MSMS	ID_level	p	d	VIP	p	d	VIP	p	d	VIP	p	d	VIP	Mean	SD	Mean	SD	Mean	SD	Mean	SD
HILIC_POS_160_03697a4_251	HILIC	POS	4.251	160.0370				9.94E-01	0.00	0.33	6.81E-01	-0.09	0.82	8.28E-01	-0.05	0.34	8.40E-01	0.04	0.28	2416353	2787981	2411541	3609413	2561018	3642688	2262064	3606499
RP_POS_220_93414a0_468	RP	POS	0.47	220.9341				6.41E-09	-0.72	1.39	6.81E-01	0.09	1.18	7.83E-05	-0.67	1.45	1.49E-05	-0.76	1.51	2876373	231817	2033507	1280842	1980518	1298394	2086495	1273985
RP_POS_364_19754a6_444	RP	POS	6.44	364.1975				9.66E-02	-0.31	0.56	6.81E-01	0.09	0.58	2.09E-01	-0.26	0.49	1.02E-01	-0.35	0.60	2644815	219570	2565191	268600	2554080	273199	2576302	266222
RP_POS_499_82596a5_14	RP	POS	5.14	499.8260				4.69E-01	0.14	0.44	6.81E-01	-0.08	0.49	6.45E-01	0.10	0.36	4.21E-01	0.18	0.57	1553367	1602769	1797108	1782730	1870827	1919706	1723390	1650682
RP_POS_134_99664a15_34	RP	POS	15.34	134.9966				1.43E-01	-0.32	1.06	6.81E-01	-0.08	0.27	1.30E-01	-0.36	0.92	2.37E-01	-0.28	0.99	34451877	12433617	30803565	10756227	31248289	10900865	30358842	10701471
RP_POS_820_07513a13_713	RP	POS	13.71	820.0751				5.83E-03	-0.55	0.99	6.81E-01	-0.08	0.81	8.16E-03	-0.59	1.06	2.10E-02	-0.51	0.98	3740102	1426293	2895061	1524378	2958084	1517943	2832039	1543575
RP_NEG_295_73599a15_599	RP	NEG	15.60	295.7360				3.46E-01	-0.19	0.76	6.82E-01	-0.08	0.47	3.05E-01	-0.23	0.53	5.13E-01	-0.15	0.66	2048918	94063	2030533	98613	2034605	99373	2026460	98685
RP_NEG_816_57745a13_558	RP	NEG	13.56	816.5775				1.17E-07	-1.42	2.29	6.82E-01	-0.05	0.75	9.30E-08	-1.45	2.18	2.39E-07	-1.39	1.97	4730108	1757716	2605128	943409	2644067	1017104	2566188	872129
HILIC_POS_159_14932a6_167	HILIC	POS	6.167	159.1493				8.94E-05	-0.77	1.30	6.82E-01	0.08	0.52	1.37E-03	-0.73	1.12	8.91E-05	-0.81	1.58	924772	299516	661744	329621	648138	278989	675350	375906
RP_NEG_487_22961a11_613	RP	NEG	11.61	487.2296				2.37E-02	-0.43	0.87	6.82E-01	-0.08	0.58	3.13E-02	-0.47	0.83	6.90E-02	-0.38	0.66	977432	93539	931191	111239	935777	108671	926605	114666
RP_POS_454_29236a10_389	RP	POS	10.39	454.2924				1.59E-01	0.25	1.05	6.82E-01	-0.09	0.83	3.50E-01	0.20	0.75	1.33E-01	0.29	0.90	3134937	953766	3438676	1310461	3492679	1165628	3384673	1450870
HILIC_NEG_201_95781a1_275	HILIC	NEG	1.275	201.9578				1.65E-01	-0.28	0.96	6.83E-01	-0.08	0.87	1.53E-01	-0.33	0.55	2.87E-01	-0.24	0.40	744190	152772	700518	153177	706824	155343	694211	152290
RP_POS_345_23718a10_962	RP	POS	10.96	345.2372				6.98E-02	-0.31	0.93	6.83E-01	0.09	0.99	1.74E-01	-0.27	0.88	8.65E-02	-0.36	0.88	504125	108504	458959	153197	452656	159957	465262	147479
RP_POS_167_07028a8_51	RP	POS	8.51	167.0703				4.95E-01	-0.11	0.52	6.83E-01	-0.09	0.44	4.71E-01	-0.16	0.45	6.96E-01	-0.07	0.76	2933422	79788	2920678	121300	2925669	97958	2915687	141707
RP_NEG_498_78275a15_66	RP	NEG	15.66	498.7828				1.07E-01	-0.26	0.78	6.83E-01	0.09	0.28	2.73E-01	-0.22	0.55	1.09E-01	-0.31	1.32	1797121	209655	1716409	327720	1702931	316125	1729888	341594
RP_POS_859_60461a11_96	RP	POS	11.96	859.6046				5.33E-01	0.13	0.64	6.84E-01	-0.08	0.79	7.00E-01	0.09	0.64	4.60E-01	0.17	0.62	9119084	3540002	9566459	3415337	9706672	3408580	9426247	3450878
RP_POS_377_32623a10_652	RP	POS	10.65	377.3262	Unknown	377.2632(70), 89.0598(100), 195.1234(65), 133.0858(45)	4	2.66E-01	-0.27	0.50	6.84E-01	-0.07	0.31	2.37E-01	-0.31	0.53	3.68E-01	-0.23	0.37	5440177	442581	5344838	321442	5358033	321476	5331643	324123
RP_NEG_322_88095a15_472	RP	NEG	15.47	322.8810				8.50E-01	0.04	0.51	6.84E-01	-0.08	0.47	9.93E-01	0.00	0.31	7.35E-01	0.08	0.52	23880221	744638	23908803	730891	23938803	789014	23878804	674481
HILIC_POS_132_1021a4_248	HILIC	POS	4.248	132.1021				3.98E-01	0.14	0.94	6.84E-01	0.09	0.86	3.75E-01	0.19	0.51	6.03E-01	0.10	0.48	76127022	25881370	81165445	37694249	79618539	34444183	82712351	40980784
RP_POS_294_93909a0_494	RP	POS	0.49	294.9391				2.43E-07	0.62	1.33	6.84E-01	-0.09	1.20	2.96E-04	0.58	1.41	2.36E-04	0.67	1.43	13699544	1228411	20773495	12620212	21291319	13468273	20255671	11825747
HILIC_POS_111_09208a3_029	HILIC	POS	3.029	111.0921				1.74E-03	0.51	1.10	6.84E-01	-0.09	0.72	1.30E-02	0.46	1.00	6.65E-03	0.55	1.13	1886544	224255	2061053	366558	2076093	390711	2046013	344028
HILIC_POS_87_09229a4_073	HILIC	POS	4.073	87.0923				2.71E-01	-0.21	0.80	6.84E-01	0.08	0.43	4.53E-01	-0.17	0.46	2.33E-01	-0.25	0.58	10381220	3075277	9660162	3551707	9514436	3343932	9805887	3776436
HILIC_NEG_115_92066a4_303	HILIC	NEG	4.303	115.9207				8.31E-02	0.26	0.77	6.84E-01	-0.09	0.88	2.93E-01	0.21	0.38	7.16E-02	0.30	0.79	37390369	2405080	38503410	4732561	38697380	4070697	38309441	5348270
HILIC_POS_144_10202a4_148	HILIC	POS	4.148	144.1020				4.69E-01	0.14	0.49	6.84E-01	0.08	0.42	3.95E-01	0.18	0.32	6.64E-01	0.10	0.21	7711013	6330150	8678584	7128385	8386518	7551704	8970650	6742584
RP_POS_526_29254a10_307	RP	POS	10.31	526.2925				1.04E-02	0.41	1.11	6.84E-01	-0.09	0.28	4.99E-02	0.36	0.91	2.41E-02	0.45	1.01	28599698	9508912	34656506	15918695	35308323	16851059	34004690	15071695
RP_POS_758_5686a15_466	RP	POS	15.47	758.5686				1.77E-01	-0.34	0.57	6.85E-01	-0.07	0.30	1.55E-01	-0.38	0.63	2.54E-01	-0.31	0.46	364013	259992	296648	168849	303554	177313	289742	161445
RP_POS_515_37292a13_136	RP	POS	13.14	515.3729				7.28E-01	-0.08	0.62	6.85E-01	-0.08	0.46	6.34E-01	-0.12	0.69	8.80E-01	-0.04	0.50	481757	310201	460226	280206	471685	266274	448767	295743
RP_POS_836_54022a11_165	RP	POS	11.17	836.5402				2.35E-02	0.28	0.59	6.85E-01	-0.09	0.39	5.46E-02	0.24	0.69	1.14E-01	0.33	0.60	924211	467540	1414251	1969845	1494843	2445549	1333658	1358603
RP_POS_413_13568a8_81	RP	POS	8.81	413.1357				1.66E-02	0.34	0.85	6.85E-01	-0.09	0.51	1.06E-01	0.29	0.63	3.36E-02	0.38	0.86	932225	707302	1428237	1613188	1494145	1607527	1362328	1632437
RP_NEG_691_50562a11_756	RP	NEG	11.76	691.5056				5.29E-04	-0.76	1.41	6.85E-01	-0.08	0.24	4.56E-04	-0.79	1.41	3.14E-03	-0.72	1.18	1140772	428267	825199	385243	840937	438653	809461	327004
RP_POS_282_90402a0_464	RP	POS	0.46	282.9040				1.16E-06	-0.65	1.31	6.85E-01	0.09	1.15	5.13E-04	-0.61	1.35	1.22E-04	-0.69	1.41	510801	86134	362663	247023	352574	251595	372752	244496
HILIC_POS_218_12877a0_542	HILIC	POS	0.542	218.1288				6.90E-05	0.69	1.40	6.85E-01	-0.08	0.65	2.28E-03	0.65	1.03	1.14E-04	0.73	1.75	164446	167416	324060	235592	333682	206382	314438	263358
HILIC_NEG_195_81091a2_951	HILIC	NEG	2.951	195.8109				5.83E-05	0.53	1.22	6.85E-01	-0.09	0.79	4.27E-03	0.48	1.19	1.77E-03	0.57	1.37	16758683	3318756	21766128	10523901	22195579	11011713	21336677	10105990
RP_POS_321_2392a11_61	RP	POS	11.61	321.2392				2.43E-03	0.53	0.88	6.86E-01	0.08	0.36	6.23E-03	0.57	1.09	1.42E-02	0.48	1.16	1955490	436805	2264881	611339	2239951	586814	2289811	639906
RP_POS_137_02957a0_454	RP	POS	0.45	137.0296				4.53E-06	-0.64	1.29	6.86E-01	-0.09	1.13	1.19E-04	-0.68	1.38	1.15E-03	-0.60	1.34	480599	73871	374214	179036	381508	184906	366919	174538
RP_POS_249_15706a3_319	RP	POS	3.32	249.1571				1.29E-04	-0.61	1.22	6.86E-01	0.09	1.11	2.69E-03	-0.57	1.22	8.08E-04	-0.66	1.28	17006370	4625852	12504967	7714106	12191000	7881568	12818934	7609798
RP_POS_510_75894a4_431	RP	POS	4.43	510.7589				9.83E-05	0.46	1.02	6.86E-01	0.09	1.06	5.07E-03	0.51	1.14	7.06E-03	0.41	1.11	130344	63157	471540	834208	437594	769241	505485	901068
RP_POS_176_12825a0_623	RP	POS	0.62	176.1283				1.06E-01	0.31	0.53	6.86E-01	0.08	0.32	1.15E-01	0.35	0.69	2.08E-01	0.27	0.48	1630353	1754582	2239191	2036185	2156353	1939157	2322029	2145314
RP_NEG_196_07428a0_538	RP	NEG	0.54	196.0743				2.98E-05	0.65	1.22	6.87E-01	-0.09	0.36	5.07E-03	0.60	0.97	1.75E-05	0.69	1.65	647048	156112	820516	283908	832064	208826	808967	344924
HILIC_POS_371_23962a4_249	HILIC	POS	4.249	371.2396				1.58E-01	0.26	0.92	6.87E-01	0.08	0.86	1.65E-01	0.30	0.49	2.89E-01	0.22	0.39	9985025	1919974	10575755	2354675	10480064	2229813	10671446	2492265
RP_POS_482_40634a10_658	RP	POS	10.66	482.4063				1.89E-01	-0.28	0.49	6.87E-01	-0.08	0.39	1.66E-01	-0.32	0.59	3.14E-01	-0.24	0.41	10739357	798656	10526941	745046	10557199	784343	10496682	710248
RP_NEG_418_89471a0_448	RP	NEG	0.45	418.8947				1.55E-04	-0.53	1.17	6.87E-01	-0.09	1.11	8.98E-04	-0.58	1.25	9.50E-03	-0.49	1.23	1744850	368314	1321357	866299	1356498	920914	1286217	815879
RP_POS_374_2103a11_159	RP	POS	11.16	374.2103				5.36E-03	-0.55	0.93	6.87E-01	0.08	0.72	2.02E-02	-0.51	0.84	7.81E-03	-0.59	1.01	912877	89498	858977	97995	855003	99149	862952	97668
HILIC_NEG_209_00395a0_7	HILIC	NEG	0.7	209.0040				1.24E-04	0.65	1.10	6.87E-01	0.08	0.80	7.16E-04	0.69	1.31	1.58E-03	0.61	1.08	458936	161134	608619	236505	599029	225836	618209	248638
RP_NEG_310_93149a0_462	RP	NEG	0.46	310.9315				2.54E-09	-0.74	1.40	6.87E-01	0.09	1.19	4.36E-05	-0.70	1.48	9.36E-06	-0.78	1.51	2244372	195200	1561398	1001162	1520808	1017848	1601987	992840
RP_POS_499_82712a6_021	RP	POS	6.02	499.8271				5.87E-01	0.09	0.62	6.87E-01	0.09	0.31	5.11E-01	0.13	0.51	8.07E-01	0.05	0.50	1553502	1330635	1720995	1974441	1640978	1901097	1801011	2061349
HILIC_NEG_171_94711a1_273	HILIC	NEG	1.273	171.9471				1.35E-01	0.28	1.06	6.87E-01	0.08	0.86	1.40E-01	0.32	0.59	2.57E-01	0.24	0.44	889034	183566	948124	217022	939331	210515	956918	225131
RP_NEG_898_58087a14_004	RP	NEG	14.00	898.5809				5.11E-02	-0.45	0.78	6.88E-01	0.08	0.37	1.02E-01	-0.41	0.71	4.65E-02	-0.48	0.79	11340482	2346527	10424940	1914389	10347421	1807930	10502459	2030686
RP_POS_838_55621a11_176	RP	POS	11.18	838.5562				7.66E-01	-0.04	0.44	6.88E-01	-0.09	0.40	4.19E-01	-0.08	0.71	9.71E-01	0.01	0.33	2084202	1042551	1964077	3581430	2109303	4716020	1818851	1905559
HILIC_POS_189_07359a5_461	HILIC	POS	5.461	189.0736				3.38E-01	-0.21	0.42	6.88E-01	-0.08	0.58	3.05E-01	-0.25	0.47	4.70E-01	-0.17	0.29	6914480	961735	6730716	845724	6764941	816487	6696491	880940
RP_POS_781_52612a10_46	RP	POS	10.46	781.5261				4.21E-01	0.13	0.35	6.88E-01	0.09	0.49	3.82E-01	0.17	0.57	6.54E-01	0.09	0.20	1558280	170890	1591501	278502	1580238	271626	1602765	287523
RP_POS_586_83374a6_307	RP	POS	6.31	586.8337				2.96E-06	0.56	1.27	6.88E-01	-0.09	1.11	1.66E-03	0.52	1.36	5.39E-04	0.61	1.34	70155	310198	1410592	2659985	1518129	2744456	1303055	2596113
RP_POS_200_90366a15_579	RP	POS	15.58	200.9037				2.84E-01	-0.18	0.44	6.89E-01	-0.09	0.25	3.19E-01	-0.23	0.51	4.18E-01	-0.14	0.52	2331444	77084	2312669	108283	2317042	79540	2308296	131621
RP_POS_407_33618a10_462	RP	POS	10.46	407.3362				2.22E-03	-0.54	1.09	6.89E-01	0.08	0.52	1.21E-02	-0.50	1.05	5.65E-03	-0.58	1.04	3322453	569914	2919998	768147	2889018	808135	2950979	732871
RP_NEG_384_93573a0_495	RP	NEG	0.50	384.9357				9.31E-07	0.59	1.32	6.89E-01	-0.09	1.20	5.02E-04	0.55	1.39	4.96E-04	0.64	1.41	28614564	2554439	39790474	20985686	40636482	22619455	38944467	19408384
RP_POS_475_41519a11_159	RP	POS	11.16	475.4152				9.02E-02	-0.28	0.88	6.89E-01	0.09	0.55	2.42E-01	-0.23	0.60	9.83E-02	-0.32	1.13	5245027	545894	5022601	867381	4987655	847293	5057548	894234
RP_POS_278_2482a10_381	RP	POS	10.38	278.2482				4.51E-04	0.55	1.00	6.89E-01	-0.09	0.35	8.21E-03	0.50	0.95	1.95E-03	0.59	1.20	3416419	2052970	5287176	3648862	5434108	3638621	5140243	3690052
RP_POS_237_22119a10_135	RP	POS	10.14	237.2212				6.78E-03	0.49	0.92	6.90E-01	-0.08	0.34	3.04E-02	0.45	0.77	1.06E-02	0.54	1.16	819273	78809	867122	99366	871121	99297	863123	100281
RP_NEG_342_73383a0_522	RP	NEG	0.52	342.7338				1.85E-07	-0.80	1.38	6.90E-01	0.08	1.06	3.79E-05	-0.76	1.40	1.12E-05	-0.84	1.46	645499	102045	499180	188362	491600	193366	506759	184869
RP_POS_244_99725a0_74	RP	POS	0.74	244.9973				2.80E-07	0.79	1.31	6.90E-01	-0.08	0.73	4.92E-05	0.75	1.42	1.54E-05	0.83	1.39	706468	599345	1551450	1106987	1595981	1139049	1506920	1083684
RP_NEG_548_85266a0_448	RP	NEG	0.45	548.8527				1.24E-03	-0.47	1.11	6.90E-01	-0.09	1.08	3.53E-03	-0.51	1.16	2.69E-02	-0.42	1.17	695204	177254	531960	380448	547249	406524	516671	355945
RP_POS_834_74548a0_499	RP	POS	0.50	834.7455				1.43E-02	-0.34	1.14	6.90E-01	-0.09	1.23	2.39E-02	-0.39	1.15	1.16E-01	-0.30	1.18	2163862	491790	1796414	1195197	1844441	1279799	1748388	1115147
RP_POS_196_00307a0_67	RP	POS	0.67	196.0031				3.85E-05	0.53	1.20	6.90E-01	-0.09	1.11	3.92E-03	0.48	1.21	1.50E-03	0.57	1.31	916157	121413	1120755	429128	1137996	446316	1103515	415036
RP_NEG_338_87381a15_658	RP	NEG	15.66	338.8738				7.17E-02	-0.35	0.77	6.90E-01	-0.08	0.42	8.49E-02	-0.39	0.68	1.42E-01	-0.31	0.75	3466570	371005	3324684	409363	3341128	376876	3308240	442706
RP_POS_221_17497a11_128	RP	POS	11.13	221.1750				1.56E-02	0.39	0.84	6.90E-01	-0.09	0.34	5.48E-02	0.35	0.73	3.71E-02	0.43	0.80	444109	541135	764883	881537	800279	976472	729486	783593
HILIC_NEG_172_8423a2_946	HILIC	NEG	2.946	172.8423				1.68E-06	0.58	1.30	6.90E-01	-0.09	0.77	8.36E-04	0.54	1.39	4.91E-04	0.63	1.50	319857	42749	458167	263072	468728	278150	447605	249461
HILIC_POS_448_05026a3_077	HILIC	POS	3.077	448.0503				2.56E-02	0.29	1.20	6.90E-01	-0.09	0.85	1.19E-01	0.25	1.22	7.35E-02	0.34	1.38	770415	45683	806421	137471	811939	150856	800904	123945
RP_POS_391_23505a11_31	RP	POS	11.31	391.2351				1.83E-02	-0.47	0.90	6.90E-01	0.08	0.75	4.57E-02	-0.43	0.83	2.61E-02	-0.51	0.92	1614261	227514	1499989	242904	1490243	261225	1509736	225336
RP_POS_438_37848a10_708	RP	POS	10.71	438.3785				8.07E-01	-0.05	0.35	6.90E-01	-0.08	0.65	6.93E-01	-0.09	0.26	9.65E-01	-0.01	0.25	8064370	842830	8022366	840018	8056067	842619	7988665	844592
RP_POS_158_96429a0_495	RP	POS	0.50	158.9643				2.60E-07	0.62	1.33	6.91E-01	-0.09	1.20	2.98E-04	0.58	1.41	2.43E-04	0.66	1.43	20323041	1468471	27981966	13668832	28529982	14578315	27433950	12819781
RP_NEG_210_90118a15_597	RP	NEG	15.60	210.9012				1.12E-01	-0.37	0.81	6.91E-01	-0.07	0.33	1.08E-01	-0.41	0.73	1.76E-01	-0.33	0.86	1552417	65092	1531989	50896	1534029	48862	1529949	53271
RP_NEG_894_54956a13_073	RP	NEG	13.07	894.5496				1.00E-01	-0.34	0.75	6.91E-01	-0.08	0.28	8.07E-02	-0.38	0.75	2.15E-01	-0.30	0.80	6986497	2110441	6268439	2123341	6353551	2417523	6183326	1802767
RP_NEG_246_07559a5_074	RP	NEG	5.07	246.0756				1.69E-01	-0.49	0.93	6.91E-01	-0.01	0.29	1.63E-01	-0.50	0.70	1.76E-01	-0.49	0.70	1557754	4730449	378297	428341	395460	458039	361134	400370
RP_POS_489_31497a11_476	RP	POS	11.48	489.3150				7.94E-01	0.05	0.40	6.91E-01	0.08	0.77	6.83E-01	0.09	0.43	9.52E-01	0.01	0.46	1666406	180315	1675988	177509	1668877	178287	1683099	178249
RP_POS_304_24869a9_527	RP	POS	9.53	304.2487				5.21E-02	-0.39	0.98	6.91E-01	0.08	0.69	1.19E-01	-0.35	0.84	5.60E-02	-0.43	0.92	881837	51127	860906	54290	858732	54599	863080	54445
RP_POS_197_01042a15_45	RP	POS	15.45	197.0104				5.69E-02	-0.36	1.07	6.92E-01	-0.08	0.27	5.40E-02	-0.40	0.83	1.49E-01	-0.32	1.54	15510403	3269517	14168117	3794746	14319653	4087928	14016582	3512271
RP_POS_337_23535a10_63	RP	POS	10.63	337.2354				3.46E-03	-0.64	1.34	6.92E-01	0.08	0.91	1.29E-02	-0.60	1.16	3.47E-03	-0.67	1.34	7957339	1603526	6978201	1450812	6920276	1328652	7036126	1574961
RP_POS_150_96906a15_627	RP	POS	15.63	150.9691				5.60E-01	0.13	1.26	6.92E-01	-0.08	0.44	7.16E-01	0.09	0.76	4.80E-01	0.17	1.07	26583079	10748014	27827447	9458977	28205053	8942989	27449841	10025088
HILIC_POS_175_10774a5_847	HILIC	POS	5.847	175.1077				2.72E-02	0.36	0.70	6.92E-01	0.09	0.66	6.12E-02	0.41	0.62	6.65E-02	0.32	0.79	1321815	736407	1711652	1144712	1665964	928381	1757340	1334661
RP_POS_196_00238a15_547	RP	POS	15.55	196.0024				6.81E-01	-0.09	0.38	6.92E-01	-0.08	0.61	5.94E-01	-0.13	0.34	8.27E-01	-0.05	0.53	83666123	8528295	82971162	7353798	83264546	7284466	82677777	7484732
HILIC_NEG_112_89616a2_948	HILIC	NEG	2.948	112.8962				1.02E-05	-0.58	1.34	6.92E-01	0.09	0.79	1.09E-03	-0.54	1.45	8.25E-04	-0.63	1.42	3825882	430106	3131844	1305646	3079761	1401278	3183927	1214535
RP_NEG_957_2063a9_727	RP	NEG	9.73	957.2063				3.75E-01	0.18	0.51	6.92E-01	-0.08	0.26	5.36E-01	0.14	0.36	3.35E-01	0.22	0.44	7258769	511520	7352321	525450	7373279	534271	7331363	521046
RP_NEG_666_84265a0_466	RP	NEG	0.47	666.8427				5.71E-09	-0.73	1.39	6.92E-01	0.09	1.20	5.11E-05	-0.68	1.47	1.56E-05	-0.77	1.49	789525	76909	550397	356323	536192	365940	564601	349571
RP_POS_802_53479a12_466	RP	POS	12.47	802.5348				3.09E-03	-0.69	1.17	6.92E-01	-0.07	0.58	4.48E-03	-0.73	1.22	6.38E-03	-0.66	1.07	2730910	1564888	1784190	1217721	1832739	1069719	1735641	1358985
RP_POS_579_29224a9_44	RP	POS	9.44	579.2922				6.11E-02	0.30	0.57	6.92E-01	-0.09	0.29	1.63E-01	0.26	0.68	9.31E-02	0.34	0.62	445636	61434	473948	102405	478028	110739	469868	94290
RP_POS_782_56866a14_258	RP	POS	14.26	782.5687				1.65E-03	0.42	0.82	6.92E-01	0.09	0.51	2.95E-02	0.46	0.81	4.20E-03	0.37	0.95	1781865	897580	2770196	2632613	2665234	1794275	2875158	3280372
HILIC_POS_230_13853a2_074	HILIC	POS	2.074	230.1385				4.45E-04	0.51	1.17	6.93E-01	0.09	0.32	4.50E-03	0.56	1.15	6.41E-03	0.47	1.21	366443	614229	977013	1290581	925758	1184300	1028268	1399023
RP_POS_410_84726a0_499	RP	POS	0.50	410.8473				1.75E-03	-0.42	1.19	6.94E-01	-0.09	1.24	5.83E-03	-0.46	1.24	4.36E-02	-0.37	1.23	8416853	1533671	6771052	4376696	6944753	4679653	6597352	4091593

Supplementary table 1: Metabolomics results (in asceding order according to p-value from progressive ALD vs non-progressive ALD comparison, with molecular features with ID_level of 1-2 first)

							all_ALD_vs_control			Prog_ALD_vs_non-prog_ALD			Prog_ALD_vs_control_ALD			Non-prog_ALD_vs_control			Healthy_control		all_ALD		Non-prog_ALD		Progressive_ALD	
							t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA								
Feature_ID	RP_HILIC	POS_NEG	Average.Rt	Average.Mz	Metabolite.name	curated_MSMS	ID_level	p	d	VIP	p	d	VIP	p	d	VIP	p	d	VIP	Mean	SD	Mean	SD	Mean	SD	Mean	SD
HILIC_POS_86_09711a4_248	HILIC	POS	4.248	86.0971				3.84E-01	0.15	0.91	6.94E-01	0.08	0.87	3.67E-01	0.19	0.48	5.81E-01	0.11	0.45	13694825	4441624	14579554	6372540	14326800	5839266	14832308	6915193
RP_POS_452_83173a0_512	RP	POS	0.51	452.8317				1.23E-05	-0.71	1.22	6.94E-01	-0.08	0.98	7.69E-05	-0.75	1.36	7.70E-04	-0.67	1.20	375889	100302	263610	164893	270147	173084	257073	157762
RP_POS_345_21573a11_609	RP	POS	11.61	345.2157				6.85E-01	-0.07	0.65	6.94E-01	0.08	0.72	8.74E-01	-0.03	0.53	6.05E-01	-0.11	0.81	1552061	366642	1519400	473390	1500630	530249	1538170	413384
RP_NEG_242_94353a0_46	RP	NEG	0.46	242.9435				1.38E-08	-0.71	1.38	6.94E-01	0.09	1.19	9.68E-05	-0.66	1.45	2.28E-05	-0.75	1.49	3256898	298077	2303624	1472663	2245253	1499255	2361995	1458429
RP_NEG_294_95297a15_288	RP	NEG	15.29	294.9530				4.77E-01	-0.15	0.51	6.94E-01	-0.08	0.26	3.82E-01	-0.19	0.46	6.64E-01	-0.11	0.40	2132944	90597	2119723	91396	2123344	106755	2116101	73848
HILIC_POS_195_12273a0_615	HILIC	POS	0.615	195.1227				8.54E-01	-0.03	1.04	6.94E-01	-0.08	0.88	7.12E-01	-0.07	0.48	9.63E-01	0.01	0.26	8138216	4377566	7957538	5939822	8192658	6185381	7722418	5736831
RP_POS_232_89619a0_515	RP	POS	0.52	232.8962				2.04E-04	-0.67	1.10	6.94E-01	0.08	0.65	3.37E-03	-0.63	1.02	3.49E-04	-0.71	1.22	1917297	410031	1562865	537999	1541570	489329	1584160	586878
RP_POS_156_0768a0_708	RP	POS	0.71	156.0768				7.12E-02	-0.63	1.15	6.94E-01	0.02	0.38	7.75E-02	-0.62	0.86	6.72E-02	-0.64	0.87	1237109	2740062	329126	433625	311966	432761	346287	438196
RP_NEG_385_63336a15_599	RP	NEG	15.60	385.6334				7.30E-01	-0.07	0.80	6.94E-01	0.08	0.42	9.14E-01	-0.02	0.30	6.07E-01	-0.11	0.69	613053	31295	610747	36704	609295	33455	612199	39979
HILIC_NEG_197_80795a3_94	HILIC	NEG	3.94	197.8080				6.53E-01	0.07	0.56	6.94E-01	0.09	0.51	5.80E-01	0.12	0.40	8.66E-01	0.03	0.21	507084	556783	566536	874287	531939	768519	601134	975341
HILIC_NEG_226_94025a5_606	HILIC	NEG	5.606	226.9403				2.54E-01	-0.23	1.07	6.95E-01	-0.08	0.51	2.42E-01	-0.27	1.02	3.94E-01	-0.19	1.14	186491	61795	171735	66498	174365	63308	169106	70088
RP_POS_198_08513a0_549	RP	POS	0.55	198.0851				2.24E-07	0.73	1.37	6.95E-01	0.08	1.19	1.88E-05	0.77	1.53	1.66E-04	0.69	1.30	447741	111675	628399	263007	617999	268575	638799	259621
HILIC_NEG_173_92632a2_947	HILIC	NEG	2.947	173.9263				6.00E-01	-0.10	0.70	6.95E-01	0.08	0.63	7.93E-01	-0.06	0.68	4.98E-01	-0.14	0.32	951293	252259	923268	288575	911857	260758	934680	316213
RP_POS_441_29733a13_475	RP	POS	13.48	441.2973				8.36E-01	-0.04	0.67	6.95E-01	-0.08	0.48	7.32E-01	-0.08	0.27	9.81E-01	-0.01	0.73	13716108	6115164	13462894	5609903	13684682	5168957	13241106	6063480
RP_POS_696_89886a6_668	RP	POS	6.67	696.8989				4.62E-07	0.60	1.30	6.95E-01	-0.09	1.12	4.99E-04	0.56	1.42	3.14E-04	0.64	1.36	26737	59480	1275463	2311537	1366829	2442611	1184097	2193643
RP_POS_846_5401a13_2	RP	POS	13.20	846.5401				2.56E-03	0.64	1.16	6.95E-01	0.08	0.63	6.71E-03	0.68	1.01	4.46E-03	0.60	1.32	2520142	795625	3027274	757316	2997353	541472	3057195	929376
RP_POS_322_95074a15_429	RP	POS	15.43	322.9507				4.50E-01	-0.17	0.32	6.95E-01	0.08	0.31	5.57E-01	-0.13	0.44	4.34E-01	-0.20	0.47	15654954	1385422	15446245	1223287	15397913	1529309	15494577	824530
HILIC_NEG_151_87407a2_949	HILIC	NEG	2.949	151.8741				5.70E-03	0.40	1.12	6.95E-01	-0.09	0.78	4.43E-02	0.36	0.94	1.91E-02	0.44	1.20	663435	128180	763741	274395	774569	286129	752913	264600
HILIC_POS_154_1591a5_647	HILIC	POS	5.647	154.1591				2.79E-01	-0.19	0.90	6.95E-01	0.08	0.85	4.59E-01	-0.14	0.70	2.80E-01	-0.23	0.95	19215010	1519907	18839296	2155566	18754286	2313257	18924307	2005455
RP_POS_475_30539a10_662	RP	POS	10.66	475.3054				1.88E-01	-0.28	0.84	6.96E-01	-0.08	0.42	1.90E-01	-0.32	0.74	2.81E-01	-0.24	0.59	908139	271375	835823	250852	845709	222634	825937	278158
RP_NEG_335_04987a0_708	RP	NEG	0.71	335.0499				3.89E-02	0.35	0.85	6.96E-01	-0.08	0.34	1.33E-01	0.31	0.83	4.40E-02	0.39	0.78	51450870	16779293	59487702	24141193	60438461	22896527	58536943	25522392
RP_NEG_134_89345a11_619	RP	NEG	11.62	134.8935				9.77E-01	-0.01	0.56	6.96E-01	0.08	0.50	8.89E-01	0.03	0.48	8.45E-01	-0.05	0.84	253678	88643	253157	84368	249835	82204	256479	87185
RP_NEG_409_31317a11_586	RP	NEG	11.59	409.3132	FA 28:7	409.3094(100)	3	2.12E-01	0.23	0.81	6.96E-01	0.08	0.81	1.89E-01	0.27	0.81	3.85E-01	0.19	0.77	860769	75247	881249	92963	877594	98370	884904	88071
HILIC_POS_199_18037a5_921	HILIC	POS	5.921	199.1804				9.97E-01	0.00	0.65	6.96E-01	-0.08	0.57	8.52E-01	-0.04	0.45	8.52E-01	0.04	0.29	3533077	921384	3532452	1053737	3573859	1019429	3491045	1095742
RP_POS_289_21606a8_256	RP	POS	8.26	289.2161				1.83E-01	0.27	0.80	6.97E-01	-0.08	0.63	3.00E-01	0.23	0.67	1.75E-01	0.31	0.72	414867	431123	533116	431494	550067	443700	516166	422750
RP_POS_531_29901a6_896	RP	POS	6.90	531.2990				8.91E-08	0.64	1.35	6.97E-01	-0.09	1.17	2.29E-04	0.60	1.46	1.30E-04	0.68	1.42	19954	24020	934793	1583866	997008	1662606	872578	1515354
RP_POS_198_18491a10_856	RP	POS	10.86	198.1849				7.10E-04	0.54	0.87	6.97E-01	0.08	0.69	6.53E-03	0.59	0.99	3.10E-03	0.50	1.03	597020	197241	764786	327079	751937	260724	777634	384487
RP_POS_444_33182a10_379	RP	POS	10.38	444.3318				3.03E-05	0.49	0.94	6.97E-01	-0.09	0.75	9.04E-03	0.45	0.97	1.05E-03	0.54	1.09	58949	55974	472460	941260	509419	912191	435502	977315
RP_NEG_129_05458a3_967	RP	NEG	3.97	129.0546				4.95E-01	0.11	0.87	6.97E-01	-0.09	0.29	7.49E-01	0.07	0.61	3.83E-01	0.15	0.46	48727724	12351919	50736165	19541701	51503306	16199988	49969023	22536835
HILIC_POS_468_30801a1_413	HILIC	POS	1.413	468.3080				6.47E-06	0.65	1.01	6.97E-01	-0.08	0.28	1.08E-03	0.61	1.05	1.08E-04	0.70	1.30	10824075	3829640	15865261	8224537	16187415	7950478	15543107	8558305
HILIC_POS_154_15919a5_12	HILIC	POS	5.12	154.1592				6.08E-01	-0.10	0.32	6.97E-01	-0.08	0.77	8.05E-01	-0.06	0.31	4.94E-01	-0.14	0.45	15984985	5177610	15422590	5957693	15189249	5002749	15655932	6824511
RP_POS_509_40408a10_663	RP	POS	10.66	509.4041				3.50E-01	-0.18	0.37	6.98E-01	-0.08	0.36	2.84E-01	-0.22	0.55	5.37E-01	-0.15	0.38	4111834	362239	4041330	387599	4056500	440220	4026161	330558
HILIC_NEG_115_92064a7_922	HILIC	NEG	7.922	115.9206				2.18E-01	-0.25	0.44	6.98E-01	-0.08	0.36	3.59E-01	-0.21	0.38	1.92E-01	-0.29	0.54	60022275	16681380	55781017	16899193	55120565	16048774	56441469	17847698
HILIC_NEG_184_99104a0_83	HILIC	NEG	0.83	184.9910				3.53E-01	0.16	0.84	6.98E-01	-0.08	0.92	5.92E-01	0.12	0.32	2.78E-01	0.20	0.46	501324	166777	536825	238931	546161	201653	527490	272945
RP_POS_356_27936a9_705	RP	POS	9.71	356.2794				5.37E-01	0.11	0.60	6.98E-01	0.08	0.38	3.75E-01	0.15	0.59	7.81E-01	0.07	0.51	366693	208701	395876	291446	384482	369039	407269	187512
RP_POS_798_59875a13_662	RP	POS	13.66	798.5988				1.05E-05	-1.04	1.75	6.98E-01	0.07	0.40	3.81E-05	-1.00	1.72	1.52E-05	-1.07	1.59	2230874	929283	1337245	720620	1309104	732950	1365385	714391
RP_POS_569_43127a15_414	RP	POS	15.41	569.4313				3.21E-01	0.20	0.39	6.98E-01	-0.08	0.36	4.89E-01	0.16	0.41	2.69E-01	0.24	0.45	14222673	6444285	15539706	6545902	15795273	5882370	15284139	7199761
RP_POS_281_91116a15_524	RP	POS	15.52	281.9112				6.66E-01	-0.08	0.31	6.98E-01	0.08	0.30	8.42E-01	-0.04	0.47	5.85E-01	-0.12	0.77	9339471	402149	9302553	466038	9284368	502994	9320738	430275
RP_POS_674_88623a6_603	RP	POS	6.60	674.8862				3.33E-07	0.61	1.31	6.99E-01	-0.09	1.14	5.22E-04	0.56	1.41	2.19E-04	0.65	1.38	32873	74311	1442399	2572566	1542706	2672887	1342092	2491264
RP_POS_197_12842a3_729	RP	POS	3.73	197.1284				2.42E-01	0.21	0.95	6.99E-01	-0.08	0.41	4.19E-01	0.17	0.58	2.30E-01	0.25	1.15	4664156	2443595	5300495	3224360	5426214	3243080	5174776	3233471
RP_POS_798_56317a11_911	RP	POS	11.91	798.5632				3.09E-01	0.15	0.55	6.99E-01	-0.09	0.44	5.72E-01	0.10	0.32	3.05E-01	0.19	0.60	1428847	1776616	1941512	3918409	2094257	3971647	1788767	3898667
HILIC_NEG_115_92075a2_169	HILIC	NEG	2.169	115.9208				7.53E-01	0.06	0.58	7.00E-01	-0.08	0.53	9.27E-01	0.02	0.20	6.27E-01	0.10	0.20	33941859	7007344	34405735	7815494	34709618	6871466	34101851	8718081
RP_NEG_264_9888a0_708	RP	NEG	0.71	264.9888				1.76E-02	0.37	0.96	7.00E-01	-0.08	0.33	6.92E-02	0.33	0.93	3.85E-02	0.42	0.80	1849732	501470	2148546	861758	2181986	923483	2115107	803310
RP_POS_271_18756a8_222	RP	POS	8.22	271.1876				6.33E-02	0.40	0.75	7.00E-01	-0.08	0.33	1.20E-01	0.36	0.64	6.69E-02	0.44	0.92	2220004	1275731	2703002	1172616	2748491	1214166	2657513	1140041
HILIC_POS_162_11247a5_457	HILIC	POS	5.457	162.1125				3.62E-03	0.47	1.04	7.01E-01	-0.08	0.56	4.41E-02	0.43	0.69	3.62E-03	0.51	1.01	1712260	453029	2040313	749924	2069357	622716	2011269	864148
RP_NEG_360_27634a9_149	RP	NEG	9.15	360.2763				1.70E-01	0.24	0.48	7.01E-01	0.08	0.42	2.30E-01	0.28	0.59	2.37E-01	0.20	0.51	453845	821269	706047	1092389	663718	701126	748377	1384105
RP_POS_243_19553a8_795	RP	POS	8.80	243.1955				5.48E-01	-0.12	0.63	7.01E-01	0.08	0.46	7.20E-01	-0.08	0.47	4.82E-01	-0.16	0.39	1146694	123672	1131231	133413	1126068	136802	1136394	131119
RP_POS_341_30481a10_643	RP	POS	10.64	341.3048				1.87E-03	-0.56	1.09	7.01E-01	0.08	0.88	1.02E-02	-0.52	1.08	4.43E-03	-0.60	1.06	1275934	225422	1116201	290330	1104966	301223	1127436	281620
RP_POS_217_10706a4_736	RP	POS	4.74	217.1071				3.19E-01	-0.18	0.56	7.01E-01	0.08	0.53	5.18E-01	-0.14	0.51	2.82E-01	-0.22	0.40	1959981	204520	1914913	266437	1904614	255399	1925211	279250
HILIC_POS_236_16452a0_819	HILIC	POS	0.819	236.1645				1.31E-01	0.17	0.47	7.02E-01	-0.09	0.54	1.39E-01	0.13	0.60	3.10E-01	0.22	0.47	11267	7309	386164	2462495	481288	3241046	291040	1314791
RP_NEG_166_08409a0_607	RP	POS	0.61	166.0841				3.39E-05	0.59	1.21	7.02E-01	-0.08	0.89	1.26E-03	0.55	1.19	1.05E-03	0.63	1.28	250341	135321	417021	303552	428729	327907	405312	279939
HILIC_NEG_295_73621a0_552	HILIC	NEG	0.552	295.7362				5.15E-01	-0.14	0.31	7.02E-01	-0.08	0.75	4.52E-01	-0.18	0.29	6.67E-01	-0.10	0.33	147441	91034	135528	84161	138769	84790	132287	84262
RP_POS_519_23932a15_438	RP	POS	15.44	519.2393				5.40E-01	-0.12	0.63	7.02E-01	-0.08	0.27	4.74E-01	-0.16	0.45	7.24E-01	-0.08	0.81	1974088	224424	1944671	264726	1954860	261337	1934482	270335
HILIC_NEG_201_80215a3_033	HILIC	NEG	3.033	201.8022				3.14E-06	0.57	1.32	7.02E-01	-0.09	0.82	9.50E-04	0.53	1.44	7.11E-04	0.62	1.49	15466803	501456	16828848	2636872	16930318	2811972	16727377	2473842
RP_POS_902_73163a0_499	RP	POS	0.50	902.7316				7.97E-03	-0.39	1.14	7.02E-01	-0.08	1.22	1.42E-02	-0.43	1.14	7.40E-02	-0.35	1.17	1850468	433928	1528771	910508	1563806	977722	1493735	846476
RP_NEG_379_17865a11_254	RP	NEG	11.25	379.1787				2.39E-06	0.92	1.78	7.03E-01	0.07	0.99	1.60E-05	0.95	1.72	2.15E-05	0.88	1.72	793269	302033	1125205	344331	1111957	318703	1138453	370967
RP_POS_248_03445a3_97	RP	POS	3.97	248.0345				3.12E-01	0.16	1.00	7.03E-01	-0.08	0.36	5.83E-01	0.12	0.74	2.32E-01	0.20	0.51	3924188	847978	4136801	1455825	4192769	1165580	4080834	1707964
RP_NEG_765_16833a9_503	RP	NEG	9.50	765.1683				9.91E-01	0.00	0.51	7.03E-01	-0.08	0.37	8.57E-01	-0.04	0.28	8.35E-01	0.04	0.36	8930190	479947	8931357	620083	8955166	596359	8907549	648114
RP_POS_285_06393a0_446	RP	POS	0.45	285.0639				1.09E-07	-0.67	1.35	7.04E-01	0.08	1.18	2.39E-04	-0.62	1.40	6.26E-05	-0.71	1.46	853694	92182	612705	395001	597563	402676	627847	390665
HILIC_NEG_226_98643a0_831	HILIC	NEG	0.831	226.9864				2.42E-01	0.20	0.84	7.04E-01	-0.08	0.93	4.80E-01	0.16	0.41	1.76E-01	0.24	0.56	384568	120642	417205	176353	423964	137321	410445	209488
RP_POS_643_29187a11_426	RP	POS	11.43	643.2919				9.27E-01	-0.02	0.18	7.04E-01	0.08	0.51	9.29E-01	0.02	0.33	7.99E-01	-0.06	0.33	885335	145913	882581	150596	876813	148627	888349	153829
HILIC_POS_96_0449a0_795	HILIC	POS	0.795	96.0449				2.46E-01	0.17	0.57	7.04E-01	0.09	0.73	3.58E-01	0.21	0.46	3.21E-01	0.12	0.42	2784613	2537531	3628432	5683598	3410599	3090451	3846265	7457754
HILIC_POS_146_98026a7_399	HILIC	POS	7.399	146.9803				6.52E-01	-0.09	0.28	7.04E-01	-0.08	0.81	5.63E-01	-0.13	0.23	8.13E-01	-0.06	0.13	1478191	213977	1458586	209327	1466591	217200	1450581	203034
RP_POS_245_18599a3_965	RP	POS	3.97	245.1860				5.26E-05	0.48	1.02	7.04E-01	0.09	1.09	1.42E-03	0.52	1.26	1.21E-02	0.43	1.00	89553	29309	1164103	2541040	1066992	2650943	1261213	2449243
RP_POS_341_35315a11_248	RP	POS	11.25	341.3532				1.89E-13	1.05	1.59	7.05E-01	0.08	0.66	5.68E-08	1.08	1.67	6.72E-10	1.01	1.79	204842	109941	469772	253063	460113	215977	479432	287319
HILIC_POS_197_08411a0_734	HILIC	POS	0.734	197.0841				8.51E-03	0.33	1.08	7.05E-01	0.09	0.87	6.87E-02	0.37	0.64	2.61E-02	0.29	0.95	640621	672475	1415549	2644010	1314590	1917819	1516508	3228842
HILIC_NEG_132_90034a1_409	HILIC	NEG	1.409	132.9003				7.57E-01	0.06	0.64	7.05E-01	-0.08	0.91	9.17E-01	0.03	0.10	6.19E-01	0.10	0.39	730873	97712	737023	95476	740663	65065	733383	118982
RP_POS_176_97488a15_38	RP	POS	15.38	176.9749				7.10E-01	0.08	0.56	7.05E-01	-0.07	0.33	8.52E-01	0.04	0.26	6.24E-01	0.12	0.53	33177518	4462664	33506935	3924705	33656423	4004237	33357447	3878333
RP_POS_132_10551a1_368	RP	POS	1.37	132.1055				2.39E-01	0.19	0.64	7.06E-01	-0.08	0.45	4.45E-01	0.14	0.49	2.48E-01	0.23	0.48	25958858	6404977	27826394	10978381	28244217	11342518	27408570	10700487
RP_POS_284_29446a11_166	RP	POS	11.17	284.2945				1.09E-10	0.93	1.56	7.06E-01	-0.08	0.85	7.08E-06	0.89	1.51	6.80E-09	0.97	1.77	75308554	24393651	124564001	54379187	126633194	46672939	122494809	61542179
RP_NEG_248_96021a14_262	RP	NEG	14.26	248.9602				2.60E-01	-0.21	0.45	7.06E-01	0.08	0.30	4.32E-01	-0.17	0.47	2.31E-01	-0.25	0.73	6432277	2531324	5822836	2957064	5710386	2798712	5935287	3131823
RP_POS_302_21472a8_219	RP	POS	8.22	302.2147				2.80E-02	0.43	1.11	7.06E-01	-0.08	1.21	6.55E-02	0.39	0.96	3.99E-02	0.47	0.96	6418905	3131622	7894522	3495197	8027199	3774108	7761845	3225259
RP_POS_365_24689a11_14	RP	POS	11.14	365.2469				8.12E-02	-0.26	0.95	7.06E-01	0.08	1.06	2.38E-01	-0.22	0.86	1.07E-01	-0.30	1.00	1223459	83201	1184905	162233	1178747	163725	1191063	162152
HILIC_POS_176_01083a4_25	HILIC	POS	4.25	176.0108				6.15E-01	-0.10	0.37	7.06E-01	-0.08	0.98	5.40E-01	-0.14	0.34	7.78E-01	-0.06	0.23	999948	1079338	887947	1118372	930394	1096202	845500	1149653
RP_POS_572_83289a0_508	RP	POS	0.51	572.8329				1.28E-06	-0.66	1.28	7.06E-01	-0.08	1.16	4.72E-05	-0.70	1.42	8.02E-04	-0.62	1.33	683372	94672	531342	247560	540736	261640	521948	234919
HILIC_NEG_290_84866a2_926	HILIC	NEG	2.926	290.8487				2.35E-06	-0.59	1.33	7.06E-01	0.08	0.78	8.12E-04	-0.54	1.45	5.33E-04	-0.63	1.51	298141	25514	235567	117928	231093	124862	240042	111653
RP_NEG_372_90158a0_456	RP	NEG	0.46	372.9016				1.62E-06	-0.63	1.29	7.07E-01	0.08	1.14	6.42E-04	-0.59	1.33	1.92E-04	-0.67	1.39	1121752	176354	804274	549278	783443	562043	825106	541101
RP_POS_323_19537a10_73	RP	POS	10.73	323.1954				1.46E-03	0.52	1.44	7.07E-01	-0.08	1.15	1.09E-02	0.48	1.28	5.49E-03	0.56	1.40	1691645	733750	2264253	1158730	2308183	1221234	2220323	1103340
RP_NEG_343_17175a6_399	RP	POS	6.40	343.1718	Magnoflorine	343.1749(100)	3	3.03E-01	-0.19	0.40	7.07E-01	0.08	0.38	4.98E-01	-0.15	0.33	2.65E-01	-0.23	0.57	1197745	64242	1183201	82069	1180090	76933	1186311	87576
RP_NEG_257_17599a8_906	RP	NEG	8.91	257.1760	Unknown	257.1742(100), 239.1642(60), 195.1735(40)	4	1.45E-01	0.29	0.78	7.07E-01	0.08	0.42	1.66E-01	0.33	0.69	2.27E-01	0.25	0.50	2645225	517570	2802939	547688	2782190	459743	2823688	627538
RP_POS_712_8197a0_472	RP	POS	0.47	712.8197				1.32E-07	-0.65	1.34	7.07E-01	0.08	1.17	2.84E-04	-0.61	1.39	8.43E-05	-0.69	1.46	604151	52639	446550	264948	436517	271110	456582	261000
RP_POS_316_12134a12_117	RP	POS	12.12	316.1213				2.96E-01	0.20	0.49	7.07E-01	-0.08	0.34	2.94E-01	0.24	0.57	4.41E-01	0.16	0.45	398362	133932	428330	156942	422388	141204	434271	172492
HILIC_NEG_199_80498a2_952	HILIC	NEG	2.952	199.8050				8.00E-05	0.52	1.22	7.07E-01	-0.08	0.79	4.47E-03	0.48	1.19	2.32E-03	0.56	1.36	9496132	1849069	12186924	5739676	12404153	6045606	11969694	5469408
RP_NEG_215_86908a15_571	RP	NEG	15.57	215.8691				2.42E-01	0.17	0.37	7.07E-01	-0.08	0.42	4.95E-01	0.12	0.64	2.49E-01	0.21	0.42	1229039	69735	1252396	155726	1258289	155275	1246503	157528
RP_POS_230_96283a15_587	RP	POS	15.59	230.9628				5.69E-01	-0.09	0.36	7.07E-01	-0.08	0.34	5.71E-01	-0.13	0.32	7.53E-01	-0.04	0.56	8107911	186596	8080294	353285	8093676	217028	8066911	452439
RP_NEG_190_9277a15_488	RP	NEG	15.49	190.9277				8.31E-01	0.04	0.37	7.08E-01	-0.08	0.39	9.80E-01	0.01	0.24	7.31E-01	0.08	0.31	36526720	699642	36557184	705812	36583854	775657	36530513	635148
RP_POS_296_25839a9_398	RP	POS	9.40	296.2584				7.15E-01	-0.11	0.75	7.08E-01	-0.05	0.28	6.60E-01	-0.13	0.56	7.88E-01	-0.08	0.46	2515724	4761683	2196018	2118233	2275958	1925654	2116077	2311754
HILIC_POS_122_92489a2_992	HILIC	POS	2.992	122.9249				1.54E-05	-0.59	1.35	7.08E-01	0.08	0.80	1.18E-03	-0.55	1.44	7.99E-04	-0.63	1.42	154992135	22941962	122285874	60377874	120008170	64279332	124563578	56771057

Supplementary table 1: Metabolomics results (in asceding order according to p-value from progressive ALD vs non-progressive ALD comparison, with molecular features with ID_level of 1-2 first)

								all_ALD_vs_control			Prog_ALD_vs_non-prog_ALD			Prog_ALD_vs_control_ALD			Non-prog_ALD_vs_control			Healthy_control		all_ALD		Non-prog_ALD		Progressive_ALD	
								t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA								
Feature_ID	RP_HILIC	POS_NEG	Average.Rt	Average.Mz	Metabolite.name	curated_MSMS	ID_level	p	d	VIP	p	d	VIP	p	d	VIP	p	d	VIP	Mean	SD	Mean	SD	Mean	SD	Mean	SD
HILIC_POS_371_2402a4_626	HILIC	POS	4.626	371.2402				6.00E-01	0.10	0.83	7.08E-01	0.08	0.70	5.52E-01	0.13	0.21	7.74E-01	0.06	0.42	6183672	1323518	6335102	1673443	6271971	1393406	6398232	1925685
RP_POS_1016_79303a0_493	RP	POS	0.49	1016.7930				1.52E-08	0.68	1.38	7.08E-01	-0.08	1.19	1.48E-04	0.64	1.45	3.29E-05	0.72	1.49	41313	42918	669270	1016476	707593	1029519	630947	1012239
RP_NEG_128_0343a0_71	RP	NEG	0.71	128.0343				1.53E-07	0.72	1.12	7.08E-01	0.08	0.70	1.61E-04	0.76	1.23	9.16E-06	0.68	1.36	3435480	544191	4371521	1379677	4319494	1123595	4423548	1605576
RP_NEG_289_89835a3_965	RP	NEG	3.97	289.8984				3.78E-01	0.15	0.87	7.08E-01	-0.08	0.32	6.23E-01	0.11	0.62	3.02E-01	0.19	0.50	1972341	669166	2110950	1024152	2149531	869557	2072369	1166197
RP_POS_175_06256a5_353	RP	POS	5.35	175.0626				4.81E-01	-0.14	0.42	7.09E-01	0.08	0.44	6.54E-01	-0.11	0.46	4.03E-01	-0.18	0.60	1023940	331579	976148	330523	963702	290591	988594	368730
HILIC_POS_142_08643a1_318	HILIC	POS	1.318	142.0864				4.97E-03	0.41	0.73	7.09E-01	0.08	0.43	9.44E-03	0.45	0.93	5.65E-02	0.37	0.69	10299266	9343694	17593764	19350304	16865743	20921250	18321786	17824974
RP_POS_530_32245a10_584	RP	POS	10.58	530.3225				5.45E-03	0.48	1.08	7.09E-01	-0.08	0.75	4.08E-02	0.44	0.89	5.55E-03	0.52	1.08	408224	168790	517039	235006	525881	200774	508197	266670
HILIC_POS_294_84357a2_992	HILIC	POS	2.992	294.8436				7.60E-06	-0.57	1.35	7.09E-01	0.08	0.78	1.34E-03	-0.53	1.47	7.65E-04	-0.61	1.51	2033095	235409	1589506	854714	1557355	900844	1621657	813850
RP_POS_643_52643a11_71	RP	POS	11.71	643.5264				2.01E-01	-0.25	0.64	7.09E-01	-0.08	0.85	1.69E-01	-0.29	0.79	3.60E-01	-0.21	0.45	2398575	2659781	1681898	2929570	1792109	3264992	1571686	2579720
RP_POS_302_24557a11_161	RP	POS	11.16	302.2456				5.90E-05	0.72	1.15	7.09E-01	0.08	0.59	5.94E-04	0.76	1.17	3.08E-04	0.68	1.31	2372502	1099130	3411608	1454075	3356912	1215619	3466304	1669725
HILIC_POS_114_12802a0_868	HILIC	POS	0.868	114.1280				2.05E-03	-0.52	1.13	7.09E-01	-0.08	0.67	4.21E-03	-0.56	1.20	1.86E-02	-0.48	1.05	504533	151912	392014	229129	400629	239789	383399	220049
RP_POS_346_00757a0_63	RP	POS	0.63	346.0076				5.18E-08	-0.66	1.36	7.09E-01	0.08	1.18	2.02E-04	-0.62	1.42	5.96E-05	-0.71	1.47	30759798	2173156	22152702	14228035	21618114	14548436	22687291	14027299
RP_POS_615_43115a15_336	RP	POS	15.34	615.4312				9.14E-01	0.02	0.85	7.09E-01	0.08	0.39	7.89E-01	0.06	0.59	9.41E-01	-0.02	0.64	7733531	2043600	7779277	2164485	7697961	2200590	7860592	2146976
RP_NEG_650_46106a11_611	RP	NEG	11.61	650.4611				7.01E-02	-0.36	0.82	7.09E-01	0.08	0.56	1.27E-01	-0.32	0.70	8.88E-02	-0.40	0.70	5151818	831421	4834640	888385	4801277	992834	4868002	778825
RP_NEG_339_20068a11_613	RP	NEG	11.61	339.2007				3.05E-01	0.18	0.61	7.10E-01	0.08	0.32	2.51E-01	0.22	0.58	5.16E-01	0.14	0.47	1842222	743273	2011478	977588	1974794	1097780	2048162	850290
RP_POS_441_297a13_631	RP	POS	13.63	441.2970				6.20E-01	-0.10	0.26	7.10E-01	-0.08	0.36	5.34E-01	-0.14	0.29	7.85E-01	-0.06	0.16	20204422	6076553	19586221	6161204	19817186	6491127	19355256	5869581
HILIC_POS_468_30814a1_267	HILIC	POS	1.267	468.3081				1.02E-04	0.59	0.90	7.10E-01	-0.08	0.30	4.93E-03	0.55	0.92	4.99E-04	0.63	1.18	1543343	520557	2094292	1004717	2131892	943077	2056693	1071090
RP_POS_239_1261a7_475	RP	POS	7.48	239.1261				8.77E-01	-0.04	0.61	7.10E-01	0.07	0.48	9.99E-01	0.00	0.30	7.77E-01	-0.07	0.60	1784200	349411	1773592	285178	1762924	300158	1784259	272003
RP_POS_590_48065a12_463	RP	POS	12.46	590.4807				4.37E-01	0.13	0.62	7.10E-01	0.08	0.30	4.29E-01	0.17	0.39	6.25E-01	0.09	0.35	2117548	349381	2181391	533913	2161424	458242	2201358	604271
RP_POS_514_63751a6_842	RP	POS	6.84	514.6375				2.83E-07	0.61	1.32	7.11E-01	-0.08	1.13	4.58E-04	0.57	1.41	2.08E-04	0.65	1.40	28701	73273	935920	1642392	997329	1706907	874511	1590196
HILIC_POS_312_20135a0_552	HILIC	POS	0.552	312.2014				4.93E-01	0.11	0.31	7.11E-01	0.08	0.63	4.84E-01	0.15	0.25	6.91E-01	0.07	0.35	354950	46862	362848	79408	359879	64941	365816	92220
RP_POS_444_76266a13_708	RP	POS	13.71	444.7627				3.22E-04	-0.76	1.46	7.11E-01	-0.07	0.51	7.15E-04	-0.79	1.37	1.16E-03	-0.72	1.40	1829214	864937	1157522	830119	1188537	771948	1126507	891287
RP_POS_480_83252a0_499	RP	POS	0.50	480.8325				1.03E-03	-0.45	1.20	7.11E-01	-0.08	1.24	4.17E-03	-0.49	1.27	2.86E-02	-0.41	1.23	2181893	396269	1762870	1031907	1801418	1095526	1724323	973749
RP_POS_639_62732a0_208	RP	POS	0.21	639.6273				4.47E-01	0.15	0.52	7.11E-01	-0.08	0.38	6.07E-01	0.12	0.50	3.99E-01	0.19	0.53	2775140	1142379	2954241	1175972	2998156	1188721	2910326	1173478
RP_POS_300_91559a0_464	RP	POS	0.46	300.9156				2.15E-06	-0.63	1.29	7.11E-01	0.08	1.14	6.28E-04	-0.59	1.33	2.13E-04	-0.67	1.39	322194	54082	231046	156814	225196	161166	236897	153751
RP_NEG_437_0553a7_855	RP	NEG	7.86	437.0553				5.14E-01	-0.14	0.60	7.11E-01	-0.07	0.82	3.83E-01	-0.18	0.49	6.93E-01	-0.11	0.50	3154236	6738239	2279781	5935410	2501534	8051242	2058028	2500861
HILIC_NEG_114_89414a2_951	HILIC	NEG	2.951	114.8941				2.56E-05	-0.54	1.31	7.11E-01	0.08	0.78	1.68E-03	-0.50	1.42	2.08E-03	-0.58	1.48	316720	33438	258378	119778	253913	131301	262843	108193
RP_POS_999_63898a10_516	RP	POS	10.52	999.6390				3.83E-05	0.63	1.30	7.11E-01	-0.08	0.28	1.05E-03	0.59	1.26	6.77E-04	0.67	1.25	232332	158466	408363	297335	419441	316485	397285	279655
RP_POS_274_87259a0_499	RP	POS	0.50	274.8726				1.45E-03	-0.42	1.18	7.12E-01	-0.08	1.23	5.12E-03	-0.46	1.24	4.00E-02	-0.38	1.23	15572909	2875319	12391066	8352728	12702205	8990675	12079926	7741456
RP_POS_716_54761a10_902	RP	POS	10.90	716.5476				3.27E-01	-0.22	0.52	7.12E-01	-0.07	0.40	2.96E-01	-0.26	0.42	4.43E-01	-0.19	0.48	1461624	396682	1385143	321493	1397105	320745	1373180	325047
HILIC_POS_171_18558a5_177	HILIC	POS	5.177	171.1856				7.48E-01	-0.06	0.59	7.12E-01	0.08	0.55	9.31E-01	-0.02	0.41	6.01E-01	-0.10	0.60	132639745	23478208	131014009	28637539	129948014	21196304	132080004	34718178
RP_POS_254_12431a0_705	RP	POS	0.71	254.1243				2.98E-13	0.90	1.72	7.12E-01	-0.08	0.61	1.32E-06	0.86	1.70	5.76E-08	0.93	1.81	78026	53982	842434	905594	876110	881757	808757	936550
HILIC_POS_508_37698a1_303	HILIC	POS	1.303	508.3770				1.53E-01	-0.31	0.74	7.12E-01	-0.07	0.87	1.49E-01	-0.35	0.56	2.42E-01	-0.28	0.60	3047323	980854	2765704	869408	2797990	851027	2733417	894870
RP_POS_357_27856a8_865	RP	POS	8.87	357.2786				6.00E-05	0.53	1.70	7.13E-01	-0.08	0.43	6.49E-04	0.49	1.61	4.89E-03	0.57	1.57	243112	245965	593115	722799	619956	858917	566273	562432
RP_POS_419_34915a11_62	RP	POS	11.62	419.3492				5.42E-02	-0.38	1.04	7.13E-01	-0.07	0.72	3.78E-02	-0.42	0.95	1.56E-01	-0.34	0.91	3309035	914110	2935906	995697	2972852	1202725	2898959	744128
RP_POS_794_56805a12_888	RP	POS	12.89	794.5681				1.78E-01	-0.25	0.86	7.13E-01	-0.08	0.55	1.83E-01	-0.29	0.65	3.15E-01	-0.21	0.50	3543853	1345500	3149211	1656083	3210617	1611978	3087805	1713192
RP_NEG_225_06955a7_846	RP	NEG	7.85	225.0696				7.96E-01	-0.04	0.43	7.13E-01	-0.08	0.28	7.04E-01	-0.08	0.36	9.84E-01	0.00	0.15	2211908	2564337	2058513	3795176	2199221	3105863	1917804	4406118
RP_NEG_738_80194a0_498	RP	NEG	0.50	738.8019				3.07E-03	-0.43	1.15	7.13E-01	-0.08	1.23	7.60E-03	-0.47	1.19	4.13E-02	-0.39	1.19	867318	203694	697227	431556	713219	458590	681235	406762
RP_POS_489_31802a10_455	RP	POS	10.46	489.3180				4.87E-01	0.14	0.69	7.13E-01	0.07	0.24	4.42E-01	0.18	0.85	6.38E-01	0.10	0.34	2269148	752942	2376469	760240	2348314	717127	2404623	807363
HILIC_POS_169_0457a7_374	HILIC	POS	7.374	169.0457				7.97E-05	-0.58	1.20	7.13E-01	-0.08	0.85	7.25E-04	-0.62	1.23	3.79E-03	-0.54	1.29	1852308	185747	1644978	384689	1659221	393430	1630735	379197
RP_NEG_638_27618a10_622	RP	NEG	10.62	638.2762				3.13E-01	0.21	1.21	7.13E-01	-0.07	0.81	4.59E-01	0.17	0.93	2.87E-01	0.24	0.97	2585591	410339	2670733	416814	2686164	418939	2655303	418351
RP_NEG_180_97238a0_497	RP	NEG	0.50	180.9724				3.30E-03	0.41	1.15	7.13E-01	-0.08	1.09	3.33E-02	0.37	1.13	1.66E-02	0.45	1.24	17253729	580331	17781826	1432736	17834825	1507637	17728827	1366988
HILIC_POS_396_31082a0_623	HILIC	POS	0.623	396.3108				1.09E-01	0.28	0.83	7.14E-01	-0.08	0.92	1.88E-01	0.24	0.65	1.56E-01	0.32	0.49	340941	180455	406543	248484	415735	292389	397350	197700
RP_NEG_530_30237a10_508	RP	NEG	10.51	530.3024				1.19E-01	-0.32	0.62	7.14E-01	-0.07	0.80	1.16E-01	-0.36	0.70	2.12E-01	-0.29	0.71	5559800	1532196	5068539	1500434	5123975	1519674	5013104	1494278
RP_NEG_352_85303a15_533	RP	NEG	15.53	352.8530				5.97E-01	0.12	0.45	7.14E-01	-0.07	0.48	7.25E-01	0.09	0.53	5.26E-01	0.16	0.31	2327598	257374	2353994	197084	2361272	189308	2346716	206230
RP_NEG_144_92288a15_618	RP	NEG	15.62	144.9229				4.34E-02	-0.41	0.88	7.14E-01	0.07	0.34	1.01E-01	-0.38	0.69	4.49E-02	-0.45	0.99	3054208	107582	3008836	109025	3004815	105298	3012857	113556
RP_POS_771_64496a11_039	RP	POS	11.04	771.6450				1.21E-01	0.25	0.66	7.15E-01	-0.08	0.24	1.94E-01	0.21	0.79	1.91E-01	0.29	0.58	422405	795022	718086	1256849	764408	1538297	671764	906003
RP_NEG_215_16521a9_161	RP	NEG	9.16	215.1652				1.23E-03	0.51	1.49	7.15E-01	0.08	1.33	1.71E-03	0.55	1.47	2.30E-02	0.47	1.20	1599735	991340	2414875	1702457	2352302	1931162	2477448	1455503
RP_POS_232_1543a2_226	RP	POS	2.23	232.1543				3.46E-03	0.37	0.66	7.16E-01	-0.08	0.78	8.14E-02	0.33	0.67	6.47E-03	0.42	0.82	1553546	580897	2226626	2013095	2300539	1730751	2152712	2276216
RP_POS_302_936a15_367	RP	POS	15.37	302.9360				6.19E-02	-0.24	0.49	7.17E-01	-0.08	0.25	1.09E-01	-0.28	0.63	2.45E-01	-0.20	0.52	6797762	232510	6630048	790029	6658926	783993	6601171	802922
RP_POS_151_144a0_536	RP	POS	0.54	151.1440				6.31E-01	0.08	0.66	7.17E-01	-0.08	0.60	5.81E-01	0.12	0.67	8.33E-01	0.04	0.40	2316801	2110769	2563086	3489290	2435544	2973359	2690628	3965438
HILIC_NEG_134_89476a0_936	HILIC	NEG	0.936	134.8948				6.55E-03	0.47	1.29	7.17E-01	-0.08	0.64	2.43E-02	0.43	0.92	1.68E-02	0.51	1.32	31862186	5886746	35582384	8267754	35884368	9020002	35280400	7520636
RP_NEG_368_68005a15_577	RP	NEG	15.58	368.6801				4.14E-02	-0.40	0.87	7.17E-01	-0.07	0.24	4.66E-02	-0.44	0.85	1.02E-01	-0.36	0.76	1954541	90272	1915276	99649	1918914	101664	1911638	98488
RP_POS_335_15131a10_731	RP	POS	10.73	335.1513				3.22E-03	0.48	1.37	7.18E-01	-0.08	1.10	1.87E-02	0.44	1.19	1.10E-02	0.52	1.34	5654861	2536158	7499032	4114220	7648864	4391820	7349200	3855536
HILIC_NEG_160_97612a7_352	HILIC	NEG	7.352	160.9761				3.04E-04	-0.61	1.17	7.18E-01	0.08	0.73	2.62E-03	-0.57	1.18	1.74E-03	-0.65	1.23	2736016	167306	2590143	247550	2581132	265456	2599154	230609
HILIC_POS_144_98228a7_4	HILIC	POS	7.4	144.9823				1.67E-01	-0.30	0.59	7.19E-01	-0.07	0.39	1.75E-01	-0.33	0.52	2.50E-01	-0.26	0.48	3068514	393233	2958528	363636	2971733	324580	2945323	401813
RP_POS_804_55054a13_288	RP	POS	13.29	804.5505				6.58E-01	0.11	0.71	7.19E-01	-0.06	0.23	7.79E-01	0.08	0.52	5.72E-01	0.14	0.75	5459658	4021259	5799876	2779403	5900742	2178598	5699011	3292531
RP_POS_233_11487a7_239	RP	POS	7.24	233.1149				3.79E-01	0.17	0.38	7.19E-01	0.07	0.55	3.59E-01	0.21	0.37	5.35E-01	0.13	0.49	486192	493147	578289	565066	557811	528166	598768	604401
RP_POS_375_20288a2_891	RP	POS	2.89	375.2029				2.68E-06	0.90	1.47	7.19E-01	0.07	0.94	1.82E-06	0.93	1.76	1.69E-04	0.86	1.26	18572579	5379793	24484255	6311351	24255509	7635068	24713000	4698741
RP_NEG_301_24066a11_16	RP	NEG	11.16	301.2407				1.20E-01	0.27	1.05	7.19E-01	-0.08	1.00	2.53E-01	0.23	0.91	1.36E-01	0.31	1.06	757769	181504	822535	257159	831848	263035	813222	253469
RP_NEG_201_80171a15_584	RP	NEG	15.58	201.8017				1.75E-01	-0.25	0.54	7.19E-01	-0.08	0.29	1.55E-01	-0.29	0.56	3.32E-01	-0.22	0.37	3537935	114837	3504208	138130	3509209	150904	3499207	125405
RP_NEG_191_01924a0_708	RP	NEG	0.71	191.0192				6.71E-02	-0.34	0.95	7.19E-01	0.07	0.76	1.63E-01	-0.31	0.84	6.84E-02	-0.38	0.89	2650306	1304774	2130995	1563586	2074397	1478203	2187592	1657672
RP_POS_649_4491a10_465	RP	POS	10.47	649.4491				4.40E-01	-0.20	0.68	7.19E-01	-0.06	0.29	3.80E-01	-0.23	0.45	5.54E-01	-0.16	0.59	8557513	1277960	8369686	834506	8399891	970550	8339481	680574
HILIC_POS_143_34065a3_53	HILIC	POS	3.53	143.3407				2.62E-01	0.20	0.48	7.20E-01	-0.08	0.52	3.96E-01	0.16	0.34	2.93E-01	0.23	0.54	356218	536271	492066	737095	518739	853101	465394	607020
HILIC_POS_134_11757a1_88	HILIC	POS	1.88	134.1176				4.07E-03	-0.47	1.07	7.20E-01	0.08	0.69	3.42E-02	-0.43	1.16	7.18E-03	-0.51	1.07	523830	149146	418594	239873	409920	224585	427267	256243
RP_NEG_222_81096a0_768	RP	NEG	0.77	222.8110				3.51E-04	-0.77	1.48	7.20E-01	-0.07	0.23	4.64E-04	-0.81	1.44	1.70E-03	-0.74	1.27	1966105	519137	1568678	476369	1585894	502883	1551461	452758
RP_POS_263_16165a9_225	RP	POS	9.23	263.1617				3.76E-01	0.14	1.23	7.20E-01	-0.08	1.45	5.60E-01	0.10	1.01	3.89E-01	0.18	1.04	715950	364141	793959	594070	815431	672149	772487	510212
RP_POS_137_04562a0_709	RP	POS	0.71	137.0456	Hypoxanthine	137.0455(100), 94.0399(1), 110.0345(1), 119.0361(1)	3	1.10E-12	0.87	1.64	7.20E-01	0.08	0.78	1.95E-06	0.91	1.67	8.69E-08	0.83	1.78	2714190	1488139	43399016	49842283	41597840	43777837	45200191	55642478
RP_POS_464_85721a0_498	RP	POS	0.50	464.8572				9.36E-07	-0.60	1.32	7.20E-01	0.08	1.19	4.82E-04	-0.56	1.39	4.45E-04	-0.64	1.41	3304389	242779	2506813	1476253	2453488	1576590	2560137	1382635
HILIC_POS_360_21661a0_555	HILIC	POS	0.555	360.2166				1.10E-02	-0.70	1.24	7.20E-01	-0.05	0.84	1.00E-02	-0.73	1.10	1.86E-02	-0.67	0.97	37530367	20207562	27540478	10777868	27929701	11555582	27151255	10042654
RP_POS_282_27957a11_159	RP	POS	11.16	282.2796				7.41E-08	0.79	1.27	7.20E-01	-0.08	0.65	1.45E-04	0.75	1.25	1.37E-06	0.82	1.54	10104724	2915843	14739949	6173663	14962714	5460318	14517184	6862194
RP_POS_382_18866a10_584	RP	POS	10.58	382.1887				1.98E-03	0.57	0.94	7.21E-01	-0.07	0.40	1.19E-02	0.53	0.91	3.71E-03	0.60	1.11	1795254	781916	2342239	983618	2377686	967248	2306791	1008275
HILIC_POS_189_16013a6_797	HILIC	POS	6.797	189.1601				5.03E-02	0.29	0.63	7.21E-01	0.08	0.58	1.09E-01	0.33	0.55	1.21E-01	0.25	0.68	4546322	2046985	5610660	3972449	5467566	3278658	5753753	4592534
RP_POS_804_55206a12_491	RP	POS	12.49	804.5521				6.83E-01	-0.07	0.89	7.21E-01	0.08	0.35	8.71E-01	-0.04	0.65	5.77E-01	-0.11	0.49	8195953	2890813	7936821	3724946	7802807	3396899	8070836	4056850
RP_NEG_401_95358a0_645	RP	NEG	0.65	401.9536				4.98E-12	-0.85	1.50	7.21E-01	0.08	1.18	1.46E-06	-0.81	1.62	7.89E-07	-0.89	1.59	3389336	172469	2323502	1339280	2275328	1385062	2371675	1304153
RP_POS_579_40063a11_598	RP	POS	11.60	579.4006				2.51E-02	-0.47	0.79	7.21E-01	0.07	0.35	4.97E-02	-0.44	0.76	3.48E-02	-0.51	0.73	787277	118907	732047	114201	727940	125927	736154	102264
RP_POS_316_77582a0_521	RP	POS	0.52	316.7758				1.43E-06	0.59	1.27	7.21E-01	-0.08	1.11	6.14E-04	0.55	1.30	5.51E-04	0.63	1.38	179513	42076	317039	259725	326374	277274	307703	243377
RP_POS_820_54456a11_906	RP	POS	11.91	820.5446				3.08E-02	0.26	0.64	7.21E-01	-0.08	0.48	1.49E-01	0.22	0.60	9.58E-02	0.30	0.71	856330	483451	1412349	2396848	1498490	2609315	1326208	2187084
RP_POS_302_24524a10_641	RP	POS	10.64	302.2452				4.29E-03	0.51	0.85	7.21E-01	-0.07	0.43	2.32E-02	0.48	0.82	7.22E-03	0.55	1.08	32915606	14995631	42656736	19589495	43360363	19088169	41953108	20247461
RP_POS_185_11501a10_578	RP	POS	10.58	185.1150				9.30E-01	-0.02	0.28	7.22E-01	-0.07	0.24	8.14E-01	-0.05	0.29	9.34E-01	0.02	0.42	2236953	685053	2224603	703268	2249845	680011	2199361	731814
RP_POS_399_76999a13_723	RP	POS	13.72	399.7700				5.10E-03	0.51	1.04	7.23E-01	0.07	0.23	1.01E-02	0.54	1.02	2.19E-02	0.47	1.08	6173007	1584470	7176468	2038655	7103647	1995029	7249290	2099067
RP_NEG_209_15465a7_723	RP	NEG	7.72	209.1547				2.41E-01	-0.23	0.56	7.23E-01	-0.07	0.35	2.09E-01	-0.26	0.57	4.04E-01	-0.19	0.51	2964676	147305	2928227	163927	2934074	180288	2922379	147374
RP_NEG_856_75732a0_498	RP	NEG	0.50	856.7573				1.94E-03	-0.42	1.18	7.24E-01	-0.08	1.23	6.87E-03	-0.46	1.24	4.14E-02	-0.38	1.22	2258783	413101	1831467	1135834	1871928	1208873	1791006	1068575
RP_POS_364_1676a10_731	RP	POS	10.73	364.1676				2.76E-03	0.49	1.38	7.24E-01	-0.08	1.13	1.81E-02	0.45	1.20	8.90E-03	0.52	1.34	1844469	825961	2453164	1329336	2500420	1387551	2405909	1280812
HILIC_NEG_448_74265a2_929	HILIC	NEG	2.929	448.7427				1.62E-06	-0.63	1.34	7.25E-01	0.08	0.76	3.58E-04	-0.60	1.45	2.97E-04	-0.67	1.47	151963	21361	114588	64054	112314	68137	116862	60302
RP_POS_291_64645a10_303	RP	POS	10.30	291.6465				3.85E-02	0.46	0.81	7.25E-01	-0.07	0.49	8.76E-02	0.43	0.69	3.34E-02	0.49	0.86	408905	127216	462187	109605	466077	94731	458296	123558
RP_POS_292_90692a15_364	RP	POS	15.36	292.9069				6.49E-01	0.09	0.50	7.25E-01	-0.07	0.26	8.13E-01	0.05	0.34	5.66E-01	0.13	0.53	1486281	278666	1512681	301671	1523388	293273	1501974	312451
RP_POS_325_12433a6_254	RP	POS	6.25	325.1243				2.79E-01	-0.22	0.48	7.25E-01	-0.07	0.29	2.56E-01	-0.25	0.48	4.24E-01	-0.18	0.34	54482280	5538297	53238947	5775737	53443910	5936904	53033985	5662730

Supplementary table 1: Metabolomics results (in asceding order according to p-value from progressive ALD vs non-progressive ALD comparison, with molecular features with ID_level of 1-2 first)

								all_ALD_vs_control			Prog_ALD_vs_non-prog_ALD			Prog_ALD_vs_control_ALD			Non-prog_ALD_vs_control			Healthy_control		all_ALD		Non-prog_ALD		Progressive_ALD	
								t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA								
Feature_ID	RP_HILIC	POS_NEG	Average.Rt	Average.Mz	Metabolite.name	curated_MSMS	ID_level	p	d	VIP	p	d	VIP	p	d	VIP	p	d	VIP	Mean	SD	Mean	SD	Mean	SD	Mean	SD
HILIC_NEG_215_97316a0_934	HILIC	NEG	0.934	215.9732				1.02E-08	0.85	1.47	7.25E-01	0.07	1.16	2.36E-05	0.89	1.39	2.33E-07	0.81	1.77	1419033	368418	2032800	743441	2006411	572178	2059190	887626
HILIC_NEG_130_99246a0_7	HILIC	NEG	0.7	130.9925				3.20E-04	0.66	1.11	7.25E-01	0.07	1.08	2.00E-03	0.69	1.12	1.15E-03	0.62	1.21	700164	259271	914433	328785	902767	270571	926100	380682
RP_POS_744_84302a0_49	RP	POS	0.49	744.8430				4.44E-08	0.66	1.36	7.25E-01	-0.08	1.20	1.53E-04	0.62	1.44	9.03E-05	0.70	1.46	500697	186756	2092436	2670228	2187134	2788272	1997739	2571572
RP_POS_291_84552a15_571	RP	POS	15.57	291.8455				7.23E-01	0.07	0.40	7.25E-01	0.07	0.22	6.44E-01	0.11	0.28	8.78E-01	0.03	0.50	884364	38386	887213	42380	885710	38968	888716	45887
RP_POS_702_53503a10_657	RP	POS	10.66	702.5350				7.36E-01	-0.07	0.27	7.25E-01	-0.07	0.28	6.46E-01	-0.11	0.36	8.78E-01	-0.04	0.25	3050330	330956	3027879	311664	3038928	321840	3016829	304008
HILIC_POS_356_35199a0_521	HILIC	POS	0.521	356.3520				4.30E-02	-0.48	0.96	7.25E-01	0.06	0.33	7.74E-02	-0.45	0.72	4.25E-02	-0.51	0.82	1891551	684374	1617073	517963	1598710	510659	1635436	529703
HILIC_POS_175_14423a6_711	HILIC	POS	6.711	175.1442				5.48E-01	0.11	0.77	7.25E-01	0.07	0.57	4.91E-01	0.15	0.55	7.29E-01	0.07	0.80	1715934	982741	1844465	1229714	1800904	1211880	1888026	1258065
RP_POS_406_20081a7_106	RP	POS	7.11	406.2008				1.63E-01	-0.32	1.06	7.25E-01	-0.07	0.49	1.55E-01	-0.35	0.82	2.45E-01	-0.29	1.04	5905887	567553	5749147	460424	5765452	458813	5732843	466105
HILIC_POS_584_35632a1_005	HILIC	POS	1.005	584.3563				1.36E-05	0.53	1.25	7.25E-01	-0.08	0.78	3.12E-03	0.49	1.42	1.15E-03	0.57	1.38	347639	923917	2923581	5425785	3115681	5576728	2731482	5320140
RP_POS_184_07391a10_822	RP	POS	10.82	184.0739				7.91E-01	-0.06	0.79	7.26E-01	-0.07	0.93	7.11E-01	-0.09	0.48	9.09E-01	-0.03	0.75	576323	224999	564713	179133	571047	165674	558379	193138
RP_NEG_1067_61292a10_304	RP	NEG	10.30	1067.6129				2.39E-04	0.59	1.21	7.26E-01	-0.07	0.30	6.14E-03	0.55	1.03	6.67E-04	0.63	1.31	506924	237343	726786	391509	740626	360160	712946	423769
HILIC_POS_146_08116a0_801	HILIC	POS	0.801	146.0812				9.27E-01	0.02	0.24	7.26E-01	0.08	0.49	7.91E-01	0.05	0.29	9.11E-01	-0.02	0.31	4572596	2797821	4631535	4071573	4487679	4061979	4775390	4117259
RP_NEG_221_94632a14_268	RP	NEG	14.27	221.9463				7.18E-01	-0.08	0.63	7.26E-01	0.07	0.25	8.53E-01	-0.05	0.46	6.29E-01	-0.11	0.55	5945104	1586112	5831937	1362594	5783800	1256363	5880073	1472426
RP_NEG_662_42291a11_254	RP	NEG	11.25	662.4229				5.85E-07	0.97	1.82	7.26E-01	0.07	1.08	5.85E-06	1.00	1.76	4.92E-06	0.94	1.79	3325787	1462328	5050110	1671839	4991082	1512192	5109139	1831201
RP_POS_420_78503a0_251	RP	POS	0.25	420.7850				5.51E-01	-0.13	0.48	7.26E-01	0.07	0.46	6.93E-01	-0.10	0.25	4.84E-01	-0.16	0.58	674040	73032	665383	64446	663108	61041	667657	68227
HILIC_POS_582_59375a10_679	HILIC	POS	10.679	582.5938				4.35E-01	-0.14	0.51	7.26E-01	-0.07	0.51	3.90E-01	-0.18	0.60	6.23E-01	-0.10	0.27	3248155	195953	3214705	248343	3223465	255258	3205946	243502
RP_NEG_400_15421a11_162	RP	NEG	11.16	400.1542				2.16E-02	0.40	1.15	7.26E-01	-0.07	1.01	7.29E-02	0.36	1.00	3.28E-02	0.44	1.20	1551548	154513	1632956	213267	1640472	215591	1625439	212835
HILIC_NEG_354_99301a7_309	HILIC	NEG	7.309	354.9930				2.48E-01	0.22	1.14	7.26E-01	-0.07	0.36	3.87E-01	0.19	0.61	2.43E-01	0.26	1.13	967818	28559	974812	32285	975950	33409	973675	31418
RP_NEG_195_81001a2_45	RP	NEG	2.45	195.8100				8.93E-01	0.03	0.59	7.27E-01	0.07	0.38	7.74E-01	0.06	0.24	9.67E-01	-0.01	0.72	8261354	3751121	8366298	4028588	8224592	4261808	8508005	3819198
RP_POS_325_27209a10_866	RP	POS	10.87	325.2721				9.66E-02	-0.31	0.66	7.28E-01	-0.07	1.10	1.09E-01	-0.35	0.83	1.90E-01	-0.28	0.54	4791111	1127673	4387483	1321728	4433869	1286298	4341097	1367708
HILIC_NEG_198_88084a7_668	HILIC	NEG	7.668	198.8808				3.11E-01	0.17	0.67	7.28E-01	-0.07	0.70	5.01E-01	0.13	0.51	3.00E-01	0.21	0.54	333542	12656	336495	18333	337137	18549	335853	18280
RP_POS_306_93033a15_367	RP	POS	15.37	306.9303				8.45E-01	-0.03	0.32	7.28E-01	0.08	0.49	9.66E-01	0.01	0.30	7.65E-01	-0.07	0.46	2303646	125655	2297781	200660	2290749	260445	2304813	115836
RP_NEG_552_85883a0_497	RP	NEG	0.50	552.8588				2.07E-07	-0.64	1.34	7.28E-01	0.08	1.20	2.25E-04	-0.60	1.42	1.98E-04	-0.67	1.42	14012282	996033	10584531	5944866	10376473	6305000	10792589	5618074
RP_POS_797_58649a13_3	RP	POS	13.30	797.5865				2.28E-05	-0.90	1.71	7.28E-01	0.06	0.58	3.67E-04	-0.87	1.59	1.38E-05	-0.93	1.72	2756416	1121746	1704835	1066759	1667491	760402	1742178	1310770
RP_POS_609_30933a10_931	RP	POS	10.93	609.3093				2.73E-04	-0.85	1.39	7.29E-01	-0.06	0.52	3.95E-04	-0.88	1.39	7.84E-04	-0.82	1.35	438837	168489	309934	131534	314530	128833	305337	135331
RP_POS_277_21381a10_629	RP	POS	10.63	277.2138				4.19E-03	-0.59	1.21	7.29E-01	0.07	0.65	1.69E-02	-0.56	1.09	4.59E-03	-0.63	1.19	742309	248068	591610	246591	582996	224626	600223	268789
RP_POS_771_64435a11_126	RP	POS	11.13	771.6444				1.30E-01	0.27	0.69	7.30E-01	-0.07	0.25	2.22E-01	0.23	0.76	1.73E-01	0.30	0.58	378494	890681	682205	1205928	724194	1385301	640216	1007744
RP_POS_218_98363a0_453	RP	POS	0.45	218.9836				3.74E-04	-0.54	1.22	7.30E-01	-0.07	1.05	1.67E-03	-0.58	1.19	8.71E-03	-0.50	1.27	355423	103084	257350	194254	264111	202302	250589	187669
RP_POS_797_58752a13_443	RP	POS	13.44	797.5875				1.65E-08	-1.25	2.20	7.30E-01	0.06	0.87	2.07E-07	-1.22	2.03	1.72E-08	-1.27	2.15	3592349	1183801	2005149	1043887	1968893	900276	2041406	1178330
HILIC_NEG_110_89904a2_948	HILIC	NEG	2.948	110.8990				1.32E-05	-0.60	1.34	7.30E-01	0.08	0.79	8.70E-04	-0.56	1.45	8.35E-04	-0.63	1.40	26651666	3429849	21760266	8915845	21450657	9591098	22069876	8271765
HILIC_NEG_155_86559a3_023	HILIC	NEG	3.023	155.8656				3.96E-01	-0.16	0.95	7.31E-01	-0.07	0.80	3.62E-01	-0.20	0.33	5.57E-01	-0.13	0.35	24633995	4555649	23819020	5091948	23995490	5124281	23642551	5105212
RP_NEG_304_91385a15_345	RP	NEG	15.35	304.9139				6.04E-01	-0.10	0.57	7.31E-01	-0.07	0.39	5.12E-01	-0.14	0.64	7.77E-01	-0.07	0.24	8774077	321771	8739100	354318	8751361	398592	8726838	307348
RP_POS_169_03601a0_98	RP	POS	0.98	169.0360	Uric acid	169.0352(100), 141.04(18), 126.0298(5), 152.009(4)	3	4.72E-04	0.55	1.04	7.31E-01	0.07	0.34	4.35E-03	0.59	1.09	3.42E-03	0.52	0.97	14025126	3384477	17052574	5823659	16851052	5094483	17254097	6518092
RP_POS_266_15909a4_09	RP	POS	4.09	266.1591				6.56E-01	0.09	0.43	7.31E-01	0.07	0.36	5.93E-01	0.13	0.33	7.94E-01	0.06	0.59	1383288	74718	1390008	71372	1387539	66205	1392477	76788
HILIC_NEG_115_92072a5_882	HILIC	NEG	5.882	115.9207				4.81E-02	-0.42	1.10	7.32E-01	0.07	0.78	9.84E-02	-0.38	0.71	5.20E-02	-0.45	0.96	43710194	7938631	40481156	7550031	40220342	7538951	40741970	7628541
RP_POS_648_80328a0_499	RP	POS	0.50	648.8033				8.37E-03	-0.36	1.18	7.32E-01	-0.08	1.21	1.75E-02	-0.39	1.20	9.14E-02	-0.32	1.23	1056217	189726	891346	516107	909162	558621	873530	474831
RP_POS_553_38934a12_462	RP	POS	12.46	553.3893	Unknown	553.454(95), 313.181(100)	4	5.62E-01	0.09	0.20	7.32E-01	-0.08	0.22	7.90E-01	0.05	0.22	4.84E-01	0.13	0.31	7150248	834736	7270533	1447388	7320486	1356083	7220581	1545499
RP_POS_646_35687a14_267	RP	POS	14.27	646.3569				8.40E-01	-0.04	0.46	7.32E-01	-0.07	0.67	7.48E-01	-0.08	0.48	9.67E-01	-0.01	0.42	2528568	748060	2498243	687976	2521976	649620	2474510	730156
RP_POS_298_27402a8_967	RP	POS	8.97	298.2740				2.27E-01	0.24	0.47	7.32E-01	0.07	0.35	2.54E-01	0.28	0.58	3.15E-01	0.21	0.47	439159	770911	633112	816754	604932	641058	661292	967063
RP_POS_548_50494a14_165	RP	POS	14.17	548.5049				5.16E-01	-0.16	0.49	7.32E-01	0.06	0.22	6.18E-01	-0.13	0.83	4.72E-01	-0.19	0.48	3939421	2253249	3658813	1567368	3604789	1646675	3712837	1498641
RP_NEG_734_83112a0_467	RP	NEG	0.47	734.8311				1.51E-09	-0.76	1.41	7.33E-01	0.07	1.17	2.39E-05	-0.72	1.50	7.90E-06	-0.80	1.51	652778	64688	448138	291384	438108	297577	458169	287723
RP_POS_400_27829a11_25	RP	POS	11.25	400.2783				2.49E-11	1.17	1.83	7.33E-01	0.06	0.44	3.48E-09	1.20	1.89	3.17E-09	1.14	1.90	1151690	490432	2022348	689189	1998624	653775	2046071	728756
RP_NEG_280_90869a0_499	RP	NEG	0.50	280.9087				1.78E-03	-0.41	1.18	7.33E-01	-0.08	1.23	6.75E-03	-0.45	1.24	4.26E-02	-0.37	1.23	2147442	373593	1733131	1118233	1771581	1196180	1694680	1045249
RP_NEG_355_15854a11_162	RP	NEG	11.16	355.1585				7.54E-02	0.31	1.07	7.33E-01	0.07	0.90	9.36E-02	0.35	0.98	1.71E-01	0.28	0.96	19053108	1485623	19647519	1987104	19579197	1947951	19715842	2042965
RP_POS_170_95744a0_468	RP	POS	0.47	170.9574				3.28E-08	-0.69	1.37	7.33E-01	0.08	1.18	1.26E-04	-0.65	1.44	4.21E-05	-0.72	1.47	491213	46214	350327	223980	342629	228879	358024	221024
RP_NEG_300_74933a0_522	RP	NEG	0.52	300.7493				7.54E-06	-0.61	1.27	7.33E-01	-0.07	1.24	1.18E-04	-0.65	1.40	2.41E-03	-0.57	1.29	653678	117434	479196	310536	489868	336264	468523	285531
HILIC_NEG_280_81897a2_932	HILIC	NEG	2.932	280.8190				1.70E-06	-0.62	1.34	7.33E-01	0.07	0.77	3.82E-04	-0.59	1.46	3.64E-04	-0.66	1.47	285891	35191	221111	113208	217225	120862	224996	106090
RP_POS_488_58948a6_727	RP	POS	6.73	488.5895				5.28E-07	0.60	1.30	7.34E-01	-0.08	1.12	5.63E-04	0.56	1.41	3.18E-04	0.64	1.36	31509	79219	1007223	1814047	1069378	1892872	945067	1748669
RP_NEG_376_12936a11_16	RP	NEG	11.16	376.1294				3.08E-03	0.53	1.30	7.34E-01	-0.07	1.17	1.60E-02	0.50	1.24	6.43E-03	0.57	1.29	714143	83825	770712	109567	774465	110512	766958	109604
RP_POS_796_52307a13_16	RP	POS	13.16	796.5231				2.65E-02	-0.48	0.88	7.34E-01	-0.07	0.27	3.25E-02	-0.51	0.94	5.37E-02	-0.45	0.75	23821781	8749218	19841606	7948111	20113630	7608254	19569582	8342518
RP_POS_561_39673a10_546	RP	POS	10.55	561.3967				5.31E-01	-0.21	0.47	7.34E-01	0.03	0.23	5.68E-01	-0.19	0.34	5.04E-01	-0.23	0.32	5220838	3454511	4829585	947525	4797184	1033175	4861986	862749
HILIC_POS_138_12769a0_668	HILIC	POS	0.668	138.1277				1.07E-01	-0.33	0.96	7.34E-01	-0.07	0.81	1.12E-01	-0.36	0.61	1.92E-01	-0.29	0.51	1025863	211617	955002	215937	962381	214717	947623	219077
RP_POS_265_90387a0_448	RP	POS	0.45	265.9039				3.63E-08	-0.68	1.36	7.35E-01	0.07	1.17	1.30E-04	-0.64	1.43	5.02E-05	-0.72	1.47	1001682	88029	718110	455246	702560	467443	733661	446913
RP_POS_335_12476a9_476	RP	POS	9.48	335.1248				4.66E-02	-0.45	0.80	7.35E-01	-0.06	0.50	4.13E-02	-0.49	0.84	9.54E-02	-0.42	0.81	1320110	139325	1264626	113457	1268501	126947	1260751	99306
RP_POS_668_82117a0_497	RP	POS	0.50	668.8212				6.15E-08	-0.66	1.36	7.35E-01	0.08	1.19	1.93E-04	-0.62	1.43	8.02E-05	-0.70	1.46	1548718	84537	1183927	609724	1163134	627769	1204720	596773
RP_POS_560_31519a6_996	RP	POS	7.00	560.3152				2.26E-07	0.62	1.33	7.35E-01	-0.08	1.12	4.27E-04	0.58	1.41	1.83E-04	0.65	1.41	9899	8744	759496	1347311	805397	1389347	713594	1316417
RP_POS_497_39578a15_235	RP	POS	15.24	497.3958				5.53E-02	-0.38	0.84	7.36E-01	-0.07	0.25	5.50E-02	-0.42	0.73	1.28E-01	-0.35	0.88	7158521	3131000	5896990	3295464	6009136	3538912	5784844	3064675
RP_POS_1084_7804a0_494	RP	POS	0.49	1084.7804				6.79E-08	0.65	1.35	7.36E-01	-0.08	1.10	3.33E-04	0.61	1.39	6.68E-05	0.68	1.48	31528	12209	484567	776149	510954	777610	458179	781672
RP_POS_199_13033a15_211	RP	POS	15.21	199.1303				7.02E-01	0.08	0.32	7.36E-01	-0.07	0.49	8.32E-01	0.05	0.26	6.25E-01	0.12	0.40	36673418	26183269	38660944	22835387	39437026	22522109	37884863	23346887
RP_POS_820_07532a13_209	RP	POS	13.21	820.0753				1.02E-02	0.48	0.86	7.36E-01	0.07	0.30	3.05E-02	0.51	0.82	1.63E-02	0.44	1.03	387999	336010	578752	406968	564924	281427	592580	505010
HILIC_NEG_194_90605a3_007	HILIC	NEG	3.007	194.9061				8.40E-01	-0.04	0.95	7.36E-01	-0.07	0.77	7.27E-01	-0.07	0.37	9.92E-01	0.00	0.44	1108869	211625	1099742	252659	1108319	266004	1091165	240972
HILIC_POS_375_32135a3_198	HILIC	POS	3.198	375.3214				9.31E-01	-0.02	0.63	7.36E-01	-0.07	0.52	8.19E-01	-0.05	0.52	9.34E-01	0.02	0.47	8016710	2532327	7971110	2774741	8065296	2635542	7876923	2931095
RP_POS_420_25281a11_31	RP	POS	11.31	420.2528				2.26E-02	-0.42	0.88	7.36E-01	0.07	0.77	6.08E-02	-0.39	0.82	3.57E-02	-0.46	0.96	802919	97787	753664	120632	749571	127251	757757	114779
RP_POS_457_34787a10_882	RP	POS	10.88	457.3479				5.13E-05	-0.73	1.24	7.36E-01	0.07	0.90	7.16E-04	-0.70	1.27	1.97E-04	-0.77	1.26	50704421	2103237	48709290	2725662	48616841	2707536	48801739	2768012
RP_POS_497_39572a13_631	RP	POS	13.63	497.3957				5.33E-01	-0.13	1.07	7.36E-01	0.07	0.87	6.54E-01	-0.10	1.14	5.01E-01	-0.17	0.66	6940597	1993979	6690761	1845071	6628180	2107106	6753342	1558897
HILIC_NEG_144_92349a1_049	HILIC	NEG	1.049	144.9235				8.97E-01	-0.03	0.65	7.36E-01	0.07	0.62	9.76E-01	0.01	0.31	7.93E-01	-0.06	0.19	34120331	8304625	33901216	8118087	33626006	8264122	34176426	8043715
RP_POS_396_87027a0_498	RP	POS	0.50	396.8703				1.75E-06	-0.59	1.31	7.37E-01	0.07	1.20	5.94E-04	-0.55	1.38	5.74E-04	-0.63	1.40	3157571	284193	2399338	1421327	2351180	1517426	2447497	1332012
RP_NEG_605_40747a12_092	RP	NEG	12.09	605.4075				5.00E-01	-0.14	0.76	7.37E-01	-0.07	0.41	4.61E-01	-0.17	0.58	6.35E-01	-0.11	0.45	1250188	632442	1163791	607272	1184315	574210	1143266	643824
HILIC_POS_160_13315a1_611	HILIC	POS	1.611	160.1332				5.92E-05	0.54	1.24	7.37E-01	0.07	0.61	5.63E-03	0.58	1.21	2.96E-04	0.51	1.54	473874	251537	814008	687396	790765	500203	837252	838667
RP_POS_812_8302a0_492	RP	POS	0.49	812.8302				3.15E-08	0.66	1.37	7.38E-01	-0.07	1.19	1.29E-04	0.63	1.45	7.62E-05	0.70	1.47	269797	136934	1552161	2125576	1623882	2212744	1480439	2054657
RP_NEG_239_16548a9_224	RP	NEG	9.22	239.1655				3.07E-01	0.17	1.30	7.38E-01	-0.07	1.42	4.77E-01	0.13	1.07	3.33E-01	0.20	1.09	950717	581761	1092671	923681	1123831	1024773	1061510	819538
RP_NEG_343_99506a0_632	RP	NEG	0.63	343.9951				1.76E-08	-0.69	1.37	7.38E-01	-0.07	1.20	1.02E-04	-0.65	1.45	3.91E-05	-0.73	1.47	61261364	4285389	43580680	28109446	42633048	28825066	44528311	27634945
HILIC_NEG_115_92065a7_352	HILIC	NEG	7.352	115.9207				2.87E-01	-0.20	0.43	7.38E-01	-0.07	0.28	2.83E-01	-0.23	0.38	4.37E-01	-0.16	0.28	83057823	5201173	81863402	6261422	82074335	6079191	81652468	6493347
RP_POS_184_99527a15_387	RP	POS	15.39	184.9953				3.73E-02	0.39	0.76	7.38E-01	-0.07	0.22	8.40E-02	0.36	0.72	5.51E-02	0.42	0.76	7379569	3564028	8998175	4262201	9141760	4591811	8854590	3946727
HILIC_NEG_157_08696a0_635	HILIC	NEG	0.635	157.0870				7.20E-02	-0.44	0.84	7.38E-01	-0.06	0.54	6.82E-02	-0.47	0.79	1.15E-01	-0.41	0.70	340926	240300	256573	167832	262224	174876	250921	162059
RP_POS_530_84827a0_498	RP	POS	0.50	530.8483				2.06E-07	-0.63	1.34	7.39E-01	0.07	1.20	2.30E-04	-0.60	1.42	2.11E-04	-0.67	1.43	14159491	917524	10671144	6087410	10466732	6450918	10875557	5759318
RP_POS_214_95479a15_564	RP	POS	15.56	214.9548				3.38E-01	-0.22	0.48	7.39E-01	0.06	0.29	4.54E-01	-0.19	0.49	3.04E-01	-0.25	0.50	1592844	63524	1580897	50999	1579185	48401	1582609	53910
RP_POS_167_10422a5_52	RP	POS	5.52	167.1042				6.05E-01	-0.11	0.40	7.39E-01	-0.07	0.26	5.55E-01	-0.14	0.49	7.44E-01	-0.07	0.33	1028686	169209	1010785	170484	1016506	155635	1005064	185562
RP_POS_158_15398a7_649	RP	POS	7.65	158.1540				6.06E-02	-0.36	0.67	7.39E-01	0.07	0.34	1.54E-01	-0.33	0.55	5.26E-02	-0.40	0.89	37964479	1257513	37461652	1399263	37414692	1184813	37508612	1596105
RP_POS_778_83624a0_491	RP	POS	0.49	778.8362				7.18E-08	0.65	1.35	7.39E-01	-0.07	1.19	2.10E-04	0.61	1.43	1.08E-04	0.68	1.45	381334	164861	1761248	2357324	1840262	2442984	1682235	2290514
RP_POS_819_57544a13_714	RP	POS	13.71	819.5754				4.19E-05	-0.77	1.34	7.40E-01	-0.07	0.93	1.63E-04	-0.81	1.40	4.04E-04	-0.74	1.31	3838571	1223378	2686933	1462871	2735911	1444564	2637955	1493987
RP_NEG_235_92618a15_548	RP	NEG	15.55	235.9262				2.68E-01	0.21	0.45	7.40E-01	-0.07	0.30	4.28E-01	0.17	0.48	2.54E-01	0.24	0.62	7465800	203279	7514492	246243	7522736	240915	7506248	253634
RP_NEG_568_83246a0_499	RP	NEG	0.50	568.8325				4.14E-04	-0.47	1.21	7.40E-01	-0.07	1.24	2.75E-03	-0.51	1.29	1.73E-02	-0.44	1.25	5013170	868626	3971706	2427306	4052972	2558154	3890440	2312193
HILIC_NEG_475_53125a1_365	HILIC	NEG	1.365	475.5313				4.55E-01	-0.11	0.38	7.40E-01	-0.07	0.34	4.59E-01	-0.15	0.32	6.53E-01	-0.08	0.45	309756	109820	288936	198769	295591	174448	282282	222040
HILIC_NEG_219_8455a2_947	HILIC	NEG	2.947	219.8455				4.49E-02	0.35	0.99	7.40E-01	-0.07	0.85	1.18E-01	0.32	0.55	6.16E-02	0.39	0.70	696002	137407	758426	185697	764641	189815	752210	183199
HILIC_POS_256_10974a0_626	HILIC	POS	0.626	256.1097				1.20E-01	0.25	0.61	7.40E-01	-0.07	0.40	1.54E-01	0.21	0.90	2.17E-01	0.29	0.59	11772580	5267325	13771030	8692672	14061965	11214565	13480096	5169911
RP_NEG_289_70337a15_584	RP	NEG	15.58	289.7034				2.24E-01	-0.24	0.72	7.40E-01	-0.07	0.20	2.01E-01	-0.27	0.58	3.70E-01	-0.21	0.58	838362	38329	828619	41172	829996	44826	827243	37571
RP_NEG_622_84503a0_497	RP	NEG	0.50	622.8450				3.94E-08	-0.67	1.36	7.40E-01	0.07	1.19	1.19E-04	-0.64	1.44	6.92E-05	-0.71	1.45	2106209	143689	1584318	848819	1555989	882840	1612647	821370

Supplementary table 1: Metabolomics results (in asceding order according to p-value from progressive ALD vs non-progressive ALD comparison, with molecular features with ID_level of 1-2 first)

								all_ALD_vs_control			Prog_ALD_vs_non-prog_ALD			Prog_ALD_vs_control_ALD			Non-prog_ALD_vs_control			Healthy_control		all_ALD		Non-prog_ALD		Progressive_ALD	
								t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA								
Feature_ID	RP_HILIC	POS_NEG	Average.Rt	Average.Mz	Metabolite.name	curated_MSMS	ID_level	p	d	VIP	p	d	VIP	p	d	VIP	p	d	VIP	Mean	SD	Mean	SD	Mean	SD	Mean	SD
RP_POS_225_14679a9_052	RP	POS	9.05	225.1468				2.14E-01	-0.25	0.61	7.40E-01	-0.07	0.35	2.04E-01	-0.29	0.75	3.38E-01	-0.22	0.58	1368855	188375	1320405	193278	1326856	198371	1313955	189840
RP_NEG_408_78726a15_5	RP	NEG	15.50	408.7873				1.59E-01	0.33	0.75	7.41E-01	-0.06	0.32	2.44E-01	0.30	0.64	1.42E-01	0.36	0.60	2144819	79583	2166832	61530	2168884	55911	2164779	67190
RP_NEG_605_15643a0_621	RP	NEG	0.62	605.1564				7.75E-04	-0.55	1.09	7.41E-01	-0.07	1.01	2.27E-03	-0.58	1.20	1.02E-02	-0.51	1.10	6877914	1912199	5284977	3072991	5387413	3213285	5182540	2955107
RP_POS_710_84906a0_49	RP	POS	0.49	710.8491				1.10E-07	0.64	1.35	7.41E-01	-0.07	1.20	2.29E-04	0.60	1.42	1.50E-04	0.67	1.44	650267	206004	2288330	2843767	2383108	2972970	2193553	2735358
RP_NEG_238_07695a8_055	RP	NEG	8.06	238.0770				2.01E-01	-0.45	0.79	7.41E-01	0.02	0.48	2.16E-01	-0.43	0.59	1.91E-01	-0.46	0.73	3737043	9379165	1563181	1670317	1507570	1398781	1618793	1916756
HILIC_NEG_270_00494a0_93	HILIC	NEG	0.93	270.0049				5.01E-09	0.82	1.32	7.41E-01	-0.07	1.18	3.76E-05	0.78	1.32	6.74E-07	0.85	1.58	589245	363635	1274456	878041	1303682	809873	1245230	948687
HILIC_POS_160_09677a4_594	HILIC	POS	4.594	160.0968				4.98E-01	0.12	0.31	7.41E-01	0.07	0.76	4.23E-01	0.16	0.34	6.97E-01	0.09	0.36	2986890	6356738	3939619	8312810	3662921	9281385	4216317	7301747
HILIC_NEG_100_93345a7_941	HILIC	NEG	7.941	100.9335				1.39E-02	-0.49	0.85	7.41E-01	-0.07	0.82	2.03E-02	-0.52	0.89	3.78E-02	-0.45	0.82	44668125	9594274	39623831	10349817	39968252	10117008	39279410	10669000
RP_POS_332_24304a6_293	RP	POS	6.29	332.2430				5.63E-01	0.11	0.91	7.41E-01	-0.07	0.80	7.40E-01	0.07	0.59	4.92E-01	0.14	0.96	2742355	1329667	2908006	1603989	2961361	1504725	2854652	1711157
HILIC_NEG_197_80791a2_952	HILIC	NEG	2.952	197.8079				8.78E-05	0.52	1.21	7.41E-01	-0.07	0.78	4.29E-03	0.48	1.17	2.62E-03	0.55	1.36	21172374	4150375	27127685	12746727	27551674	13422828	26703696	12154621
HILIC_POS_193_09491a0_544	HILIC	POS	0.544	193.0949				2.32E-01	0.15	0.73	7.41E-01	0.08	0.40	3.11E-01	0.19	0.55	4.77E-01	0.11	0.44	291381	1170676	939012	4982672	773367	4536728	1104657	5433490
HILIC_NEG_132_92345a4_723	HILIC	NEG	4.723	132.9235				1.64E-02	0.42	0.81	7.41E-01	0.07	0.94	3.99E-02	0.46	0.70	3.68E-02	0.39	0.77	2333718	575374	2648369	776087	2622569	635759	2674168	900758
RP_POS_406_23849a11_162	RP	POS	11.16	406.2385				6.57E-01	0.08	0.76	7.42E-01	-0.07	0.74	8.20E-01	0.05	0.64	5.96E-01	0.12	0.77	8675611	509997	8725006	641528	8746294	690292	8703719	595052
RP_NEG_367_24722a10_962	RP	NEG	10.96	367.2472				2.01E-04	-0.58	1.24	7.42E-01	0.07	0.80	2.35E-03	-0.55	1.25	2.22E-03	-0.62	1.15	3210471	364169	2858018	644471	2836640	700507	2879397	589507
RP_NEG_832_79498a0_495	RP	NEG	0.50	832.7950				1.42E-07	-0.65	1.34	7.42E-01	0.07	1.18	3.30E-04	-0.62	1.40	6.85E-05	-0.69	1.45	1920898	157166	1480287	737537	1455830	738427	1504744	743323
RP_POS_310_08942a6_862	RP	POS	6.86	310.0894				6.92E-02	-0.35	0.74	7.42E-01	0.07	0.60	1.27E-01	-0.32	0.74	9.17E-02	-0.39	0.81	1952618	181141	1882389	203244	1875652	224137	1889126	182015
RP_POS_271_22598a9_193	RP	POS	9.19	271.2260				3.41E-01	-0.19	0.51	7.42E-01	0.07	0.77	4.79E-01	-0.16	0.37	3.17E-01	-0.23	0.61	2999506	311528	2938565	313603	2928172	313403	2948958	316636
RP_POS_474_2847a8_659	RP	POS	8.66	474.2847				2.15E-02	0.35	0.75	7.42E-01	-0.07	0.73	1.20E-01	0.31	0.67	2.78E-02	0.38	0.85	480404	216820	612036	413230	625730	369659	598341	456040
HILIC_NEG_136_89165a5_388	HILIC	NEG	5.388	136.8917				7.95E-01	0.05	0.90	7.43E-01	0.07	0.31	7.05E-01	0.09	0.61	9.32E-01	0.02	0.31	4328242	1775842	4422996	1812095	4363049	1808608	4482944	1831936
HILIC_POS_59_06127a0_684	HILIC	POS	0.684	59.0613				1.04E-02	-0.62	1.02	7.43E-01	-0.06	0.91	1.49E-02	-0.65	0.96	1.57E-02	-0.60	1.28	2774567	563550	2486195	403127	2499536	319711	2472854	475143
RP_NEG_334_91953a0_497	RP	NEG	0.50	334.9195				1.70E-06	-0.59	1.30	7.43E-01	0.07	1.17	5.51E-04	-0.55	1.35	6.16E-04	-0.63	1.39	1560936	121617	1225212	630649	1204355	676188	1246069	587737
HILIC_NEG_134_89478a2_953	HILIC	NEG	2.953	134.8948				1.09E-02	0.39	1.10	7.43E-01	-0.07	0.80	5.30E-02	0.35	0.84	2.93E-02	0.42	1.11	165544034	25840824	182757791	48053990	184346902	50417307	181168680	46026511
RP_POS_1051_79895a14_269	RP	POS	14.27	1051.7990				5.22E-01	0.10	0.29	7.43E-01	0.07	0.21	5.50E-01	0.13	0.33	6.79E-01	0.06	0.19	199456688	19203251	202662783	36623278	201450740	23987330	203874827	46168298
RP_POS_724_54303a12_325	RP	POS	12.33	724.5430				1.59E-05	-0.95	1.62	7.43E-01	-0.06	0.37	3.74E-05	-0.98	1.57	6.33E-05	-0.92	1.57	7495296	1846240	5741045	1639390	5795249	1564058	5686842	1725623
HILIC_POS_129_10237a0_792	HILIC	POS	0.792	129.1024				1.64E-04	-0.57	1.32	7.43E-01	0.07	0.79	3.48E-03	-0.53	1.40	1.71E-03	-0.60	1.35	2810019	682120	2108898	1325887	2065063	1377056	2152732	1285157
RP_NEG_294_8855a0_446	RP	NEG	0.45	294.8855				4.61E-07	-0.64	1.32	7.43E-01	0.07	1.18	3.08E-04	-0.61	1.38	1.68E-04	-0.68	1.41	738637	92191	536283	344135	524921	357750	547646	333205
HILIC_NEG_202_96536a0_93	HILIC	NEG	0.93	202.9654				5.00E-09	0.85	1.38	7.44E-01	-0.07	1.24	3.15E-05	0.81	1.34	2.76E-07	0.88	1.65	3717122	2140304	7521534	4671764	7675335	4185810	7367733	5150426
HILIC_NEG_130_95763a2_912	HILIC	NEG	2.912	130.9576				1.06E-04	-0.58	1.33	7.44E-01	0.07	0.80	2.46E-03	-0.54	1.37	1.43E-03	-0.62	1.35	13323078	2498775	10657062	4927177	10494952	5171849	10819172	4716773
RP_POS_955_57971a10_339	RP	POS	10.34	955.5797				4.77E-03	0.43	1.05	7.44E-01	0.07	0.52	3.21E-02	0.47	0.86	1.03E-02	0.40	1.14	371900	268941	570403	496488	554059	356286	586748	608724
RP_POS_221_98213a1_199	RP	POS	1.20	221.9821				2.29E-12	0.92	1.46	7.44E-01	0.07	0.28	1.61E-06	0.96	1.48	6.67E-09	0.89	1.69	2029890	708290	4019504	2240308	3945860	1845262	4093149	2593131
RP_POS_568_89178a0_496	RP	POS	0.50	568.8918				5.04E-07	0.61	1.32	7.44E-01	-0.07	1.15	4.28E-04	0.57	1.39	3.21E-04	0.64	1.41	180300	73362	497987	579905	517042	610318	478931	553365
RP_POS_359_315a11_264	RP	POS	11.26	359.3150				5.61E-01	0.10	0.36	7.44E-01	0.07	0.36	5.22E-01	0.14	0.45	7.38E-01	0.07	0.44	943178	945533	1067691	1322566	1024235	1229126	1111148	1421076
HILIC_NEG_270_79047a2_937	HILIC	NEG	2.937	270.7905				1.13E-04	-0.58	1.33	7.45E-01	0.07	0.78	2.59E-03	-0.54	1.39	1.54E-03	-0.61	1.37	284431	63768	216410	126765	212249	133225	220571	121172
RP_POS_236_07108a6_993	RP	POS	6.99	236.0711				2.88E-03	-0.51	1.08	7.45E-01	0.07	0.84	1.28E-02	-0.47	0.97	9.90E-03	-0.54	1.28	2319338	108305	2243053	157059	2237899	170794	2248207	143575
RP_NEG_249_15019a10_291	RP	NEG	10.29	249.1502				7.50E-01	0.07	0.64	7.45E-01	0.07	0.65	6.76E-01	0.10	0.57	8.83E-01	0.03	0.59	1371715	105708	1378594	105557	1375133	97508	1382056	113928
HILIC_NEG_173_92603a6_275	HILIC	NEG	6.275	173.9260				7.85E-01	0.06	0.16	7.45E-01	-0.07	0.52	9.16E-01	0.02	0.11	6.97E-01	0.09	0.28	8108044	2764529	8260689	2642588	8347313	2589329	8174066	2718293
RP_POS_350_98758a8_122	RP	POS	8.12	350.9876				1.43E-01	-0.31	0.81	7.45E-01	-0.06	0.81	1.42E-01	-0.34	0.70	2.36E-01	-0.28	0.53	1729033	538893	1567869	515891	1584773	524321	1550964	512077
RP_POS_296_22165a9_141	RP	POS	9.14	296.2217				9.78E-04	-0.71	1.17	7.45E-01	0.06	0.89	4.02E-03	-0.67	1.11	1.32E-03	-0.74	1.23	2774571	158782	2663288	148273	2658431	141693	2668145	155863
HILIC_NEG_118_92398a4_811	HILIC	NEG	4.811	118.9240				6.43E-01	0.09	0.52	7.45E-01	0.07	0.65	5.93E-01	0.13	0.30	7.77E-01	0.06	0.30	2348100	785866	2422905	802780	2396606	698891	2449205	901223
HILIC_POS_540_33026a0_99	HILIC	POS	0.99	540.3303				5.40E-05	0.50	1.21	7.45E-01	-0.07	0.76	6.40E-03	0.46	1.35	1.92E-03	0.54	1.33	294807	910088	2189771	4231304	2328344	4267321	2051198	4233679
RP_NEG_288_93591a15_331	RP	NEG	15.33	288.9359				6.68E-01	-0.08	0.65	7.45E-01	-0.07	0.39	5.87E-01	-0.12	0.66	8.25E-01	-0.05	0.40	3832710	116206	3822302	127397	3826474	134793	3818130	120775
RP_POS_151_00519a10_666	RP	POS	10.67	151.0052				2.36E-01	0.24	0.54	7.45E-01	0.07	0.45	2.25E-01	0.27	0.51	3.67E-01	0.20	0.65	1939674	606708	2089017	635766	2068209	653178	2109826	623795
HILIC_NEG_94_92467a3_017	HILIC	NEG	3.017	94.9247				8.30E-01	-0.04	0.73	7.45E-01	0.07	0.63	9.61E-01	-0.01	0.33	7.37E-01	-0.08	0.61	741962	236065	731608	236726	723860	238443	739356	237160
RP_NEG_554_85638a0_497	RP	NEG	0.50	554.8564				5.05E-07	-0.61	1.32	7.45E-01	0.07	1.19	3.64E-04	-0.58	1.40	3.07E-04	-0.65	1.41	2055890	153860	1555094	900073	1525640	951305	1584548	854425
RP_POS_433_28128a12_127	RP	POS	12.13	433.2813				7.44E-02	-0.32	0.99	7.45E-01	0.07	0.86	1.42E-01	-0.29	0.89	1.06E-01	-0.36	0.90	1051056	192528	974889	246410	966826	273928	982952	217958
RP_POS_166_98492a15_398	RP	POS	15.40	166.9849				5.59E-01	-0.12	0.68	7.45E-01	0.07	0.23	7.02E-01	-0.08	0.52	5.12E-01	-0.15	0.42	105686192	38102296	101108992	39211940	99826678	41107638	102391305	37594385
RP_NEG_291_89355a3_965	RP	NEG	3.97	291.8936				3.49E-01	0.16	0.87	7.46E-01	-0.07	0.29	5.75E-01	0.12	0.61	2.92E-01	0.19	0.50	1786873	625245	1924393	951418	1955508	806147	1893278	1084904
RP_NEG_369_00574a0_678	RP	NEG	0.68	369.0057				3.59E-09	-0.72	1.40	7.46E-01	0.07	1.18	5.31E-05	-0.68	1.48	1.66E-05	-0.75	1.50	4615379	263414	3285973	2016434	3220047	2050657	3351898	2000232
HILIC_NEG_132_90038a7_673	HILIC	NEG	7.673	132.9004				4.29E-02	-0.38	0.76	7.46E-01	-0.07	0.38	4.18E-02	-0.42	0.90	1.20E-01	-0.35	0.56	1597849	296072	1468076	345876	1479362	383723	1456790	306918
RP_POS_979_57941a10_332	RP	POS	10.33	979.5794				4.69E-08	0.72	1.31	7.46E-01	0.07	0.31	6.61E-05	0.76	1.36	2.80E-05	0.69	1.27	208760	119977	454983	367396	443012	336095	466954	399327
HILIC_POS_175_10776a4_792	HILIC	POS	4.792	175.1078				1.09E-01	0.28	0.76	7.47E-01	0.07	0.62	1.07E-01	0.31	0.65	2.51E-01	0.25	0.41	958993	182367	1025189	249807	1017059	271959	1033318	228001
RP_POS_341_30447a11_264	RP	POS	11.26	341.3045				9.36E-01	0.01	0.34	7.47E-01	0.07	0.40	8.23E-01	0.05	0.41	9.24E-01	-0.02	0.45	401205	401927	408232	500271	391971	464916	424494	537554
RP_POS_285_06412a15_342	RP	POS	15.34	285.0641				8.34E-01	0.04	0.36	7.47E-01	0.07	0.27	7.38E-01	0.08	0.37	9.66E-01	0.01	0.32	1937354	533773	1960258	542338	1942638	555573	1977877	533825
HILIC_POS_375_3212a1_017	HILIC	POS	1.017	375.3212				3.31E-01	-0.17	0.32	7.47E-01	-0.07	0.26	3.22E-01	-0.20	0.39	5.05E-01	-0.14	0.24	4282236	1098677	4042194	1494125	4090656	1482771	3993732	1518872
RP_POS_160_13335a4_294	RP	POS	4.29	160.1334	Unknown	160.1337(5), 114.1282(100)	4	4.03E-01	-0.19	0.36	7.48E-01	0.06	0.20	5.14E-01	-0.16	0.35	3.73E-01	-0.22	0.36	2372772	1832644	2072220	1483377	2024147	1513695	2120293	1466197
RP_POS_751_51599a10_655	RP	POS	10.66	751.5160				3.02E-01	0.22	0.78	7.48E-01	0.06	0.29	2.82E-01	0.25	0.69	4.25E-01	0.19	0.71	4529116	386627	4609829	362467	4598092	367515	4621566	360691
HILIC_NEG_119_90752a6_272	HILIC	NEG	6.272	119.9075				2.50E-01	-0.26	0.44	7.48E-01	-0.06	0.45	2.28E-01	-0.29	0.47	3.59E-01	-0.23	0.45	1852964	822350	1665030	696315	1687568	736876	1642492	659985
HILIC_POS_59_06131a0_934	HILIC	POS	0.934	59.0613				2.69E-01	-0.25	0.47	7.49E-01	-0.06	0.69	2.51E-01	-0.28	0.47	3.71E-01	-0.22	0.35	3705000	1089321	3467314	894940	3496181	910621	3438447	887271
RP_POS_244_86719a0_246	RP	POS	0.25	244.8672				9.19E-01	0.02	0.40	7.49E-01	0.07	0.65	8.04E-01	0.05	0.36	9.48E-01	-0.01	0.48	409356	60257	410664	70686	408384	73451	412944	68479
HILIC_NEG_179_8828a7_667	HILIC	NEG	7.667	179.8828				9.45E-02	0.28	0.78	7.49E-01	0.07	0.79	1.12E-01	0.32	0.61	2.19E-01	0.25	0.49	1176403	57101	1198660	84237	1195945	85624	1201375	83607
HILIC_POS_292_84528a2_991	HILIC	POS	2.991	292.8453				6.91E-06	-0.58	1.35	7.49E-01	0.07	0.78	1.01E-03	-0.54	1.47	8.35E-04	-0.61	1.50	20010893	2373848	15637446	8332125	15368993	8839799	15905900	7872504
RP_POS_369_38422a11_247	RP	POS	11.25	369.3842				5.95E-10	0.89	1.43	7.49E-01	0.07	0.96	1.73E-05	0.92	1.42	4.65E-09	0.85	1.79	486658	222687	917877	502992	901682	349144	934071	623480
HILIC_NEG_157_90068a1_328	HILIC	NEG	1.328	157.9007				7.16E-04	-0.55	0.97	7.50E-01	-0.07	0.55	2.71E-03	-0.58	1.00	8.28E-03	-0.52	0.88	866494	93498	787825	151379	792693	153236	782956	150894
HILIC_POS_666_33441a0_855	HILIC	POS	0.855	666.3344				8.69E-01	0.03	0.37	7.50E-01	0.06	0.36	7.47E-01	0.07	0.36	9.93E-01	0.00	0.29	4931198	2827253	5025523	2738408	4937509	3431430	5113537	1833105
HILIC_POS_130_0977a6_968	HILIC	POS	6.968	130.0977				8.44E-02	0.23	1.07	7.50E-01	-0.07	0.76	2.64E-01	0.20	0.95	1.29E-01	0.27	1.14	530243	165169	622153	440327	636290	442482	608017	442192
RP_NEG_643_11218a0_621	RP	NEG	0.62	643.1122				7.18E-06	-0.66	1.27	7.50E-01	-0.07	1.11	7.73E-05	-0.70	1.41	1.19E-03	-0.63	1.26	1092188	230648	797568	473364	812755	509908	782380	438455
HILIC_NEG_342_72574a2_938	HILIC	NEG	2.938	342.7257				2.75E-07	-0.67	1.35	7.50E-01	0.07	0.77	1.38E-04	-0.63	1.49	1.43E-04	-0.70	1.49	403637	50365	301401	166130	296073	176468	306729	156725
HILIC_NEG_315_04199a5_607	HILIC	NEG	5.607	315.0420				2.30E-01	-0.25	0.81	7.50E-01	-0.06	0.67	2.35E-01	-0.28	0.47	3.34E-01	-0.22	0.61	6607011	1151307	6323398	1143155	6360050	1067955	6286746	1223522
RP_NEG_268_98413a8_316	RP	NEG	8.32	268.9841				4.67E-02	-0.41	0.85	7.50E-01	0.06	0.39	9.58E-02	-0.38	0.66	5.30E-02	-0.44	0.78	3517898	147440	3457136	144811	3452496	145374	3461777	145572
RP_POS_644_49445a10_46	RP	POS	10.46	644.4945				3.93E-01	-0.22	0.49	7.50E-01	0.05	0.69	4.76E-01	-0.20	0.37	3.60E-01	-0.25	0.52	2899895	463188	2825131	279885	2816165	273193	2834097	288914
RP_POS_169_9856a0_522	RP	POS	0.52	169.9856				1.09E-06	0.59	1.22	7.51E-01	0.07	1.12	4.34E-04	0.62	1.32	7.43E-04	0.55	1.27	295900	65601	598248	572924	579898	553487	616597	596780
RP_POS_147_01398a0_45	RP	POS	0.45	147.0140				2.43E-06	-0.63	1.30	7.51E-01	-0.07	1.13	1.28E-04	-0.67	1.37	1.00E-03	-0.60	1.35	598569	86435	455655	246007	463530	255148	447781	238845
RP_POS_316_13089a6_074	RP	POS	6.07	316.1309				6.41E-01	0.09	0.40	7.51E-01	0.07	0.54	5.65E-01	0.12	0.47	8.05E-01	0.05	0.62	584786	135972	598323	160467	593191	169224	603455	152756
RP_POS_1050_78564a0_493	RP	POS	0.49	1050.7856				1.65E-08	0.68	1.39	7.51E-01	-0.07	1.19	1.45E-04	0.64	1.46	3.67E-05	0.71	1.49	37438	29279	586083	891240	614580	898476	557586	892139
RP_NEG_381_19635a11_611	RP	NEG	11.61	381.1964				2.45E-01	-0.22	0.54	7.51E-01	-0.07	0.91	2.49E-01	-0.25	0.62	3.85E-01	-0.18	0.45	1099176	139144	1064116	169157	1069524	165032	1058708	174692
RP_NEG_265_14908a11_966	RP	NEG	11.97	265.1491				1.82E-01	0.20	0.39	7.51E-01	-0.07	0.44	3.74E-01	0.16	0.32	2.16E-01	0.23	0.54	257020	137264	305865	271031	314514	276742	297216	267725
RP_POS_564_82123a6_221	RP	POS	6.22	564.8212				1.09E-05	0.53	1.25	7.52E-01	-0.07	1.09	3.29E-03	0.50	1.32	9.02E-04	0.57	1.31	80288	344821	1150265	2241755	1221756	2252513	1078774	2251498
HILIC_POS_90_97712a5_463	HILIC	POS	5.463	90.9771				2.53E-01	-0.24	0.40	7.52E-01	0.06	0.55	3.74E-01	-0.21	0.35	2.32E-01	-0.28	0.47	1365399	111163	1339803	102223	1336546	96178	1343061	108814
RP_NEG_318_98199a9_425	RP	NEG	9.43	318.9820				2.72E-01	0.17	0.63	7.52E-01	-0.07	0.31	4.46E-01	0.14	0.57	3.05E-01	0.21	0.75	2854597	839193	3081626	1423629	3126964	1543413	3036288	1307089
RP_POS_514_97168a6_842	RP	POS	6.84	514.9717				2.99E-07	0.61	1.32	7.52E-01	-0.07	1.12	5.15E-04	0.58	1.41	1.99E-04	0.65	1.41	22732	33010	679656	1193579	717586	1221130	641725	1176538
RP_POS_226_21646a8_727	RP	POS	8.73	226.2165				6.46E-05	0.47	0.96	7.52E-01	-0.07	0.84	1.99E-03	0.43	1.09	8.02E-03	0.51	1.07	53368	67941	1042654	2368095	1117908	2722000	967400	1977209
RP_POS_798_56305a11_8	RP	POS	11.80	798.5631				2.70E-01	0.16	0.55	7.53E-01	-0.07	0.45	4.98E-01	0.13	0.35	2.79E-01	0.20	0.64	1366940	1854506	1920470	3764633	2039752	3695625	1801188	3866197
RP_POS_487_27258a6_73	RP	POS	6.73	487.2726				2.58E-07	0.61	1.32	7.54E-01	-0.07	1.13	4.06E-04	0.58	1.42	2.16E-04	0.65	1.39	25462	58478	925083	1623729	976422	1681666	873743	1579055
RP_POS_814_56927a13_509	RP	POS	13.51	814.5693				7.59E-01	-0.06	0.51	7.54E-01	0.07	0.70	9.14E-01	-0.02	0.46	6.77E-01	-0.09	0.47	5310910	1298252	5224073	1641032	5172189	1695739	5275957	1599971
RP_POS_358_11896a3_317	RP	POS	3.32	358.1190				6.33E-04	-0.66	1.20	7.54E-01	0.06	1.03	3.05E-03	-0.63	1.18	1.70E-03	-0.69	1.19	1380257	598983	924656	687466	902924	717054	946388	663124
RP_POS_527_77814a10_339	RP	POS	10.34	527.7781				4.74E-02	0.35	0.81	7.54E-01	-0.07	0.42	1.42E-01	0.32	0.74	4.76E-02	0.39	0.80	361023	164519	434185	216041	441013	191090	427357	240185
RP_POS_314_77866a0_522	RP	POS	0.52	314.7787				2.47E-06	0.57	1.26	7.54E-01	-0.07	1.10	8.99E-04	0.54	1.27	7.13E-04	0.61	1.37	292900	62135	502547	407682	515419	430337	489676	387650
RP_POS_522_35571a11_16	RP	POS	11.16	522.3557				1.06E-01	0.31	0.94	7.55E-01	-0.06	0.58	2.43E-01	0.28	0.76	7.95E-02	0.34	1.03	954544	440619	1105983	496197	1121620	366989	1090345	601887

Supplementary table 1: Metabolomics results (in asceding order according to p-value from progressive ALD vs non-progressive ALD comparison, with molecular features with ID_level of 1-2 first)

							all_ALD_vs_control			Prog_ALD_vs_non-prog_ALD			Prog_ALD_vs_control_ALD			Non-prog_ALD_vs_control			Healthy_control		all_ALD		Non-prog_ALD		Progressive_ALD	
							t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA								
Feature_ID	RP_HILIC	POS_NEG	Average.Rt	Average.Mz	Metabolite.name	curated_MSMS	ID_level	p	d	VIP	p	d	VIP	p	d	VIP	p	d	VIP	Mean	SD	Mean	SD	Mean	SD	Mean	SD
HILIC_POS_375_32129a0_686	HILIC	POS	0.686	375.3213				7.23E-02	-0.37	0.74	7.55E-01	-0.06	0.51	8.23E-02	-0.40	0.64	1.34E-01	-0.34	0.77	2956069	815355	2652345	815286	2677998	797957	2626692	839565
RP_POS_627_43268a10_978	RP	POS	10.98	627.4327				7.45E-03	0.44	1.29	7.55E-01	-0.07	1.21	3.79E-02	0.41	1.12	1.64E-02	0.47	1.26	196195	123927	276343	193220	282419	194474	270267	193739
RP_NEG_594_39551a11_163	RP	NEG	11.16	594.3955				5.66E-03	0.48	1.16	7.55E-01	-0.07	1.06	2.40E-02	0.44	1.09	1.39E-02	0.51	1.13	3287035	311724	3488273	441595	3502159	462564	3474387	423831
HILIC_POS_170_11766a0_549	HILIC	POS	0.549	170.1177				1.84E-01	-0.30	0.74	7.55E-01	-0.06	0.55	1.92E-01	-0.33	0.66	2.56E-01	-0.27	0.56	2807184	1738102	2348078	1467680	2394194	1317273	2301963	1616349
RP_POS_278_24802a9_417	RP	POS	9.42	278.2480				9.43E-01	-0.02	0.70	7.55E-01	-0.06	0.32	8.54E-01	-0.05	0.46	9.56E-01	0.01	0.41	2469329	1938970	2442083	1582636	2491757	1507429	2392408	1668296
RP_POS_234_89365a0_515	RP	POS	0.52	234.8937				3.63E-04	-0.64	1.04	7.56E-01	0.06	0.66	4.21E-03	-0.61	0.99	7.71E-04	-0.67	1.18	689569	156456	560134	206008	553671	192073	566596	220833
HILIC_POS_171_18549a7_15	HILIC	POS	7.15	171.1855				3.64E-02	0.39	0.82	7.56E-01	0.06	0.67	6.44E-02	0.42	0.79	6.91E-02	0.36	0.75	4215169	1449674	4878956	1753109	4823968	1465328	4933944	2013989
HILIC_NEG_144_92325a2_939	HILIC	NEG	2.939	144.9233				6.67E-07	0.64	1.32	7.56E-01	-0.07	0.77	1.39E-04	0.60	1.49	4.02E-04	0.67	1.44	11270424	843474	13039141	3035237	13134326	3347796	12943957	2717924
RP_POS_608_84674a6_388	RP	POS	6.39	608.8467				2.89E-06	0.56	1.27	7.56E-01	-0.07	1.10	1.64E-03	0.53	1.36	5.45E-04	0.60	1.34	92326	324401	1613719	3023193	1708488	3069078	1518951	3004721
RP_POS_385_23587a11_149	RP	POS	11.15	385.2359				5.81E-01	-0.08	1.01	7.56E-01	0.07	1.10	7.78E-01	-0.05	0.91	5.58E-01	-0.12	1.08	4597599	212759	4567163	401410	4554583	443497	4579744	358518
RP_POS_738_50494a10_464	RP	POS	10.46	738.5049				2.05E-01	-0.28	0.93	7.56E-01	0.06	0.33	2.90E-01	-0.25	0.60	2.03E-01	-0.31	0.82	1212287	283052	1141014	239455	1133513	249897	1148516	230834
RP_POS_155_15419a2_78	RP	POS	2.78	155.1542				1.85E-02	0.36	0.84	7.56E-01	-0.07	0.67	5.30E-02	0.33	0.87	5.59E-02	0.40	0.85	2920513	1090154	3580748	1971105	3642490	2248980	3519006	1668565
RP_NEG_144_9989a15_302	RP	NEG	15.30	144.9989				1.19E-01	0.28	0.65	7.56E-01	0.07	0.27	1.27E-01	0.32	0.64	2.39E-01	0.25	0.64	1347742	201107	1416812	254654	1408838	263671	1424786	247726
RP_NEG_765_1684a9_804	RP	NEG	9.80	765.1684				4.56E-01	-0.16	0.51	7.56E-01	0.06	0.53	5.76E-01	-0.13	0.31	4.22E-01	-0.19	0.44	5349113	348428	5297453	304787	5287918	311863	5306989	300403
RP_POS_256_26309a10_731	RP	POS	10.73	256.2631				6.10E-06	0.71	1.19	7.56E-01	-0.07	0.82	1.18E-03	0.68	1.16	1.48E-05	0.74	1.41	157953919	47916688	215405209	84813491	218057863	69911572	212752555	98140057
RP_POS_532_84973a0_498	RP	POS	0.50	532.8497				1.93E-07	-0.63	1.34	7.56E-01	0.07	1.19	2.12E-04	-0.60	1.43	2.16E-04	-0.67	1.42	1998235	125934	1509420	851694	1482792	902491	1536049	805998
RP_NEG_315_86319a15_786	RP	NEG	15.79	315.8632				1.37E-01	0.27	0.58	7.57E-01	-0.06	0.26	2.48E-01	0.24	0.54	1.52E-01	0.31	0.67	851108	394257	978968	483264	994060	496068	963876	474665
HILIC_POS_282_81635a3_009	HILIC	POS	3.009	282.8164				2.99E-05	-0.56	1.35	7.57E-01	0.07	0.78	1.93E-03	-0.53	1.46	1.26E-03	-0.60	1.47	3722495	588210	2887417	1624651	2836733	1706717	2938100	1553938
RP_POS_334_17252a10_979	RP	POS	10.98	334.1725				3.63E-02	0.39	1.44	7.57E-01	-0.06	1.24	1.06E-01	0.35	1.23	4.07E-02	0.42	1.30	1577660	384123	1754909	475351	1769735	441016	1740084	511454
RP_POS_459_3075a10_705	RP	POS	10.71	459.3075				2.81E-02	-0.37	0.59	7.57E-01	-0.07	0.40	4.37E-02	-0.40	0.79	9.06E-02	-0.34	0.55	3416985	723988	3044940	1061493	3078041	1067098	3011840	1065643
RP_NEG_801_08136a9_224	RP	NEG	9.22	801.0814				9.09E-01	0.02	0.75	7.57E-01	0.07	0.46	7.84E-01	0.05	0.68	9.41E-01	-0.01	0.36	1327618	101419	1330345	157464	1325436	165985	1335254	149986
RP_POS_523_37915a13_755	RP	POS	13.76	523.3792				2.47E-03	-0.58	1.00	7.57E-01	-0.06	0.37	1.01E-02	-0.61	0.90	4.12E-03	-0.55	1.08	3234633	770161	2722048	878702	2749460	623316	2694636	1081636
RP_POS_517_94098a6_841	RP	POS	6.84	517.9410				1.64E-07	0.62	1.33	7.57E-01	-0.07	1.15	3.20E-04	0.59	1.45	1.75E-04	0.66	1.39	16563	32355	962514	1677530	1014809	1737106	910218	1631725
RP_POS_294_92075a15_626	RP	POS	15.63	294.9208				1.87E-01	0.25	0.60	7.57E-01	-0.06	0.20	3.19E-01	0.22	0.62	1.81E-01	0.29	0.64	11296584	2794139	12077592	3141914	12175441	2991733	11979744	3312809
RP_POS_800_57812a11_832	RP	POS	11.83	800.5781				7.75E-02	0.22	0.56	7.57E-01	-0.07	0.38	2.54E-01	0.18	0.48	1.53E-01	0.26	0.59	1054908	1326270	2102850	5400985	2271045	5701853	1934654	5134952
HILIC_POS_201_06108a4_868	HILIC	POS	4.868	201.0611				9.20E-01	0.02	0.41	7.57E-01	0.06	0.27	8.01E-01	0.05	0.49	9.66E-01	-0.01	0.15	341952	230540	346689	229398	339540	282124	353837	163164
RP_NEG_174_95537a0_448	RP	NEG	0.45	174.9554				4.71E-08	-0.68	1.36	7.57E-01	0.07	1.19	1.39E-04	-0.64	1.43	5.92E-05	-0.71	1.46	27438693	2508913	19643510	12599847	19251288	12922115	20035731	12387784
RP_NEG_598_85529a0_466	RP	NEG	0.47	598.8553				1.06E-08	-0.72	1.39	7.58E-01	0.07	1.20	5.20E-05	-0.68	1.47	2.60E-05	-0.75	1.47	877755	90865	614971	397082	602627	409165	627315	388379
RP_POS_149_02388a7_493	RP	POS	7.49	149.0239	Unknown	149.0228(70), 121.0287(10), 84.9604(100)	4	7.20E-01	0.06	0.64	7.58E-01	0.07	0.53	6.52E-01	0.10	0.35	8.78E-01	0.03	0.39	3928527	289577	3951511	381269	3939674	359837	3963348	404884
HILIC_NEG_272_95865a7_347	HILIC	NEG	7.347	272.9587				2.51E-03	-0.57	1.15	7.58E-01	-0.06	0.91	5.73E-03	-0.61	0.98	9.62E-03	-0.54	0.97	627305	168296	514746	197311	520871	189128	508621	206910
RP_POS_201_79674a10_848	RP	POS	10.85	201.7967				5.99E-05	0.68	1.16	7.58E-01	-0.06	0.65	3.44E-03	0.64	1.06	4.96E-05	0.71	1.47	946277	312191	1253284	468384	1267831	353724	1238736	563641
HILIC_NEG_228_98117a0_831	HILIC	NEG	0.831	228.9812				3.64E-01	0.15	0.86	7.58E-01	-0.07	0.92	5.86E-01	0.12	0.37	3.04E-01	0.19	0.47	8310802	2698346	8881984	4050393	9007623	3358823	8756345	4672501
HILIC_NEG_212_92065a2_91	HILIC	NEG	2.91	212.9207				2.39E-07	-0.63	1.35	7.58E-01	-0.07	0.78	2.19E-04	-0.60	1.49	2.48E-04	-0.66	1.54	8575672	497138	6748024	3203332	6648717	3407681	6847330	3016566
HILIC_POS_200_05412a1_385	HILIC	POS	1.385	200.0541				1.87E-14	0.95	1.64	7.58E-01	-0.07	0.61	4.74E-07	0.91	1.60	8.27E-09	0.98	2.07	127368	73304	1035006	1008170	1066259	955871	1003752	1066711
RP_POS_282_9201a15_454	RP	POS	15.45	282.9201				7.20E-01	-0.08	1.03	7.58E-01	0.06	0.34	8.41E-01	-0.05	0.82	6.53E-01	-0.11	0.72	2704329	704656	2654062	631486	2634490	644865	2673634	623742
HILIC_POS_160_13338a2_295	HILIC	POS	2.295	160.1334				1.59E-03	0.51	0.93	7.58E-01	0.07	0.58	6.51E-03	0.54	0.97	1.14E-02	0.48	0.86	1722676	709280	2277612	1149969	2241993	1105657	2313231	1202822
HILIC_POS_444_05597a3_076	HILIC	POS	3.076	444.0560				1.22E-02	0.33	1.21	7.59E-01	-0.07	0.84	7.05E-02	0.30	1.26	4.81E-02	0.37	1.39	1059588	66942	1116840	191674	1122774	205322	1110907	178882
RP_POS_363_28598a10_845	RP	POS	10.85	363.2860				1.65E-04	-0.62	1.18	7.59E-01	0.06	0.97	2.93E-03	-0.59	1.18	7.50E-04	-0.65	1.22	1489979	347134	1166828	541461	1150080	530859	1183576	556739
RP_NEG_288_93677a0_449	RP	NEG	0.45	288.9368				5.53E-06	-0.60	1.26	7.59E-01	-0.07	1.16	1.81E-04	-0.63	1.36	2.06E-03	-0.57	1.32	3909743	651909	2820238	1988701	2881707	2107962	2758768	1881319
RP_POS_313_32086a10_848	RP	POS	10.85	313.3209				4.37E-01	-0.14	0.32	7.60E-01	-0.06	0.26	3.94E-01	-0.18	0.35	6.10E-01	-0.11	0.36	1724842	372052	1662280	454197	1676278	483834	1648281	426971
RP_POS_669_49329a11_752	RP	POS	11.75	669.4933				8.32E-04	-0.69	1.29	7.60E-01	-0.06	0.21	1.09E-03	-0.72	1.28	4.53E-03	-0.66	1.07	524714	213848	370321	216295	376988	235420	363655	197506
RP_POS_546_82196a0_499	RP	POS	0.50	546.8220				4.80E-04	-0.46	1.22	7.60E-01	-0.07	1.23	3.02E-03	-0.49	1.29	2.16E-02	-0.42	1.26	6275813	1025702	4961859	3188557	5060100	3414393	4863619	2977163
RP_POS_299_25803a9_865	RP	POS	9.87	299.2580				3.27E-02	-0.42	0.83	7.60E-01	-0.06	0.72	3.56E-02	-0.45	0.81	8.43E-02	-0.39	0.86	3427640	426311	3234660	456249	3248710	488562	3220609	426004
RP_POS_329_24155a11_609	RP	POS	11.61	329.2416				4.96E-01	-0.13	0.57	7.60E-01	0.06	0.61	6.30E-01	-0.10	0.49	4.81E-01	-0.16	0.71	3718468	853925	3595248	975861	3565231	1097607	3625265	847033
RP_NEG_166_98578a0_45	RP	POS	0.45	166.9858				2.59E-07	-0.65	1.33	7.60E-01	0.07	1.17	2.54E-04	-0.61	1.40	1.45E-04	-0.68	1.44	4849034	475554	3655844	2021323	3593690	2096127	3717998	1962968
HILIC_NEG_128_9597a2_912	HILIC	NEG	2.912	128.9597				1.34E-04	-0.57	1.33	7.60E-01	0.07	0.80	2.76E-03	-0.54	1.36	1.74E-03	-0.60	1.35	160069215	29963627	128616249	59022444	126802201	61983405	130430297	56477734
RP_POS_303_14374a6_254	RP	POS	6.25	303.1437				3.56E-01	-0.19	0.43	7.60E-01	-0.06	0.28	3.31E-01	-0.22	0.39	4.95E-01	-0.16	0.31	3524320	378141	3452430	386404	3464297	398075	3440563	378038
HILIC_POS_634_875a4_325	HILIC	POS	4.325	634.8750				2.61E-03	0.40	1.23	7.61E-01	-0.07	0.91	2.35E-02	0.37	1.28	2.12E-02	0.44	1.41	5314370	355603	5676222	996915	5706823	1087100	5645620	907889
HILIC_POS_208_88416a2_991	HILIC	POS	2.991	208.8842				8.56E-05	-0.56	1.34	7.61E-01	0.07	0.79	2.50E-03	-0.53	1.40	1.73E-03	-0.60	1.39	12708261	2449504	9866242	5475089	9698292	5777360	10034192	5208600
RP_NEG_174_08777a0_548	RP	NEG	0.55	174.0878				2.19E-05	0.72	1.50	7.61E-01	0.06	0.96	1.40E-04	0.75	1.53	5.54E-04	0.69	1.39	748047	200129	956067	294287	947060	300588	965074	290617
RP_POS_479_37039a11_166	RP	POS	11.17	479.3704				1.58E-01	-0.21	0.94	7.62E-01	0.07	0.91	3.18E-01	-0.17	0.82	2.21E-01	-0.24	0.95	328808	61462	304815	129107	300876	140221	308754	118253
RP_POS_270_27859a10_958	RP	POS	10.96	270.2786				9.83E-09	0.78	1.27	7.62E-01	0.06	0.84	1.01E-04	0.81	1.30	1.63E-07	0.75	1.58	846847	249879	1337208	665435	1316899	485114	1357517	811460
RP_NEG_612_26489a10_511	RP	NEG	10.51	612.2649				5.24E-02	-0.43	0.87	7.62E-01	0.06	0.55	9.84E-02	-0.40	0.77	5.34E-02	-0.46	0.81	2365002	607725	2127607	517387	2111833	495894	2143382	542608
RP_NEG_325_185a9_979	RP	NEG	9.98	325.1850				8.17E-01	-0.05	0.47	7.62E-01	-0.06	0.19	7.39E-01	-0.08	0.20	9.24E-01	-0.02	0.44	1656715	1470994	1589926	1205749	1626645	1244441	1553208	1177262
RP_POS_253_11765a0_716	RP	POS	0.72	253.1177				3.58E-08	0.66	1.28	7.63E-01	0.07	1.14	1.40E-04	0.69	1.39	7.33E-05	0.63	1.41	35214	26861	377189	570700	359815	529311	394563	614213
RP_POS_462_30243a12_124	RP	POS	12.12	462.3024				2.49E-01	-0.21	1.02	7.63E-01	0.06	0.80	3.73E-01	-0.18	0.85	2.74E-01	-0.24	0.85	630278	128393	597735	163258	592767	179618	602703	146756
RP_POS_553_45959a12_89	RP	POS	12.89	553.4596				4.58E-02	0.34	0.85	7.63E-01	0.06	0.54	6.37E-02	0.37	0.93	1.25E-01	0.31	0.61	14218528	1775452	15038201	2537044	14961230	2559499	15115172	2537995
RP_POS_181_98769a0_677	RP	POS	0.68	181.9877				8.85E-08	0.67	1.33	7.63E-01	-0.07	1.18	1.95E-04	0.64	1.40	6.58E-05	0.70	1.44	2053556	246411	2722232	1091924	2755354	1108933	2689111	1084877
RP_POS_172_09679a3_969	RP	POS	3.97	172.0968				1.68E-01	0.16	0.69	7.63E-01	-0.07	0.26	3.21E-01	0.12	0.86	3.22E-01	0.19	0.45	7827	9238	1888247	13531850	2298811	16189246	1477684	10369339
RP_POS_213_14603a7_439	RP	POS	7.44	213.1460				8.60E-01	0.03	0.54	7.63E-01	0.06	0.68	7.71E-01	0.07	0.22	9.89E-01	0.00	0.66	3801582	224250	3809879	250637	3802280	239958	3817478	263101
RP_POS_204_06316a0_704	RP	POS	0.70	204.0632				4.33E-03	-0.43	1.18	7.63E-01	-0.07	0.66	1.16E-02	-0.47	1.12	3.64E-02	-0.40	1.29	830110	193877	683939	364969	695003	377658	672875	355313
HILIC_POS_278_21115a0_578	HILIC	POS	0.578	278.2112				3.49E-03	0.38	0.73	7.64E-01	0.07	0.51	1.46E-02	0.41	0.80	5.67E-02	0.34	0.77	6712434	9527836	17652933	32676556	16662664	34201274	18643202	31393904
RP_POS_173_07843a10_572	RP	POS	10.57	173.0784				3.89E-02	0.38	0.70	7.64E-01	-0.06	0.24	1.06E-01	0.35	0.66	4.51E-02	0.42	0.81	1898955	741215	2234030	898502	2261257	848277	2206802	953940
RP_NEG_229_9019a1_466	RP	NEG	1.47	229.9019				3.56E-10	0.89	1.49	7.64E-01	0.06	0.61	1.12E-06	0.92	1.63	8.47E-07	0.86	1.52	1202202	953261	3093669	2188566	3027352	2082796	3159986	2308763
RP_POS_136_95326a0_255	RP	POS	0.26	136.9533				3.82E-01	0.17	0.35	7.64E-01	-0.06	0.49	5.34E-01	0.13	0.23	3.65E-01	0.20	0.34	20888005	2004780	21262269	2347485	21333395	2379302	21191144	2337184
HILIC_POS_130_08653a3_843	HILIC	POS	3.843	130.0865				1.01E-03	-0.87	1.92	7.64E-01	0.05	0.49	2.17E-03	-0.85	1.42	9.68E-04	-0.89	1.72	25028932	13172289	16283625	7814072	16046892	7053498	16520358	8573176
RP_POS_607_29266a10_619	RP	POS	10.62	607.2927				1.47E-01	-0.32	0.76	7.64E-01	0.06	0.24	2.45E-01	-0.29	0.63	1.31E-01	-0.35	0.70	765736	291867	680721	257026	672934	223577	688508	288726
HILIC_NEG_132_92365a5_606	HILIC	NEG	5.606	132.9237				3.97E-01	-0.19	0.81	7.64E-01	-0.06	0.74	3.63E-01	-0.22	0.42	5.20E-01	-0.16	0.52	1427666	280543	1380430	245089	1387853	258004	1373007	233848
RP_POS_204_95728a0_468	RP	POS	0.47	204.9573				5.98E-04	-0.59	1.20	7.64E-01	-0.06	1.01	2.06E-03	-0.62	1.16	5.50E-03	-0.56	1.25	386988	73609	326776	106309	329995	107086	323556	106513
RP_NEG_299_22354a9_889	RP	NEG	9.89	299.2235				8.31E-01	0.04	0.54	7.64E-01	0.06	0.39	7.38E-01	0.07	0.19	9.51E-01	0.01	0.59	1734209	315843	1747801	299404	1738736	331906	1756867	266057
HILIC_POS_208_03973a7_963	HILIC	POS	7.963	208.0397				1.94E-05	-0.65	1.28	7.65E-01	0.06	0.72	8.89E-04	-0.62	1.29	3.05E-04	-0.69	1.35	12907136	3081928	9351833	5753158	9178217	5812555	9525450	5746811
RP_POS_248_89961a15_43	RP	POS	15.43	248.8996				8.04E-01	-0.04	0.22	7.65E-01	-0.07	0.57	6.99E-01	-0.07	0.32	9.67E-01	-0.01	0.30	3087109	297250	3069882	450835	3083488	481833	3056277	422033
RP_POS_478_83469a0_499	RP	POS	0.50	478.8347				8.87E-04	-0.44	1.20	7.65E-01	-0.07	1.23	4.60E-03	-0.47	1.26	2.79E-02	-0.41	1.25	10328994	1788429	8214084	5350339	8375380	5716173	8052789	5010861
HILIC_NEG_203_7989a3_032	HILIC	NEG	3.032	203.7989				7.34E-05	0.50	1.32	7.65E-01	-0.07	0.77	3.56E-03	0.47	1.41	3.65E-03	0.54	1.52	1235549	55490	1330681	210350	1337020	226416	1324342	195067
HILIC_NEG_234_82027a5_575	HILIC	NEG	5.575	234.8203				5.36E-01	-0.09	0.64	7.65E-01	0.07	0.57	6.89E-01	-0.06	0.79	5.68E-01	-0.12	0.44	556655	51933	547996	104891	544841	130438	551150	72072
RP_POS_167_05641a1_973	RP	POS	1.97	167.0564				5.01E-04	-0.97	1.77	7.66E-01	-0.04	0.42	5.26E-04	-0.99	1.55	8.51E-04	-0.94	1.66	767627	662246	301594	342748	311887	344554	291300	344116
RP_NEG_659_07574a9_006	RP	NEG	9.01	659.0757				9.20E-01	-0.02	0.60	7.66E-01	-0.06	0.55	8.33E-01	-0.05	0.34	9.71E-01	0.01	0.26	3303946	209148	3299704	194735	3305547	175538	3293862	213855
RP_POS_641_59399a11_248	RP	POS	11.25	641.5940				1.78E-13	0.98	1.51	7.66E-01	0.06	0.67	3.15E-07	1.01	1.60	2.45E-09	0.94	1.71	3189550	2255080	9741143	6898905	9534176	5897303	9948110	7829144
RP_POS_370_7402a0_52	RP	POS	0.52	370.7402				5.73E-07	0.61	1.30	7.66E-01	-0.07	1.12	5.10E-04	0.57	1.32	2.96E-04	0.64	1.39	99709	26708	203194	189070	208858	196054	197531	183636
RP_POS_282_40607a10_845	RP	POS	10.85	282.4061				1.86E-04	0.59	1.05	7.67E-01	-0.06	0.68	5.98E-03	0.56	1.02	5.31E-04	0.62	1.28	306954	133645	435497	230371	442385	206005	428609	254342
RP_NEG_908_77045a0_496	RP	NEG	0.50	908.7705				7.66E-07	-0.61	1.32	7.67E-01	0.07	1.20	5.18E-04	-0.58	1.38	3.10E-04	-0.64	1.41	3861207	325786	2909962	1727362	2858357	1793549	2961567	1675173
RP_POS_295_22427a10_017	RP	POS	10.02	295.2243				6.25E-02	-0.38	0.81	7.67E-01	0.06	0.71	1.21E-01	-0.35	0.73	7.30E-02	-0.41	0.84	2443390	246067	2347650	253218	2340087	257466	2355213	251279
HILIC_POS_290_84735a2_99	HILIC	POS	2.99	290.8474				5.07E-06	-0.59	1.36	7.67E-01	0.07	0.77	8.18E-04	-0.55	1.47	7.29E-04	-0.62	1.50	75532028	9021591	58682730	31585652	57741085	33456394	59624375	29908648
RP_POS_399_34448a11_162	RP	POS	11.16	399.3445				1.36E-03	-0.62	1.04	7.67E-01	0.06	0.52	6.41E-03	-0.59	1.07	2.70E-03	-0.65	1.07	643015	107668	567067	121379	563450	121118	570683	122760
RP_POS_359_24121a9_041	RP	POS	9.04	359.2412				6.29E-03	-0.51	1.19	7.68E-01	-0.06	0.54	1.20E-02	-0.54	1.14	2.18E-02	-0.48	0.98	2785349	88030	2732142	105712	2735289	103467	2728995	108870
HILIC_POS_113_10762a0_549	HILIC	POS	0.549	113.1076				4.94E-05	-0.79	1.38	7.68E-01	-0.06	0.51	1.63E-04	-0.82	1.34	4.01E-04	-0.76	1.29	2671205	426389	2278599	484754	2293028	484536	2264170	489457
RP_NEG_428_18729a11_611	RP	NEG	11.61	428.1873				7.26E-02	-0.33	0.97	7.68E-01	-0.06	0.71	7.76E-02	-0.36	0.84	1.67E-01	-0.30	0.76	2189833	232430	2098863	281551	2107220	300863	2090506	263627
RP_POS_458_3237a9_678	RP	POS	9.68	458.3237				8.57E-01	-0.05	0.33	7.68E-01	-0.05	0.25	8.02E-01	-0.07	0.35	9.28E-01	-0.03	0.19	590834	844655	562519	463209	576259	392350	548778	528375

Supplementary table 1: Metabolomics results (in asceding order according to p-value from progressive ALD vs non-progressive ALD comparison, with molecular features with ID_level of 1-2 first)

							all_ALD_vs_control			Prog_ALD_vs_non-prog_ALD			Prog_ALD_vs_control_ALD			Non-prog_ALD_vs_control			Healthy_control		all_ALD		Non-prog_ALD		Progressive_ALD	
							t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA								
Feature_ID	RP_HILIC	POS_NEG	Average.Rt	Average.Mz	Metabolite.name	curated_MSMS	p	d	VIP	p	d	VIP	p	d	VIP	p	d	VIP	Mean	SD	Mean	SD	Mean	SD	Mean	SD
RP_POS_954_7467a0_497	RP	POS	0.50	954.7467			3.34E-07	-0.62	1.33	7.69E-01	0.07	1.19	3.72E-04	-0.59	1.40	2.18E-04	-0.65	1.43	2955460	206885	2204349	1334850	2164798	1383392	2243901	1297322
RP_POS_548_82056a0_499	RP	POS	0.50	548.8206			4.99E-04	-0.46	1.20	7.69E-01	-0.07	1.24	3.10E-03	-0.50	1.28	1.97E-02	-0.43	1.24	1356756	216025	1096016	622191	1114423	663645	1077609	583977
RP_POS_140_90327a0_521	RP	POS	0.52	140.9033			2.92E-05	0.51	1.21	7.69E-01	-0.07	1.09	3.07E-03	0.48	1.19	2.46E-03	0.54	1.35	234216	28250	305598	156273	310220	165335	300977	148195
RP_NEG_316_9483a0_496	RP	NEG	0.50	316.9483			4.19E-06	0.56	1.30	7.69E-01	-0.07	1.20	8.68E-04	0.53	1.37	1.19E-03	0.59	1.38	49315114	3092171	59339887	19982300	59930419	21534790	58749355	18500664
RP_POS_195_09996a5_581	RP	POS	5.58	195.1000			5.65E-01	0.10	0.37	7.69E-01	-0.06	0.46	7.29E-01	0.07	0.38	5.26E-01	0.13	0.59	1146233	124689	1162175	165665	1167067	171049	1157282	161689
RP_POS_245_07825a7_493	RP	POS	7.49	245.0783			5.88E-01	0.10	0.46	7.69E-01	0.06	0.72	5.49E-01	0.13	0.32	7.38E-01	0.07	0.44	11972984	902824	12078560	1101194	12046048	1041875	12111071	1167195
RP_POS_397_22189a9_072	RP	POS	9.07	397.2219			1.21E-09	0.73	1.20	7.70E-01	-0.06	0.38	3.49E-05	0.70	1.41	1.09E-05	0.77	1.31	74246	175516	2999141	4350531	3127540	4403187	2870742	4338065
HILIC_POS_387_21359a3_927	HILIC	POS	3.927	387.2136			3.28E-02	-0.39	0.96	7.70E-01	0.06	0.78	8.62E-02	-0.36	0.77	4.72E-02	-0.42	0.76	4472596	982600	4006201	1249140	3969354	1267040	4043047	1242734
RP_POS_344_01434a0_631	RP	POS	0.63	344.0143			2.63E-08	-0.68	1.36	7.70E-01	0.06	1.17	1.13E-04	-0.65	1.44	4.74E-05	-0.72	1.47	1828004	135700	1339406	781829	1316370	799141	1362441	771543
RP_POS_512_33423a8_761	RP	POS	8.76	512.3342			1.43E-03	-0.50	1.31	7.70E-01	0.06	0.63	3.65E-02	-0.47	1.25	4.84E-04	-0.53	1.30	849368	249201	646077	434105	633274	278430	658879	550347
RP_NEG_325_18503a15_464	RP	NEG	15.46	325.1850			7.86E-01	-0.06	0.43	7.70E-01	0.06	0.37	8.99E-01	-0.03	0.51	7.03E-01	-0.09	0.23	7162562	2596075	7023649	2203404	6958741	1892046	7088558	2494118
RP_NEG_371_19043a9_565	RP	NEG	9.57	371.1904			1.12E-02	0.40	0.76	7.70E-01	0.06	0.69	3.83E-02	0.43	0.83	3.50E-02	0.37	0.82	1167551	1320760	2010435	2270563	1943579	1953672	2077290	2567132
RP_POS_605_45154a10_976	RP	POS	10.98	605.4515			1.09E-02	0.43	1.33	7.70E-01	-0.06	1.17	5.44E-02	0.40	1.14	1.72E-02	0.46	1.27	552315	268832	714943	403957	726834	379663	703052	430420
RP_POS_478_38873a10_785	RP	POS	10.79	478.3887			6.30E-01	-0.10	1.04	7.70E-01	-0.06	0.59	5.74E-01	-0.13	0.90	7.56E-01	-0.07	0.81	1301536	460086	1257013	428574	1269617	437411	1244410	423613
RP_POS_472_26309a6_668	RP	POS	6.67	472.2631			2.03E-07	0.62	1.34	7.70E-01	-0.07	1.14	4.43E-04	0.59	1.44	1.58E-04	0.65	1.42	17822	20337	1284906	2267663	1351578	2303321	1218234	2252814
RP_NEG_326_83194a15_519	RP	NEG	15.52	326.8319			1.67E-01	0.32	0.56	7.70E-01	0.05	0.38	1.40E-01	0.35	0.62	2.68E-01	0.29	0.47	2183056	335007	2274216	266961	2266363	320019	2282069	203599
HILIC_POS_274_78516a3_016	HILIC	POS	3.016	274.7852			1.42E-04	-0.50	1.34	7.71E-01	0.06	0.77	5.29E-03	-0.47	1.44	3.41E-03	-0.54	1.47	386654	59429	306463	175459	301307	183920	311619	168283
HILIC_NEG_153_86874a0_675	HILIC	NEG	0.675	153.8687			5.27E-04	-0.71	1.13	7.71E-01	0.06	1.47	1.80E-03	-0.69	1.26	1.32E-03	-0.74	1.18	964686	168634	837976	169864	832987	181507	842965	159062
RP_POS_293_28351a11_246	RP	POS	11.25	293.2835			9.80E-11	0.92	1.44	7.71E-01	0.06	0.85	7.54E-06	0.95	1.45	1.80E-09	0.89	1.82	858432	414138	1718766	966157	1690381	694457	1747151	1184083
HILIC_NEG_298_8804a2_91	HILIC	NEG	2.91	298.8804			3.08E-07	-0.63	1.35	7.71E-01	0.06	0.78	2.33E-04	-0.60	1.50	2.65E-04	-0.66	1.54	4236438	296095	3302813	1636722	3254796	1737751	3350830	1545284
RP_POS_684_79498a0_499	RP	POS	0.50	684.7950			1.65E-03	-0.42	1.21	7.71E-01	-0.06	1.24	7.20E-03	-0.46	1.27	3.37E-02	-0.39	1.25	1209617	197218	1003698	537301	1019457	568678	987939	509289
RP_NEG_314_98926a7_717	RP	NEG	7.72	314.9893			2.20E-01	-0.28	0.60	7.71E-01	-0.06	0.17	2.14E-01	-0.30	0.58	3.09E-01	-0.25	0.41	9841051	508677	9717134	428397	9729689	430413	9704579	430368
HILIC_POS_129_06601a5_5	HILIC	POS	5.5	129.0660			3.41E-01	0.15	0.47	7.71E-01	0.06	0.97	3.95E-01	0.18	0.36	4.89E-01	0.12	0.31	361763	435096	465698	766848	443255	624665	488142	892680
RP_POS_860_75238a0_5	RP	POS	0.50	860.7524			3.43E-04	-0.49	1.22	7.72E-01	-0.06	1.22	2.19E-03	-0.52	1.27	1.40E-02	-0.46	1.26	1046151	175435	845031	449720	858188	478758	831873	423156
RP_POS_167_716a11_165	RP	POS	11.17	167.7160			4.75E-11	1.11	1.76	7.72E-01	-0.06	0.53	7.25E-08	1.08	1.74	1.61E-09	1.13	1.89	220681	90099	380447	136972	384452	126922	376442	147525
RP_POS_616_80725a0_499	RP	POS	0.50	616.8073			5.22E-04	-0.47	1.22	7.72E-01	-0.06	1.23	3.18E-03	-0.50	1.29	1.88E-02	-0.44	1.26	1299593	215316	1049072	592019	1066364	629558	1031780	557829
RP_NEG_405_19357a6_795	RP	NEG	6.80	405.1936			3.22E-02	0.37	1.39	7.72E-01	0.06	0.33	3.78E-02	0.40	0.97	1.09E-01	0.34	1.34	753908	160515	832885	224104	826343	244497	839427	203972
HILIC_NEG_115_92069a3_008	HILIC	NEG	3.008	115.9207			8.48E-01	0.04	0.88	7.72E-01	-0.05	0.67	9.45E-01	0.02	0.43	7.71E-01	0.07	0.43	17426681	2105672	17505188	1638413	17552955	1542064	17457421	1743834
RP_POS_312_91617a15_483	RP	POS	15.48	312.9162			2.07E-01	-0.23	0.78	7.72E-01	0.06	0.31	3.53E-01	-0.20	0.56	2.04E-01	-0.26	0.71	2427593	323451	2338324	403375	2326569	384068	2350080	425386
RP_NEG_461_14453a11_611	RP	NEG	11.61	461.1445			5.22E-01	0.15	0.98	7.72E-01	0.06	0.58	4.79E-01	0.17	0.77	6.35E-01	0.12	0.98	818573	117410	833313	95676	830525	99160	836100	92985
RP_NEG_508_87665a0_46	RP	NEG	0.46	508.8767			3.05E-07	-0.67	1.32	7.73E-01	0.06	1.14	2.12E-04	-0.64	1.38	8.65E-05	-0.71	1.41	526686	81805	369570	252385	362228	257598	376913	249458
HILIC_NEG_316_94769a4_232	HILIC	NEG	4.232	316.9477			1.02E-01	0.24	1.07	7.73E-01	-0.06	0.87	2.46E-01	0.21	0.76	1.51E-01	0.27	1.07	46409867	6254097	49190424	12721298	49559655	13221475	48821192	12323955
RP_POS_419_31558a12_242	RP	POS	12.24	419.3156			7.32E-01	0.07	0.32	7.73E-01	-0.06	0.68	8.64E-01	0.04	0.58	6.59E-01	0.10	0.65	10329837	4534451	10650744	4771535	10789232	4628615	10512255	4953435
RP_POS_581_27832a10_517	RP	POS	10.52	581.2783			6.77E-02	-0.38	0.77	7.74E-01	-0.06	0.44	7.96E-02	-0.41	0.75	1.19E-01	-0.35	0.57	684772	199419	609862	191743	615420	184944	604304	200034
RP_NEG_384_16144a11_162	RP	NEG	11.16	384.1614			2.91E-01	0.18	0.86	7.74E-01	0.06	0.70	2.88E-01	0.21	0.76	4.59E-01	0.15	0.74	836035	69768	852678	96195	849895	98819	855461	94418
RP_POS_239_16145a8_561	RP	POS	8.56	239.1615			4.83E-01	0.13	0.54	7.74E-01	-0.06	0.68	6.62E-01	0.10	0.22	4.17E-01	0.16	0.52	4663057	564749	4748763	691505	4768763	583729	4728763	790291
RP_NEG_440_88895a0_458	RP	NEG	0.46	440.8890			1.73E-06	-0.63	1.28	7.74E-01	0.06	1.13	4.91E-04	-0.60	1.34	2.38E-04	-0.66	1.37	821081	135166	585729	404188	574061	415501	597396	396423
RP_POS_249_13313a4_569	RP	POS	4.57	249.1331			2.25E-01	-0.24	0.54	7.75E-01	-0.06	0.33	2.37E-01	-0.27	0.50	3.29E-01	-0.21	0.51	1635068	116127	1605657	123434	1609217	116424	1602097	131158
RP_POS_297_0293a3_622	RP	POS	3.62	297.0293			1.65E-02	-0.51	0.91	7.75E-01	0.06	0.83	4.62E-02	-0.49	0.79	1.55E-02	-0.54	1.12	1082177	919886	626542	849490	602043	723928	651041	965763
RP_NEG_915_1272a9_56	RP	NEG	9.56	915.1272			8.48E-01	-0.04	0.51	7.75E-01	-0.06	0.32	7.64E-01	-0.07	0.43	9.60E-01	-0.01	0.49	3350670	245336	3341216	230910	3347873	243173	3334558	220235
RP_NEG_211_91736a15_562	RP	NEG	15.56	211.9174			9.14E-04	-0.63	1.61	7.75E-01	-0.06	0.27	1.03E-03	-0.66	1.61	8.30E-03	-0.60	1.12	6013615	797713	5421510	947540	5448832	1086269	5394187	795287
RP_POS_524_83057a0_474	RP	POS	0.47	524.8306			2.51E-05	-0.57	1.26	7.75E-01	-0.06	1.23	4.40E-04	-0.60	1.35	3.59E-03	-0.54	1.32	359408	64283	268236	174760	273272	184887	263200	165742
RP_NEG_224_06203a6_51	RP	NEG	6.51	224.0620			3.22E-01	-0.36	0.70	7.75E-01	0.01	0.44	3.29E-01	-0.35	0.50	3.16E-01	-0.36	0.58	95338903	443431971	16379572	34638819	15383105	25168561	17376039	42293018
RP_NEG_324_87967a15_474	RP	NEG	15.47	324.8797			9.20E-01	-0.02	0.55	7.75E-01	0.06	0.43	9.51E-01	0.01	0.24	8.10E-01	-0.05	0.81	4262564	559231	4250044	753130	4228395	718834	4271693	792657
RP_NEG_226_96576a15_292	RP	NEG	15.29	226.9658			2.45E-01	-0.22	0.46	7.75E-01	-0.06	0.44	2.38E-01	-0.25	0.51	3.90E-01	-0.19	0.78	3813513	109774	3786150	129593	3789874	136286	3782426	123810
RP_POS_330_27655a10_985	RP	POS	10.99	330.2766			2.43E-04	0.60	0.94	7.76E-01	0.06	0.44	3.12E-03	0.63	1.01	1.30E-03	0.57	1.11	728943	576789	1258391	933451	1231597	784830	1285184	1069121
RP_POS_407_258a13_724	RP	POS	13.72	407.2580			1.46E-03	0.64	1.04	7.76E-01	0.06	0.37	3.45E-03	0.67	1.06	4.47E-03	0.62	1.02	1192904	580581	1592094	603074	1574794	559511	1609394	648965
RP_POS_321_06982a8_805	RP	POS	8.81	321.0698			5.54E-02	0.32	0.81	7.76E-01	0.06	1.11	2.41E-02	0.35	1.05	2.20E-01	0.29	0.81	84769674	29191663	98007419	44420146	96731982	57889577	99282857	25140486
RP_POS_793_5575a13_277	RP	POS	13.28	793.5575			9.30E-01	-0.02	0.30	7.76E-01	0.06	0.32	9.60E-01	0.01	0.23	8.39E-01	-0.05	0.31	3172370	1022450	3153864	1049034	3123781	1105579	3183947	999625
HILIC_NEG_118_93065a2_931	HILIC	NEG	2.931	118.9307			4.17E-04	-0.53	1.32	7.76E-01	-0.06	0.78	5.68E-03	-0.50	1.34	3.71E-03	-0.56	1.33	17692367	3362204	14466678	6551497	14278998	6875654	14654359	6274846
HILIC_NEG_100_93346a4_797	HILIC	NEG	4.797	100.9335			2.00E-01	-0.26	0.75	7.76E-01	-0.06	0.62	2.14E-01	-0.29	0.55	2.90E-01	-0.23	0.49	52407041	11865522	49278834	11862065	49618625	11005626	48939042	12764377
HILIC_NEG_253_79393a0_55	HILIC	NEG	0.55	253.7939			3.45E-03	-0.55	0.94	7.76E-01	0.06	0.89	2.21E-02	-0.52	0.79	3.54E-03	-0.58	1.08	255778	74552	207350	89389	204791	74334	209909	102980
RP_NEG_200_8588a15_618	RP	NEG	15.62	200.8588			5.33E-01	-0.13	0.62	7.76E-01	-0.06	0.32	5.04E-01	-0.16	0.65	6.54E-01	-0.10	0.62	629171	37317	624428	36807	625481	34354	623375	39430
RP_POS_774_56281a11_525	RP	POS	11.53	774.5628			1.69E-01	0.19	0.55	7.76E-01	-0.06	0.61	3.50E-01	0.16	0.54	2.43E-01	0.22	0.57	506942	368649	666458	949750	693623	1021358	639293	881918
RP_POS_167_97215a0_676	RP	POS	0.68	167.9722			4.94E-07	0.62	1.30	7.77E-01	-0.06	1.16	5.83E-04	0.59	1.35	1.56E-04	0.65	1.42	979347	120823	1316900	597662	1333964	598861	1299836	602047
RP_POS_530_96454a6_895	RP	POS	6.90	530.9645			1.72E-07	0.62	1.32	7.77E-01	-0.06	1.13	3.67E-04	0.59	1.42	1.61E-04	0.66	1.40	13550	29404	1235927	2172459	1297851	2221323	1174004	2143215
RP_POS_420_25281a11_613	RP	POS	11.61	420.2528			1.29E-03	-0.55	1.02	7.77E-01	0.06	0.80	4.31E-03	-0.52	1.13	7.81E-03	-0.58	1.02	795281	50334	756827	72938	754747	84078	758906	60585
HILIC_NEG_82_97139a2_985	HILIC	NEG	2.985	82.9714			9.35E-01	0.02	0.97	7.77E-01	-0.06	0.83	9.45E-01	-0.01	0.24	8.34E-01	0.04	0.57	2372768	442789	2380583	538001	2395904	549313	2365262	531577
HILIC_POS_562_34326a0_998	HILIC	POS	0.998	562.3433			3.10E-05	0.51	1.22	7.78E-01	-0.06	0.78	5.99E-03	0.47	1.36	1.34E-03	0.54	1.36	348062	952908	2922941	5689671	3084909	5591814	2760974	5838102
HILIC_POS_113_1076a0_681	HILIC	POS	0.681	113.1076			1.10E-01	-0.37	0.72	7.78E-01	-0.05	0.31	1.16E-01	-0.40	0.62	1.60E-01	-0.35	0.58	3135377	637136	2935125	490759	2949091	469032	2921158	515961
HILIC_NEG_520_91058a4_232	HILIC	NEG	4.232	520.9106			1.92E-03	0.40	1.25	7.78E-01	-0.06	0.92	2.54E-02	0.37	1.30	1.86E-02	0.43	1.45	9951626	626547	10721705	2164828	10783249	2299710	10660161	2042597
HILIC_NEG_296_88248a2_91	HILIC	NEG	2.91	296.8825			1.74E-07	-0.64	1.35	7.78E-01	0.06	0.78	1.69E-04	-0.61	1.50	2.16E-04	-0.67	1.54	21439631	1383180	16640611	8265995	16405633	8787365	16875589	7792131
RP_NEG_297_82843a15_552	RP	NEG	15.55	297.8284			2.96E-01	-0.20	0.58	7.78E-01	-0.06	0.17	3.03E-01	-0.23	0.52	4.18E-01	-0.17	0.45	2559108	89652	2539356	99999	2542193	94803	2536520	105828
RP_POS_148_97606a0_45	RP	POS	0.45	148.9761			5.59E-07	-0.64	1.32	7.79E-01	0.06	1.16	3.21E-04	-0.61	1.38	1.68E-04	-0.68	1.42	12100383	1639699	8713461	5737673	8550924	5908540	8875997	5616840
HILIC_POS_366_26379a0_665	HILIC	POS	0.665	366.2638			9.91E-01	0.00	0.50	7.79E-01	-0.06	0.67	8.83E-01	-0.03	0.16	9.02E-01	0.03	0.41	1067331	538225	1066110	619771	1083650	650119	1048570	593959
HILIC_NEG_360_78674a2_93	HILIC	NEG	2.93	360.7867			1.14E-06	-0.62	1.34	7.79E-01	0.06	0.77	3.32E-04	-0.59	1.47	3.54E-04	-0.66	1.50	870717	98969	670275	351147	660353	372346	680198	332088
RP_NEG_512_26764a7_388	RP	NEG	7.39	512.2676			2.43E-01	-0.38	1.03	7.79E-01	0.03	0.58	2.68E-01	-0.37	0.90	2.31E-01	-0.40	0.76	653756	1214368	395224	357497	385122	352387	405325	365831
HILIC_POS_198_85435a3_011	HILIC	POS	3.011	198.8544			1.45E-04	-0.55	1.34	7.79E-01	0.06	0.78	3.52E-03	-0.52	1.40	2.03E-03	-0.58	1.43	531559	113019	408544	240458	401750	249573	415337	233323
RP_POS_380_24667a10_455	RP	POS	10.46	380.2467			7.72E-01	0.05	0.67	7.79E-01	0.06	0.24	7.18E-01	0.08	0.56	9.20E-01	0.02	0.27	978830	116976	986725	176430	981742	144471	991708	204861
RP_POS_652_87286a6_534	RP	POS	6.53	652.8729			2.95E-07	0.61	1.33	7.79E-01	-0.06	1.14	6.22E-04	0.58	1.41	1.57E-04	0.64	1.41	41218	114294	1653117	2924778	1735685	2922731	1570550	2954144
RP_NEG_1021_21887a9_76	RP	NEG	9.76	1021.2189			1.63E-01	0.24	0.43	7.79E-01	0.06	0.42	2.07E-01	0.27	0.49	2.78E-01	0.21	0.50	4788232	420099	4924043	614068	4906707	559139	4941379	669781
RP_POS_876_56958a14	RP	POS	14.00	876.5696			2.99E-01	-0.20	0.44	7.81E-01	0.06	0.26	4.46E-01	-0.18	0.46	2.73E-01	-0.23	0.45	9928087	2900765	9298468	3129043	9210647	2817372	9386289	3439231
RP_POS_294_21915a10_732	RP	POS	10.73	294.2192			5.07E-07	0.70	1.12	7.81E-01	-0.06	0.58	9.85E-04	0.67	1.10	2.08E-06	0.73	1.46	1218843	302837	1701195	734627	1721809	580579	1680581	867426
RP_POS_130_96547a0_45	RP	POS	0.45	130.9655			1.18E-06	-0.64	1.31	7.81E-01	0.06	1.15	4.17E-04	-0.61	1.36	2.24E-04	-0.67	1.41	8251994	1235259	5962191	3924946	5852176	4045022	6072206	3838996
HILIC_POS_209_09174a4_124	HILIC	POS	4.124	209.0917			2.72E-02	-0.36	1.01	7.81E-01	-0.06	1.31	7.59E-02	-0.39	0.60	4.81E-02	-0.33	1.16	2306663	493977	2045292	766521	2066775	575425	2023810	924686
HILIC_POS_374_80884a2_99	HILIC	POS	2.99	374.8088			1.46E-05	-0.57	1.35	7.82E-01	0.06	0.77	1.28E-03	-0.54	1.47	1.16E-03	-0.60	1.49	8536433	1174773	6635405	3673831	6532920	3892341	6737889	3478185
HILIC_NEG_382_84122a2_91	HILIC	NEG	2.91	382.8412			2.95E-07	-0.63	1.35	7.82E-01	0.06	0.78	2.14E-04	-0.60	1.50	2.66E-04	-0.66	1.54	3100347	228947	2397021	1227750	2362798	1304630	2431244	1158038
HILIC_NEG_458_77112a2_923	HILIC	NEG	2.923	458.7711			4.58E-07	-0.65	1.34	7.82E-01	0.06	0.76	1.83E-04	-0.62	1.47	2.23E-04	-0.68	1.50	195745	23116	147781	80498	145538	85559	150024	75904
RP_POS_462_85864a0_498	RP	POS	0.50	462.8586			5.31E-07	-0.61	1.33	7.82E-01	0.06	1.19	3.09E-04	-0.58	1.41	3.84E-04	-0.64	1.41	24392526	1731296	18539615	10571707	18245172	11247989	18834057	9955331
RP_POS_553_45837a13_631	RP	POS	13.63	553.4584			5.69E-02	-0.40	0.74	7.82E-01	-0.05	0.70	5.93E-02	-0.42	0.90	1.16E-01	-0.37	0.61	16192373	2533630	15197210	2456814	15265546	2627112	15128874	2298654
HILIC_POS_113_10769a3_032	HILIC	POS	3.032	113.1077			4.68E-05	0.50	1.19	7.83E-01	-0.06	0.75	2.68E-03	0.47	1.27	3.71E-03	0.53	1.33	2652702	136019	2938376	632301	2955942	686574	2920810	579443
RP_POS_955_70135a14_271	RP	POS	14.27	955.7014			6.45E-01	-0.09	0.74	7.83E-01	-0.06	0.36	6.01E-01	-0.12	0.57	7.81E-01	-0.06	0.75	2491307	859007	2406986	1002629	2434814	951493	2379158	1060248
HILIC_NEG_136_89175a7_674	HILIC	NEG	7.674	136.8918			5.45E-02	-0.36	0.56	7.83E-01	-0.06	0.58	6.59E-02	-0.39	0.75	1.24E-01	-0.33	0.56	11600333	1903996	10805802	2258960	10868466	2329100	10743137	2208442
RP_POS_1064_7146a0_496	RP	POS	0.50	1064.7146			2.99E-01	-0.24	0.47	7.83E-01	0.05	0.72	3.92E-01	-0.22	0.67	2.81E-01	-0.27	0.50	571025	131002	544449	101476	541634	98103	547264	105663
RP_POS_742_79657a0_496	RP	POS	0.50	742.7966			1.71E-07	-0.65	1.35	7.83E-01	0.06	1.17	2.61E-04	-0.62	1.42	1.23E-04	-0.68	1.44	2352111	190748	1778953	974630	1751928	998181	1805978	959863
RP_POS_487_36023a10_71	RP	POS	10.71	487.3602			6.85E-03	-0.57	1.00	7.84E-01	0.05	0.20	1.84E-02	-0.54	0.88	1.01E-02	-0.59	1.09	64763919	5597341	61580950	5445274	61430389	5493371	61731512	5448280
RP_POS_443_33395a13_099	RP	POS	13.10	443.3340			7.68E-01	-0.04	0.77	7.84E-01	0.06	0.36	9.46E-01	-0.01	0.97	6.55E-01	-0.08	0.37	4527910	588557	4482780	1116980	4451892	946727	4513667	1273779

Supplementary table 1: Metabolomics results (in asceding order according to p-value from progressive ALD vs non-progressive ALD comparison, with molecular features with ID_level of 1-2 first)

								all_ALD_vs_control			Prog_ALD_vs_non-prog_ALD			Prog_ALD_vs_control_ALD			Non-prog_ALD_vs_control			Healthy_control		all_ALD		Non-prog_ALD		Progressive_ALD	
								t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA								
Feature_ID	RP_HILIC	POS_NEG	Average.Rt	Average.Mz	Metabolite.name	curated_MSMS	ID_level	p	d	VIP	p	d	VIP	p	d	VIP	p	d	VIP	Mean	SD	Mean	SD	Mean	SD	Mean	SD
RP_POS_191_08553a9_449	RP	POS	9.45	191.0855	6-methoxy-4-methyl-2H-chromen-2-one	191.0847(100)	3	9.77E-01	0.00	0.30	7.84E-01	0.06	0.39	9.04E-01	0.03	0.29	8.01E-01	-0.03	0.53	2653271	238464	2651343	509036	2637263	334860	2665423	641084
RP_POS_120_97961a10_572	RP	POS	10.57	120.9796				4.45E-01	-0.17	0.48	7.84E-01	-0.05	0.20	4.16E-01	-0.20	0.57	5.54E-01	-0.14	0.39	2200995	891510	2066614	748914	2087289	765540	2045939	739098
RP_POS_228_19649a8_755	RP	POS	8.76	228.1965				3.53E-02	-0.37	0.59	7.84E-01	0.06	0.46	8.85E-02	-0.34	0.60	5.76E-02	-0.40	0.76	1776981	105913	1726315	143891	1722346	150610	1730284	138263
RP_POS_716_79022a0_498	RP	POS	0.50	716.7902				6.39E-04	-0.45	1.18	7.84E-01	-0.06	1.20	4.11E-03	-0.48	1.24	2.29E-02	-0.42	1.24	1588079	223954	1309745	689819	1328769	734323	1290722	649188
HILIC_POS_460_7677a2_992	HILIC	POS	2.992	460.7677				1.18E-05	-0.58	1.35	7.85E-01	0.06	0.77	1.11E-03	-0.55	1.47	9.90E-04	-0.61	1.49	4236226	610629	3251842	1870609	3200311	1977063	3303372	1776392
RP_NEG_766_85376a0_49	RP	NEG	0.49	766.8538				6.61E-08	0.65	1.36	7.85E-01	-0.06	1.20	1.46E-04	0.62	1.45	1.32E-04	0.68	1.44	630510	218047	2021897	2360008	2086860	2471698	1956933	2266063
RP_POS_411_09268a9_625	RP	POS	9.63	411.0927	Artemitin	411.0932(100)	3	2.15E-01	0.25	0.66	7.85E-01	-0.05	0.48	3.20E-01	0.23	0.50	2.17E-01	0.28	0.73	924649	203975	976609	203632	982213	203856	971006	205321
RP_POS_150_01347a0_518	RP	POS	0.52	150.0135				5.08E-03	0.35	1.07	7.85E-01	0.06	1.03	4.45E-02	0.38	1.08	3.36E-02	0.32	1.10	296097	67446	380892	272335	373397	236805	388387	306031
RP_NEG_226_96593a0_462	RP	NEG	0.46	226.9659				1.30E-06	-0.65	1.30	7.85E-01	-0.06	1.16	8.16E-05	-0.68	1.41	7.37E-04	-0.62	1.35	956016	124289	744228	354356	753971	371876	734485	339430
HILIC_NEG_200_97098a0_93	HILIC	NEG	0.93	200.9710				3.62E-09	0.83	1.37	7.86E-01	-0.06	1.23	3.95E-05	0.80	1.31	2.30E-07	0.86	1.66	164656	94692	341951	222318	348029	194816	335873	248657
HILIC_NEG_408_62604a2_947	HILIC	NEG	2.947	408.6260				1.28E-05	-0.60	1.31	7.86E-01	0.06	0.76	1.01E-03	-0.57	1.43	7.37E-04	-0.63	1.45	417689	67270	321377	175510	316582	183720	326171	168631
RP_POS_241_17737a7_525	RP	POS	7.53	241.1774				8.98E-01	0.02	0.28	7.86E-01	0.06	0.19	8.16E-01	0.05	0.27	9.85E-01	0.00	0.21	3183123	473304	3196002	549391	3180998	496889	3211007	602049
RP_NEG_301_88419a15_686	RP	NEG	15.69	301.8842				2.93E-01	-0.21	0.86	7.87E-01	-0.06	0.33	2.78E-01	-0.24	0.60	4.27E-01	-0.18	1.00	1267658	472940	1164095	502302	1177786	532406	1150404	475316
RP_POS_206_88542a0_5	RP	POS	0.50	206.8854				8.84E-03	-0.41	1.09	7.87E-01	-0.06	1.12	1.50E-02	-0.44	1.10	5.90E-02	-0.38	1.12	1556926	432075	1269521	755912	1290066	823356	1248976	689704
RP_POS_280_15436a3_352	RP	POS	3.35	280.1544	Likely acylcarnitine	280.1533(65), 221.0797(5), 85.0288(100)	3	7.72E-01	-0.06	0.42	7.87E-01	0.06	0.58	9.05E-01	-0.03	0.30	6.80E-01	-0.08	0.38	780140	801104	731402	898943	706974	748727	755830	1034833
RP_POS_323_25598a10_96	RP	POS	10.96	323.2560				1.06E-02	-0.42	1.06	7.88E-01	0.06	0.96	3.57E-02	-0.39	1.03	2.98E-02	-0.45	0.99	12872053	1756994	11785379	2756855	11710659	2991885	11860098	2528407
HILIC_POS_553_40698a2_224	HILIC	POS	2.224	553.4070				3.66E-01	0.17	0.76	7.88E-01	0.06	0.77	3.77E-01	0.20	0.35	4.90E-01	0.14	0.29	1111481	309919	1171522	366521	1161592	333461	1181451	400025
RP_POS_530_35797a10_868	RP	POS	10.87	530.3580				1.21E-03	-0.78	1.27	7.88E-01	-0.05	0.90	1.35E-03	-0.80	1.30	3.22E-03	-0.76	1.27	2319735	989904	1661691	729982	1681431	784952	1641951	677995
RP_NEG_691_12634a9_222	RP	NEG	9.22	691.1263				9.45E-02	0.29	0.57	7.88E-01	-0.06	0.44	2.41E-01	0.26	0.41	8.60E-02	0.31	0.66	1485949	97749	1523672	140532	1527473	116361	1519871	162272
RP_POS_185_1149a5_77	RP	POS	5.77	185.1149				2.37E-02	-0.79	1.70	7.88E-01	-0.02	0.58	2.28E-02	-0.79	1.29	2.54E-02	-0.78	1.14	5864384	2562392	4783568	394868	4794243	399725	4772892	393715
RP_POS_280_13837a0_709	RP	POS	0.71	280.1384				4.69E-01	0.12	0.66	7.89E-01	0.06	0.63	4.87E-01	0.15	0.50	6.07E-01	0.09	0.69	412154	129725	433765	188516	428677	157877	438854	216388
RP_NEG_320_8082a15_378	RP	NEG	15.38	320.8082				5.62E-01	-0.10	0.42	7.89E-01	-0.06	0.72	4.86E-01	-0.13	0.56	7.39E-01	-0.07	0.23	818827	68515	810008	90429	812448	104467	807568	74809
RP_POS_421_23212a9_679	RP	POS	9.68	421.2321				9.30E-01	-0.02	0.35	7.89E-01	-0.04	0.23	8.74E-01	-0.05	0.35	9.97E-01	0.00	0.18	537932	709752	526313	410726	537366	344090	515260	471367
HILIC_POS_372_15857a0_552	HILIC	POS	0.552	372.1586				1.52E-03	0.50	0.92	7.90E-01	0.06	0.79	1.07E-02	0.53	1.03	7.21E-03	0.47	1.03	69598702	30637600	94326537	52825067	92906575	45872338	95746499	59409915
HILIC_NEG_99_92558a2_951	HILIC	NEG	2.951	99.9256				8.05E-01	0.05	0.78	7.90E-01	-0.05	0.53	9.11E-01	0.03	0.21	7.36E-01	0.08	0.52	6577330	2582111	6704527	2357222	6767867	2336636	6641188	2399652
HILIC_NEG_259_83615a1_362	HILIC	NEG	1.362	259.8362				1.08E-15	1.05	1.66	7.90E-01	0.05	0.64	5.25E-08	1.08	1.69	4.73E-11	1.03	2.10	118365	44345	266909	142357	263088	118491	270731	163935
HILIC_POS_87_09224a0_684	HILIC	POS	0.684	87.0922				6.13E-03	-0.55	0.93	7.90E-01	0.05	0.52	1.52E-02	-0.52	0.90	1.25E-02	-0.57	1.04	5154371	1014235	4557373	1083525	4528295	1175514	4586450	994211
RP_POS_331_05368a0_62	RP	POS	0.62	331.0537				5.96E-06	-0.61	1.26	7.90E-01	-0.06	1.18	1.62E-04	-0.64	1.38	1.91E-03	-0.58	1.30	11020357	1957834	7935362	5537912	8083841	5926782	7786883	5176011
RP_POS_534_31622a8_913	RP	POS	8.91	534.3162				1.11E-03	-0.51	1.31	7.91E-01	0.06	0.59	3.04E-02	-0.48	1.24	4.40E-04	-0.54	1.32	671304	201211	503019	351188	493611	230427	512426	442612
RP_POS_457_58731a6_606	RP	POS	6.61	457.5873				3.90E-07	0.60	1.31	7.91E-01	-0.06	1.13	5.31E-04	0.57	1.40	2.54E-04	0.63	1.38	32406	54162	1024569	1822972	1073346	1865001	975791	1797552
RP_NEG_458_86832a0_511	RP	NEG	0.51	458.8683				2.08E-03	-0.57	0.98	7.91E-01	-0.05	0.68	6.89E-03	-0.59	0.93	6.97E-03	-0.54	0.99	603624	145198	502918	180736	507750	163074	498087	198386
HILIC_POS_206_88622a2_991	HILIC	POS	2.991	206.8862				6.65E-05	-0.57	1.34	7.91E-01	0.06	0.78	1.95E-03	-0.54	1.41	1.58E-03	-0.60	1.40	62798179	12147094	48513284	27022969	47791261	28506175	49235306	25723892
HILIC_NEG_372_81213a2_924	HILIC	NEG	2.924	372.8121				2.75E-07	-0.65	1.35	7.91E-01	0.06	0.77	1.57E-04	-0.62	1.49	2.08E-04	-0.68	1.52	1380588	136034	1058395	542107	1043912	576184	1072879	511216
HILIC_POS_482_32538a1_83	HILIC	POS	1.83	482.3254				5.80E-02	0.32	0.83	7.91E-01	0.06	0.58	1.16E-01	0.35	0.53	9.58E-02	0.29	0.65	675628	223211	773741	322642	765124	250486	782358	383959
HILIC_POS_90_05559a5_648	HILIC	POS	5.648	90.0556				3.71E-01	-0.18	1.00	7.91E-01	-0.05	0.62	3.74E-01	-0.20	0.85	4.87E-01	-0.15	0.96	15903732	6674281	14659507	7148113	14850151	6621596	14468863	7701564
RP_POS_239_08968a4_735	RP	POS	4.74	239.0897				1.11E-01	-0.25	0.85	7.91E-01	-0.06	0.55	1.89E-01	-0.28	0.82	1.97E-01	-0.22	0.54	1753365	138959	1697475	246067	1704040	203920	1690911	284011
RP_POS_293_89764a0_448	RP	POS	0.45	293.8976				4.72E-08	-0.68	1.35	7.92E-01	0.06	1.17	1.22E-04	-0.65	1.43	6.20E-05	-0.71	1.46	527335	49811	379842	237184	373537	242963	386146	233557
RP_NEG_701_15558a9_55	RP	NEG	9.55	701.1556				1.15E-01	-0.37	0.67	7.92E-01	-0.05	0.58	1.14E-01	-0.40	0.65	1.73E-01	-0.35	0.65	9156693	989139	8850267	755633	8870340	789712	8830193	727425
RP_POS_315_15643a9_707	RP	POS	9.71	315.1564				1.96E-01	-0.26	0.63	7.92E-01	-0.05	0.60	1.94E-01	-0.29	0.55	3.09E-01	-0.23	0.60	4136516	138762	4099218	144940	4103068	152534	4095369	138373
RP_POS_503_26544a6_787	RP	POS	6.79	503.2654				2.41E-07	0.62	1.35	7.92E-01	-0.06	1.15	7.46E-04	0.59	1.42	9.88E-05	0.64	1.45	14037	13518	995998	1769560	1042913	1716043	949084	1837741
HILIC_NEG_221_84229a3_02	HILIC	NEG	3.02	221.8423				3.02E-04	-0.70	1.07	7.92E-01	-0.05	0.70	9.08E-04	-0.73	1.21	1.50E-03	-0.68	1.16	744270	69891	688016	78337	690092	76175	685939	81161
RP_POS_247_08498a15_339	RP	POS	15.34	247.0850				4.86E-01	-0.14	0.43	7.93E-01	-0.05	0.42	4.61E-01	-0.17	0.41	6.11E-01	-0.12	0.68	1812144	458508	1746747	462081	1758985	460777	1734509	467732
RP_POS_181_00143a0_45	RP	POS	0.45	181.0014				9.60E-08	-0.67	1.35	7.93E-01	0.06	1.18	1.51E-04	-0.64	1.42	9.38E-05	-0.70	1.45	1683236	175204	1206658	781202	1185968	806241	1227347	762961
HILIC_POS_148_13315a1_378	HILIC	POS	1.378	148.1332				4.07E-02	-0.38	1.11	7.93E-01	0.05	0.71	8.88E-02	-0.35	1.07	6.23E-02	-0.40	1.17	875238	208477	781356	256970	774554	271527	788159	244116
RP_NEG_638_8183a0_498	RP	NEG	0.50	638.8183				2.67E-04	-0.48	1.22	7.93E-01	-0.06	1.21	2.67E-03	-0.51	1.29	1.24E-02	-0.45	1.26	1365401	200404	1107697	589172	1123264	616639	1092130	566209
RP_NEG_319_98438a3_698	RP	NEG	3.70	319.9844				8.46E-01	0.04	0.44	7.93E-01	0.05	0.68	7.75E-01	0.06	0.28	9.63E-01	0.01	0.26	1127360	385679	1143279	445644	1131517	411599	1155041	481200
HILIC_NEG_194_10326a1_446	HILIC	NEG	1.446	194.1033				2.41E-02	0.34	0.54	7.94E-01	-0.06	0.50	1.31E-01	0.31	0.52	2.86E-02	0.37	0.74	377934	73290	422171	143372	425947	121631	418394	163424
RP_NEG_199_8046a0_723	RP	NEG	0.72	199.8046				4.07E-01	-0.17	0.76	7.94E-01	-0.05	0.32	3.93E-01	-0.20	0.44	5.28E-01	-0.14	0.66	5830706	2991143	5322152	3008155	5401353	2986889	5242951	3057508
RP_NEG_333_09457a0_71	RP	NEG	0.71	333.0946				2.76E-01	0.17	0.62	7.94E-01	-0.06	0.65	4.75E-01	0.14	0.58	2.77E-01	0.20	0.74	880723	296136	960727	508056	974080	476264	947373	542512
HILIC_NEG_116_92847a4_727	HILIC	NEG	4.727	116.9285				2.68E-02	0.45	0.95	7.95E-01	-0.05	0.69	5.46E-02	0.43	0.76	3.82E-02	0.48	0.91	10456057	2040413	11402555	2063489	11456698	2170353	11348411	1971409
RP_POS_271_22568a9_581	RP	POS	9.58	271.2257				6.74E-01	0.09	0.82	7.95E-01	-0.05	0.78	7.85E-01	0.06	0.56	6.23E-01	0.12	0.80	4230314	762225	4294593	701617	4312995	703090	4276190	706789
RP_POS_642_86206a0_489	RP	POS	0.49	642.8621				1.40E-07	0.63	1.35	7.95E-01	-0.06	1.20	2.37E-04	0.60	1.43	1.77E-04	0.66	1.44	836642	246998	2358610	2657526	2428304	2760869	2288917	2576182
HILIC_NEG_146_96136a7_948	HILIC	NEG	7.948	146.9614				1.85E-03	-0.60	1.09	7.95E-01	-0.05	0.60	2.82E-03	-0.63	1.13	9.76E-03	-0.58	1.06	2918580	834281	2347419	943294	2372157	1017472	2322681	872506
HILIC_NEG_384_93555a4_232	HILIC	NEG	4.232	384.9356				1.41E-01	0.24	1.04	7.95E-01	-0.06	0.86	2.70E-01	0.21	0.64	1.82E-01	0.27	0.95	23573087	4528036	25170717	7186956	25359106	7466600	24982327	6966795
RP_POS_215_16426a7_185	RP	POS	7.19	215.1643				6.95E-01	0.09	0.65	7.95E-01	0.05	0.73	6.46E-01	0.12	0.61	7.88E-01	0.07	0.47	900069	134516	910311	103742	907593	102818	913029	105631
RP_POS_309_20279a9_594	RP	POS	9.59	309.2028				3.07E-01	0.21	0.64	7.95E-01	0.05	0.29	3.14E-01	0.24	0.49	4.04E-01	0.19	0.61	2640441	384818	2720517	372457	2710759	344378	2730275	401856
HILIC_POS_376_80582a2_992	HILIC	POS	2.992	376.8058				8.63E-06	-0.57	1.35	7.95E-01	0.06	0.77	9.46E-04	-0.55	1.47	1.05E-03	-0.60	1.49	3035698	385878	2350462	1312025	2316129	1396150	2384794	1235438
RP_POS_736_80988a0_497	RP	POS	0.50	736.8099				3.25E-08	-0.67	1.37	7.95E-01	0.06	1.17	1.28E-04	-0.64	1.44	6.20E-05	-0.70	1.48	1669395	89930	1280523	634172	1263935	648045	1297110	626125
RP_POS_384_84512a0_513	RP	POS	0.51	384.8451				9.85E-06	-0.71	1.22	7.95E-01	-0.05	0.95	1.00E-04	-0.74	1.34	5.07E-04	-0.68	1.22	375434	99144	262409	165437	266733	171969	258085	160269
RP_NEG_243_16a8_496	RP	NEG	8.50	243.1600				9.06E-01	0.03	0.57	7.95E-01	0.05	0.47	8.27E-01	0.05	0.27	1.00E+00	0.00	0.55	3400792	595835	3414871	540398	3400750	564122	3428992	520940
HILIC_POS_370_29559a0_631	HILIC	POS	0.631	370.2956				7.98E-02	0.30	0.68	7.95E-01	-0.06	0.83	1.37E-01	0.28	0.74	1.32E-01	0.33	0.52	7113682	4414794	8874926	6112029	9034675	7010858	8715178	5125619
RP_NEG_347_89267a15_686	RP	NEG	15.69	347.8927				4.58E-01	-0.14	0.61	7.95E-01	-0.05	0.47	4.27E-01	-0.17	0.48	6.03E-01	-0.12	0.47	1053117	314320	1003905	353247	1013130	373355	994680	335480
HILIC_POS_154_15901a5_783	HILIC	POS	5.783	154.1590				2.35E-01	-0.25	0.94	7.96E-01	0.05	0.55	3.40E-01	-0.22	0.47	2.36E-01	-0.27	0.81	7705552	1790539	7270577	1759142	7224660	1749566	7316494	1785226
RP_POS_413_20303a11_609	RP	POS	11.61	413.2030				9.86E-01	0.00	0.68	7.96E-01	0.05	0.66	8.78E-01	0.03	0.54	9.14E-01	-0.02	0.80	1137617	213546	1138458	266287	1131538	296524	1145379	235033
RP_POS_500_27444a10_34	RP	POS	10.34	500.2744				1.80E-03	0.54	1.13	7.97E-01	-0.05	0.43	1.77E-02	0.52	1.04	2.29E-03	0.57	1.19	6946859	1883323	8317824	2609359	8385619	2195530	8250028	2987764
RP_POS_132_95859a0_675	RP	POS	0.68	132.9586				1.96E-02	0.38	0.91	7.97E-01	0.06	0.56	3.93E-02	0.41	0.96	6.64E-02	0.36	0.71	1223629	131718	1297451	204987	1292128	201581	1302774	210248
RP_NEG_235_92621a1_04	RP	NEG	1.04	235.9262				1.18E-01	0.25	0.68	7.97E-01	-0.06	0.38	2.52E-01	0.22	0.65	1.51E-01	0.28	0.64	3532520	1376445	4057438	2264816	4116145	2266923	3998731	2284183
RP_NEG_142_0862a0_708	RP	POS	0.71	142.0862				5.59E-04	0.49	0.75	7.97E-01	0.06	0.20	2.20E-03	0.52	1.03	1.70E-02	0.46	0.72	720233	637691	1371677	1449388	1334159	1586054	1409196	1313729
HILIC_NEG_234_81987a5_828	HILIC	NEG	5.828	234.8199				2.92E-01	-0.23	0.57	7.97E-01	0.05	0.70	3.91E-01	-0.21	0.50	2.85E-01	-0.26	0.41	1063405	403670	978431	355778	969223	354589	987638	360323
RP_POS_281_17181a9_529	RP	POS	9.53	281.1718				2.83E-02	-0.48	0.90	7.97E-01	-0.05	0.60	3.10E-02	-0.50	0.92	6.07E-02	-0.45	0.80	27494738	1337795	26894769	1202871	26925895	1281780	26863644	1130659
RP_POS_193_09491a3_143	RP	POS	3.14	193.0949		193.0948(100), 134.0588(5)	4	3.98E-01	0.10	0.73	7.98E-01	-0.06	0.27	6.47E-01	0.07	0.72	4.61E-01	0.13	0.52	2734568	4213803	5031342	25999698	5703160	27764884	4359524	24371177
HILIC_POS_458_76917a2_991	HILIC	POS	2.991	458.7692				1.41E-05	-0.57	1.36	7.98E-01	0.06	0.77	1.21E-03	-0.54	1.46	1.11E-03	-0.60	1.48	9989565	1453523	7679310	4427030	7565200	4671208	7793420	4213123
RP_POS_338_1499a3_701	RP	POS	3.70	338.1499				1.33E-01	0.23	0.78	7.98E-01	0.06	0.72	1.98E-01	0.25	0.69	2.64E-01	0.20	0.85	19494438	4671882	21347708	9026572	21115465	8343807	21579951	9741236
RP_POS_419_31564a11_827	RP	POS	11.83	419.3156				7.39E-01	0.05	0.33	7.99E-01	0.06	0.55	7.13E-01	0.08	0.26	8.92E-01	0.02	0.62	201212983	15578599	202586698	30493857	201802736	23478060	203370660	36417772
RP_NEG_178_05038a3_625	RP	NEG	3.63	178.0504				1.79E-02	-0.51	0.90	7.99E-01	0.05	0.78	4.58E-02	-0.49	0.79	1.82E-02	-0.54	1.11	18699386	15940152	10931462	14526944	10558497	12766504	11304427	16220464
HILIC_POS_90_05548a5_48	HILIC	POS	5.48	90.0555				1.01E-01	0.25	0.87	7.99E-01	0.06	0.47	1.56E-01	0.28	0.60	2.26E-01	0.22	0.49	369952	93323	410284	179298	405685	171201	414883	188677
RP_POS_300_2301a10_395	RP	POS	10.40	300.2301				2.72E-02	0.45	0.81	7.99E-01	-0.05	0.32	6.15E-02	0.43	0.68	3.36E-02	0.48	1.00	743947	463250	957611	462612	969474	451705	945748	477558
RP_POS_335_25574a10_412	RP	POS	10.41	335.2557				2.84E-03	-0.52	0.98	7.99E-01	0.05	0.71	1.04E-02	-0.49	0.99	1.07E-02	-0.54	0.99	2526499	302112	2315839	424191	2304973	465341	2326704	383100
RP_NEG_186_11313a4_74	RP	NEG	4.74	186.1131				6.54E-01	-0.08	0.54	8.00E-01	0.05	0.40	8.22E-01	-0.06	0.55	5.27E-01	-0.11	0.65	2214924	2257334	1994538	2821906	1922265	1612303	2066811	3671326
RP_POS_422_80295a0_25	RP	POS	0.25	422.8030				8.41E-01	0.04	0.34	8.00E-01	-0.05	0.38	9.40E-01	0.02	0.21	7.75E-01	0.07	0.38	571417	76064	574463	69731	576247	71602	572680	68488
HILIC_NEG_364_78018a2_931	HILIC	NEG	2.931	364.7802				1.07E-05	-0.57	1.32	8.00E-01	0.06	0.76	1.07E-03	-0.54	1.43	1.18E-03	-0.60	1.47	235447	29197	184142	99357	181601	105616	186683	93688
HILIC_NEG_380_84409a2_91	HILIC	NEG	2.91	380.8441				2.20E-07	-0.64	1.35	8.00E-01	0.06	0.78	1.77E-04	-0.61	1.50	2.49E-04	-0.66	1.54	11467523	806319	8843108	4545137	8726935	4830331	8959281	4287015
RP_NEG_287_83652a0_772	RP	NEG	0.77	287.8365				3.71E-10	0.88	1.35	8.00E-01	0.05	0.43	5.14E-06	0.91	1.42	1.45E-07	0.85	1.68	456691	678284	1831956	1619143	1790567	1387775	1873345	1835031
HILIC_NEG_189_97369a0_933	HILIC	NEG	0.933	189.9737				1.89E-07	0.80	1.36	8.00E-01	-0.05	1.20	1.17E-04	0.77	1.29	2.51E-06	0.82	1.55	352742	110864	512401	207065	517686	183515	507115	229984
RP_POS_437_19315a8_659	RP	POS	8.66	437.1932				1.28E-02	0.37	0.77	8.00E-01	-0.06	0.74	8.35E-02	0.35	0.71	2.03E-02	0.40	0.87	634445	285577	824035	551960	838124	492126	809945	610692
RP_NEG_829_18073a9_56	RP	NEG	9.56	829.1807				4.86E-01	0.12	0.59	8.00E-01	-0.05	0.33	6.59E-01	0.09	0.28	4.54E-01	0.15	0.62	6370204	345219	6424940	487881	6437386	459922	6412494	518718
RP_POS_633_14893a10_813	RP	POS	10.81	633.1489				1.44E-02	0.43	0.97	8.00E-01	-0.05	0.51	2.98E-02	0.40	0.93	4.08E-02	0.45	1.00	379305	173266	476729	238633	482818	277556	470640	194783

Supplementary table 1: Metabolomics results (in asceding order according to p-value from progressive ALD vs non-progressive ALD comparison, with molecular features with ID_level of 1-2 first)

							all_ALD_vs_control			Prog_ALD_vs_non-prog_ALD			Prog_ALD_vs_control_ALD			Non-prog_ALD_vs_control			Healthy_control		all_ALD		Non-prog_ALD		Progressive_ALD	
							t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA								
Feature_ID	RP_HILIC	POS_NEG	Average.Rt	Average.Mz	Metabolite.name	curated_MSMS	ID_level	p	d	VIP	p	d	VIP	p	d	VIP	p	d	VIP	Mean	SD	Mean	SD	Mean	SD	Mean	SD
RP_POS_168_98029a10_662	RP	POS	10.66	168.9803				3.62E-01	0.21	0.49	8.00E-01	-0.05	0.75	4.62E-01	0.18	0.31	3.41E-01	0.23	0.52	4669548	1268851	4896469	1022414	4922529	971862	4870410	1079858
RP_POS_309_12933a0_573	RP	POS	0.57	309.1293				1.01E-03	0.40	0.85	8.00E-01	0.06	0.70	4.16E-02	0.43	0.79	1.36E-03	0.37	1.20	362964	44081	454429	259499	447810	169622	461049	327403
HILIC_POS_566_8894a4_324	HILIC	POS	4.324	566.8894				2.05E-03	0.41	1.23	8.01E-01	-0.06	0.87	2.00E-02	0.38	1.28	1.96E-02	0.44	1.40	9527712	617776	10187743	1790476	10233264	1934284	10142222	1652679
HILIC_NEG_374_81015a2_924	HILIC	NEG	2.924	374.8102				4.67E-07	-0.63	1.34	8.01E-01	0.06	0.76	1.97E-04	-0.61	1.49	3.03E-04	-0.66	1.51	261037	25492	200607	104336	197961	111393	203253	97834
RP_NEG_319_92706a6_867	RP	NEG	6.87	319.9271				7.47E-02	-0.36	0.65	8.01E-01	0.05	0.73	1.28E-01	-0.33	0.62	9.43E-02	-0.39	0.59	1815137	220510	1733064	227906	1727287	241273	1738842	216013
HILIC_NEG_452_92413a4_232	HILIC	NEG	4.232	452.9241				1.32E-01	0.24	1.04	8.02E-01	-0.05	0.86	2.56E-01	0.22	0.65	1.76E-01	0.27	0.98	16234313	3136986	17373652	5041972	17501294	5257320	17246011	4867145
RP_POS_419_31528a10_573	RP	POS	10.57	419.3153				8.45E-01	0.04	0.26	8.02E-01	0.05	0.16	7.75E-01	0.07	0.24	9.39E-01	0.02	0.60	1082347	396551	1097665	339512	1089094	366198	1106236	314067
RP_POS_372_88251a0_471	RP	POS	0.47	372.8825				5.80E-07	-0.63	1.32	8.02E-01	0.06	1.18	3.23E-04	-0.61	1.39	2.28E-04	-0.66	1.41	1054818	113846	797580	445120	786361	461379	808799	432641
RP_POS_151_00874a0_45	RP	POS	0.45	151.0087				1.68E-06	-0.64	1.31	8.03E-01	-0.05	1.13	1.40E-04	-0.67	1.38	6.25E-04	-0.61	1.37	968916	130422	750742	368376	760011	377284	741472	362840
HILIC_NEG_80_91625a1_363	HILIC	NEG	1.363	80.9163				3.77E-06	0.62	1.01	8.03E-01	0.05	0.70	1.30E-03	0.64	1.00	9.91E-05	0.59	1.22	1522265	385391	2158016	1125813	2129689	922837	2186344	1306717
RP_POS_193_13132a5_931	RP	POS	5.93	193.1313				2.74E-01	-0.18	1.04	8.03E-01	-0.05	1.06	2.60E-01	-0.21	0.90	4.66E-01	-0.15	1.07	2745836	733587	2556570	1128845	2584968	1253809	2528173	1000452
RP_POS_387_20505a10_173	RP	POS	10.17	387.2051				6.80E-01	-0.08	0.78	8.03E-01	0.05	0.73	8.05E-01	-0.05	0.58	6.40E-01	-0.10	0.83	1208539	201052	1190879	236224	1184940	251935	1196818	221808
HILIC_POS_450_73837a3_007	HILIC	POS	3.007	450.7384				4.07E-05	-0.54	1.36	8.03E-01	0.06	0.79	2.17E-03	-0.52	1.48	1.91E-03	-0.57	1.46	965571	151611	744193	446747	732979	471082	755406	425516
HILIC_NEG_144_92349a7_425	HILIC	NEG	7.425	144.9235				3.31E-01	0.18	0.68	8.03E-01	0.05	0.34	3.35E-01	0.21	0.59	4.68E-01	0.15	0.82	34829112	8919411	36706073	10877475	36433074	10835349	36979073	11022556
HILIC_POS_124_92298a2_992	HILIC	POS	2.992	124.9230				5.72E-07	-0.63	1.37	8.03E-01	0.05	0.78	2.15E-04	-0.61	1.52	3.22E-04	-0.66	1.52	23623814	2200441	18611428	8680757	18393615	9261152	18829241	8147588
RP_POS_416_78769a13_869	RP	POS	13.87	416.7877				1.90E-01	-0.26	0.49	8.04E-01	0.05	0.51	3.02E-01	-0.24	0.59	1.88E-01	-0.29	0.50	2024317	597810	1861808	620253	1846259	580059	1877358	663563
HILIC_POS_154_15889a5_921	HILIC	POS	5.921	154.1589				1.42E-02	-0.53	1.22	8.04E-01	-0.05	0.70	1.70E-02	-0.55	1.17	3.45E-02	-0.50	1.16	6967396	1843255	6033652	1693886	6076096	1789463	5991207	1609721
RP_NEG_146_96024a0_448	RP	NEG	0.45	146.9602				7.30E-08	-0.67	1.35	8.04E-01	0.05	1.18	1.40E-04	-0.64	1.43	8.30E-05	-0.70	1.45	1452960	143612	1040426	673058	1023572	691698	1057280	660480
RP_POS_866_526a13_713	RP	POS	13.71	866.5260				8.64E-05	0.66	1.38	8.04E-01	-0.05	0.57	7.61E-04	0.64	1.33	8.85E-04	0.69	1.23	726854	372533	1083100	553091	1096929	597451	1069270	510613
RP_NEG_425_91077a15_704	RP	NEG	15.70	425.9108				4.85E-01	-0.14	0.79	8.04E-01	-0.05	0.37	4.73E-01	-0.16	0.46	6.05E-01	-0.11	0.82	1374021	353701	1322691	377870	1332133	360201	1313250	398193
HILIC_POS_159_02786a1_385	HILIC	POS	1.385	159.0279				9.91E-14	0.92	1.59	8.04E-01	-0.05	0.63	8.04E-07	0.89	1.57	2.87E-08	0.94	2.01	1035984	570334	8680159	8822465	8900517	8431090	8459801	9277818
RP_POS_408_16074a4_144	RP	POS	4.14	408.1607				7.81E-01	0.04	0.32	8.05E-01	0.06	0.22	6.83E-01	0.06	0.43	9.67E-01	0.01	0.74	2007522	295231	2037214	931122	2014005	1028425	2060422	832415
RP_POS_390_21472a10_733	RP	POS	10.73	390.2147				1.40E-02	0.40	1.16	8.05E-01	0.05	1.09	4.66E-02	0.42	1.01	3.47E-02	0.37	1.21	414197	164121	513072	267128	506413	223475	519730	306823
HILIC_POS_171_18552a5_566	HILIC	POS	5.566	171.1855				4.20E-01	-0.11	0.76	8.05E-01	-0.06	0.73	5.09E-01	-0.14	0.21	5.59E-01	-0.08	0.20	98172906	4795114	96955241	12423004	97264809	9148807	96645673	15096868
RP_POS_627_26166a7_624	RP	POS	7.62	627.2617				2.47E-01	-0.22	0.46	8.05E-01	-0.05	0.68	2.62E-01	-0.25	0.48	3.65E-01	-0.19	0.40	1675612	180832	1630845	210624	1636088	207161	1625602	216005
RP_POS_339_16129a10_978	RP	POS	10.98	339.1613				3.26E-02	0.40	1.44	8.05E-01	-0.05	1.16	9.32E-02	0.37	1.23	3.85E-02	0.42	1.29	9427085	2488253	10597519	3055429	10673566	2792333	10521471	3324589
HILIC_NEG_300_87851a2_911	HILIC	NEG	2.911	300.8785				4.51E-05	-0.60	1.34	8.05E-01	0.05	0.76	1.14E-03	-0.58	1.48	1.12E-03	-0.63	1.46	284220	56895	219060	115602	216183	122769	221937	109139
HILIC_NEG_195_81087a4_1	HILIC	NEG	4.1	195.8109				5.49E-01	-0.14	0.71	8.05E-01	0.05	0.66	6.45E-01	-0.12	0.72	5.14E-01	-0.16	0.58	362408	445429	310419	347062	301790	339601	319049	357605
RP_POS_367_9902a0_639	RP	POS	0.64	367.9902				3.54E-10	-0.77	1.43	8.05E-01	0.05	1.17	1.22E-05	-0.75	1.53	5.87E-06	-0.80	1.53	4574560	314795	3175193	1957422	3126529	1994110	3223858	1939043
HILIC_POS_126_92099a2_993	HILIC	POS	2.993	126.9210				1.33E-06	-0.61	1.36	8.05E-01	0.05	0.79	3.54E-04	-0.59	1.52	4.58E-04	-0.64	1.52	821894	84660	641674	321953	633670	342200	649678	303629
HILIC_NEG_130_92897a4_279	HILIC	NEG	4.279	130.9290				9.61E-01	-0.01	0.75	8.05E-01	0.05	0.82	9.43E-01	0.02	0.07	8.74E-01	-0.04	0.17	1177235	284805	1174290	312796	1166515	314426	1182066	314155
RP_POS_223_09406a13_263	RP	POS	13.26	223.0941				6.81E-01	-0.08	0.53	8.05E-01	-0.05	0.49	6.31E-01	-0.11	0.45	7.98E-01	-0.06	0.88	13381343	4157544	13030868	4237090	13136152	4312538	12925583	4201386
RP_POS_631_40112a15_097	RP	POS	15.10	631.4011				9.53E-01	0.01	0.33	8.05E-01	-0.05	0.33	9.53E-01	-0.01	0.42	8.69E-01	0.04	0.48	7964920	1964061	7989039	2049098	8039935	2062678	7938142	2055082
RP_POS_630_85986a6_463	RP	POS	6.46	630.8599				6.16E-07	0.59	1.32	8.05E-01	-0.06	1.14	9.38E-04	0.57	1.40	2.17E-04	0.62	1.40	50652	96790	1650403	2997153	1724819	2961339	1575987	3060776
HILIC_POS_402_35745a0_526	HILIC	POS	0.526	402.3575				5.41E-01	0.10	0.65	8.06E-01	-0.05	0.56	7.05E-01	0.08	0.50	5.20E-01	0.13	0.33	129932	151635	151484	227197	157119	229443	145848	227115
RP_NEG_311_16943a10_051	RP	NEG	10.05	311.1694				6.66E-01	0.08	0.63	8.06E-01	0.05	0.42	6.17E-01	0.11	0.37	7.98E-01	0.06	0.18	12747189	12269188	13880623	14501660	13520921	14803841	14240324	14334237
HILIC_POS_542_73163a2_992	HILIC	POS	2.992	542.7316				2.64E-05	-0.56	1.35	8.06E-01	0.05	0.77	1.57E-03	-0.54	1.46	1.44E-03	-0.59	1.47	7695778	1218874	5918088	3461645	5832267	3651484	6003910	3295780
HILIC_NEG_108_90194a2_948	HILIC	NEG	2.948	108.9019				5.56E-07	-0.62	1.34	8.06E-01	0.05	0.77	2.37E-04	-0.59	1.47	3.91E-04	-0.65	1.52	28040867	1803003	23177381	8624638	22963772	9229056	23390989	8063388
RP_POS_486_13574a8_699	RP	POS	8.70	486.1357				2.25E-01	0.19	0.87	8.06E-01	-0.05	0.24	4.25E-01	0.16	0.56	2.19E-01	0.22	0.72	1893763	717433	2109604	1227736	2140003	1082010	2079205	1368503
RP_POS_393_29587a10_987	RP	POS	10.99	393.2959				6.41E-01	-0.09	0.58	8.06E-01	0.05	0.60	7.58E-01	-0.07	0.60	6.03E-01	-0.12	0.54	2125465	370761	2089830	385353	2080298	397503	2099361	376603
RP_NEG_343_99524a15_554	RP	NEG	15.55	343.9952				8.39E-06	-0.67	1.31	8.06E-01	0.05	1.20	4.12E-04	-0.64	1.36	2.88E-04	-0.69	1.37	1169286	252545	856237	496922	843962	516131	868512	481874
RP_POS_229_11835a0_621	RP	POS	0.62	229.1184				9.49E-01	0.01	0.65	8.06E-01	-0.05	0.73	9.40E-01	-0.02	0.64	8.14E-01	0.04	0.41	382002	165418	384632	282661	391613	199264	377651	348739
RP_POS_146_93704a0_251	RP	POS	0.25	146.9370				2.76E-01	0.22	0.43	8.07E-01	-0.05	0.25	3.81E-01	0.19	0.38	2.86E-01	0.24	0.45	7206791	693870	7363790	726434	7381705	757554	7345874	701169
RP_POS_463_37509a11_958	RP	POS	11.96	463.3751				1.36E-01	-0.24	0.79	8.07E-01	0.05	0.77	2.65E-01	-0.21	0.73	1.83E-01	-0.26	0.77	504546	134650	455076	226609	449491	235619	460662	219480
HILIC_NEG_153_86855a2_949	HILIC	NEG	2.949	153.8686				1.64E-03	0.45	1.14	8.07E-01	-0.05	0.79	1.63E-02	0.42	0.98	1.12E-02	0.48	1.20	14060125	2665180	16496966	5908285	16642502	6176781	16351431	5686142
HILIC_NEG_144_92342a5_882	HILIC	NEG	5.882	144.9234				9.44E-01	-0.02	0.23	8.08E-01	-0.05	0.34	8.74E-01	-0.04	0.19	9.75E-01	0.01	0.08	33691820	9659433	33559035	8036399	33755970	7862688	33362099	8281573
RP_NEG_787_10187a9_222	RP	NEG	9.22	787.1019				9.41E-01	-0.01	0.34	8.08E-01	-0.05	0.57	8.53E-01	-0.04	0.26	9.56E-01	0.01	0.09	5132718	332834	5127403	402547	5137263	408878	5117542	400021
RP_POS_455_18875a7_265	RP	POS	7.27	455.1888				4.01E-01	-0.16	0.47	8.08E-01	-0.05	0.54	3.98E-01	-0.19	0.35	5.28E-01	-0.14	0.39	791807	74551	778579	84176	780640	82625	776519	86489
HILIC_NEG_153_86879a6_295	HILIC	NEG	6.295	153.8688				4.60E-03	-0.66	1.21	8.08E-01	-0.04	0.19	5.73E-03	-0.68	1.14	1.06E-02	-0.63	1.26	1660276	679658	1266909	540846	1280126	560100	1253692	526242
RP_NEG_311_16962a9_368	RP	NEG	9.37	311.1696				6.16E-01	0.09	0.63	8.09E-01	-0.05	0.16	7.42E-01	0.07	0.58	5.92E-01	0.12	0.53	2848740	3889544	3269428	4716737	3384430	5083432	3154426	4368178
RP_POS_223_20511a8_812	RP	POS	8.81	223.2051				8.66E-01	0.03	0.39	8.09E-01	-0.05	0.56	7.89E-01	0.06	0.31	9.76E-01	0.01	0.34	511326	234827	519805	277023	513051	282955	526558	273665
RP_POS_418_74771a13_069	RP	POS	13.07	418.7477				8.58E-02	-0.32	1.30	8.09E-01	-0.05	0.27	1.03E-01	-0.34	0.96	1.70E-01	-0.29	1.16	16169930	2556182	15213787	3095524	15289210	3169216	15138364	3050336
RP_POS_532_61633a6_895	RP	POS	6.90	532.6163				2.08E-07	0.62	1.32	8.09E-01	-0.05	1.14	3.85E-04	0.59	1.43	1.86E-04	0.65	1.39	19276	24866	863408	1511628	900207	1540500	826609	1496920
RP_POS_469_36566a12_33	RP	POS	12.33	469.3657				6.80E-01	0.09	0.81	8.09E-01	-0.05	0.36	7.96E-01	0.06	0.63	6.18E-01	0.11	0.37	2840137	866960	2912011	811186	2931738	701121	2892284	914937
HILIC_NEG_588_89764a4_232	HILIC	NEG	4.232	588.8976				8.84E-04	0.43	1.24	8.10E-01	-0.05	0.89	1.39E-02	0.40	1.29	1.39E-02	0.45	1.42	5921665	367695	6414879	1294827	6446303	1390033	6383455	1205471
RP_POS_405_3335a11_419	RP	POS	11.42	405.3335				4.07E-02	-0.38	0.96	8.10E-01	-0.05	0.92	3.93E-02	-0.40	0.96	1.21E-01	-0.35	0.93	1139309	243356	1029587	301263	1036896	347646	1022277	249807
RP_POS_930_18707a0_621	RP	POS	0.62	930.1871				3.79E-01	-0.17	0.77	8.10E-01	-0.05	0.79	3.55E-01	-0.20	0.65	5.17E-01	-0.15	0.77	421466	226254	380068	241072	385913	262673	374223	219887
RP_POS_818_56561a13_395	RP	POS	13.40	818.5656				1.38E-02	0.45	0.74	8.10E-01	0.05	0.49	1.55E-02	0.48	0.95	5.54E-02	0.43	0.69	2933860	1196376	3588920	1488756	3552831	1682494	3625010	1282409
RP_POS_279_91782a0_448	RP	POS	0.45	279.9178				3.43E-08	-0.68	1.36	8.10E-01	0.05	1.17	9.22E-05	-0.66	1.45	6.60E-05	-0.71	1.46	529739	47364	377885	243125	372001	251075	383770	237311
HILIC_NEG_99_92554a4_207	HILIC	NEG	4.207	99.9255				8.18E-01	0.04	0.69	8.11E-01	0.05	0.35	7.49E-01	0.07	0.71	9.34E-01	0.02	0.69	1025731	135724	1032383	159954	1028523	164146	1036243	157222
RP_POS_676_85571a0_489	RP	POS	0.49	676.8557				1.07E-07	0.64	1.35	8.11E-01	-0.05	1.20	2.06E-04	0.61	1.43	1.60E-04	0.66	1.44	794072	240190	2487609	2932246	2558297	3039878	2416920	2849658
HILIC_NEG_112_98579a5_429	HILIC	NEG	5.429	112.9858				3.24E-01	-0.20	0.63	8.11E-01	0.05	1.05	4.49E-01	-0.18	0.30	3.10E-01	-0.22	0.92	11876436	1132912	11646349	1153223	11618568	1078433	11674131	1233854
RP_POS_163_97684a0_251	RP	POS	0.25	163.9768				5.93E-01	-0.11	0.55	8.11E-01	-0.05	0.72	5.40E-01	-0.13	0.37	7.27E-01	-0.08	0.37	22973623	4609787	22461895	4912961	22580225	5446743	22343566	4367079
RP_NEG_344_86771a15_682	RP	NEG	15.68	344.8677				3.17E-02	-0.46	0.84	8.11E-01	0.05	0.22	6.03E-02	-0.44	0.84	4.01E-02	-0.48	0.79	894560	320111	753509	294136	746427	299485	760592	291554
RP_POS_315_25217a9_594	RP	POS	9.59	315.2522				1.86E-01	0.25	0.72	8.11E-01	0.05	0.36	2.14E-01	0.28	0.55	2.81E-01	0.23	0.70	1325446	183092	1377030	209738	1371984	198090	1382076	222679
HILIC_NEG_186_82896a2_951	HILIC	NEG	2.951	186.8290				6.46E-07	-0.64	1.33	8.11E-01	0.05	0.77	2.11E-04	-0.62	1.45	2.65E-04	-0.67	1.51	668617	71853	524393	244445	518518	258682	530267	231817
HILIC_NEG_278_82208a2_932	HILIC	NEG	2.932	278.8221				6.40E-07	-0.63	1.34	8.12E-01	0.05	0.76	2.04E-04	-0.61	1.48	3.50E-04	-0.66	1.50	1053942	107965	815798	412231	805894	441406	825702	385094
RP_POS_1022_73462a0_496	RP	POS	0.50	1022.7346				4.04E-07	-0.63	1.32	8.12E-01	0.05	1.16	3.47E-04	-0.60	1.38	2.23E-04	-0.65	1.42	1928643	132041	1551172	663780	1535227	683916	1567116	649569
RP_NEG_215_12943a7_471	RP	NEG	7.47	215.1294				8.47E-01	-0.04	0.58	8.12E-01	0.05	0.47	9.34E-01	-0.02	0.33	7.90E-01	-0.07	0.47	2770098	574549	2748286	488114	2736563	517721	2760010	461581
RP_POS_277_88074a0_246	RP	POS	0.25	277.8807				5.37E-01	0.13	0.33	8.12E-01	-0.05	0.15	6.41E-01	0.11	0.30	5.14E-01	0.16	0.63	1274463	152192	1293326	140288	1296695	145957	1289957	135780
RP_POS_181_04898a9_441	RP	POS	9.44	181.0490	fragment fo Di-n-butyl phtalate	149.0226(100), 163.0377(45), 84.9603(80)	3	6.66E-01	0.09	0.37	8.12E-01	0.05	0.84	6.28E-01	0.11	0.71	7.71E-01	0.07	0.31	1460514	126185	1471510	120673	1468613	116090	1474408	126202
HILIC_NEG_255_82204a2_946	HILIC	NEG	2.946	255.8220				1.63E-03	0.44	1.11	8.12E-01	-0.05	0.79	1.90E-02	0.41	0.95	1.15E-02	0.47	1.13	3868370	603482	4449607	1454349	4484463	1499585	4414751	1422040
RP_NEG_829_18103a9_838	RP	NEG	9.84	829.1810				5.63E-01	-0.12	0.44	8.12E-01	0.05	0.55	6.76E-01	-0.09	0.26	5.40E-01	-0.14	0.45	5252076	333291	5212435	341006	5204272	357637	5220598	326962
RP_POS_248_97632a0_453	RP	POS	0.45	248.9763				1.81E-04	-0.55	1.21	8.12E-01	-0.05	1.08	1.24E-03	-0.57	1.24	6.30E-03	-0.52	1.26	624932	148513	467323	310529	474754	328800	459892	294283
HILIC_POS_247_09232a7_688	HILIC	POS	7.688	247.0923				5.59E-01	0.11	0.37	8.13E-01	-0.05	0.52	6.95E-01	0.09	0.19	5.25E-01	0.14	0.26	869122	71654	877999	82594	879972	80040	876026	85838
RP_NEG_310_93307a15_326	RP	NEG	15.33	310.9331				7.84E-01	0.05	0.61	8.13E-01	-0.05	0.20	9.03E-01	0.02	0.61	7.31E-01	0.07	0.33	2158899	69869	2163069	87977	2165170	94128	2160969	82273
HILIC_NEG_262_75821a2_947	HILIC	NEG	2.947	262.7582				7.64E-07	-0.67	1.35	8.13E-01	0.05	0.76	1.30E-04	-0.64	1.48	2.25E-04	-0.69	1.47	296545	44288	221740	120623	218861	129250	224619	112580
RP_POS_1047_73303a10_828	RP	POS	10.83	1047.7330				1.81E-03	0.56	1.21	8.13E-01	0.05	0.91	9.25E-03	0.59	1.00	4.22E-03	0.54	1.27	689383	554864	1084806	721241	1067597	578651	1102016	845904
HILIC_NEG_120_92785a2_931	HILIC	NEG	2.931	120.9279				1.84E-04	-0.56	1.33	8.13E-01	0.05	0.77	2.96E-03	-0.53	1.36	2.47E-03	-0.59	1.33	5246855	1023544	4196044	2017588	4147923	2125873	4244165	1923626
HILIC_POS_522_67371a3_013	HILIC	POS	3.013	522.6737				3.18E-05	-0.60	1.32	8.13E-01	-0.05	0.76	4.46E-04	-0.62	1.45	2.43E-03	-0.57	1.41	271642	52794	206692	117401	209490	123247	203894	112434
HILIC_NEG_160_84204a3_002	HILIC	NEG	3.002	160.8420				4.84E-01	0.14	0.50	8.13E-01	0.05	0.64	4.43E-01	0.16	0.35	6.29E-01	0.11	0.19	43605422	6738492	44598781	7541300	44419349	8372559	44778213	6688617
RP_POS_197_05724a6_418	RP	POS	6.42	197.0572				1.04E-01	-0.31	0.52	8.14E-01	0.05	0.24	1.94E-01	-0.28	0.49	1.20E-01	-0.33	0.53	650345	88761	619274	104194	616801	102057	621746	107268
HILIC_NEG_286_85382a2_924	HILIC	NEG	2.924	286.8538				7.42E-07	-0.62	1.35	8.14E-01	0.05	0.77	2.55E-04	-0.59	1.49	4.18E-04	-0.65	1.52	4005809	358201	3138190	1538086	3101713	1643887	3174667	1440353
RP_NEG_435_10196a0_709	RP	NEG	0.71	435.1020				8.33E-02	0.23	0.71	8.14E-01	0.05	0.51	1.86E-01	0.26	0.63	1.83E-01	0.21	1.04	1113014	355168	1315886	978257	1292690	835169	1339082	1111260
RP_POS_503_59991a6_788	RP	POS	6.79	503.5999				1.92E-07	0.62	1.33	8.14E-01	-0.05	1.13	4.38E-04	0.59	1.42	1.49E-04	0.65	1.41	10787	15594	689660	1211906	718376	1216557	660944	1218898
RP_NEG_179_05702a2_929	RP	NEG	2.93	179.0570				6.97E-01	-0.07	0.42	8.14E-01	-0.05	0.16	6.53E-01	-0.10	0.28	8.20E-01	-0.05	0.53	1455632	1386234	1340579	1634657	1379293	1610133	1301865	1674262
RP_POS_248_90034a0_449	RP	POS	0.45	248.9003				2.14E-06	-0.64	1.31	8.14E-01	0.05	1.13	4.05E-04	-0.61	1.36	2.67E-04	-0.67	1.42	1057759	181654	763854	497127	752086	513022	775622	485634
HILIC_NEG_464_80627a2_909	HILIC	NEG	2.909	464.8063				2.20E-07	-0.64	1.35	8.14E-01	0.05	0.77	1.60E-04	-0.61	1.52	2.43E-04	-0.67	1.54	5318895	422278	4065981	2151552	4015078	2285632	4116883	2030621

Supplementary table 1: Metabolomics results (in asceding order according to p-value from progressive ALD vs non-progressive ALD comparison, with molecular features with ID_level of 1-2 first)

							all_ALD_vs_control			Prog_ALD_vs_non-prog_ALD			Prog_ALD_vs_control_ALD			Non-prog_ALD_vs_control			Healthy_control		all_ALD		Non-prog_ALD		Progressive_ALD	
							t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA								
Feature_ID	RP_HILIC	POS_NEG	Average.Rt	Average.Mz	Metabolite.name	curated_MSMS	ID_level	p	d	VIP	p	d	VIP	p	d	VIP	p	d	VIP	Mean	SD	Mean	SD	Mean	SD	Mean	SD
RP_POS_794_50836a12_76	RP	POS	12.76	794.5084				1.18E-01	0.28	0.64	8.15E-01	-0.05	0.45	1.70E-01	0.26	0.55	1.79E-01	0.31	0.57	995585	782041	1266536	1005871	1290317	1186754	1242755	796657
RP_POS_424_77634a13_872	RP	POS	13.87	424.7763				3.96E-01	-0.17	0.56	8.15E-01	0.05	1.00	5.32E-01	-0.15	0.57	3.63E-01	-0.20	0.42	4566870	983545	4394779	1006882	4371039	877809	4418520	1129874
RP_POS_257_21057a8_795	RP	POS	8.80	257.2106				7.13E-01	0.08	0.54	8.15E-01	0.05	0.55	6.71E-01	0.10	0.40	8.14E-01	0.05	0.51	2914418	345444	2940054	330161	2932273	315465	2947835	347269
RP_POS_319_16531a3_83	RP	POS	3.83	319.1653				4.63E-03	0.40	0.64	8.15E-01	-0.05	0.41	5.30E-02	0.38	0.74	1.12E-02	0.43	0.98	626545	358616	926347	822664	945728	743669	906966	901971
RP_POS_276_89288a0_248	RP	POS	0.25	276.8929				5.40E-01	-0.12	0.41	8.15E-01	0.05	0.37	6.68E-01	-0.09	0.30	5.14E-01	-0.14	0.33	444182	58320	436650	65406	435111	65233	438188	66204
HILIC_NEG_197_80783a3_033	HILIC	NEG	3.033	197.8078				4.62E-02	0.30	1.06	8.16E-01	-0.05	0.81	1.34E-01	0.28	0.69	8.78E-02	0.33	0.95	146737461	22408641	158459372	42455359	159457432	43828057	157461311	41458033
HILIC_POS_141_13853a1_074	HILIC	POS	1.074	141.1385				8.81E-03	-0.47	1.03	8.16E-01	-0.05	0.71	1.99E-02	-0.49	0.93	2.84E-02	-0.44	0.87	6466565	1208920	5746639	1600966	5784257	1542521	5709022	1672194
RP_POS_553_4588a10_458	RP	POS	10.46	553.4588				4.57E-02	-0.45	0.93	8.16E-01	0.04	0.30	8.44E-02	-0.42	0.77	4.92E-02	-0.47	0.82	1108136	449251	926925	384833	917889	364108	935960	408012
RP_NEG_282_77814a0_522	RP	NEG	0.52	282.7781				1.60E-08	-0.80	1.41	8.16E-01	0.05	1.14	9.64E-06	-0.77	1.49	1.33E-05	-0.82	1.46	1270793	172768	962702	406300	953167	427840	972238	387681
RP_NEG_213_02271a6_441	RP	NEG	6.44	213.0227				8.74E-02	0.24	0.55	8.17E-01	0.05	0.18	1.49E-01	0.27	0.59	2.18E-01	0.22	0.56	1097512	1170190	1669374	2593001	1608814	2514834	1729933	2693074
RP_NEG_322_89328a0_512	RP	NEG	0.51	322.8933				8.54E-05	-0.69	1.20	8.17E-01	0.05	0.96	8.82E-04	-0.66	1.19	5.40E-04	-0.71	1.25	604584	156352	458306	216907	453253	223215	463358	212557
RP_POS_282_88321a0_254	RP	POS	0.25	282.8832				3.89E-01	0.18	0.57	8.17E-01	-0.05	0.18	5.14E-01	0.15	0.35	3.68E-01	0.20	0.44	3123147	492198	3209984	493109	3221467	457352	3198501	530882
RP_POS_693_45184a10_905	RP	POS	10.91	693.4518				4.95E-01	0.12	0.60	8.17E-01	-0.05	0.60	6.32E-01	0.09	0.44	5.02E-01	0.14	0.81	779918	350895	834168	490415	845586	530475	822750	451943
HILIC_POS_173_09183a5_188	HILIC	POS	5.188	173.0918				4.33E-07	-0.76	1.39	8.17E-01	0.05	0.76	5.68E-05	-0.73	1.51	4.07E-05	-0.78	1.46	5727339	1298625	3873785	2559421	3814228	2645797	3933342	2495492
RP_POS_619_75122a6_197	RP	POS	6.20	619.7512				1.05E-04	0.46	1.05	8.17E-01	-0.05	0.93	9.81E-03	0.43	1.13	3.99E-03	0.48	1.21	230666	75081	663518	1063735	688270	1067417	638765	1070292
HILIC_NEG_288_85132a2_924	HILIC	NEG	2.924	288.8513				7.72E-07	-0.62	1.34	8.17E-01	0.05	0.77	2.69E-04	-0.59	1.48	4.39E-04	-0.64	1.52	1942485	168584	1522082	749914	1504633	800970	1539532	702884
RP_POS_486_93842a6_729	RP	POS	6.73	486.9384				1.65E-07	0.62	1.33	8.17E-01	-0.05	1.14	3.58E-04	0.60	1.42	1.58E-04	0.65	1.41	27895	46337	1424534	2477802	1482182	2511797	1366886	2467468
RP_POS_550_29034a10_456	RP	POS	10.46	550.2903				1.48E-13	1.03	1.80	8.17E-01	0.05	0.52	1.36E-07	1.05	1.75	3.40E-10	1.01	1.93	644568	263786	1306889	646059	1291857	541139	1321920	741627
RP_POS_429_31851a13_016	RP	POS	13.02	429.3185				3.04E-01	-0.21	1.02	8.18E-01	-0.05	0.27	2.98E-01	-0.24	1.09	4.14E-01	-0.19	0.44	2778401	1089041	2550630	1050743	2575027	1095998	2526233	1014016
HILIC_POS_126_02219a5_325	HILIC	POS	5.325	126.0222				1.39E-04	0.49	1.14	8.18E-01	0.05	0.69	5.03E-03	0.51	1.26	5.01E-03	0.46	1.27	2966642	929057	4437964	3366331	4359829	3178104	4516099	3575309
HILIC_NEG_538_7373a2_922	HILIC	NEG	2.922	538.7373				8.77E-07	-0.62	1.34	8.18E-01	0.05	0.77	3.07E-04	-0.59	1.48	4.24E-04	-0.64	1.51	989237	95748	759197	410726	749669	435973	768725	388042
HILIC_NEG_656_88708a4_232	HILIC	NEG	4.232	656.8871				6.28E-04	0.44	1.25	8.18E-01	-0.05	0.90	1.10E-02	0.42	1.31	1.12E-02	0.47	1.42	2654840	171808	2882950	575694	2896278	615847	2869621	538498
RP_POS_800_57666a14_261	RP	POS	14.26	800.5767				3.42E-01	0.15	0.46	8.18E-01	0.05	0.18	4.47E-01	0.18	0.34	3.85E-01	0.13	1.02	414706	279924	479771	467052	468947	264603	490595	608666
RP_POS_267_15591a8_499	RP	POS	8.50	267.1559				4.27E-01	0.18	0.69	8.18E-01	0.04	0.43	4.11E-01	0.20	0.43	5.22E-01	0.16	0.65	2754550	482254	2830208	404452	2820854	408038	2839561	404757
RP_POS_158_96312a15_379	RP	POS	15.38	158.9631				3.55E-01	0.20	0.55	8.18E-01	0.05	0.26	3.36E-01	0.22	0.42	4.66E-01	0.18	0.79	7287835	1160718	7502817	1047295	7478601	1130504	7527034	967885
HILIC_NEG_57_03372a0_927	HILIC	NEG	0.927	57.0337				1.44E-06	0.68	1.11	8.19E-01	-0.05	1.25	1.23E-03	0.65	1.03	8.22E-06	0.70	1.43	89170	53580	169397	12667	172326	103198	166468	147476
RP_POS_441_29691a13_797	RP	POS	13.80	441.2969				6.39E-01	0.10	0.24	8.19E-01	-0.04	0.49	7.29E-01	0.08	0.29	6.11E-01	0.13	0.37	19261710	6781479	19891355	5838171	20026252	6317300	19756459	5377608
RP_POS_253_1263a0_551	RP	POS	0.55	253.1263				6.60E-01	0.08	0.30	8.19E-01	-0.05	0.27	7.93E-01	0.06	0.19	6.16E-01	0.10	0.66	946326	240123	969230	297663	976107	290690	962353	307274
RP_POS_783_0658a13_23	RP	POS	13.23	783.0658				3.48E-01	0.17	0.45	8.19E-01	-0.05	0.30	4.67E-01	0.15	0.34	3.73E-01	0.20	0.50	1010626	1065102	1228958	1337879	1259858	1447213	1198058	1232881
HILIC_NEG_134_89481a3_128	HILIC	NEG	3.128	134.8948				2.66E-04	-0.58	1.04	8.19E-01	0.05	0.63	3.65E-03	-0.55	1.06	1.91E-03	-0.60	1.09	106519762	21149052	86767725	36236650	85931625	36840305	87603826	35977114
RP_POS_553_4585a11_693	RP	POS	11.69	553.4585				6.89E-01	-0.09	0.41	8.20E-01	-0.04	0.26	6.46E-01	-0.11	0.31	7.81E-01	-0.07	0.40	11328276	5569474	10890190	4619458	10996105	4728272	10784275	4553552
HILIC_POS_146_11775a3_338	HILIC	POS	3.338	146.1178				4.79E-01	0.12	0.65	8.20E-01	-0.05	0.65	6.52E-01	0.10	0.39	4.39E-01	0.15	0.47	70867146	22140112	74415236	30891907	75123538	26986989	73706935	34623318
RP_NEG_321_13254a7_723	RP	NEG	7.72	321.1325				5.43E-02	-0.36	0.74	8.20E-01	-0.05	0.41	6.39E-02	-0.39	0.76	1.23E-01	-0.34	0.60	899143	47704	879299	55783	880578	59537	878020	52334
HILIC_NEG_155_86565a2_95	HILIC	NEG	2.95	155.8657				2.19E-03	0.44	1.15	8.20E-01	-0.05	0.79	1.91E-02	0.41	0.99	1.37E-02	0.46	1.20	8585850	1641784	10040724	3623448	10123774	3785031	9957674	3490869
HILIC_POS_120_06582a5_785	HILIC	POS	5.785	120.0658				2.75E-01	-0.20	0.95	8.20E-01	0.05	0.65	4.50E-01	-0.17	0.66	2.38E-01	-0.22	0.82	7800729	2675338	7159692	3398170	7081967	2648854	7237416	4037578
RP_POS_148_03964a3_947	RP	POS	3.95	148.0396				1.41E-02	-0.64	1.23	8.21E-01	0.04	0.88	2.57E-02	-0.62	0.94	1.29E-02	-0.66	1.36	5314290	3773505	3500202	2294646	3447752	1867937	3552652	2672724
HILIC_POS_407_16473a5_723	HILIC	POS	5.723	407.1647				1.34E-02	0.33	0.57	8.21E-01	-0.05	0.46	6.80E-02	0.31	0.58	5.47E-02	0.36	0.64	193102	332843	470176	935517	491519	994703	448832	881975
RP_POS_632_49078a13_505	RP	POS	13.51	632.4908				8.89E-01	-0.03	0.28	8.21E-01	0.05	0.30	9.94E-01	0.00	0.26	7.91E-01	-0.05	0.23	432506	108128	429222	133964	426168	100908	432276	161423
HILIC_NEG_141_92374a0_593	HILIC	NEG	0.593	141.9237				2.46E-01	0.24	0.80	8.21E-01	-0.05	0.73	3.33E-01	0.22	0.42	2.60E-01	0.26	0.63	445697	154582	482335	150328	485760	157842	478909	143944
RP_POS_629_40137a11_978	RP	POS	11.98	629.4014				7.54E-01	-0.06	0.68	8.22E-01	0.05	0.21	8.65E-01	-0.04	0.51	6.94E-01	-0.09	0.30	1114741	528344	1080474	558982	1067801	516587	1093147	603415
RP_POS_517_34979a10_889	RP	POS	10.89	517.3498				4.02E-01	0.14	0.77	8.22E-01	0.05	0.48	4.32E-01	0.17	0.65	5.38E-01	0.12	0.51	2683308	707461	2820900	1048622	2797141	954491	2844659	1144312
HILIC_POS_366_77661a3_008	HILIC	POS	3.008	366.7766				1.18E-05	-0.59	1.35	8.22E-01	0.05	0.77	9.68E-04	-0.56	1.47	9.39E-04	-0.61	1.47	711469	111677	540300	319444	533073	335834	547528	305418
HILIC_NEG_370_81476a2_923	HILIC	NEG	2.923	370.8148				6.51E-07	-0.62	1.35	8.23E-01	0.05	0.77	2.40E-04	-0.60	1.49	3.99E-04	-0.65	1.52	2417911	219509	1875493	958205	1853841	1022528	1897145	899183
HILIC_POS_263_0867a7_689	HILIC	POS	7.689	263.0867				8.54E-03	-0.50	0.90	8.23E-01	0.05	0.63	2.48E-02	-0.48	0.83	1.66E-02	-0.52	0.90	1538949	110710	1475064	130129	1472123	134208	1478004	127213
HILIC_POS_362_92596a4_324	HILIC	POS	4.324	362.9260				1.33E-01	0.25	1.03	8.23E-01	-0.05	0.85	2.47E-01	0.22	0.59	1.79E-01	0.27	0.92	34527024	6625448	36885437	10236912	37116687	10676100	36654187	9881252
RP_POS_394_87268a0_498	RP	POS	0.50	394.8727				1.25E-06	-0.59	1.32	8.23E-01	0.05	1.20	4.30E-04	-0.57	1.39	6.48E-04	-0.62	1.40	24028214	1782128	18397241	10539309	18159671	11224834	18634811	9915082
RP_POS_310_2373a9_788	RP	POS	9.79	310.2373				6.23E-03	-0.47	1.14	8.23E-01	0.05	0.51	2.76E-02	-0.44	0.85	1.45E-02	-0.49	1.30	5585408	191542	5462311	276922	5456070	276933	5468553	279580
RP_POS_600_83197a0_498	RP	POS	0.50	600.8320				6.76E-08	-0.66	1.36	8.23E-01	0.05	1.18	1.42E-04	-0.64	1.45	1.06E-04	-0.68	1.45	1801587	116138	1368945	720117	1352718	743278	1385172	703363
RP_POS_278_88828a0_249	RP	POS	0.25	278.8883				7.80E-01	-0.06	0.54	8.23E-01	0.04	0.24	8.77E-01	-0.04	0.42	7.28E-01	-0.08	0.28	4271961	505039	4243404	488059	4232424	489548	4254385	491285
RP_POS_195_10164a8_51	RP	POS	8.51	195.1016				5.33E-01	-0.11	0.54	8.23E-01	0.05	0.42	6.93E-01	-0.09	0.46	4.78E-01	-0.14	0.70	16690327	543561	16616395	686610	16600949	567200	16631840	793905
RP_POS_337_16782a10_978	RP	POS	10.98	337.1678				3.04E-02	0.40	1.44	8.24E-01	-0.05	1.15	8.73E-02	0.37	1.23	3.77E-02	0.42	1.28	25458620	6540283	28586585	8122823	28768900	7441095	28404270	8824359
HILIC_POS_76_07645a1_509	HILIC	POS	1.509	76.0765				7.30E-01	0.06	0.32	8.24E-01	0.05	0.88	7.06E-01	0.08	0.15	8.50E-01	0.03	0.10	121835579	76300708	127860276	109947102	125393958	91536939	130326594	126617562
RP_POS_820_58411a13_312	RP	POS	13.31	820.5841				2.27E-11	-1.42	2.49	8.24E-01	-0.04	0.84	7.78E-11	-1.44	2.39	1.33E-10	-1.40	2.26	3008226	1011724	1271217	961453	1292743	949686	1249692	982242
RP_POS_599_36584a14_266	RP	POS	14.27	599.3658				2.94E-01	-0.22	0.52	8.24E-01	-0.04	0.78	2.91E-01	-0.24	0.56	4.04E-01	-0.19	0.35	3088573	960576	2882271	950769	2903533	991472	2861008	917842
HILIC_NEG_263_10385a1_832	HILIC	NEG	1.832	263.1039				1.71E-01	-0.25	0.53	8.25E-01	0.05	0.52	3.38E-01	-0.23	0.33	1.27E-01	-0.28	0.81	1057862	680141	855374	830860	836839	541841	873909	1049024
RP_NEG_343_68149a15_599	RP	NEG	15.60	343.6815				5.53E-01	-0.12	0.55	8.25E-01	-0.05	0.16	5.40E-01	-0.14	0.37	6.62E-01	-0.10	0.40	1301934	60403	1294492	64173	1295922	60520	1293063	68217
RP_NEG_218_98579a7_148	RP	NEG	7.15	218.9858				3.35E-01	-0.22	0.53	8.25E-01	0.04	0.22	4.12E-01	-0.20	0.36	3.41E-01	-0.24	0.86	3220331	1509276	2933109	1259372	2905060	1358977	2961158	1164464
RP_POS_273_20645a8_499	RP	POS	8.50	273.2065				9.20E-01	-0.02	0.57	8.25E-01	0.04	0.39	9.95E-01	0.00	0.22	8.59E-01	-0.04	0.56	2007422	367892	2000190	304758	1993411	312372	2006970	299967
HILIC_POS_430_91431a4_324	HILIC	POS	4.324	430.9143				1.45E-01	0.24	1.02	8.25E-01	-0.05	0.84	2.60E-01	0.22	0.57	1.91E-01	0.27	0.91	25638178	4948425	27339323	7550140	27507280	7885791	27171366	7275254
RP_POS_253_88002a0_249	RP	POS	0.25	253.8800				2.63E-01	0.22	0.41	8.26E-01	0.04	0.45	2.61E-01	0.25	0.68	3.78E-01	0.20	0.39	1036690	138567	1068867	144315	1065663	152577	1072072	137032
HILIC_POS_106_05019a6_165	HILIC	POS	6.165	106.0502				5.08E-01	-0.10	1.15	8.26E-01	-0.05	0.70	5.37E-01	-0.13	1.07	6.53E-01	-0.08	1.16	1543151	445283	1469226	785303	1486666	687232	1451785	879249
RP_POS_282_16006a6_888	RP	POS	6.89	282.1601				1.20E-02	0.38	0.66	8.26E-01	-0.05	0.57	1.03E-02	0.36	0.98	7.41E-02	0.41	0.75	1231277	594956	1623825	1116453	1648617	1447804	1599032	648832
RP_NEG_730_81561a0_499	RP	NEG	0.50	730.8156				4.67E-06	-0.58	1.30	8.26E-01	0.05	1.19	5.35E-04	-0.56	1.39	1.04E-03	-0.61	1.36	1815803	190793	1444375	699503	1428862	755508	1459887	645995
RP_NEG_241_75789a0_57	RP	NEG	0.57	241.7579				1.71E-04	0.51	0.90	8.26E-01	-0.05	0.81	1.37E-02	0.49	0.97	6.66E-04	0.53	1.17	2164414	618545	2933805	1658015	2970509	1403914	2897101	1892195
HILIC_POS_317_056a5_463	HILIC	POS	5.463	317.0560				1.35E-01	-0.29	0.77	8.26E-01	0.05	0.32	2.00E-01	-0.27	0.52	1.72E-01	-0.31	0.69	7838974	1059979	7504242	1166984	7478415	1287489	7530069	1045232
RP_POS_496_41922a10_88	RP	POS	10.88	496.4192				2.74E-01	-0.19	0.55	8.26E-01	0.05	0.48	3.87E-01	-0.17	0.76	3.15E-01	-0.22	0.46	7042410	581981	6901095	765987	6884155	832873	6918034	700845
RP_POS_177_0546a7_494	RP	POS	7.49	177.0546				5.73E-01	0.10	0.43	8.27E-01	0.05	0.59	5.53E-01	0.13	0.30	7.03E-01	0.08	0.34	4375046	373330	4420673	462326	4410465	458727	4430880	470331
RP_POS_182_95851a0_258	RP	POS	0.26	182.9585				2.23E-01	0.23	0.57	8.27E-01	-0.05	0.17	3.44E-01	0.21	0.34	2.29E-01	0.26	0.76	1117283	285264	1191159	325096	1198327	309179	1183991	343271
RP_POS_171_14877a5_931	RP	POS	5.93	171.1488				3.35E-01	-0.16	1.01	8.27E-01	-0.05	1.04	3.19E-01	-0.18	0.87	5.18E-01	-0.14	1.04	16534477	4229499	15582181	6354425	15722207	7092148	15442154	5589537
RP_POS_736_54028a13_57	RP	POS	13.57	736.5403				5.93E-01	0.13	0.62	8.27E-01	-0.04	0.30	6.75E-01	0.11	0.46	5.56E-01	0.15	0.65	2757166	315826	2789452	218617	2794267	198570	2784637	238923
HILIC_NEG_100_93345a5_606	HILIC	NEG	5.606	100.9335				1.77E-01	-0.22	0.75	8.27E-01	-0.05	0.65	2.24E-01	-0.24	0.50	3.11E-01	-0.19	0.48	33154881	3032277	32158908	4968913	32268274	4844901	32049542	5136788
HILIC_NEG_271_99994a0_93	HILIC	NEG	0.93	271.9999				1.83E-08	0.80	1.33	8.27E-01	-0.05	1.19	7.02E-05	0.78	1.28	1.03E-06	0.82	1.58	12471019	8109958	26706582	18717167	27118450	16631147	26294714	20757484
HILIC_NEG_426_6882a2_935	HILIC	NEG	2.935	426.6882				5.67E-06	-0.61	1.31	8.27E-01	0.05	0.75	5.77E-04	-0.58	1.43	6.60E-04	-0.63	1.48	142232	21820	107510	62357	106138	65867	108882	59278
HILIC_NEG_136_89165a4_165	HILIC	NEG	4.165	136.8917				8.51E-01	-0.04	0.43	8.27E-01	0.05	0.50	9.53E-01	-0.01	0.16	7.85E-01	-0.06	0.15	4626951	2215466	4539047	2537400	4483254	2469637	4594839	2627307
HILIC_POS_115_12332a3_024	HILIC	POS	3.024	115.1233				3.00E-07	0.66	1.30	8.27E-01	0.05	0.80	6.98E-05	0.68	1.47	3.90E-04	0.63	1.44	1249437	95940	1457499	345368	1449911	357402	1465088	336362
RP_POS_275_07907a5_873	RP	POS	5.87	275.0791	Unknown	275.0778(100)	4	1.59E-01	-0.20	0.46	8.28E-01	-0.05	0.32	4.33E-02	-0.22	0.95	4.54E-01	-0.17	0.48	4256796	2321578	3284517	5503152	3405511	7448823	3163524	2381716
RP_NEG_299_25934a10_962	RP	NEG	10.96	299.2593				3.98E-03	-0.49	1.09	8.28E-01	-0.05	0.84	1.38E-02	-0.46	1.09	1.54E-02	-0.51	1.02	25740713	3395215	23417210	5023390	23307027	5508293	23527393	4540683
RP_POS_467_80005a0_245	RP	POS	0.25	467.8001				8.82E-02	0.32	0.58	8.28E-01	-0.05	0.20	1.04E-01	0.34	0.76	1.76E-01	0.29	0.78	522692	228950	607893	279597	601763	292266	614023	269162
RP_NEG_304_91425a0_448	RP	NEG	0.45	304.9143				9.80E-06	-0.60	1.26	8.28E-01	0.05	1.13	9.34E-04	-0.57	1.31	6.69E-04	-0.62	1.34	10733442	2006522	7737873	5450827	7618525	5635887	7857221	5313859
HILIC_POS_429_36749a1_071	HILIC	POS	1.071	429.3675				1.16E-02	-0.41	1.15	8.28E-01	-0.05	0.68	2.80E-02	-0.44	1.25	4.50E-02	-0.39	1.06	1321326	377657	1089726	600099	1102847	593649	1076604	612222
RP_POS_169_11946a4_931	RP	POS	4.93	169.1195				5.25E-01	0.12	0.50	8.28E-01	0.05	0.35	5.28E-01	0.14	0.46	6.30E-01	0.10	0.44	2601333	292714	2640727	332975	2633450	294293	2648004	370529
HILIC_NEG_446_74567a2_929	HILIC	NEG	2.929	446.7457				1.31E-06	-0.63	1.34	8.28E-01	-0.05	0.76	2.76E-04	-0.60	1.46	4.31E-04	-0.65	1.49	425019	52024	324097	176323	320247	187855	327947	165813
HILIC_NEG_167_8343a3_01	HILIC	NEG	3.01	167.8343				3.40E-01	0.18	0.96	8.29E-01	-0.05	0.77	4.67E-01	0.15	0.66	3.55E-01	0.20	0.53	3810572	838418	3984632	1038937	4007303	1065693	3961960	1021793
RP_POS_248_86255a0_245	RP	POS	0.25	248.8626				9.27E-01	0.02	0.30	8.29E-01	-0.05	0.29	9.81E-01	-0.01	0.19	8.57E-01	0.04	0.66	366397	50164	367376	58216	368645	61421	366107	55421
RP_POS_524_29944a10_502	RP	POS	10.50	524.2994				1.92E-03	-0.55	1.07	8.29E-01	-0.04	0.22	4.36E-03	-0.57	1.10	1.20E-02	-0.53	1.09	12915064	2068749	11432077	2790582	11492812	2933696	11371342	2668242
RP_POS_338_26642a8_966	RP	POS	8.97	338.2664				1.59E-01	0.28	0.52	8.29E-01	0.04	0.26	1.93E-01	0.31	0.61	2.22E-01	0.26	0.53	1402781	2175552	2039440	2245367	1990628	1991177	2088251	2493309
HILIC_NEG_532_70422a2_927	HILIC	NEG	2.927	532.7042				3.45E-06	-0.61	1.33	8.29E-01	0.05	0.76	4.52E-04	-0.58	1.45	6.65E-04	-0.63	1.46	152919	20578	116359	66005	114925	70346	117792	62045
RP_POS_321_2399a10_265	RP	POS	10.27	321.2399				3.13E-01	-0.21	0.71	8.29E-01	0.04	0.46	4.05E-01	-0.19	0.55	3.21E-01	-0.23	0.66	9691333	2223015	9237585	2097110	9192054	2179854	9283116	2032118

Supplementary table 1: Metabolomics results (in asceding order according to p-value from progressive ALD vs non-progressive ALD comparison, with molecular features with ID_level of 1-2 first)

							all_ALD_vs_control			Prog_ALD_vs_non-prog_ALD			Prog_ALD_vs_control_ALD			Non-prog_ALD_vs_control			Healthy_control		all_ALD		Non-prog_ALD		Progressive_ALD	
							t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA								
Feature_ID	RP_HILIC	POS_NEG	Average.Rt	Average.Mz	Metabolite.name	curated_MSMS	ID_level	p	d	VIP	p	d	VIP	p	d	VIP	p	d	VIP	Mean	SD	Mean	SD	Mean	SD	Mean	SD
RP_POS_846_5399Ba13_373	RP	POS	13.37	846.5400				4.81E-02	0.40	0.85	8.30E-01	-0.04	0.22	9.87E-02	0.38	0.77	5.52E-02	0.43	0.79	1517360	742983	1823328	749292	1839573	705644	1807083	797409
HILIC_POS_155_0928a1_236	HILIC	POS	1.236	155.0928				5.52E-02	-0.36	0.92	8.30E-01	-0.04	0.66	8.39E-02	-0.38	0.90	1.05E-01	-0.33	1.01	1045514	112152	998544	136051	1001484	128127	995605	144788
RP_NEG_349_23743a11_255	RP	NEG	11.26	349.2374				1.19E-03	0.61	1.39	8.30E-01	0.04	0.82	3.42E-03	0.64	1.30	4.82E-03	0.59	1.26	2606231	730404	3134197	862363	3115568	836917	3152826	895198
RP_POS_577_36945a10_464	RP	POS	10.46	577.3695				1.64E-03	0.51	0.87	8.30E-01	0.05	0.36	7.01E-03	0.54	1.20	1.07E-02	0.49	1.01	1570765	383959	1869116	616846	1855791	603898	1882441	635380
HILIC_POS_438_71259a3_013	HILIC	POS	3.013	438.7126				3.34E-04	-0.50	1.33	8.30E-01	-0.05	0.76	2.37E-03	-0.53	1.43	1.09E-02	-0.48	1.44	368543	70679	290953	168935	294602	179366	287305	159566
RP_POS_293_20853a9_675	RP	POS	9.68	293.2085				3.92E-05	0.57	1.08	8.31E-01	0.05	0.43	2.43E-03	0.59	1.13	8.15E-04	0.55	1.26	3159323	415148	3700879	1035867	3678553	914467	3723205	1153547
RP_POS_415_21124a8_658	RP	POS	8.66	415.2112				1.69E-02	0.35	0.75	8.31E-01	-0.05	0.71	1.02E-01	0.33	0.70	2.50E-02	0.38	0.84	378910	168005	488279	339160	495578	293690	480979	382156
HILIC_NEG_132_90039a1_329	HILIC	NEG	1.329	132.9004				3.56E-06	-0.85	1.31	8.31E-01	-0.04	0.57	4.48E-05	-0.87	1.38	3.67E-05	-0.83	1.45	732033	102051	619367	130565	622174	122556	616559	139307
RP_POS_140_06808a11_224	RP	POS	11.22	140.0681				9.16E-01	0.02	0.53	8.31E-01	-0.04	0.23	9.92E-01	0.00	0.19	8.47E-01	0.04	0.64	1977723	803609	1995677	929153	2015630	952167	1975725	914786
HILIC_POS_368_21994a2_934	HILIC	POS	2.934	368.2199				2.74E-01	-0.22	1.00	8.31E-01	-0.04	0.83	2.85E-01	-0.24	0.48	3.82E-01	-0.19	0.34	3309356	605236	3171293	647402	3185188	649880	3157399	651210
RP_NEG_264_93466a0_498	RP	NEG	0.50	264.9347				1.59E-06	-0.59	1.31	8.31E-01	0.05	1.20	3.94E-04	-0.57	1.39	7.05E-04	-0.62	1.38	1440698	1185576	11362499	5653152	11241199	6055045	11483798	5279664
RP_NEG_851_11444a9_605	RP	NEG	9.61	851.1144				1.70E-01	-0.31	0.67	8.32E-01	0.04	0.54	2.17E-01	-0.29	0.55	1.96E-01	-0.33	0.52	5540572	409284	5428476	349634	5420991	397367	5435961	298275
RP_POS_452_39294a10_881	RP	POS	10.88	452.3929				6.71E-01	-0.08	0.57	8.32E-01	0.05	0.44	7.87E-01	-0.05	0.56	6.53E-01	-0.10	0.55	4775982	436047	4734921	573765	4722645	632972	4747198	513974
HILIC_POS_280_8183a3_007	HILIC	POS	3.007	280.8183				2.39E-05	-0.56	1.35	8.32E-01	0.05	0.77	1.42E-03	-0.54	1.46	1.58E-03	-0.58	1.47	6761346	997045	5254150	2952208	5191090	3123708	5317209	2800584
HILIC_NEG_371_61011a1_364	HILIC	NEG	1.364	371.6101				5.58E-06	0.63	0.96	8.32E-01	-0.05	0.57	2.48E-03	0.60	0.95	3.77E-05	0.65	1.30	822733	398780	1406933	1008866	1428466	840773	1385401	1161269
RP_POS_440_86914a0_471	RP	POS	0.47	440.8691				1.63E-07	-0.66	1.34	8.32E-01	0.05	1.17	1.71E-04	-0.63	1.41	1.33E-04	-0.68	1.43	1318122	123175	1001999	526024	990777	543079	1013221	513671
HILIC_POS_642_15289a0_508	HILIC	POS	0.508	642.1529				3.84E-01	0.14	0.79	8.33E-01	-0.05	0.56	5.56E-01	0.12	0.41	3.80E-01	0.17	0.84	151300	75202	166647	114543	169080	106986	164213	122678
HILIC_POS_371_2395a4_007	HILIC	POS	4.007	371.2395				5.15E-01	0.14	0.60	8.33E-01	-0.04	0.56	6.10E-01	0.12	0.21	5.05E-01	0.16	0.28	12209483	4167683	12755022	3884091	12837432	4086611	12672612	3710249
HILIC_NEG_278_98145a4_988	HILIC	NEG	4.988	278.9815				5.45E-01	-0.12	0.65	8.33E-01	0.04	0.49	6.40E-01	-0.10	0.23	5.39E-01	-0.15	0.84	29200815	17838429	27000983	17639905	26626757	19312282	27375210	15982264
HILIC_NEG_204_88899a2_928	HILIC	NEG	2.928	204.8890				1.60E-06	-0.60	1.33	8.34E-01	0.05	0.76	3.83E-04	-0.58	1.46	6.38E-04	-0.62	1.51	389581	34001	309574	146862	306464	156771	312684	137768
RP_POS_181_07216a3_264	RP	POS	3.26	181.0722				9.58E-01	0.01	0.38	8.34E-01	-0.04	0.16	9.48E-01	-0.01	0.18	8.78E-01	0.03	0.56	3755586	3276040	3794396	4462192	3888627	4544896	3700165	4422044
RP_POS_235_99773a1_2	RP	POS	1.20	235.9977				4.35E-10	0.83	1.33	8.34E-01	0.04	0.20	1.76E-05	0.85	1.34	2.02E-07	0.81	1.53	1181008	574225	2531543	1722583	2495201	1441806	2567885	1978292
HILIC_NEG_350_75714a2_935	HILIC	NEG	2.935	350.7571				2.64E-06	-0.61	1.33	8.34E-01	0.05	0.76	3.85E-04	-0.58	1.48	6.56E-04	-0.63	1.48	415988	51047	320319	172508	316687	184596	323951	161315
HILIC_POS_296_00943a4_863	HILIC	POS	4.863	296.0094				8.98E-01	-0.03	0.83	8.35E-01	0.04	0.32	9.68E-01	-0.01	0.61	8.47E-01	-0.05	0.47	322399	220231	316904	175583	313213	191759	320594	159651
RP_POS_442_91208a6_535	RP	POS	6.54	442.9121				6.21E-07	0.60	1.32	8.35E-01	-0.05	1.13	8.05E-04	0.57	1.40	2.49E-04	0.62	1.40	37438	89624	762148	1353113	790563	1344358	733732	1374863
RP_POS_407_31213a11_162	RP	POS	11.16	407.3121				7.47E-01	-0.05	0.76	8.35E-01	0.05	0.66	8.81E-01	-0.03	0.72	7.08E-01	-0.07	0.62	2958866	477233	2920941	811335	2903940	843642	2937942	785902
RP_POS_627_26184a7_514	RP	POS	7.51	627.2618				5.03E-01	-0.12	0.47	8.35E-01	-0.04	0.69	5.08E-01	-0.15	0.40	6.21E-01	-0.10	0.36	1473446	147873	1452053	180747	1455839	169131	1448267	193317
RP_POS_175_07539a6_419	RP	POS	6.42	175.0754				2.59E-01	-0.22	0.45	8.35E-01	0.04	0.18	3.72E-01	-0.20	0.39	2.74E-01	-0.24	0.39	1012961	127048	982598	143750	979588	143790	985609	145107
HILIC_NEG_144_92349a5_607	HILIC	NEG	5.607	144.9235				1.33E-01	-0.32	1.18	8.35E-01	0.04	0.63	2.16E-01	-0.30	0.56	1.31E-01	-0.34	0.93	43376471	6809572	41298849	6307381	41166814	5601914	41430883	6997213
RP_NEG_248_9606a0_497	RP	NEG	0.50	248.9606				1.62E-04	0.47	1.25	8.36E-01	-0.05	1.18	5.37E-03	0.45	1.29	6.49E-03	0.50	1.32	54342739	2285249	58322472	9399645	58518788	10048540	58126157	8801022
HILIC_POS_246_17014a1_31	HILIC	POS	1.31	246.1701				2.44E-01	0.19	0.42	8.36E-01	-0.05	0.69	3.76E-01	0.17	0.40	2.99E-01	0.21	0.35	7333424	3668341	8364608	5929834	8488394	6333441	8240822	5558753
RP_POS_199_1692a8_616	RP	POS	8.62	199.1692				7.24E-03	0.47	0.96	8.36E-01	0.04	0.24	2.39E-02	0.49	0.76	1.80E-02	0.45	1.11	1234017	138068	1319357	188944	1315415	163587	1323298	212921
RP_NEG_369_17432a10_358	RP	NEG	10.36	369.1743				3.99E-02	0.26	0.52	8.36E-01	-0.05	0.28	2.04E-01	0.24	0.42	6.83E-02	0.28	0.81	11713452	15435175	24627107	55913649	25792688	50087079	23461525	61684576
RP_NEG_696_82062a0_496	RP	NEG	0.50	696.8206				5.12E-04	-0.54	1.21	8.36E-01	-0.04	1.21	3.35E-03	-0.56	1.21	6.33E-03	-0.52	1.21	1015919	156269	873951	282061	879823	281946	868080	284914
RP_NEG_135_03026a0_71	RP	NEG	0.71	135.0303				7.90E-13	0.88	1.62	8.36E-01	0.04	0.67	2.17E-06	0.90	1.64	5.41E-08	0.86	1.80	168902	119293	2135807	2387408	2086121	2112809	2185494	2654572
HILIC_POS_355_01123a7_33	HILIC	POS	7.33	355.0112				3.64E-02	-0.40	0.98	8.37E-01	0.04	0.31	7.78E-02	-0.38	0.73	5.38E-02	-0.42	0.97	5478625	138996	5415858	159999	5412534	163311	5419181	158205
HILIC_POS_293_09732a7_687	HILIC	POS	7.687	293.0973				5.15E-01	-0.12	0.46	8.37E-01	0.04	0.46	6.21E-01	-0.10	0.19	5.25E-01	-0.14	0.23	30653375	2268801	30337660	2680823	30281967	2973381	30393353	2381798
RP_POS_722_52686a12_991	RP	POS	12.99	722.5269				6.72E-02	-0.39	0.75	8.37E-01	-0.04	0.23	8.25E-02	-0.41	0.75	1.10E-01	-0.37	0.62	1495390	393846	1348060	367498	1355679	359601	1340441	378728
RP_POS_769_55811a13_157	RP	POS	13.16	769.5581				4.43E-02	-0.42	0.69	8.37E-01	0.04	0.21	8.49E-02	-0.40	0.68	5.54E-02	-0.44	0.82	26314940	3502989	24852824	3459557	24781167	3426993	24924480	3525133
RP_POS_778_53552a12_82	RP	POS	12.82	778.5355				1.22E-04	0.61	1.03	8.37E-01	0.04	0.21	1.63E-03	0.64	1.11	1.26E-03	0.59	1.14	14406606	7363674	21619807	12366812	21363701	11472965	21875914	13312944
RP_NEG_324_89612a15_46	RP	NEG	15.46	324.8961				3.21E-02	-0.42	0.96	8.37E-01	-0.04	0.26	3.86E-02	-0.44	0.84	7.72E-02	-0.40	0.90	3281319	241530	3171408	260378	3176800	280894	3166016	240866
RP_NEG_360_27655a8_963	RP	NEG	8.96	360.2766				2.85E-01	0.22	0.49	8.37E-01	0.04	0.27	3.18E-01	0.25	0.56	3.50E-01	0.20	0.47	502981	970565	713546	923992	694418	769985	732674	1063636
HILIC_NEG_466_80344a2_91	HILIC	NEG	2.91	466.8034				1.59E-07	-0.65	1.36	8.37E-01	0.05	0.77	1.20E-04	-0.63	1.52	2.20E-04	-0.67	1.54	1873288	151390	1427452	754108	1411847	801934	1443057	710893
HILIC_NEG_205_83957a2_943	HILIC	NEG	2.943	205.8396				2.49E-02	0.36	1.03	8.37E-01	-0.04	0.77	7.64E-02	0.34	0.72	5.42E-02	0.38	0.97	474898	93621	526778	155882	530001	161382	523554	151753
RP_POS_271_11563a4_09	RP	POS	4.09	271.1156				2.82E-01	0.20	0.49	8.38E-01	-0.04	0.32	4.21E-01	0.18	0.45	2.72E-01	0.22	0.94	3949534	174809	3989821	205110	3994053	182263	3985589	227469
HILIC_POS_74_09716a5_481	HILIC	POS	5.481	74.0972				8.76E-01	-0.03	0.37	8.38E-01	-0.04	0.34	8.23E-01	-0.05	0.21	9.58E-01	-0.01	0.32	14482436	2651101	14398140	2612505	14451942	2424090	14344339	2812033
RP_NEG_824_54669a12_463	RP	NEG	12.46	824.5467				5.15E-03	-0.62	1.06	8.38E-01	-0.04	0.57	1.07E-02	-0.63	1.14	8.49E-03	-0.60	1.02	2345081	1247886	1621828	1101174	1644508	920290	1599148	1265675
RP_NEG_356_92645a15_32	RP	NEG	15.32	356.9265				6.69E-01	-0.08	0.74	8.38E-01	-0.04	0.43	6.33E-01	-0.10	0.69	7.89E-01	-0.06	0.46	1084718	34596	1081538	41782	1082399	42912	1080678	41039
HILIC_NEG_131_91556a2_963	HILIC	NEG	2.963	131.9156				6.68E-01	-0.10	0.40	8.38E-01	-0.04	0.72	6.41E-01	-0.12	0.29	7.50E-01	-0.08	0.16	576520	193068	560148	164062	563524	154535	556772	174579
RP_POS_501_61377a6_787	RP	POS	6.79	501.6138				2.75E-07	0.61	1.33	8.38E-01	-0.05	1.13	5.10E-04	0.59	1.42	1.83E-04	0.64	1.41	26522	53022	1459222	2595044	1512592	2595349	1405851	2619978
RP_NEG_239_76036a0_569	RP	NEG	0.57	239.7604				2.77E-04	0.50	0.88	8.38E-01	-0.05	0.85	1.48E-02	0.48	0.99	1.11E-03	0.52	1.09	1120013	341313	1512994	859254	1530664	741720	1495323	970009
RP_NEG_286_97781a7_698	RP	NEG	7.70	286.9778				9.84E-01	0.00	0.88	8.38E-01	-0.04	0.15	9.49E-01	-0.02	0.66	9.20E-01	0.02	0.78	2550043	206430	2550874	178025	2554532	180650	2547216	177117
RP_POS_274_90555a15_367	RP	POS	15.37	274.9056				1.62E-01	-0.20	0.62	8.39E-01	-0.05	0.34	2.44E-01	-0.22	0.99	3.17E-01	-0.17	0.67	3567226	115416	3518996	275280	3524642	261970	3513351	290536
RP_POS_553_4585a12_268	RP	POS	12.27	553.4585				5.16E-02	-0.42	0.73	8.39E-01	0.04	0.44	9.64E-02	-0.41	0.77	5.53E-02	-0.44	0.93	13569585	5147074	11535633	4582625	11441715	4208936	11629551	4969541
HILIC_POS_294_93857a4_323	HILIC	POS	4.323	294.9386				1.42E-01	0.24	1.03	8.39E-01	-0.04	0.84	2.54E-01	0.22	0.58	1.90E-01	0.27	0.91	30103976	5735528	32097763	8817428	32278262	9151746	31917264	8559194
HILIC_POS_199_18044a5_783	HILIC	POS	5.783	199.1804				2.99E-01	-0.22	0.71	8.39E-01	0.04	0.55	4.05E-01	-0.20	0.37	2.93E-01	-0.24	0.52	3834276	839801	3657123	802993	3640704	750530	3673541	859599
RP_NEG_207_93144a0_104	RP	NEG	0.10	207.9314				4.22E-01	0.16	0.54	8.39E-01	0.04	0.31	4.18E-01	0.18	0.47	5.41E-01	0.14	0.57	3498477	1392848	3732752	1527481	3701525	1559064	3763979	1510411
RP_POS_223_0943a7_165	RP	POS	7.17	223.0943	Unknown	223.0946(100)	4	1.05E-01	-0.36	0.64	8.39E-01	0.04	0.32	1.45E-01	-0.34	0.62	1.29E-01	-0.38	0.61	7728072	4557994	6240204	4000028	6158499	4426670	6321910	3566224
RP_POS_371_22498a11_608	RP	POS	11.61	371.2250				3.65E-02	-0.40	0.78	8.40E-01	0.04	0.58	5.26E-02	-0.38	0.80	7.29E-02	-0.43	0.84	3716549	360815	3554809	405260	3546542	483656	3563076	312666
HILIC_POS_226_95108a4_323	HILIC	POS	4.323	226.9511				1.65E-01	0.23	1.02	8.40E-01	-0.04	0.85	2.82E-01	0.21	0.58	2.12E-01	0.25	0.90	324962027	61958734	345230486	94220010	347151385	97835426	343309587	91414942
HILIC_POS_357_00858a7_33	HILIC	POS	7.33	357.0086				9.51E-03	-0.53	1.25	8.40E-01	0.04	0.54	2.28E-02	-0.51	1.03	1.52E-02	-0.55	1.32	2935666	115069	2872760	114936	2870418	116681	2875103	114299
HILIC_NEG_214_0769a0_929	HILIC	NEG	0.929	214.0769				2.36E-08	0.72	1.22	8.40E-01	-0.04	1.00	2.42E-04	0.74	1.13	1.25E-06	0.70	1.57	1179442	946347	3389754	3316441	3322149	2586499	3457359	3939889
HILIC_NEG_115_92069a2_939	HILIC	NEG	2.939	115.9207				1.52E-04	0.50	1.11	8.40E-01	-0.04	0.78	2.80E-03	0.48	1.06	5.84E-03	0.53	1.18	23305151	1550772	25364828	4507639	25456651	4965924	25273005	4046565
RP_POS_226_95076a15_422	RP	POS	15.42	226.9508				3.91E-01	0.16	0.39	8.40E-01	-0.04	0.43	4.14E-01	0.18	0.37	5.03E-01	0.14	0.42	2748088	1044734	2941682	1271285	2915795	1183931	2967570	1364645
HILIC_NEG_301_68372a1_368	HILIC	NEG	1.368	301.6837				9.96E-11	-0.90	1.70	8.40E-01	-0.04	0.45	9.47E-07	-0.92	1.70	4.67E-07	-0.88	1.92	338354	39852	252382	99072	254398	94746	250367	104142
HILIC_NEG_201_80197a2_952	HILIC	NEG	2.952	201.8020				1.10E-06	0.60	1.32	8.40E-01	-0.04	0.77	4.86E-04	0.57	1.46	4.95E-04	0.62	1.52	1961349	180439	2501276	999683	2521586	1043846	2480965	963676
HILIC_POS_448_74155a3_007	HILIC	POS	3.007	448.7416				3.20E-05	-0.55	1.36	8.41E-01	0.04	0.78	1.85E-03	-0.52	1.47	1.87E-03	-0.57	1.49	1368659	204412	1056609	627363	1043891	659441	1069327	600006
RP_NEG_294_98242a7_424	RP	NEG	7.42	294.9824				8.59E-03	-0.49	0.91	8.41E-01	0.04	0.21	2.85E-02	-0.47	0.78	1.53E-02	-0.51	0.93	8065436	1444065	7225993	1747782	7190564	1716681	7261422	1795069
RP_POS_352_24429a11_609	RP	POS	11.61	352.2443				1.46E-01	-0.32	0.67	8.41E-01	0.04	0.19	1.92E-01	-0.31	0.60	1.70E-01	-0.34	0.52	3958098	805257	3724799	682319	3710988	757769	3738610	604992
HILIC_POS_274_20102a0_963	HILIC	POS	0.963	274.2010				7.09E-01	-0.08	0.42	8.41E-01	-0.04	0.56	8.10E-01	-0.06	0.10	6.45E-01	-0.10	0.41	746359	611251	701188	533271	690395	378063	711980	656802
HILIC_NEG_276_84253a7_667	HILIC	NEG	7.667	276.8425				4.18E-01	0.15	0.77	8.41E-01	-0.04	0.72	4.22E-01	0.17	0.55	5.53E-01	0.13	0.65	2570137	191341	2604146	244539	2599203	248184	2609090	243256
HILIC_POS_394_31659a3_166	HILIC	POS	3.166	394.3166				2.98E-07	0.62	1.31	8.41E-01	-0.04	0.76	3.00E-04	0.59	1.44	2.90E-04	0.64	1.51	1239904	421222	3474128	4012185	3555190	4171680	3393067	3886831
RP_POS_543_34448a10_931	RP	POS	10.93	543.3445				7.26E-02	-0.45	0.98	8.42E-01	-0.03	1.14	8.18E-02	-0.47	0.86	9.68E-02	-0.43	0.86	424237	208326	351582	140213	354406	130721	348758	150388
HILIC_NEG_144_92342a2_172	HILIC	NEG	2.172	144.9234				5.14E-01	0.13	0.71	8.42E-01	-0.04	0.52	6.36E-01	0.11	0.40	4.92E-01	0.15	0.38	28479391	6517882	29367960	7088502	29510630	6710952	29225290	7512705
HILIC_NEG_118_92426a2_171	HILIC	NEG	2.171	118.9243				4.41E-01	0.15	0.60	8.42E-01	-0.04	0.66	5.63E-01	0.13	0.21	4.34E-01	0.17	0.33	2118905	528433	2204786	592873	2216701	579122	2192870	611961
RP_POS_508_85791a0_472	RP	POS	0.47	508.8579				1.29E-07	-0.66	1.34	8.42E-01	0.04	1.18	1.52E-04	-0.63	1.42	1.46E-04	-0.68	1.43	849971	74028	634655	360445	627414	374153	641896	349850
RP_POS_286_77121a0_52	RP	POS	0.52	286.7712				4.59E-06	-0.63	1.27	8.43E-01	0.04	1.14	3.92E-04	-0.61	1.35	5.23E-04	-0.65	1.31	375640	65007	277962	168399	274591	178380	281333	159539
HILIC_POS_524_67102a3_012	HILIC	POS	3.012	524.6710				3.51E-05	-0.59	1.32	8.43E-01	-0.04	0.77	4.77E-04	-0.61	1.48	2.59E-03	-0.57	1.40	297437	58674	225440	131218	228066	138937	222815	124379
HILIC_POS_240_18048a0_625	HILIC	POS	0.625	240.1805				8.91E-01	0.02	1.00	8.43E-01	-0.04	0.85	9.86E-01	0.00	0.28	8.31E-01	0.05	0.08	787281	1366961	828293	1754362	863381	1841655	793205	1680529
RP_POS_222_86752a0_519	RP	POS	0.52	222.8675				4.83E-06	-0.79	1.37	8.43E-01	0.04	1.04	7.16E-05	-0.77	1.42	9.17E-05	-0.81	1.36	511287	102428	396241	147497	393292	156875	399190	139023
RP_POS_202_04749a3_625	RP	POS	3.63	202.0475				2.12E-02	-0.50	0.89	8.43E-01	0.04	0.78	5.02E-02	-0.48	0.77	2.23E-02	-0.52	1.07	5208975	4371076	3139687	3969802	3060352	3449522	3219023	4464104
HILIC_NEG_255_82175a3_026	HILIC	NEG	3.026	255.8218				1.26E-02	-0.43	1.13	8.43E-01	0.04	0.82	4.25E-02	-0.41	0.87	2.61E-02	-0.45	0.82	9198269	1404745	8386723	1976686	8347243	1990734	8426203	1981946
RP_POS_295_18796a9_812	RP	POS	9.81	295.1880				3.99E-03	-0.54	0.93	8.43E-01	-0.04	0.51	8.93E-03	-0.56	1.03	1.41E-02	-0.52	0.98	1575596	59302	1537680	71337	1539103	70968	1536256	72395
RP_POS_765_3783a13_57	RP	POS	13.57	765.3783				4.00E-01	0.22	0.45	8.43E-01	0.03	0.47	3.86E-01	0.23	0.68	4.65E-01	0.20	0.47	1334657	294266	1381686	186180	1377975	193176	1385396	180800
RP_NEG_299_25961a10_652	RP	NEG	10.65	299.2596				8.72E-03	-0.51	0.98	8.43E-01	-0.04	0.74	1.25E-02	-0.53	1.01	2.94E-02	-0.49	0.90	6898892	849525	6415620	956474	6434678	1028770	6396562	888395
RP_POS_415_28122a10_705	RP	POS	10.71	415.2812				3.77E-02	-0.40	0.78	8.43E-01	0.04	0.51	9.53E-02	-0.38	0.69	4.43E-02	-0.42	0.89	2794032	765821	2449970	888055	2432280	801060	2467659	975214
RP_POS_658_51111a10_658	RP	POS	10.66	658.5111				3.41E-01	-0.19	0.47	8.43E-01	0.04	0.47	4.52E-01	-0.17	0.49	3.49E-01	-0.21	0.55	4794378	380662	4718664	410828	4710487	411135	4726841	414530
RP_POS_276_19904a7_791	RP	POS	7.79	276.1990				2.89E-04	0.64	1.38	8.44E-01	-0.04	1.12	1.77E-03	0.62	1.31	1.57E-03	0.66	1.22	694006	349059	989945	469489	999278	494146	980612	448309

Supplementary table 1: Metabolomics results (in asceding order according to p-value from progressive ALD vs non-progressive ALD comparison, with molecular features with ID_level of 1-2 first)

							all_ALD_vs_control			Prog_ALD_vs_non-prog_ALD			Prog_ALD_vs_control_ALD			Non-prog_ALD_vs_control			Healthy_control		all_ALD		Non-prog_ALD		Progressive_ALD	
							t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA								
Feature_ID	RP_HILIC	POS_NEG	Average.Rt	Average.Mz	Metabolite.name	curated_MSMS	ID_level	p	d	VIP	p	d	VIP	p	d	VIP	p	d	VIP	Mean	SD	Mean	SD	Mean	SD	Mean	SD
RP_NEG_313_0658a0_622	RP	NEG	0.62	313.0658				1.14E-09	-0.77	1.41	8.44E-01	0.04	1.16	1.10E-05	-0.75	1.53	1.12E-05	-0.79	1.49	24946427	2638932	16902830	11283330	16678678	11671328	17126983	10995584
RP_NEG_563_09882a9_006	RP	NEG	9.01	563.0988				4.86E-01	0.14	0.71	8.44E-01	-0.04	0.20	6.10E-01	0.12	0.64	4.56E-01	0.16	0.45	1629724	116795	1646507	120905	1648904	106863	1644111	134548
RP_POS_252_95801a15_499	RP	POS	15.50	252.9580				3.39E-01	-0.19	0.54	8.44E-01	0.04	0.28	4.22E-01	-0.17	0.47	3.65E-01	-0.21	0.57	2102891	85022	2086164	86547	2084449	95812	2087879	77120
RP_POS_165_02408a0_45	RP	POS	0.45	165.0241				1.31E-06	-0.65	1.30	8.44E-01	-0.04	1.11	1.37E-04	-0.67	1.38	4.44E-04	-0.63	1.36	690334	92100	537169	253837	542187	258863	532152	251236
RP_NEG_367_15869a8_933	RP	NEG	8.93	367.1587				1.31E-01	0.25	0.89	8.45E-01	0.04	0.67	2.13E-01	0.28	0.58	1.87E-01	0.23	0.68	161252875	128541918	206545925	190451670	202784833	150681620	210307016	224833492
RP_NEG_319_05618a8_812	RP	NEG	8.81	319.0562				3.51E-02	0.29	0.61	8.45E-01	0.04	0.64	3.54E-02	0.31	0.77	1.93E-01	0.27	0.56	38756826	4497943	41751171	11592359	41522283	13773870	41980058	9037791
RP_POS_432_23804a8_659	RP	POS	8.66	432.2380				1.84E-02	0.36	0.76	8.45E-01	-0.04	0.74	9.85E-02	0.33	0.69	2.83E-02	0.38	0.85	318485	150782	412820	289821	418525	254604	407114	323755
RP_NEG_437_16223a9_327	RP	NEG	9.33	437.1622				6.30E-01	0.09	0.39	8.45E-01	-0.04	0.58	7.67E-01	0.07	0.23	5.67E-01	0.11	0.55	1256572	1305285	1392079	1580634	1423196	1240176	1360962	1872908
HILIC_NEG_215_07324a0_929	HILIC	NEG	0.929	215.0732				1.96E-08	0.72	1.22	8.45E-01	0.04	0.99	2.72E-04	0.74	1.12	7.27E-07	0.70	1.61	5033655	3871106	14449342	14147218	14170820	10770367	14727864	16976836
RP_POS_363_30911a10_535	RP	POS	10.54	363.3091				4.85E-01	-0.16	0.65	8.45E-01	0.04	0.65	5.67E-01	-0.14	0.54	4.79E-01	-0.17	0.75	935159	222748	904331	190812	900583	201128	908079	181879
RP_NEG_573_12897a9_006	RP	NEG	9.01	573.1290				9.70E-01	-0.01	0.58	8.46E-01	-0.04	0.74	9.00E-01	-0.03	0.25	9.52E-01	0.01	0.34	16879032	951954	16871550	1090904	16892907	1089527	16850192	1102919
HILIC_NEG_248_96017a4_232	HILIC	NEG	4.232	248.9602				1.83E-01	0.22	1.03	8.46E-01	-0.04	0.85	3.04E-01	0.20	0.58	2.30E-01	0.24	0.89	69498304	13219343	73632138	20013623	74023525	20650373	73240751	19557968
HILIC_NEG_132_92331a4_278	HILIC	NEG	4.278	132.9233				6.50E-01	0.09	0.94	8.47E-01	-0.04	0.80	7.62E-01	0.06	0.12	6.26E-01	0.11	0.37	26445327	4883974	26919169	5782963	27031869	5870640	26806469	5751304
HILIC_NEG_196_8856a7_667	HILIC	NEG	7.667	196.8856				6.14E-01	0.10	0.71	8.47E-01	0.04	0.71	5.94E-01	0.12	0.48	7.27E-01	0.08	0.41	8160090	306648	8192908	355192	8185988	355441	8199828	358415
RP_POS_132_99835a0_45	RP	POS	0.45	132.9984				1.17E-06	-0.65	1.31	8.47E-01	-0.04	1.12	1.26E-04	-0.67	1.38	4.74E-04	-0.63	1.38	1378301	194429	1046032	553170	1056796	567871	1035268	543622
RP_POS_796_61877a14_278	RP	POS	14.28	796.6188				5.59E-01	0.09	0.22	8.47E-01	-0.04	0.14	6.97E-01	0.07	0.26	5.83E-01	0.11	0.26	3996212	2692643	4394442	4844323	4488640	5337157	4300244	4348621
RP_POS_262_87753a0_249	RP	POS	0.25	262.8775				8.71E-01	0.03	0.56	8.47E-01	0.04	0.16	8.11E-01	0.05	0.31	9.56E-01	0.01	0.26	1023477	109805	1027147	114392	1024929	123021	1029365	106272
RP_POS_138_90623a0_521	RP	POS	0.52	138.9062				5.41E-05	0.50	1.21	8.48E-01	-0.04	1.11	4.17E-03	0.48	1.20	3.16E-03	0.52	1.33	342440	48648	447049	234596	451591	242450	442506	228843
HILIC_NEG_436_71536a2_933	HILIC	NEG	2.933	436.7154				8.47E-07	-0.65	1.33	8.48E-01	0.04	0.75	1.65E-04	-0.62	1.48	3.42E-04	-0.67	1.46	240532	32198	180430	101266	178469	108484	182390	94564
RP_POS_261_10995a7_349	RP	POS	7.35	261.1100				3.74E-01	0.16	0.49	8.48E-01	-0.04	0.32	5.01E-01	0.14	0.36	3.97E-01	0.18	0.52	701757	809579	862609	1084878	883589	1122530	841628	1056867
HILIC_NEG_550_76477a2_91	HILIC	NEG	2.91	550.7648				3.37E-07	-0.63	1.35	8.48E-01	0.04	0.77	1.82E-04	-0.61	1.51	3.15E-04	-0.65	1.54	1490118	125979	1136347	615696	1124454	653436	1148240	581922
RP_POS_284_88412a0_251	RP	POS	0.25	284.8841				3.09E-01	0.23	0.68	8.48E-01	0.04	0.13	3.16E-01	0.25	0.52	3.87E-01	0.21	0.49	374258	77074	389807	65566	388543	64344	391070	67395
RP_POS_288_76837a0_522	RP	POS	0.52	288.7684				1.88E-05	-0.57	1.24	8.48E-01	0.04	1.15	1.14E-03	-0.54	1.29	1.52E-03	-0.59	1.29	538562	85274	406660	255755	401733	271681	411587	241445
HILIC_POS_462_76495a2_992	HILIC	POS	2.992	462.7650				1.14E-05	-0.57	1.36	8.49E-01	0.04	0.77	9.28E-04	-0.55	1.49	1.28E-03	-0.59	1.49	740096	102298	568255	330094	561905	350539	574604	311749
RP_POS_366_1864a10_978	RP	POS	10.98	366.1864				2.60E-02	0.41	1.47	8.49E-01	-0.04	1.18	7.51E-02	0.39	1.27	3.41E-02	0.43	1.31	7947614	2015894	8938305	2488838	8986038	2280846	8890572	2703357
RP_POS_508_33978a10_261	RP	POS	10.26	508.3398				1.29E-03	0.54	1.17	8.49E-01	0.04	0.80	9.06E-03	0.56	1.07	4.06E-03	0.52	1.13	664955	278933	880743	417782	872736	352533	888750	477740
RP_NEG_146_93761a15_662	RP	NEG	15.66	146.9376				8.31E-01	0.05	0.46	8.49E-01	0.04	0.60	7.76E-01	0.06	0.25	9.11E-01	0.03	0.60	6645537	1464650	6708099	1325434	6682712	1469188	6733486	1178803
RP_NEG_636_82013a0_498	RP	NEG	0.50	636.8201				6.03E-05	-0.52	1.25	8.49E-01	-0.04	1.23	1.20E-03	-0.54	1.34	6.56E-03	-0.50	1.30	6056277	835371	4716469	2872524	4771417	3051459	4661522	2711755
RP_NEG_297_24393a10_54	RP	NEG	10.54	297.2439				6.68E-02	-0.37	0.74	8.50E-01	-0.04	0.66	7.59E-02	-0.39	0.77	1.27E-01	-0.35	0.74	2183731	324499	2059691	332219	2066031	355509	2053350	310682
HILIC_NEG_115_04009a0_999	HILIC	NEG	0.999	115.0401				8.43E-02	0.26	0.92	8.50E-01	-0.04	1.07	1.98E-01	0.24	0.44	1.33E-01	0.28	0.72	7342123	1902831	8191901	3525470	8259129	3543472	8124674	3542050
RP_POS_534_38629a14_267	RP	POS	14.27	534.3863				7.50E-01	0.06	0.43	8.50E-01	0.04	0.27	7.25E-01	0.08	0.35	8.33E-01	0.05	0.62	2084836	609260	2124598	619519	2112800	536315	2136395	698227
RP_POS_784_58496a13_572	RP	POS	13.57	784.5850				5.09E-08	0.76	1.32	8.50E-01	0.04	0.27	1.91E-05	0.78	1.37	4.24E-05	0.74	1.36	15193814	11871484	36260441	29607819	35696792	29670712	36824091	29835157
RP_POS_239_06401a0_612	RP	POS	0.61	239.0640				1.46E-07	-0.71	1.35	8.50E-01	0.04	1.14	8.39E-05	-0.68	1.42	6.65E-05	-0.73	1.42	688268	111033	482025	314380	476041	323534	488008	308122
HILIC_NEG_213_87982a2_945	HILIC	NEG	2.945	213.8798				4.93E-01	0.13	0.78	8.50E-01	-0.04	0.75	6.06E-01	0.11	0.19	4.95E-01	0.15	0.26	272650	59796	281396	69920	282726	72080	280065	68397
RP_POS_323_21811a10_083	RP	POS	10.08	323.2181				4.06E-04	-0.77	1.20	8.50E-01	-0.04	0.96	9.02E-04	-0.79	1.23	1.15E-03	-0.75	1.17	2454852	203033	2301559	184401	2305067	178268	2298052	192085
RP_POS_576_53491a15_1	RP	POS	15.10	576.5349				9.23E-01	-0.02	0.22	8.50E-01	0.04	0.12	9.92E-01	0.00	0.38	8.69E-01	-0.04	0.33	30219667	10392557	30021057	9254651	29845062	9308325	30197052	9291767
HILIC_NEG_260_76074a2_947	HILIC	NEG	2.947	260.7607				7.44E-06	-0.59	1.33	8.50E-01	0.04	0.76	6.83E-04	-0.57	1.45	8.90E-04	-0.61	1.48	1023989	136085	802313	409283	794529	432763	810096	388633
HILIC_NEG_528_70941a2_928	HILIC	NEG	2.928	528.7094				1.06E-05	-0.55	1.33	8.50E-01	0.04	0.77	1.08E-03	-0.53	1.45	1.57E-03	-0.58	1.50	367362	39869	287149	159954	284109	170146	290189	150745
RP_POS_475_41525a11_263	RP	POS	11.26	475.4153				3.63E-01	-0.16	0.75	8.51E-01	-0.04	1.06	3.99E-01	-0.18	0.73	4.70E-01	-0.14	0.56	4283370	935324	4096586	1191202	4119201	1089758	4073971	1295479
RP_POS_328_88492a0_498	RP	POS	0.50	328.8849				7.35E-06	-0.56	1.29	8.51E-01	0.04	1.21	9.10E-04	-0.54	1.36	1.37E-03	-0.58	1.36	1885786	203293	1448476	862393	1432108	917525	1464845	812541
HILIC_POS_147_14922a4_831	HILIC	POS	4.831	147.1492				5.57E-01	-0.11	0.86	8.51E-01	-0.04	0.72	5.42E-01	-0.13	0.37	6.69E-01	-0.09	0.17	17971886	2795752	17626639	3111204	17685669	3157997	17567609	3094618
RP_POS_249_1458a8_4	RP	POS	8.40	249.1458	Pterosin A	249.1438(100)	3	7.41E-01	0.06	0.60	8.51E-01	-0.04	0.35	8.32E-01	0.05	0.40	7.13E-01	0.08	0.48	685418	201476	699286	218842	703436	235458	695136	203188
RP_POS_263_9006a15_512	RP	POS	15.51	263.9006				4.21E-02	0.47	1.10	8.51E-01	0.03	0.80	5.15E-02	0.49	1.00	6.52E-02	0.46	0.95	1436785	336622	1573105	264695	1568097	257321	1578112	274392
RP_POS_436_3403a11_391	RP	POS	11.39	436.3403				2.02E-01	0.21	0.54	8.51E-01	-0.04	0.30	2.62E-01	0.19	0.51	2.98E-01	0.23	0.58	1668193	547738	1832038	829002	1847705	999107	1816371	624337
RP_POS_135_03207a15_303	RP	POS	15.30	135.0321				1.76E-01	-0.29	0.72	8.51E-01	0.04	0.44	2.43E-01	-0.27	0.49	1.95E-01	-0.31	0.69	17600349	5908465	15988203	5383441	15886552	5569777	16089853	5245077
HILIC_NEG_182_8345a2_95	HILIC	NEG	2.95	182.8345				8.21E-07	-0.63	1.34	8.52E-01	0.04	0.77	1.91E-04	-0.61	1.47	4.29E-04	-0.65	1.50	1782082	174040	1416763	633991	1404818	680523	1428709	590499
RP_POS_271_22675a9_961	RP	POS	9.96	271.2268				8.03E-02	-0.37	0.78	8.52E-01	-0.04	0.74	8.89E-02	-0.39	0.70	1.36E-01	-0.36	0.83	1440339	162359	1382494	150114	1385320	158633	1379667	142646
RP_POS_631_401a15_431	RP	POS	15.43	631.4010				7.37E-01	-0.06	0.35	8.52E-01	0.04	0.37	8.41E-01	-0.04	0.32	7.00E-01	-0.08	0.51	5501029	682970	5451921	815232	5436576	809750	5467266	828610
HILIC_NEG_226_86159a0_837	HILIC	NEG	0.837	226.8616				3.72E-01	-0.20	0.92	8.52E-01	-0.04	0.74	3.79E-01	-0.21	0.34	4.54E-01	-0.18	0.47	152378	33652	146394	29609	146952	28593	145837	30872
RP_POS_154_08643a2_879	RP	POS	2.88	154.0864				1.62E-01	0.16	0.72	8.52E-01	-0.04	0.21	3.23E-01	0.14	0.86	3.22E-01	0.18	0.45	9318	9575	2298503	16263416	2604404	18358290	1992601	14041993
RP_NEG_636_08643a0_624	RP	NEG	0.62	636.0864				2.71E-03	-0.47	1.08	8.52E-01	-0.04	1.01	7.44E-03	-0.49	1.10	2.36E-02	-0.45	1.12	2992099	753253	2417059	1307621	2441615	1398795	2392503	1223430
RP_POS_801_03644a13_152	RP	POS	13.15	801.0364				3.40E-02	-0.47	0.94	8.52E-01	0.04	0.30	6.57E-02	-0.45	0.77	3.88E-02	-0.48	0.96	1107470	446741	914735	394111	907339	368638	922131	421677
RP_POS_563_55054a10_848	RP	POS	10.85	563.5505				1.12E-08	0.81	1.26	8.53E-01	0.04	0.74	5.35E-05	0.83	1.31	4.46E-07	0.79	1.51	133071935	70183115	259530967	164535070	256451655	131778081	262610278	193161201
RP_POS_184_13326a5_662	RP	POS	5.66	184.1333				5.37E-01	-0.15	0.63	8.53E-01	-0.03	0.24	5.51E-01	-0.16	0.61	5.80E-01	-0.13	0.50	485260	680041	403804	516817	413449	328438	394159	656955
RP_POS_149_96095a0_678	RP	POS	0.68	149.9610				3.78E-08	0.69	1.33	8.53E-01	-0.04	1.16	9.79E-05	0.67	1.40	5.60E-05	0.71	1.44	1914522	217750	2533947	982197	2552236	997640	2515658	976290
RP_POS_223_09398a13_11	RP	POS	13.11	223.0940				3.19E-01	0.18	0.55	8.53E-01	-0.04	0.62	4.31E-01	0.16	0.42	3.46E-01	0.20	0.48	9387315	991686	9601207	1209163	9623706	1253282	9578708	1175686
HILIC_POS_112_89601a3_017	HILIC	POS	3.017	112.8960				1.54E-04	-0.55	1.34	8.54E-01	0.04	0.78	2.72E-03	-0.53	1.40	2.79E-03	-0.57	1.38	41962648	8446995	32818481	17939650	32484893	18904843	33152070	17105844
RP_NEG_203_88588a14_274	RP	NEG	14.27	203.8859				2.28E-01	-0.24	0.62	8.54E-01	0.04	0.24	3.33E-01	-0.22	0.38	2.37E-01	-0.26	0.62	883402	457233	768429	486418	759388	461266	777470	514879
HILIC_POS_544_73077a2_992	HILIC	POS	2.992	544.7308				2.55E-05	-0.56	1.35	8.54E-01	0.04	0.76	1.41E-03	-0.54	1.46	1.71E-03	-0.58	1.47	3936308	603810	3027309	1786522	2994129	1887889	3060489	1697670
RP_POS_289_15405a9_356	RP	POS	9.36	289.1541				4.88E-01	0.13	0.49	8.54E-01	-0.04	0.35	4.86E-01	0.15	0.42	6.08E-01	0.11	0.50	476792	71814	487495	86053	485897	86883	489092	86067
RP_POS_265_25104a10_848	RP	POS	10.85	265.2510				5.22E-06	0.80	1.26	8.54E-01	-0.04	0.65	2.82E-04	0.79	1.26	1.25E-05	0.82	1.47	11241735	3645938	15256530	4981813	15348998	4194342	15164061	5703811
RP_POS_165_06042a15_299	RP	POS	15.30	165.0604				5.65E-02	-0.33	0.56	8.54E-01	-0.04	0.18	8.65E-02	-0.35	0.62	1.24E-01	-0.31	0.54	29026576	6154170	26353150	8480436	26510364	8454510	26195935	8589187
HILIC_POS_336_69052a3_023	HILIC	POS	3.023	336.6905				5.46E-04	-0.50	1.31	8.54E-01	-0.04	0.76	3.25E-03	-0.52	1.41	1.22E-02	-0.48	1.40	731590	158506	572149	349904	578636	370984	565663	331133
HILIC_POS_421_36954a7_689	HILIC	POS	7.689	421.3695				3.72E-01	0.18	0.49	8.54E-01	0.04	0.38	3.93E-01	0.19	0.31	4.68E-01	0.16	0.38	1006511	83260	1022070	90527	1020392	84978	1023748	96594
RP_POS_576_84497a0_472	RP	POS	0.47	576.8450				5.40E-08	-0.68	1.35	8.54E-01	0.04	1.17	7.60E-05	-0.66	1.45	1.01E-04	-0.70	1.43	692652	65270	509149	294837	503685	308472	514613	283577
HILIC_NEG_273_01746a0_579	HILIC	NEG	0.579	273.0175				9.52E-01	0.01	0.60	8.54E-01	0.04	0.58	8.83E-01	0.03	0.18	9.71E-01	-0.01	0.11	559046	126412	560687	151893	557875	161953	563499	142720
RP_POS_441_17322a6_81	RP	POS	6.81	441.1732				6.54E-02	-0.34	0.75	8.54E-01	0.04	0.55	1.32E-01	-0.32	0.61	8.82E-02	-0.36	0.69	1062427	78782	1030633	96763	1028843	95891	1032422	98567
RP_POS_512_33459a8_913	RP	POS	8.91	512.3346				6.64E-04	-0.54	1.33	8.55E-01	0.04	0.60	1.90E-02	-0.53	1.27	3.50E-04	-0.56	1.34	7454333	2152298	5608216	3591450	5541899	2392433	5674533	4508609
RP_POS_614_80927a0_499	RP	POS	0.50	614.8093				1.97E-04	-0.49	1.23	8.55E-01	-0.04	1.22	2.28E-03	-0.51	1.30	1.09E-02	-0.47	1.28	6164065	988288	4815637	3054661	4871953	3254869	4759321	2872575
RP_POS_409_18735a2_489	RP	POS	2.49	409.1874				2.09E-03	-0.64	1.23	8.55E-01	-0.04	1.10	8.74E-03	-0.62	1.14	2.69E-03	-0.65	1.28	917168	404746	651205	403323	643780	353343	658630	451326
RP_NEG_732_86047a0_491	RP	NEG	0.49	732.8605				1.41E-07	0.63	1.35	8.55E-01	-0.04	1.21	2.00E-04	0.61	1.44	2.02E-04	0.65	1.43	781470	235714	2055649	2218903	2096430	2301416	2014868	2155837
RP_POS_415_28177a9_935	RP	POS	9.94	415.2818				7.80E-02	0.28	1.09	8.55E-01	-0.04	0.36	1.47E-01	0.26	0.64	1.51E-01	0.30	1.22	2846335	2434954	3924154	4247772	4002222	4736837	3846086	3742367
RP_NEG_462_88031a0_465	RP	NEG	0.47	462.8803				1.30E-07	-0.67	1.35	8.55E-01	0.04	1.20	1.20E-04	-0.65	1.43	1.16E-04	-0.69	1.43	790046	95388	565336	364668	558640	377630	572032	354941
RP_POS_408_36716a10_881	RP	POS	10.88	408.3672				1.63E-05	-0.69	1.07	8.55E-01	-0.04	0.57	1.62E-04	-0.71	1.28	6.85E-04	-0.67	1.09	4438033	420510	3970082	708358	3983088	742788	3957077	679488
RP_POS_279_03922a6_074	RP	POS	6.07	279.0392				7.04E-01	0.07	0.43	8.56E-01	0.04	0.55	6.65E-01	0.09	0.42	8.12E-01	0.05	0.61	622619	155087	635093	178772	631814	191067	638372	167459
HILIC_NEG_632_72791a2_91	HILIC	NEG	2.91	632.7279				5.25E-07	-0.63	1.36	8.56E-01	0.04	0.78	2.19E-04	-0.60	1.52	3.77E-04	-0.65	1.54	1712263	157048	1306159	714393	1293062	757628	1319256	675855
RP_NEG_172_86778a15_568	RP	NEG	15.57	172.8678				1.96E-02	-0.43	0.77	8.56E-01	-0.04	0.44	2.70E-02	-0.45	0.80	6.00E-02	-0.41	0.88	1066936	74237	1028663	91253	1030332	98910	1026995	83877
HILIC_NEG_134_89478a3_013	HILIC	NEG	3.013	134.8948				3.85E-01	0.16	0.96	8.56E-01	-0.04	0.80	5.05E-01	0.14	0.25	3.98E-01	0.18	0.33	241512667	38664308	248752196	46652711	249604657	46826528	247899735	46937852
RP_POS_296_99902a6_797	RP	POS	6.80	296.9990				5.47E-01	0.18	0.89	8.56E-01	-0.03	0.58	5.86E-01	0.17	0.78	5.30E-01	0.19	0.57	5753301	695643	5830264	298902	5835723	299824	5824804	300919
RP_NEG_384_93628a14_265	RP	NEG	14.27	384.9363				5.07E-01	-0.15	0.48	8.56E-01	-0.04	0.21	4.84E-01	-0.16	0.48	6.05E-01	-0.13	0.42	3226751	1801899	2988814	1589035	3017837	1729053	2959791	1452670
RP_NEG_329_03979a0_621	RP	NEG	0.62	329.0398				2.21E-07	-0.66	1.33	8.56E-01	-0.04	1.22	4.67E-05	-0.68	1.46	4.68E-04	-0.64	1.38	6306349	757853	4500039	3011107	4555003	3199504	4445076	2841756
RP_POS_617_33704a14_267	RP	POS	14.27	617.3370				6.63E-01	-0.09	0.62	8.56E-01	0.04	0.20	7.60E-01	-0.07	0.57	6.33E-01	-0.11	0.31	9294091	2187064	9099236	2195602	9059191	2122555	9139282	2287183
HILIC_POS_116_08198a2_131	HILIC	POS	2.131	116.0820				2.74E-01	-0.28	0.54	8.57E-01	0.03	0.47	3.39E-01	-0.27	0.39	2.58E-01	-0.30	0.48	225424	313917	160092	195669	156529	162987	163655	225306
RP_POS_304_26071a11_608	RP	POS	11.61	304.2607				3.75E-06	0.75	1.20	8.57E-01	0.04	0.48	2.84E-04	0.77	1.21	2.58E-05	0.73	1.47	11480856	3971554	16197236	6464308	16079627	5309382	16314845	7497306
HILIC_NEG_480_56104a2_946	HILIC	NEG	2.946	480.5610				1.10E-04	-0.54	1.30	8.57E-01	-0.04	0.76	9.49E-04	-0.56	1.44	6.21E-03	-0.52	1.39	252709	46312	197914	109875	199911	118894	195917	101230
RP_POS_296_25821a9_495	RP	POS	9.50	296.2582				3.37E-01	-0.28	0.86	8.57E-01	0.03	0.45	3.85E-01	-0.27	0.66	3.17E-01	-0.30	0.74	3971033	9103691	2356831	4035616	2283491	2930695	2430172	4929992
RP_NEG_197_04224a3_698	RP	NEG	3.70	197.0422				2.98E-01	0.19	0.67	8.57E-01	0.04	0.80	3.48E-01	0.21	0.55	3.85E-01	0.17	0.37	1286983	392758	1375503	480282	1366800	419075	1384206	538767
RP_POS_553_45856a13_013	RP	POS	13.01	553.4586				4.83E-02	-0.43	0.98	8.58E-01	0.03	0.16	9.03E-02	-0.41	0.99	5.38E-02	-0.44	0.77	6736800	1195390	6255625	1084234	6236053	1001599	6275197	1170954

Supplementary table 1: Metabolomics results (in asceding order according to p-value from progressive ALD vs non-progressive ALD comparison, with molecular features with ID_level of 1-2 first)

							all_ALD_vs_control			Prog_ALD_vs_non-prog_ALD			Prog_ALD_vs_control_ALD			Non-prog_ALD_vs_control			Healthy_control		all_ALD		Non-prog_ALD		Progressive_ALD	
							t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA								
Feature_ID	RP_HILIC	POS_NEG	Average.Rt	Average.Mz	Metabolite.name	curated_MSMS	p	d	VIP	p	d	VIP	p	d	VIP	p	d	VIP	Mean	SD	Mean	SD	Mean	SD	Mean	SD
HILIC_NEG_384_83936a2_911	HILIC	NEG	2.911	384.8394			1.62E-06	-0.59	1.34	8.58E-01	0.04	0.77	4.28E-04	-0.57	1.48	7.39E-04	-0.61	1.54	305350	24517	238364	125396	236110	133337	240619	118237
RP_POS_250_89377a0_257	RP	POS	0.26	250.8938			5.80E-01	0.11	0.58	8.58E-01	0.04	0.34	5.72E-01	0.13	0.47	6.79E-01	0.09	0.58	2895412	1208738	3035009	1311301	3011442	1272924	3058575	1361119
RP_POS_502_29239a10_324	RP	POS	10.32	502.2924			7.83E-10	1.07	1.80	8.58E-01	-0.03	0.23	4.61E-07	1.05	1.68	6.83E-09	1.09	1.91	32604540	8682680	46484972	12334014	46706640	10749378	46263304	13845975
HILIC_NEG_180_97305a4_232	HILIC	NEG	4.232	180.9731			2.49E-01	0.20	1.02	8.59E-01	-0.04	0.85	3.74E-01	0.18	0.53	2.93E-01	0.21	0.85	39505128	7478103	41499345	10929325	41695406	11249818	41303285	10709864
RP_POS_124_92249a0_498	RP	POS	0.50	124.9225			7.00E-05	-0.52	1.25	8.59E-01	-0.04	1.22	1.11E-03	-0.54	1.32	6.40E-03	-0.50	1.30	1485627	239897	1138297	731293	1151394	781998	1125200	684560
RP_NEG_1043_15271a9_73	RP	NEG	9.73	1043.1527			4.14E-01	-0.17	0.43	8.59E-01	-0.04	1.06	4.03E-01	-0.19	0.48	5.22E-01	-0.15	0.34	3957047	307694	3905722	302990	3911134	326727	3900310	280481
RP_POS_184_07294a10_618	RP	POS	10.62	184.0729			1.02E-01	0.34	1.09	8.59E-01	-0.04	0.90	1.90E-01	0.32	0.86	9.61E-02	0.35	0.99	615375	244970	698360	245866	702747	198792	693973	287362
HILIC_POS_158_96407a4_322	HILIC	POS	4.322	158.9641			2.06E-01	0.21	1.02	8.60E-01	-0.04	0.84	3.24E-01	0.19	0.55	2.56E-01	0.23	0.87	102545558	19500429	108282861	28914325	108797715	29958753	107768008	28125975
RP_NEG_484_87112a0_498	RP	NEG	0.50	484.8711			1.53E-06	-0.60	1.31	8.60E-01	0.04	1.21	3.93E-04	-0.58	1.39	6.96E-04	-0.62	1.38	14054298	1305605	10678287	6262137	10566829	6662379	10789745	5900539
HILIC_POS_90_97725a4_322	HILIC	POS	4.322	90.9773			2.49E-01	0.20	1.01	8.60E-01	-0.04	0.84	3.71E-01	0.18	0.50	2.93E-01	0.22	0.81	265878856	50022827	279125642	71837018	280401710	74074487	277849574	70257234
HILIC_NEG_193_81575a3_034	HILIC	NEG	3.034	193.8158			5.52E-05	0.50	1.20	8.60E-01	0.04	0.77	1.48E-03	0.52	1.43	7.78E-03	0.48	1.25	6251790	252621	6800273	1233148	6778369	1309886	6822177	1164285
RP_NEG_701_15546a9_222	RP	NEG	9.22	701.1555			4.39E-01	0.13	0.71	8.60E-01	-0.04	0.52	5.73E-01	0.11	0.39	4.54E-01	0.15	0.57	12372954	678587	12491741	946716	12508537	950247	12474945	952518
HILIC_POS_448_36249a1_071	HILIC	POS	1.071	448.3625			4.39E-02	-0.33	1.15	8.60E-01	-0.04	0.66	7.95E-02	-0.35	1.22	1.05E-01	-0.32	1.06	390753	121969	332456	186086	335757	181754	329156	192108
RP_POS_210_10957a11_609	RP	POS	11.61	210.1096			7.51E-02	-0.34	0.79	8.60E-01	0.04	0.43	1.12E-01	-0.32	0.67	1.22E-01	-0.36	0.73	1594943	164046	1532038	191191	1528648	218208	1535427	161913
RP_POS_403_78049a13_394	RP	POS	13.39	403.7805			3.78E-01	0.21	0.60	8.60E-01	0.03	0.21	3.66E-01	0.22	0.60	4.59E-01	0.19	0.65	2038442	965030	2204339	745229	2191134	803613	2217544	689868
RP_NEG_362_9415a0_465	RP	NEG	0.47	362.9415			5.70E-07	-0.72	1.33	8.61E-01	-0.04	1.10	4.57E-05	-0.74	1.42	1.53E-04	-0.70	1.37	1221994	183382	947353	404541	954509	414208	940198	398715
RP_POS_589_427a10_875	RP	POS	10.88	589.4270			9.09E-01	0.02	0.64	8.61E-01	0.04	0.49	8.53E-01	0.04	0.37	9.83E-01	0.00	0.79	16406138	1011714	16430221	1078373	16411166	1116554	16449275	1049796
RP_POS_248_87036a0_515	RP	POS	0.52	248.8704			7.51E-06	-0.66	1.23	8.61E-01	-0.04	1.05	1.55E-04	-0.68	1.32	7.32E-04	-0.64	1.27	1062744	245632	751012	500183	759833	524698	742192	479588
RP_POS_313_27362a10_25	RP	POS	10.25	313.2736			9.82E-01	0.00	0.45	8.61E-01	0.03	0.20	9.58E-01	0.01	0.53	9.24E-01	-0.02	0.52	5688088	985980	5683621	917172	5667454	904609	5699788	938470
RP_POS_255_97752a0_51	RP	POS	0.51	255.9775			1.09E-05	0.55	1.20	8.62E-01	0.04	1.15	1.12E-03	0.57	1.30	2.01E-03	0.53	1.27	236022	86342	430960	396449	423991	395682	437929	401109
RP_POS_240_23146a10_846	RP	POS	10.85	240.2315			4.89E-04	0.58	0.92	8.62E-01	-0.04	0.49	3.34E-03	0.56	1.04	3.23E-03	0.60	0.93	317940	171882	464161	263825	468796	277945	459526	251655
RP_NEG_326_98917a7_342	RP	NEG	7.34	326.9892			6.65E-01	-0.08	0.29	8.62E-01	-0.04	0.21	6.40E-01	-0.10	0.39	7.69E-01	-0.06	0.37	5461895	1420191	5332168	1610959	5360469	1656117	5303866	1580818
HILIC_POS_196_85735a3_011	HILIC	POS	3.011	196.8574			6.54E-05	-0.58	1.34	8.62E-01	0.04	0.77	1.62E-03	-0.56	1.42	1.61E-03	-0.60	1.40	1225094	255781	930455	547967	920832	573546	940077	526801
RP_NEG_271_22867a10_283	RP	NEG	10.28	271.2287			5.15E-01	-0.12	0.59	8.62E-01	0.04	0.53	6.30E-01	-0.10	0.46	5.29E-01	-0.13	0.72	1822764	172869	1797850	227741	1793851	240274	1801848	216855
HILIC_POS_354_75095a3_014	HILIC	POS	3.014	354.7510			7.81E-05	-0.54	1.35	8.62E-01	0.04	0.79	2.57E-03	-0.52	1.46	2.68E-03	-0.56	1.46	375830	65297	290325	174720	287260	183374	293390	167427
HILIC_POS_375_3212a1_393	HILIC	POS	1.393	375.3212			1.55E-04	-0.63	1.12	8.62E-01	-0.04	0.35	1.19E-03	-0.65	1.10	1.53E-03	-0.62	1.37	8542574	1545837	7114083	2335970	7155047	2281733	7073119	2411461
HILIC_NEG_128_95969a3_046	HILIC	NEG	3.046	128.9597			7.35E-04	-0.54	1.27	8.62E-01	0.04	0.76	5.96E-03	-0.52	1.28	4.87E-03	-0.55	1.32	4145025	1106672	3195085	1887040	3162058	1959849	3228113	1830650
RP_POS_307_22415a9_865	RP	POS	9.87	307.2242			2.40E-01	-0.21	0.74	8.62E-01	0.04	0.73	3.42E-01	-0.19	0.56	2.84E-01	-0.23	0.89	4342464	487574	4216076	627258	4205104	661564	4227049	597513
HILIC_POS_145_09697a5_188	HILIC	POS	5.188	145.0970			1.49E-06	-0.73	1.37	8.62E-01	0.04	0.75	1.01E-04	-0.71	1.49	1.01E-04	-0.75	1.41	738249	156333	529237	301484	523966	313332	534509	292244
RP_POS_472_59756a6_667	RP	POS	6.67	472.5976			3.37E-07	0.61	1.31	8.62E-01	-0.04	1.11	4.42E-04	0.59	1.40	2.65E-04	0.63	1.38	15753	29147	860567	1543411	887541	1567415	833593	1534463
RP_POS_185_03215a0_52	RP	POS	0.52	185.0322			1.58E-05	-0.68	1.23	8.63E-01	-0.04	1.07	4.05E-04	-0.70	1.25	3.14E-04	-0.67	1.31	1579824	368927	1165022	634454	1176094	601354	1153951	671864
HILIC_POS_131_08162a5_648	HILIC	POS	5.648	131.0816			4.79E-01	-0.14	0.98	8.63E-01	-0.04	0.62	4.98E-01	-0.16	0.80	5.69E-01	-0.12	0.92	456107	166717	431387	182957	434578	165018	428196	200942
RP_POS_230_22221a5_932	RP	POS	5.93	230.2222			2.92E-01	-0.18	1.01	8.63E-01	-0.04	1.01	2.95E-01	-0.20	0.86	4.53E-01	-0.16	1.03	663575	189926	617470	275814	622267	305662	612674	245404
HILIC_POS_58_06571a4_831	HILIC	POS	4.831	58.0657			1.81E-02	0.41	0.98	8.63E-01	-0.04	0.58	7.33E-02	0.39	0.64	2.23E-02	0.43	0.84	2646557	645146	2999238	908621	3015029	771375	2983447	1035618
RP_POS_335_24301a10_978	RP	POS	10.98	335.2430			5.49E-02	0.36	1.41	8.63E-01	-0.04	1.21	1.26E-01	0.34	1.21	6.52E-02	0.38	1.22	1431330	356941	1580821	431207	1588309	390099	1573333	472633
RP_POS_126_0916a2_88	RP	POS	2.88	126.0916			1.59E-01	0.16	0.72	8.63E-01	-0.04	0.21	3.19E-01	0.14	0.86	3.20E-01	0.18	0.45	45925	51405	5107331	35681283	5726920	39975274	4487742	31200715
HILIC_NEG_169_96764a0_93	HILIC	NEG	0.93	169.9676			1.89E-08	0.79	1.31	8.64E-01	-0.04	1.23	5.99E-05	0.77	1.29	1.74E-06	0.81	1.53	351542	201096	708560	473855	716743	429132	700377	519007
RP_POS_311_00858a3_622	RP	POS	3.62	311.0086			2.29E-02	-0.49	0.87	8.64E-01	0.03	0.73	5.23E-02	-0.48	0.78	2.44E-02	-0.51	1.06	959636	838668	568187	758205	555097	653358	581276	856888
RP_NEG_167_02037a0_982	RP	NEG	0.98	167.0204			2.23E-02	0.39	0.94	8.64E-01	-0.04	0.28	7.92E-02	0.37	0.97	3.41E-02	0.40	0.77	15386854	3917253	17493937	5806281	17594144	5327060	17393730	6302044
RP_NEG_297_73343a15_599	RP	NEG	15.60	297.7334			3.65E-02	-0.45	0.89	8.65E-01	0.03	0.36	6.73E-02	-0.43	0.74	4.53E-02	-0.47	0.88	2516882	125435	2463230	114308	2461267	111542	2465193	118110
HILIC_POS_284_81412a3_009	HILIC	POS	3.009	284.8141			2.15E-05	-0.58	1.35	8.65E-01	0.04	0.77	1.04E-03	-0.56	1.46	1.33E-03	-0.60	1.46	733211	124870	558424	328746	552793	347099	564055	312748
RP_POS_309_23941a10_744	RP	POS	10.74	309.2394			4.24E-04	-0.58	1.14	8.65E-01	-0.04	1.00	1.15E-03	-0.60	1.24	7.02E-03	-0.56	1.14	1486665	166446	1341651	263612	1346163	292448	1337140	234165
RP_POS_285_24237a9_854	RP	POS	9.85	285.2424			8.54E-01	-0.04	0.68	8.65E-01	-0.04	0.71	8.05E-01	-0.05	0.43	9.36E-01	-0.02	0.82	2413672	274754	2403059	306233	2408290	320246	2397828	294717
RP_POS_682_79657a0_499	RP	POS	0.50	682.7966			1.63E-04	-0.48	1.24	8.65E-01	-0.04	1.21	2.43E-03	-0.50	1.31	1.04E-02	-0.47	1.29	6058505	856545	4763239	2971416	4813975	3148975	4712503	2813809
RP_POS_752_78241a0_498	RP	POS	0.50	752.7824			9.79E-05	-0.50	1.25	8.66E-01	-0.04	1.22	1.89E-03	-0.52	1.32	7.12E-03	-0.49	1.30	1375552	185523	1096452	611839	1106892	641494	1086012	587023
RP_POS_293_12561a9_356	RP	POS	9.36	293.1256			3.43E-05	0.61	1.22	8.66E-01	0.04	0.72	1.22E-03	0.63	1.16	7.88E-04	0.59	1.17	514386	142550	682611	296898	677561	277844	687661	317563
RP_POS_126_09157a3_143	RP	POS	3.14	126.0916			1.62E-01	0.16	0.72	8.66E-01	-0.04	0.21	3.22E-01	0.14	0.86	3.23E-01	0.18	0.45	13910	26342	6578748	46562561	7370733	52074759	5786763	40832952
RP_NEG_451_29416a11_612	RP	NEG	11.61	451.2942			5.73E-02	-0.34	0.99	8.66E-01	-0.04	0.89	6.72E-02	-0.36	0.91	1.42E-01	-0.32	0.92	841841	127061	787643	167649	790494	186700	784791	148030
RP_POS_325_21362a10_704	RP	POS	10.70	325.2136			1.46E-07	0.75	1.63	8.66E-01	-0.04	0.51	3.83E-05	0.77	1.51	4.40E-05	0.73	1.57	2464004	1325131	4608881	3036177	4557261	2975213	4660501	3125307
HILIC_NEG_159_06624a0_576	HILIC	NEG	0.576	159.0662			8.96E-01	-0.03	0.84	8.66E-01	0.03	0.76	9.71E-01	-0.01	0.09	8.48E-01	-0.04	0.40	252316	55696	250794	61248	249754	62961	251835	60107
RP_POS_263_87595a0_242	RP	POS	0.24	263.8760			8.29E-02	0.27	0.79	8.67E-01	-0.04	0.14	1.64E-01	0.25	0.95	1.49E-01	0.29	0.58	835327	69145	865453	120791	867497	130081	863408	112023
RP_POS_154_95532a15_566	RP	POS	15.57	154.9553			5.04E-01	-0.13	0.60	8.67E-01	0.03	0.51	6.06E-01	-0.11	0.33	5.07E-01	-0.15	0.61	29786675	1680985	29550495	1868685	29518893	1911896	29582097	1843325
RP_NEG_551_12665a8_312	RP	NEG	8.31	551.1267			6.82E-01	-0.08	0.36	8.67E-01	-0.03	0.50	6.53E-01	-0.10	0.30	7.83E-01	-0.06	0.30	899521	51531	895071	57948	896050	60891	894093	55451
RP_NEG_297_1543a15_107	RP	NEG	15.11	297.1543			2.76E-01	0.20	0.34	8.67E-01	0.04	0.13	3.24E-01	0.22	0.39	3.62E-01	0.18	0.51	3203513	2604993	3817274	3152499	3764093	2839722	3870455	3465477
RP_POS_308_12863a8_874	RP	POS	8.87	308.1286			8.06E-01	0.05	0.44	8.67E-01	-0.03	0.20	8.93E-01	0.03	0.31	7.60E-01	0.07	0.23	2505325	399943	2525739	433351	2533045	398551	2518432	469540
RP_POS_322_24994a11_166	RP	POS	11.17	322.2499			4.20E-09	1.04	1.61	8.67E-01	-0.03	0.53	9.25E-07	1.02	1.61	4.12E-08	1.05	1.77	1072909	366008	1621361	503989	1629847	455248	1612875	552988
RP_POS_309_91843a15_439	RP	POS	15.44	309.9184			9.12E-01	0.03	1.10	8.68E-01	-0.03	0.42	9.65E-01	0.01	0.75	8.72E-01	0.04	0.72	3244998	712882	3260062	515378	3268719	528688	3251404	506937
RP_POS_152_96909a15_42	RP	POS	15.42	152.9691			8.94E-01	-0.03	0.36	8.68E-01	-0.03	0.48	8.40E-01	-0.04	0.16	9.67E-01	-0.01	0.25	5900970	2442058	5833732	2578067	5876914	2800230	5790551	2362924
RP_NEG_529_46448a15_123	RP	NEG	15.12	529.4645			1.47E-01	-0.24	0.51	8.68E-01	-0.04	0.35	2.13E-01	-0.26	0.46	2.36E-01	-0.22	0.46	16323246	2647841	15422813	3991547	15489647	3660041	15355978	4334170
RP_POS_349_2699a10_645	RP	POS	10.65	349.2699			7.56E-02	-0.34	0.98	8.68E-01	0.03	0.92	1.35E-01	-0.32	0.88	1.02E-01	-0.36	0.85	1684815	352339	1550412	405577	1543635	411930	1557189	403190
RP_POS_413_30258a11_306	RP	POS	11.31	413.3026			3.33E-02	-0.40	0.73	8.68E-01	-0.03	0.68	3.96E-02	-0.42	0.87	8.67E-02	-0.39	0.63	1100159	85715	1060639	99762	1062306	111003	1058973	88209
RP_POS_418_24918a13_07	RP	POS	13.07	418.2492			1.61E-01	-0.29	0.61	8.68E-01	-0.03	0.22	1.81E-01	-0.31	0.66	2.30E-01	-0.28	0.58	1787006	473946	1651266	454706	1658856	455036	1643675	458867
HILIC_NEG_552_76215a2_91	HILIC	NEG	2.91	552.7622			2.40E-07	-0.64	1.35	8.68E-01	0.04	0.76	1.22E-04	-0.63	1.51	2.87E-04	-0.66	1.52	266355	24453	200667	111958	198798	119491	202536	105069
HILIC_POS_371_2402a5_16	HILIC	POS	5.16	371.2402			8.32E-01	-0.05	0.58	8.68E-01	0.03	0.47	9.04E-01	-0.03	0.12	7.89E-01	-0.06	0.36	14437567	6290894	14169844	5786278	14073278	5465984	14266410	6144045
RP_POS_336_18341a10_581	RP	POS	10.58	336.1834			1.11E-02	0.49	0.80	8.69E-01	-0.03	0.35	3.38E-02	0.47	0.79	1.71E-02	0.50	1.00	521068	248614	658377	285065	663119	269571	653635	302437
RP_POS_443_33432a13_004	RP	POS	13.00	443.3343			5.22E-01	0.13	0.43	8.69E-01	0.03	0.31	5.22E-01	0.15	0.56	6.15E-01	0.11	0.40	4258277	1960646	4515913	2000107	4482752	1967553	4549074	2051582
RP_POS_609_15918a9_666	RP	POS	9.67	609.1592			2.46E-01	-0.22	0.56	8.69E-01	-0.03	0.59	2.80E-01	-0.23	0.44	3.44E-01	-0.20	0.82	2213479	122663	2182874	145613	2185286	142691	2180462	149887
RP_POS_203_08086a5_411	RP	POS	5.41	203.0809			8.67E-01	0.03	0.28	8.70E-01	-0.03	0.12	9.45E-01	0.02	0.19	8.16E-01	0.05	0.11	2025563	333760	2037259	367133	2043328	337244	2031190	398140
RP_POS_192_90997a0_498	RP	POS	0.50	192.9100			3.90E-04	-0.46	1.22	8.70E-01	-0.04	1.21	3.96E-03	-0.47	1.27	1.66E-02	-0.44	1.28	1130689	162633	901558	559618	910808	597158	892308	525323
RP_POS_316_2847a8_965	RP	POS	8.97	316.2847			3.23E-01	0.21	0.47	8.70E-01	0.03	0.23	3.54E-01	0.23	0.54	3.86E-01	0.19	0.44	1050098	1854754	1420116	1724597	1391625	1502407	1448607	1936566
RP_POS_542_80774a6_133	RP	POS	6.13	542.8077			1.26E-05	0.53	1.24	8.70E-01	-0.04	1.06	3.86E-03	0.51	1.32	8.68E-04	0.54	1.30	69462	283183	1033303	2046497	1067003	1964472	999603	2144833
HILIC_POS_178_0722a1_387	HILIC	POS	1.387	178.0722			3.55E-16	1.02	1.68	8.70E-01	-0.03	0.60	1.02E-07	1.00	1.65	3.71E-10	1.03	2.20	55380	35470	313214	261478	317519	236793	308909	286406
HILIC_POS_532_70203a3_006	HILIC	POS	3.006	532.7020			6.31E-05	-0.54	1.34	8.71E-01	0.04	0.77	2.11E-03	-0.53	1.46	2.45E-03	-0.56	1.45	1010134	177919	775363	471981	767617	496885	783110	450623
HILIC_POS_270_78946a3_016	HILIC	POS	3.016	270.7895			7.92E-05	-0.53	1.35	8.71E-01	0.04	0.77	2.69E-03	-0.51	1.45	3.13E-03	-0.54	1.48	1500877	238380	1172587	686114	1161330	722772	1183844	654565
HILIC_POS_387_21396a4_248	HILIC	POS	4.248	387.2140			4.14E-01	-0.14	0.93	8.71E-01	-0.03	0.88	4.39E-01	-0.16	0.67	5.36E-01	-0.13	0.38	1848017	364357	1781469	491715	1789532	485245	1773405	502899
RP_POS_399_30795a10_705	RP	POS	10.71	399.3080			1.28E-01	-0.31	0.70	8.71E-01	-0.03	0.55	1.61E-01	-0.33	0.60	1.82E-01	-0.30	1.07	61204383	6397368	59200357	6352272	59304483	5910906	59096231	6823876
RP_POS_294_92041a15_445	RP	POS	15.45	294.9204			1.67E-01	-0.34	0.69	8.71E-01	-0.03	0.48	1.77E-01	-0.36	0.65	2.09E-01	-0.33	0.64	18658753	2199752	18071425	1514864	18096201	1487184	18046649	1556757
RP_POS_313_27353a10_173	RP	POS	10.17	313.2735			7.31E-01	-0.07	0.69	8.71E-01	-0.03	0.70	6.93E-01	-0.08	0.48	8.24E-01	-0.05	0.81	27990889	4075079	27698929	4392977	27770764	4786957	27627094	4008097
HILIC_NEG_134_89476a0_71	HILIC	NEG	0.71	134.8948			1.78E-01	0.28	0.75	8.71E-01	-0.03	0.57	2.74E-01	0.26	0.88	1.76E-01	0.30	0.55	16109788	4492462	17346618	4360370	17417900	3756053	17275336	4929033
HILIC_POS_682_32935a1_245	HILIC	POS	1.245	682.3294			8.55E-01	0.04	0.57	8.71E-01	0.03	0.69	8.11E-01	0.05	0.77	9.31E-01	0.02	0.29	476425	291912	487468	310223	482402	321355	492534	301861
HILIC_POS_546_729a2_992	HILIC	POS	2.992	546.7290			1.85E-05	-0.58	1.35	8.71E-01	0.04	0.77	9.60E-04	-0.56	1.47	1.43E-03	-0.59	1.47	856215	139321	651542	388532	645202	412543	657881	367043
HILIC_NEG_299_68469a1_365	HILIC	NEG	1.365	299.6847			1.12E-02	-0.33	0.94	8.72E-01	0.04	0.40	1.05E-01	-0.31	0.67	2.22E-02	-0.35	1.12	364008	39805	327809	121805	325824	104074	329794	138333
HILIC_NEG_296_68744a1_363	HILIC	NEG	1.363	296.6874			3.44E-05	0.58	0.88	8.72E-01	0.04	0.59	3.53E-03	0.59	0.92	2.86E-04	0.56	1.16	105233	41429	159242	102026	157583	82425	160901	119295
HILIC_POS_186_82828a3_023	HILIC	POS	3.023	186.8283			5.51E-05	-0.55	1.35	8.72E-01	0.04	0.77	1.97E-03	-0.53	1.45	2.34E-03	-0.56	1.46	1124991	182516	879249	492502	871244	518876	887254	469791
RP_POS_341_0549a8_805	RP	POS	8.81	341.0549			4.50E-01	0.11	0.74	8.72E-01	0.04	1.00	3.20E-01	0.12	1.02	6.94E-01	0.09	0.47	26081454	8338395	27936425	19555561	27618348	25406691	28254503	11266678
RP_POS_139_05435a15_491	RP	POS	15.49	139.0544			2.73E-03	-0.49	0.83	8.72E-01	0.03	0.22	1.69E-02	-0.47	0.82	8.73E-03	-0.51	1.01	17223043	2021932	15742022	3195435	15690125	3140803	15793919	3280223
HILIC_NEG_548_76624a2_909	HILIC	NEG	2.909	548.7662			4.73E-07	-0.62	1.35	8.72E-01	0.04	0.77	1.98E-04	-0.60	1.50	4.17E-04	-0.64	1.53	3455761	286785	2646830	1430835	2623650	1523212	2670010	1347253
RP_POS_309_20303a9_912	RP	POS	9.91	309.2030			8.00E-01	0.05	0.48	8.72E-01	0.03	0.55	7.61E-01	0.06	0.26	8.92E-01	0.03	0.46	12339784	2495820	12478027	3170957	12426695	3275419	12529360	3095383

Supplementary table 1: Metabolomics results (in asceding order according to p-value from progressive ALD vs non-progressive ALD comparison, with molecular features with ID_level of 1-2 first)

							all_ALD_vs_control			Prog_ALD_vs_non-prog_ALD			Prog_ALD_vs_control_ALD			Non-prog_ALD_vs_control			Healthy_control		all_ALD		Non-prog_ALD		Progressive_ALD	
							t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA								
Feature_ID	RP_HILIC	POS_NEG	Average.Rt	Average.Mz	Metabolite.name	curated_MSMS	ID_level	p	d	VIP	p	d	VIP	p	d	VIP	p	d	VIP	Mean	SD	Mean	SD	Mean	SD	Mean	SD
RP_POS_397_14792a6_593	RP	POS	6.59	397.1479				1.64E-01	-0.27	0.56	8.72E-01	-0.03	0.24	1.82E-01	-0.29	0.61	2.59E-01	-0.25	0.43	16703217	1774747	16179772	1987987	16211950	2102091	16147594	1887840
HILIC_NEG_404_63226a2_947	HILIC	NEG	2.947	404.6323				1.22E-05	-0.61	1.30	8.72E-01	0.03	0.74	4.81E-04	-0.59	1.44	9.71E-04	-0.63	1.41	183572	33211	138343	79868	137050	85919	139636	74178
RP_NEG_297_15411a11_61	RP	NEG	11.61	297.1541				6.73E-02	-0.34	0.70	8.72E-01	0.03	0.72	1.17E-01	-0.32	0.88	1.05E-01	-0.36	0.65	2173768	288031	2058541	351758	2052853	376490	2064229	328911
HILIC_NEG_87_00832a1_688	HILIC	NEG	1.688	87.0083				3.12E-02	-0.45	1.01	8.73E-01	0.03	0.60	5.35E-02	-0.43	0.75	4.87E-02	-0.46	1.06	4954468	2532178	3819032	2497732	3778679	2671628	3859384	2337462
RP_POS_511_51904a10_731	RP	POS	10.73	511.5190				1.81E-05	0.58	1.05	8.73E-01	0.04	0.87	3.33E-03	0.60	1.08	1.68E-04	0.56	1.19	2537599	1552062	4806762	4291638	4737463	3408712	4876060	5057971
RP_POS_267_15607a9_21	RP	POS	9.21	267.1561				2.82E-01	0.17	0.45	8.73E-01	0.03	0.36	3.20E-01	0.19	0.51	4.29E-01	0.16	0.66	471714	157750	512561	253718	508468	260847	516653	248965
HILIC_POS_338_68753a3_023	HILIC	POS	3.023	338.6875				4.27E-04	-0.50	1.31	8.73E-01	-0.04	0.76	2.90E-03	-0.52	1.40	1.04E-02	-0.49	1.40	476068	102713	369905	229571	373604	243548	366205	217112
RP_POS_310_23422a9_36	RP	POS	9.36	310.2342				7.60E-03	-0.58	0.94	8.73E-01	0.03	0.33	1.60E-02	-0.57	1.00	1.19E-02	-0.60	0.91	3307219	291938	3146020	260999	3141829	264926	3150212	259632
RP_POS_266_87213a0_249	RP	POS	0.25	266.8721				5.88E-01	0.12	0.50	8.73E-01	-0.03	0.14	6.67E-01	0.10	0.29	5.80E-01	0.13	0.40	760358	88938	770004	80860	771302	83563	768705	78890
HILIC_POS_628_69232a2_992	HILIC	POS	2.992	628.6923				5.82E-06	-0.60	1.35	8.74E-01	0.04	0.76	5.27E-04	-0.58	1.47	8.40E-04	-0.62	1.47	1759035	265348	1323786	792090	1311095	839900	1336478	749572
HILIC_NEG_157_90071a1_414	HILIC	NEG	1.414	157.9007				2.82E-01	0.21	0.58	8.74E-01	0.03	0.66	3.46E-01	0.23	0.40	3.33E-01	0.19	0.62	1085263	134684	1115808	149770	1113416	115312	1118200	178917
RP_POS_988_73529a0_495	RP	POS	0.50	988.7353				4.72E-01	-0.17	0.61	8.74E-01	-0.03	0.33	4.47E-01	-0.18	0.46	5.62E-01	-0.15	0.43	864991	104794	850230	84066	851569	96711	848891	70156
HILIC_NEG_244_8483a5_465	HILIC	NEG	5.465	244.8483				9.05E-01	-0.02	0.09	8.75E-01	-0.03	0.30	8.61E-01	-0.04	0.26	9.70E-01	-0.01	0.18	1317239	449316	1306258	450937	1313433	442826	1299083	463291
RP_POS_271_20554a8_691	RP	POS	8.69	271.2055				4.17E-01	0.15	0.53	8.75E-01	0.03	0.20	4.63E-01	0.16	0.38	5.10E-01	0.13	0.45	127226	213263	165495	278203	161069	244430	169922	310784
RP_NEG_435_14615a8_933	RP	NEG	8.93	435.1462				1.54E-01	0.25	0.88	8.75E-01	-0.03	0.65	2.79E-01	0.24	0.56	1.65E-01	0.27	0.69	7869065	5533504	9626965	7289639	9742674	6448862	9511255	8108451
HILIC_NEG_362_7836a2_93	HILIC	NEG	2.93	362.7836				2.15E-06	-0.60	1.34	8.75E-01	0.03	0.76	3.48E-04	-0.58	1.48	7.75E-04	-0.62	1.49	753652	79568	585235	308533	580346	330528	590123	288150
HILIC_NEG_336_69138a2_947	HILIC	NEG	2.947	336.6914				1.13E-05	-0.58	1.32	8.75E-01	-0.03	0.79	2.80E-04	-0.59	1.45	2.90E-03	-0.56	1.46	527515	70797	411578	220755	415065	240583	408091	201383
RP_POS_608_86865a0_489	RP	POS	0.49	608.8687				1.69E-07	0.63	1.35	8.76E-01	-0.03	1.20	2.47E-04	0.61	1.43	2.02E-04	0.65	1.43	790724	221363	2006653	2134260	2040312	2187433	1972995	2101408
RP_POS_163_12274a0_71	RP	POS	0.71	163.1227				1.35E-08	0.75	1.49	8.76E-01	-0.03	0.30	5.95E-05	0.73	1.40	9.16E-06	0.76	1.62	36621	116104	289783	363607	295516	350999	284049	379277
RP_NEG_243_75516a0_57	RP	NEG	0.57	243.7552				3.98E-04	0.49	0.86	8.76E-01	-0.03	0.85	1.76E-02	0.47	0.96	1.46E-03	0.50	1.09	1452108	434912	1942141	1105232	1959551	939020	1924732	1259218
HILIC_NEG_98_93902a7_354	HILIC	NEG	7.354	98.9390				6.14E-01	0.08	0.46	8.76E-01	0.03	0.50	6.30E-01	0.10	0.32	7.19E-01	0.07	0.58	2246957	152451	2264842	227638	2261259	205590	2268424	249805
RP_POS_193_09488a2_877	RP	POS	2.88	193.0949		193.0942(100), 134.0682(8)	4	2.30E-01	0.14	0.70	8.76E-01	-0.04	0.27	3.79E-01	0.12	0.81	3.99E-01	0.16	0.52	925915	1108964	2174456	10153545	2334214	11613176	2014697	8565920
HILIC_NEG_155_86562a7_678	HILIC	NEG	7.678	155.8656				2.08E-01	-0.25	0.50	8.76E-01	-0.03	0.24	2.49E-01	-0.27	0.50	2.77E-01	-0.23	0.63	1014542	265048	944699	283766	949159	260712	940239	307698
RP_POS_826_53394a12_487	RP	POS	12.49	826.5339				6.72E-01	-0.08	0.92	8.76E-01	-0.03	0.21	6.70E-01	-0.10	0.67	7.54E-01	-0.07	0.49	2511616	1130042	2410632	1280047	2430743	1138677	2390520	1418826
RP_POS_318_21945a10_59	RP	POS	10.59	318.2195				5.96E-04	0.54	0.94	8.76E-01	0.03	0.33	7.43E-03	0.56	0.90	2.34E-03	0.53	1.06	3560260	1300476	4696338	2215277	4661541	1867860	4731135	2534499
RP_POS_180_02762a15_527	RP	POS	15.53	180.0276				5.72E-01	-0.12	0.50	8.77E-01	0.03	0.13	6.68E-01	-0.10	0.41	5.53E-01	-0.13	0.33	1895248	545597	1832790	527874	1824534	487871	1841047	569940
RP_POS_290_8786a15_426	RP	POS	15.43	290.8786				6.75E-01	-0.07	0.49	8.77E-01	0.03	0.35	7.84E-01	-0.05	0.56	6.79E-01	-0.09	0.51	1866349	209266	1845430	332875	1840231	359937	1850629	307022
RP_POS_349_01547a0_623	RP	POS	0.62	349.0155				3.86E-03	-0.44	1.04	8.77E-01	0.03	0.98	2.22E-02	-0.42	1.02	1.72E-02	-0.46	1.06	1056836	344981	794007	646168	783918	665273	804096	633081
HILIC_NEG_179_05746a0_562	HILIC	NEG	0.562	179.0575				6.41E-01	-0.09	0.43	8.77E-01	-0.03	0.40	6.35E-01	-0.11	0.29	7.32E-01	-0.07	0.19	2320705	2073626	2115802	2372806	2152835	2277297	2078770	2487255
RP_NEG_242_17572a7_71	RP	NEG	7.71	242.1757				8.02E-01	0.06	0.37	8.77E-01	-0.03	0.18	8.64E-01	0.04	0.39	7.65E-01	0.07	0.35	4058594	894434	4102071	680605	4112662	604295	4091479	755312
HILIC_POS_189_07315a5_921	HILIC	POS	5.921	189.0732				3.36E-01	-0.20	0.97	8.78E-01	0.03	0.76	4.26E-01	-0.18	0.73	3.54E-01	-0.21	0.88	3955090	1051497	3746783	1070487	3730186	1084742	3763379	1066792
RP_POS_370_29483a8_585	RP	POS	8.59	370.2948				5.96E-05	0.67	1.28	8.78E-01	0.03	0.83	5.37E-04	0.68	1.28	8.83E-04	0.65	1.30	1302152	613124	1910672	942585	1896079	943404	1925265	951115
HILIC_NEG_340_72769a2_938	HILIC	NEG	2.938	340.7277				6.03E-06	-0.59	1.32	8.78E-01	0.03	0.76	4.69E-04	-0.58	1.45	1.04E-03	-0.61	1.47	260756	35984	200142	111588	198415	119957	201868	103741
HILIC_POS_58_06611a1_509	HILIC	POS	1.509	58.0661				9.65E-01	-0.01	0.35	8.78E-01	0.03	0.94	9.68E-01	0.01	0.10	8.99E-01	-0.02	0.05	2588134	1178766	2576559	1609193	2551728	1371648	2601390	1830075
HILIC_NEG_276_8248a2_931	HILIC	NEG	2.931	276.8248				1.30E-06	-0.61	1.34	8.78E-01	0.03	0.76	2.83E-04	-0.59	1.47	6.11E-04	-0.63	1.50	1337358	129576	1045145	526904	1037016	562405	1053274	494458
HILIC_POS_102_05539a5_784	HILIC	POS	5.784	102.0554				3.25E-01	-0.18	0.96	8.78E-01	0.03	0.64	4.77E-01	-0.16	0.67	3.04E-01	-0.20	0.75	746947	240309	695387	300191	690755	238117	700019	354012
HILIC_NEG_268_79288a2_937	HILIC	NEG	2.937	268.7929				7.06E-06	-0.56	1.33	8.79E-01	0.03	0.76	7.02E-04	-0.55	1.45	1.58E-03	-0.58	1.49	715529	70234	565748	294250	561217	316557	570279	273282
RP_POS_162_99109a0_45	RP	POS	0.45	162.9911				6.02E-07	-0.65	1.32	8.79E-01	0.03	1.16	2.02E-04	-0.63	1.40	2.45E-04	-0.66	1.40	2917202	405777	2116007	1346786	2095385	1402187	2136629	1302954
RP_POS_240_23224a10_244	RP	POS	10.24	240.2322				3.64E-04	0.61	0.97	8.79E-01	-0.03	0.54	7.02E-03	0.59	0.95	5.15E-04	0.62	1.24	491459	218225	678477	320192	683373	255069	673582	376868
RP_POS_347_19598a10_704	RP	POS	10.70	347.1960				2.06E-07	0.69	1.56	8.79E-01	0.03	0.53	1.14E-04	0.71	1.43	7.85E-05	0.68	1.55	280466	167089	592153	484987	584740	466451	599565	507481
RP_POS_802_5946a12_043	RP	POS	12.04	802.5946				6.37E-01	0.07	0.36	8.80E-01	-0.03	0.29	7.67E-01	0.06	0.24	6.38E-01	0.09	0.39	1629580	2256588	1897601	4013989	1958915	4046494	1836287	4021349
RP_POS_585_53223a10_848	RP	POS	10.85	585.5322				3.17E-05	0.79	1.26	8.80E-01	0.03	0.35	3.44E-04	0.80	1.24	1.04E-04	0.77	1.49	35180138	12954156	47576552	15399839	47341399	13118468	47811706	17519787
RP_POS_199_16925a9_912	RP	POS	9.91	199.1693				6.74E-01	0.08	0.45	8.80E-01	0.03	0.53	6.57E-01	0.09	0.26	7.79E-01	0.06	0.37	2520024	511120	2567321	663341	2557201	683493	2577441	649347
RP_POS_191_1799a8_812	RP	POS	8.81	191.1799				9.29E-01	0.02	0.37	8.80E-01	0.03	0.52	8.78E-01	0.03	0.29	9.96E-01	0.00	0.34	585771	256973	590671	301360	586074	313221	595267	292127
RP_POS_808_07715a13_68	RP	POS	13.68	808.0772				7.21E-03	0.56	1.16	8.80E-01	-0.03	0.27	1.49E-02	0.54	0.97	1.40E-02	0.57	1.07	582053	458434	841365	449203	848200	477618	834529	423639
HILIC_NEG_510_64792a2_934	HILIC	NEG	2.934	510.6479				1.11E-05	-0.57	1.32	8.80E-01	-0.03	0.77	3.01E-04	-0.59	1.47	2.94E-03	-0.56	1.47	137270	19156	105015	61870	105954	67319	104077	56572
RP_NEG_485_20923a11_258	RP	NEG	11.26	485.2092				3.41E-04	0.72	1.51	8.81E-01	0.03	1.04	1.16E-03	0.73	1.42	1.15E-03	0.70	1.42	932249	218674	1104381	231520	1100875	219907	1107887	244771
RP_POS_1027_66565a10_932	RP	POS	10.93	1027.6657				1.84E-01	0.23	1.01	8.81E-01	-0.03	0.84	3.08E-01	0.21	0.74	2.15E-01	0.25	0.88	291374	163882	340972	230235	344444	219143	337501	243001
HILIC_NEG_410_62479a2_947	HILIC	NEG	2.947	410.6248				2.41E-05	-0.61	1.31	8.81E-01	0.03	0.75	7.47E-04	-0.59	1.43	1.10E-03	-0.62	1.43	227035	44178	171821	98173	170341	104116	173301	92888
RP_POS_898_55011a13_21	RP	POS	13.21	898.5501				7.17E-04	0.65	1.07	8.81E-01	0.03	0.29	3.77E-03	0.67	1.12	1.48E-03	0.64	1.25	1213465	366798	1488725	416809	1482439	341856	1495011	483797
RP_POS_859_60193a11_839	RP	POS	11.84	859.6019				2.89E-01	0.23	0.49	8.81E-01	-0.03	0.20	3.76E-01	0.22	0.38	2.88E-01	0.25	0.62	26671717	5927337	27928472	5226997	28007031	4768699	27849913	5696270
HILIC_POS_553_40704a5_647	HILIC	POS	5.647	553.4070				3.40E-01	-0.16	1.02	8.82E-01	-0.03	0.77	3.80E-01	-0.18	0.66	4.61E-01	-0.15	0.89	586259	98246	564946	138341	567024	136551	562868	141463
HILIC_NEG_197_73663a3_033	HILIC	NEG	3.033	197.7366				7.14E-05	0.53	1.16	8.82E-01	-0.03	0.82	2.18E-03	0.52	1.39	3.11E-03	0.55	1.18	749307	51694	819489	144493	821656	153494	817322	136429
RP_POS_928_73901a0_499	RP	POS	0.50	928.7390				1.93E-05	-0.57	1.26	8.82E-01	-0.03	1.18	4.90E-04	-0.59	1.34	2.69E-03	-0.56	1.31	868957	124075	686267	348355	691487	370884	681047	327976
HILIC_NEG_99_92547a4_289	HILIC	NEG	4.289	99.9255				9.15E-01	0.02	0.84	8.82E-01	0.03	0.81	8.70E-01	0.04	0.07	9.82E-01	0.00	0.59	2609224	446259	2619246	507862	2611650	506392	2626841	514355
RP_POS_307_04355a0_71	RP	POS	0.71	307.0436				1.92E-03	0.43	1.36	8.82E-01	-0.03	0.91	2.30E-02	0.41	1.40	1.25E-02	0.44	1.32	292201	160613	449026	404987	455082	401973	442970	411969
RP_POS_532_38806a11_442	RP	POS	11.44	532.3881				3.61E-01	-0.18	0.61	8.82E-01	-0.03	0.23	3.97E-01	-0.19	0.61	4.44E-01	-0.16	0.51	2425581	293269	2369217	325164	2374078	298624	2364356	352699
RP_POS_304_89594a0_47	RP	POS	0.47	304.8959				1.63E-06	-0.61	1.31	8.82E-01	0.03	1.19	4.42E-04	-0.59	1.37	4.72E-04	-0.63	1.40	2014819	223300	1545570	845394	1532943	876557	1558197	821760
RP_NEG_285_24496a10_747	RP	NEG	10.75	285.2450				2.33E-02	-0.39	0.99	8.82E-01	-0.03	0.93	3.50E-02	-0.41	0.98	7.64E-02	-0.38	0.97	2453381	338072	2276179	477337	2283306	519712	2269053	436058
RP_POS_122_92949a15_568	RP	POS	15.57	122.9295				1.05E-01	0.27	0.54	8.82E-01	-0.03	0.09	1.38E-01	0.26	0.56	1.98E-01	0.29	0.51	5560573	179515	5628826	268750	5632838	323586	5624813	202944
HILIC_NEG_315_04196a7_355	HILIC	NEG	7.355	315.0420				2.11E-01	0.18	0.35	8.82E-01	-0.03	0.42	3.52E-01	0.16	0.31	3.06E-01	0.19	0.45	1989682	125361	2034924	282945	2039146	300644	2030702	267071
RP_POS_852_76514a0_497	RP	POS	0.50	852.7651				5.52E-04	-0.49	1.21	8.82E-01	-0.03	1.14	2.88E-03	-0.51	1.25	1.40E-02	-0.47	1.26	1325478	156079	1165731	355285	1171029	386720	1160434	324686
HILIC_POS_345_19946a4_846	HILIC	POS	4.846	345.1995				7.28E-05	0.57	0.94	8.82E-01	0.03	0.42	3.82E-03	0.59	0.92	5.02E-04	0.56	1.15	223982	133698	377332	287721	373043	237467	381621	332909
RP_POS_268_14008a0_71	RP	POS	0.71	268.1401				1.87E-12	0.86	1.65	8.83E-01	-0.03	0.66	2.04E-06	0.85	1.64	2.43E-07	0.88	1.76	238524	154152	2127445	2339146	2162267	2267867	2092622	2430880
RP_POS_222_18231a9_477	RP	POS	9.48	222.1823				1.12E-01	0.31	0.87	8.83E-01	-0.03	0.54	2.16E-01	0.29	0.78	1.05E-01	0.32	0.79	1704535	228693	1781615	253578	1785380	196686	1777851	301996
RP_POS_181_98721a0_257	RP	POS	0.26	181.9872				7.57E-01	-0.06	0.27	8.83E-01	-0.03	0.58	7.25E-01	-0.08	0.38	8.39E-01	-0.05	0.55	4006331	849580	3951760	904032	3965123	962523	3938397	851124
RP_POS_478_38901a12_889	RP	POS	12.89	478.3890				8.76E-01	-0.03	0.36	8.83E-01	-0.03	0.24	8.37E-01	-0.05	0.24	9.41E-01	-0.02	0.41	7965849	2636139	7882076	2653923	7921296	2725839	7842857	2607109
HILIC_POS_271_20557a0_507	HILIC	POS	0.507	271.2056				1.20E-02	0.40	0.77	8.83E-01	0.03	0.44	4.89E-02	0.41	0.70	2.78E-02	0.38	0.77	394798	317012	594398	540189	586414	456491	602382	617292
HILIC_NEG_456_77396a2_923	HILIC	NEG	2.923	456.7740				1.26E-06	-0.60	1.35	8.83E-01	0.03	0.77	2.90E-04	-0.59	1.50	7.14E-04	-0.62	1.52	828378	72599	642352	341240	637312	365645	647393	318618
RP_POS_540_88171a0_496	RP	POS	0.50	540.8817				3.18E-07	0.62	1.34	8.84E-01	0.03	1.22	1.36E-04	0.64	1.45	5.21E-04	0.61	1.41	106570	62729	326356	388891	320631	401831	332081	379505
RP_NEG_656_31952a10_301	RP	NEG	10.30	656.3195				2.60E-03	0.66	1.17	8.84E-01	0.03	0.28	5.28E-03	0.68	1.10	5.18E-03	0.65	1.12	2324921	666260	2743636	589250	2734971	548121	2752301	633188
RP_POS_153_00705a0_451	RP	POS	0.45	153.0071				3.00E-07	-0.66	1.34	8.85E-01	-0.03	1.17	1.54E-04	-0.64	1.42	1.91E-04	-0.67	1.42	834149	105018	605696	379436	600146	394518	611245	367660
RP_POS_677_36371a6_603	RP	POS	6.60	677.3637				7.42E-07	0.59	1.29	8.85E-01	-0.03	1.11	8.40E-04	0.57	1.39	2.97E-04	0.61	1.37	29829	76222	1083514	1989456	1112491	1963578	1054536	2034524
RP_POS_486_13669a8_805	RP	POS	8.81	486.1367				2.46E-04	0.44	0.82	8.85E-01	-0.03	0.33	1.13E-02	0.42	0.79	8.09E-03	0.45	0.92	579989	619157	2823211	5808171	2907774	5920148	2738648	5752862
RP_POS_628_49567a10_873	RP	POS	10.87	628.4957				3.25E-03	-0.52	0.95	8.85E-01	-0.03	0.79	1.25E-02	-0.54	0.94	9.46E-03	-0.51	0.92	3736473	397798	3467753	531530	3475491	482388	3460014	581372
HILIC_NEG_294_68777a1_363	HILIC	NEG	1.363	294.6878				1.36E-05	0.62	0.95	8.85E-01	-0.03	0.61	3.29E-03	0.61	0.93	3.87E-05	0.64	1.33	86570	39842	138162	89059	139458	69830	136866	105572
RP_POS_304_26126a11_161	RP	POS	11.16	304.2613				6.09E-07	0.84	1.30	8.86E-01	0.03	0.58	9.07E-05	0.85	1.33	2.37E-06	0.82	1.62	15796929	6038619	23431486	9187707	23298375	7097829	23564597	10960626
RP_NEG_238_07845a8_301	RP	NEG	8.30	238.0785				1.91E-01	-0.46	0.85	8.86E-01	0.01	0.20	1.97E-01	-0.45	0.68	1.89E-01	-0.46	0.63	14111335	39851183	4656769	6736757	4559363	7144932	4754175	6373741
RP_POS_359_15128a10_703	RP	POS	10.70	359.1513				2.42E-07	0.73	1.58	8.86E-01	-0.03	0.54	5.67E-05	0.71	1.49	6.68E-05	0.74	1.53	585805	317582	1099188	750809	1109999	778751	1088378	729549
RP_POS_372_24884a10_851	RP	POS	10.85	372.2488				4.90E-03	0.55	0.99	8.86E-01	0.03	0.75	8.96E-03	0.56	1.03	1.58E-02	0.53	1.04	4077031	1297426	4869743	1440795	4849001	1499254	4890485	1394813
HILIC_POS_169_98592a5_325	HILIC	POS	5.325	169.9859				4.40E-03	0.39	1.28	8.86E-01	-0.03	0.64	4.14E-02	0.37	1.32	2.08E-02	0.40	1.36	619156	83696	696810	223167	700022	217900	693599	230481
RP_POS_199_13063a14_343	RP	POS	14.34	199.1306				6.17E-01	-0.11	0.78	8.87E-01	-0.03	0.38	6.09E-01	-0.12	0.50	6.89E-01	-0.10	0.67	31428861	11916218	30242796	10552355	30394120	10438315	30091472	10769017
HILIC_POS_164_02905a5_783	HILIC	POS	5.783	164.0291				1.01E-01	-0.29	1.23	8.87E-01	-0.03	0.68	1.72E-01	-0.31	1.09	1.39E-01	-0.28	1.15	540721	90385	507769	117350	509451	95129	506086	136995
HILIC_POS_94_06577a1_23	HILIC	POS	1.23	94.0658				1.90E-01	-0.25	0.44	8.87E-01	-0.03	0.87	2.82E-01	-0.27	0.39	1.99E-01	-0.24	0.55	4094590	5438926	2576048	6209460	2665055	3769159	2487041	7979009
RP_NEG_610_39313a11_163	RP	NEG	11.16	610.3931				1.48E-02	0.46	1.22	8.87E-01	0.03	0.93	2.75E-02	0.47	1.12	3.76E-02	0.44	1.19	4189734	356795	4380807	426928	4374701	427307	4386914	430798
RP_NEG_311_16949a11_158	RP	NEG	11.16	311.1695				4.76E-01	-0.15	0.37	8.87E-01	0.03	0.28	5.85E-01	-0.13	0.27	4.55E-01	-0.16	0.46	2117718	871313	1990751	867817	1978339	727294	2003163	996148
RP_POS_574_87494a0_492	RP	POS	0.49	574.8749				3.97E-07	0.61	1.33	8.88E-01	-0.03	1.21	3.53E-04	0.60	1.41	3.04E-04	0.63	1.42	521896	164384	1206675	1234894	1224254	1265553	1189096	1216056
RP_POS_553_45868a10_982	RP	POS	10.98	553.4587				2.83E-02	0.43	1.23	8.88E-01	-0.03	1.23	6.59E-02	0.41	1.09	3.85E-02	0.44	1.06	5929858	1597235	6678174	1757767	6703190	1650673	6653159	1875246

Supplementary table 1: Metabolomics results (in asceding order according to p-value from progressive ALD vs non-progressive ALD comparison, with molecular features with ID_level of 1-2 first)

							all_ALD_vs_control			Prog_ALD_vs_non-prog_ALD			Prog_ALD_vs_control_ALD			Non-prog_ALD_vs_control			Healthy_control		all_ALD		Non-prog_ALD		Progressive_ALD	
							t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA								
Feature_ID	RP_HILIC	POS_NEG	Average.Rt	Average.Mz	Metabolite.name	curated_MSMS	ID_level	p	d	VIP	p	d	VIP	p	d	VIP	p	d	VIP	Mean	SD	Mean	SD	Mean	SD	Mean	SD
HILIC_POS_136_11208a0_636	HILIC	POS	0.636	136.1121			1.14E-01	-0.33	0.85	8.88E-01	-0.03	0.73	1.20E-01	-0.34	0.84	1.89E-01	-0.31	0.49	2166434	172222	2110365	169186	2112769	188224	2107960	149639
HILIC_NEG_375_60498a1_363	HILIC	NEG	1.363	375.6050			6.62E-06	0.62	0.95	8.88E-01	-0.03	0.58	2.61E-03	0.60	0.94	4.26E-05	0.64	1.30	4371337	2160130	7523515	5504907	7601480	4506281	7445550	6395895
HILIC_NEG_257_8194a3_026	HILIC	NEG	3.026	257.8194			9.82E-03	-0.45	1.14	8.88E-01	0.03	0.79	3.26E-02	-0.43	0.90	2.36E-02	-0.46	0.84	9736922	1339437	8933162	1894323	8906390	1916730	8959935	1890724
HILIC_POS_371_24091a3_93	HILIC	POS	3.93	371.2409			6.87E-01	0.07	0.79	8.89E-01	0.03	0.75	6.84E-01	0.09	0.39	7.76E-01	0.06	0.63	14466856	3297276	14756853	4184121	14697752	3980821	14815953	4417801
RP_POS_785_6521a14_567	RP	POS	14.57	785.6521			4.39E-01	-0.15	0.51	8.89E-01	0.03	0.12	5.46E-01	-0.13	0.47	4.50E-01	-0.16	0.38	1779422	1039251	1608222	1206142	1591211	1177937	1625233	1245440
HILIC_NEG_354_75201a2_935	HILIC	NEG	2.935	354.7520			1.50E-06	-0.63	1.34	8.89E-01	0.03	0.76	1.98E-04	-0.61	1.49	5.50E-04	-0.64	1.50	226369	29602	171859	94560	170526	101748	173193	87803
RP_NEG_177_95628a15_476	RP	NEG	15.48	177.9563			1.46E-01	-0.28	0.59	8.89E-01	0.03	0.19	2.06E-01	-0.27	0.62	1.93E-01	-0.29	0.61	1772005	617203	1581613	693778	1571832	753155	1591393	636430
RP_POS_273_08359a0_709	RP	POS	0.71	273.0836			1.00E-02	0.32	0.81	8.89E-01	0.03	0.62	7.88E-02	0.34	0.72	3.75E-02	0.31	1.25	200808	87589	301968	354644	296975	300421	306961	404733
HILIC_NEG_199_73282a3_033	HILIC	NEG	3.033	199.7328			2.21E-01	0.24	0.59	8.89E-01	0.03	0.82	2.38E-01	0.26	0.63	3.18E-01	0.23	0.51	314406	65830	331269	70966	330270	75355	332267	67042
RP_POS_663_45386a14_26	RP	POS	14.26	663.4539			8.81E-01	0.03	0.42	8.89E-01	0.03	0.33	8.34E-01	0.04	0.37	9.53E-01	0.01	0.57	2008425	1081972	2043055	1289300	2024912	1427791	2061198	1148588
RP_NEG_205_83942a3_116	RP	NEG	3.12	205.8394			4.08E-01	0.16	0.65	8.89E-01	-0.03	0.29	4.95E-01	0.15	0.40	4.34E-01	0.18	0.49	2165679	1688105	2457067	1821980	2482664	1914860	2431470	1743255
RP_POS_280_65439a10_615	RP	POS	10.62	280.6544			1.38E-02	-0.49	0.79	8.89E-01	0.03	0.62	2.97E-02	-0.48	0.80	2.53E-02	-0.50	0.81	815672	173282	724650	185398	722046	192531	727255	179902
RP_NEG_698_86639a0_49	RP	NEG	0.49	698.8664			3.86E-07	0.61	1.33	8.89E-01	-0.03	1.20	3.07E-04	0.60	1.41	3.50E-04	0.63	1.41	850228	231009	1898570	1894775	1925176	1962821	1871963	1843774
RP_POS_258_89948a0_498	RP	POS	0.50	258.8995			2.64E-06	-0.58	1.31	8.90E-01	0.03	1.20	4.73E-04	-0.56	1.39	1.06E-03	-0.59	1.38	48786385	4316532	37482694	21603062	37180323	23091127	37785065	20236653
RP_NEG_196_94128a15_779	RP	NEG	15.78	196.9413			8.00E-01	0.05	0.36	8.90E-01	0.03	0.75	7.80E-01	0.07	0.23	8.66E-01	0.04	0.18	909451	357613	928118	371369	922920	340350	933316	403425
RP_NEG_233_01889a8_812	RP	NEG	8.81	233.0189			1.77E-02	0.32	0.77	8.90E-01	0.03	0.70	5.90E-03	0.34	1.09	1.63E-01	0.31	0.54	3820842	4052387	6940013	10825161	6788394	13983205	7091632	6417383
RP_POS_322_14294a9_357	RP	POS	9.36	322.1429			4.96E-06	0.66	1.29	8.90E-01	0.03	0.81	4.48E-04	0.67	1.23	2.25E-04	0.64	1.26	934265	254196	1277286	556967	1269495	522723	1285077	594469
HILIC_NEG_542_73218a2_922	HILIC	NEG	2.922	542.7322			4.98E-06	-0.60	1.32	8.90E-01	0.03	0.76	4.33E-04	-0.59	1.44	9.13E-04	-0.62	1.49	197243	27323	150940	84323	149765	90123	152116	78999
HILIC_POS_387_21368a5_784	HILIC	POS	5.784	387.2137			2.49E-01	-0.23	1.02	8.90E-01	-0.03	0.76	2.85E-01	-0.24	0.78	3.29E-01	-0.21	0.67	1534486	352518	1449198	382982	1454535	369259	1443862	399917
RP_POS_718_91187a6_73	RP	POS	6.73	718.9119			4.49E-07	0.60	1.30	8.90E-01	-0.03	1.12	6.30E-04	0.59	1.39	2.39E-04	0.62	1.38	26317	75527	1044386	1880245	1070585	1860700	1018187	1918121
RP_POS_170_20627a10_847	RP	POS	10.85	170.2063			4.58E-07	0.92	1.49	8.90E-01	-0.03	0.14	1.47E-05	0.91	1.46	3.38E-06	0.94	1.74	3065324	739267	3967104	943951	3980256	898116	3953952	996648
RP_POS_680_47876a13_57	RP	POS	13.57	680.4788			8.18E-01	-0.05	0.43	8.90E-01	-0.03	0.25	7.83E-01	-0.06	0.44	8.88E-01	-0.03	0.36	3457934	293046	3444169	293350	3448245	317005	3440092	270810
HILIC_POS_171_1857a5_921	HILIC	POS	5.921	171.1857			8.24E-01	0.05	0.69	8.90E-01	-0.03	0.59	8.89E-01	0.03	0.49	7.95E-01	0.06	0.34	58608600	16086042	59336711	15859153	59556804	15998875	59116618	15877516
RP_POS_255_23184a10_283	RP	POS	10.28	255.2318			2.26E-01	-0.24	0.86	8.91E-01	0.03	0.77	3.01E-01	-0.23	0.61	2.63E-01	-0.25	0.94	1617148	163515	1575928	173220	1573526	181991	1578331	165800
RP_POS_267_05847a0_706	RP	POS	0.71	267.0585			5.53E-01	-0.08	1.07	8.91E-01	0.03	0.77	7.08E-01	-0.07	0.72	5.94E-01	-0.10	1.30	772120	121692	749559	312428	745226	320821	753892	307003
RP_POS_266_17294a7_715	RP	POS	7.72	266.1729			4.02E-01	-0.20	0.77	8.91E-01	0.03	0.21	4.88E-01	-0.19	0.56	3.78E-01	-0.21	0.53	2688094	597835	2590702	453535	2584425	345443	2596979	544219
RP_POS_166_98488a11_672	RP	POS	11.67	166.9849			1.19E-01	0.34	1.46	8.91E-01	0.03	0.61	1.29E-01	0.35	1.32	1.79E-01	0.33	1.01	11519014	4573392	12952846	4031932	12897085	4339048	13008608	3743132
RP_NEG_264_99155a6_739	RP	NEG	6.74	264.9916			3.14E-01	-0.22	0.55	8.91E-01	-0.03	0.31	3.47E-01	-0.23	0.42	3.70E-01	-0.21	0.56	12922011	803318	12760204	716628	12770114	636876	12750294	794846
HILIC_POS_188_82552a3_023	HILIC	POS	3.023	188.8255			1.94E-05	-0.58	1.34	8.91E-01	0.03	0.76	8.94E-04	-0.57	1.46	1.38E-03	-0.60	1.46	837032	137145	643164	363194	638160	384520	648167	344391
RP_NEG_231_02188a8_812	RP	NEG	8.81	231.0219			6.45E-03	0.33	0.72	8.91E-01	-0.03	0.85	3.02E-04	0.31	1.36	1.20E-01	0.34	0.51	7184529	5703142	16602470	32413009	17049278	43540565	16155662	15048555
RP_POS_437_27682a11_612	RP	POS	11.61	437.2768			5.39E-02	-0.36	1.11	8.91E-01	0.03	0.81	8.41E-02	-0.35	1.16	9.56E-02	-0.38	0.84	1594053	150277	1531342	176745	1528909	198184	1533774	154358
RP_POS_311_21909a10_825	RP	POS	10.83	311.2191			6.83E-01	0.07	0.74	8.91E-01	-0.03	0.17	7.90E-01	0.06	0.92	6.53E-01	0.09	0.27	4481297	1829362	4644467	2324628	4676446	2030248	4612489	2606546
HILIC_POS_144_98228a3_101	HILIC	POS	3.101	144.9823			4.92E-01	0.12	0.95	8.92E-01	-0.03	0.83	6.11E-01	0.10	0.57	5.13E-01	0.13	0.75	3292171	646723	3393463	917555	3406069	921434	3380857	922839
HILIC_POS_147_14917a5_888	HILIC	POS	5.888	147.1492			2.82E-01	0.23	0.45	8.92E-01	-0.03	0.57	2.98E-01	0.24	0.50	3.63E-01	0.21	0.34	136504568	55962662	148732675	53217451	148002169	54552471	149463180	52392088
RP_POS_462_30725a9_945	RP	POS	9.95	462.3073			1.27E-03	-0.61	1.11	8.92E-01	-0.03	0.65	3.44E-03	-0.62	1.14	5.42E-03	-0.59	1.01	654330	38592	626555	45874	627184	46512	625927	45690
RP_NEG_272_95886a15_304	RP	NEG	15.30	272.9589			2.10E-01	-0.24	0.53	8.92E-01	-0.03	0.13	2.12E-01	-0.25	0.52	3.27E-01	-0.23	0.47	1223351	44047	1211585	50365	1212275	57273	1210895	42941
RP_NEG_459_19745a11_166	RP	NEG	11.17	459.1975			4.46E-01	-0.15	0.58	8.92E-01	-0.03	0.14	4.13E-01	-0.16	0.38	5.80E-01	-0.13	0.47	715639	89965	701079	103217	702492	124007	699666	78378
RP_NEG_296_99893a7_376	RP	NEG	7.38	296.9989			1.95E-01	0.28	0.71	8.92E-01	-0.03	0.27	2.23E-01	0.29	0.59	2.57E-01	0.26	0.58	2717355	1052012	2993436	980782	2980022	951846	3006850	1018391
RP_NEG_152_978a15_497	RP	NEG	15.50	152.9780			8.97E-01	-0.03	0.30	8.92E-01	0.03	0.62	9.53E-01	-0.01	0.36	8.62E-01	-0.04	0.35	989134	36886	988163	35921	987672	37301	988654	34859
RP_POS_296_89929a15_46	RP	POS	15.46	296.8993			2.94E-01	0.24	0.70	8.92E-01	0.03	0.15	3.03E-01	0.26	0.52	3.58E-01	0.23	0.58	13108032	3714722	13871140	2913044	13831359	2975624	13910922	2878761
HILIC_POS_396_03836a4_799	HILIC	POS	4.799	396.0384			3.77E-02	0.43	0.78	8.92E-01	0.03	0.70	5.46E-02	0.44	0.71	6.71E-02	0.41	0.70	368530	86731	406095	86789	404911	85698	407278	88721
HILIC_POS_96_08138a0_505	HILIC	POS	0.505	96.0814			2.15E-05	-0.70	1.27	8.92E-01	-0.03	0.75	2.06E-04	-0.72	1.41	5.49E-04	-0.69	1.33	815376	187884	615338	294685	619355	305014	611321	287026
RP_NEG_896_56488a13_369	RP	NEG	13.37	896.5649			1.80E-01	0.23	0.64	8.92E-01	-0.03	0.24	2.30E-01	0.25	0.69	2.78E-01	0.22	0.49	4673603	1395240	5095460	1905229	5069496	1877721	5121424	1951067
HILIC_POS_137_13249a5_647	HILIC	POS	5.647	137.1325			6.59E-02	-0.33	1.03	8.92E-01	-0.03	0.70	1.13E-01	-0.35	0.61	1.08E-01	-0.32	0.92	2619627	294590	2499792	373432	2504879	336605	2494705	410356
RP_POS_223_13063a8_072	RP	POS	8.07	223.1306			7.89E-01	-0.05	0.37	8.93E-01	-0.03	0.09	7.59E-01	-0.07	0.33	8.60E-01	-0.04	0.47	1258408	301024	1241909	302409	1246017	319175	1237800	287857
RP_NEG_851_11438a9_503	RP	NEG	9.50	851.1144			4.63E-01	-0.14	0.46	8.93E-01	-0.03	0.27	4.75E-01	-0.15	0.31	5.65E-01	-0.13	0.33	4016287	240688	3978811	276188	3982560	282370	3975062	272682
HILIC_NEG_373_6073a1_363	HILIC	NEG	1.363	373.6073			6.97E-06	0.62	0.95	8.93E-01	-0.03	0.59	2.62E-03	0.60	0.94	4.60E-05	0.63	1.29	3043629	1507664	5235433	3835418	5287437	3146083	5183428	4451710
HILIC_POS_421_37097a3_173	HILIC	POS	3.173	421.3710			5.97E-02	0.34	0.87	8.93E-01	0.03	0.82	7.88E-02	0.36	0.71	1.29E-01	0.33	0.86	1757451	701538	2049304	884331	2037326	946574	2061281	826890
RP_POS_327_29028a10_412	RP	POS	10.41	327.2903			1.53E-02	-0.44	0.95	8.93E-01	-0.03	0.80	2.09E-02	-0.45	0.95	5.47E-02	-0.42	0.93	1539368	226750	1415964	292064	1419918	327462	1412010	255110
RP_POS_473_91483a6_667	RP	POS	6.67	473.9148			4.31E-07	0.60	1.33	8.93E-01	0.03	1.15	7.95E-04	0.62	1.44	1.38E-04	0.59	1.41	23849	47667	995391	1792950	971156	1618979	1019625	1967905
HILIC_NEG_530_70685a2_928	HILIC	NEG	2.928	530.7069			9.57E-07	-0.64	1.35	8.94E-01	0.03	0.76	1.69E-04	-0.63	1.49	4.03E-04	-0.66	1.47	382921	50642	287765	161791	285582	172619	289947	151920
HILIC_POS_312_20139a0_779	HILIC	POS	0.779	312.2014			4.30E-01	-0.16	0.72	8.94E-01	-0.03	0.78	4.45E-01	-0.17	0.35	5.17E-01	-0.15	0.79	752347	166955	725244	170324	727540	169896	722948	172446
HILIC_NEG_379_60126a1_363	HILIC	NEG	1.363	379.6013			5.66E-06	0.63	0.96	8.94E-01	-0.03	0.59	2.45E-03	0.61	0.95	3.40E-05	0.64	1.32	635650	311373	1091759	788448	1102374	639628	1081145	920127
RP_POS_422_32602a8_861	RP	POS	8.86	422.3260			1.91E-03	0.49	0.88	8.94E-01	-0.03	0.11	1.04E-02	0.47	1.07	1.15E-02	0.50	1.04	545342	219281	719816	384736	724994	407253	714639	364903
RP_NEG_299_92615a3_96	RP	NEG	3.96	299.9262			4.09E-01	0.14	0.78	8.94E-01	-0.03	0.21	5.67E-01	0.12	0.59	4.07E-01	0.15	0.42	965037	341462	1031121	520438	1038121	449597	1024121	587368
RP_POS_533_50092a10_731	RP	POS	10.73	533.5009			2.61E-06	0.68	1.11	8.94E-01	-0.03	0.71	1.07E-03	0.67	1.13	1.34E-05	0.70	1.35	1825820	936284	3107555	1989451	3134233	1613232	3080877	2322206
RP_POS_264_8728a0_249	RP	POS	0.25	264.8728			5.29E-01	0.13	0.56	8.95E-01	0.03	0.11	5.21E-01	0.14	0.36	6.22E-01	0.12	0.29	8095653	866653	8207304	869299	8195742	934819	8218866	807852
RP_POS_694_47803a10_463	RP	POS	10.46	694.4780			5.11E-01	-0.15	0.49	8.95E-01	0.03	0.44	5.91E-01	-0.14	0.36	4.96E-01	-0.16	0.86	1884835	312139	1844543	255484	1841146	225083	1847941	284939
RP_POS_214_91756a0_453	RP	POS	0.45	214.9176			9.94E-04	-0.51	1.16	8.95E-01	0.03	1.06	7.58E-03	-0.49	1.15	7.10E-03	-0.52	1.22	1926212	593684	1416145	1074572	1401893	1116552	1430397	1042053
HILIC_NEG_377_60303a1_363	HILIC	NEG	1.363	377.6030			5.83E-06	0.62	0.95	8.95E-01	-0.03	0.59	2.47E-03	0.61	0.95	3.94E-05	0.64	1.30	2716405	1333104	4685304	3426137	4730730	2801409	4639878	3983000
RP_POS_638_09833a0_624	RP	POS	0.62	638.0983			6.36E-03	-0.43	1.06	8.96E-01	-0.03	1.00	1.74E-02	-0.44	1.05	3.57E-02	-0.41	1.10	1761423	478912	1429429	834938	1440473	877006	1418384	799426
RP_NEG_266_93259a0_498	RP	NEG	0.50	266.9326			3.25E-06	-0.58	1.30	8.96E-01	0.03	1.19	3.91E-04	-0.57	1.39	1.16E-03	-0.60	1.36	1137467	125829	861246	521282	854367	563253	868124	481316
RP_POS_140_94911a0_25	RP	POS	0.25	140.9491			1.49E-01	0.26	0.57	8.96E-01	0.03	0.11	1.86E-01	0.28	0.52	2.38E-01	0.25	0.41	665804	170671	719578	211697	716788	215484	722367	209992
RP_POS_322_91418a0_254	RP	POS	0.25	322.9142			7.14E-01	0.08	0.47	8.96E-01	-0.03	0.17	7.72E-01	0.07	0.21	7.02E-01	0.09	0.66	764195	158579	775670	134042	777434	141024	773906	128091
RP_POS_420_26498a13_99	RP	POS	13.99	420.2650			2.89E-02	-0.50	0.83	8.96E-01	-0.02	0.56	3.26E-02	-0.51	0.91	5.36E-02	-0.49	0.74	1463681	603288	1198525	493356	1205016	542804	1192034	443897
RP_POS_381_79999a0_254	RP	POS	0.25	381.8000			2.74E-01	0.22	0.54	8.96E-01	-0.03	0.14	3.76E-01	0.21	0.37	2.82E-01	0.23	0.51	358912	70435	374834	72757	375790	65738	373877	79823
HILIC_POS_126_09152a0_617	HILIC	POS	0.617	126.0915			1.33E-01	0.18	0.53	8.97E-01	-0.03	0.33	2.25E-01	0.16	0.66	3.21E-01	0.19	0.45	420748	218649	693818	1763446	716920	2070702	670715	1412110
RP_POS_727_57397a12_445	RP	POS	12.45	727.5740			1.43E-05	-1.04	1.69	8.97E-01	-0.02	0.48	2.28E-05	-1.05	1.68	4.13E-05	-1.03	1.52	2512257	1156107	1425150	865513	1436479	907213	1413821	830793
RP_POS_250_93854a0_454	RP	POS	0.45	250.9385			2.04E-04	-0.54	1.20	8.97E-01	0.03	1.09	3.21E-03	-0.53	1.22	3.18E-03	-0.56	1.27	3161689	815617	2305855	1697262	2283695	1762542	2328015	1647006
HILIC_NEG_186_11357a0_546	HILIC	NEG	0.546	186.1136			5.27E-01	-0.13	0.51	8.97E-01	-0.03	0.50	5.49E-01	-0.15	0.45	5.87E-01	-0.12	0.39	202238	210959	175334	198656	177927	171890	172742	223995
RP_POS_154_08638a3_143	RP	POS	3.14	154.0864			1.60E-01	0.16	0.74	8.97E-01	-0.03	0.20	3.22E-01	0.15	0.86	3.22E-01	0.18	0.45	6456	10230	3184245	22446586	3477179	24539804	2891310	20386368
RP_POS_316_22458a9_231	RP	POS	9.23	316.2246			3.60E-01	-0.18	0.92	8.97E-01	0.03	0.69	4.69E-01	-0.17	0.66	3.60E-01	-0.20	1.01	831678	690550	700350	731020	690812	650529	709889	810132
HILIC_NEG_112_98553a4_233	HILIC	NEG	4.233	112.9855			3.68E-01	0.16	0.99	8.97E-01	-0.03	0.84	4.79E-01	0.14	0.40	4.08E-01	0.17	0.71	537457571	99738422	557568216	134754689	559321637	137685153	555814794	133134387
HILIC_POS_210_11008a0_549	HILIC	POS	0.549	210.1101			5.85E-01	-0.12	0.52	8.97E-01	-0.03	0.56	6.06E-01	-0.13	0.44	6.30E-01	-0.11	0.41	264056	321488	229067	285581	232781	216464	225353	343355
RP_POS_380_25436a10_058	RP	POS	10.06	380.2544			3.77E-03	0.51	0.96	8.97E-01	-0.03	0.60	1.74E-02	0.50	0.85	9.07E-03	0.52	1.00	928834	475644	1247112	649508	1255543	625661	1238680	678773
RP_POS_260_89597a0_498	RP	POS	0.50	260.8960			5.00E-06	-0.56	1.30	8.98E-01	0.03	1.20	6.82E-04	-0.55	1.37	1.45E-03	-0.58	1.37	7325014	662763	5636894	3329565	5593679	3553813	5680109	3124877
HILIC_POS_342_18304a0_851	HILIC	POS	0.851	342.1830			8.33E-01	0.04	0.34	8.98E-01	0.03	0.44	7.83E-01	0.06	0.17	9.04E-01	0.03	0.20	2504970	1553415	2571760	1544420	2551737	1920250	2591782	1063467
RP_NEG_468_80865a15_474	RP	NEG	15.47	468.8087			2.45E-01	0.24	0.51	8.98E-01	0.03	0.35	2.67E-01	0.25	0.52	3.26E-01	0.23	0.51	3039683	109201	3065733	108794	3064327	111389	3067140	107250
RP_NEG_394_89273a0_465	RP	NEG	0.47	394.8927			8.30E-07	-0.65	1.34	8.98E-01	0.03	1.22	2.14E-04	-0.63	1.40	2.79E-04	-0.66	1.40	782688	111618	573952	351512	569416	365778	578488	340305
RP_NEG_772_79541a0_497	RP	NEG	0.50	772.7954			4.36E-06	-0.58	1.30	8.98E-01	0.03	1.21	6.03E-04	-0.57	1.38	1.01E-03	-0.60	1.37	6028069	716673	4568694	2763316	4533054	2916312	4604335	2630626
RP_POS_391_20697a8_101	RP	POS	8.10	391.2070			9.12E-03	-0.46	0.81	8.98E-01	-0.03	0.67	2.03E-02	-0.47	0.88	3.10E-02	-0.44	0.85	3348606	108464	3283703	147756	3285604	150775	3281803	146180
HILIC_POS_537_53601a10_681	HILIC	POS	10.681	537.5360			2.06E-01	-0.22	0.60	8.98E-01	-0.03	0.44	2.89E-01	-0.21	0.47	2.73E-01	-0.23	0.61	2151099	129216	2114263	176578	2111992	191328	2116533	162415
RP_NEG_275_91916a15_699	RP	NEG	15.70	275.9192			4.11E-01	-0.17	0.35	8.99E-01	-0.03	0.14	4.25E-01	-0.18	0.33	4.96E-01	-0.16	0.26	793783	263893	749559	259807	752892	263486	746226	258706
HILIC_NEG_540_73511a2_922	HILIC	NEG	2.922	540.7351			4.83E-07	-0.63	1.35	8.99E-01	0.03	0.76	1.43E-04	-0.62	1.51	4.11E-04	-0.65	1.52	714102	72588	542519	296601	538729	317595	546308	277206
RP_POS_546_35236a10_82	RP	POS	10.82	546.3524			2.81E-01	-0.24	0.85	8.99E-01	-0.02	0.95	3.08E-01	-0.26	0.59	3.32E-01	-0.23	0.87	18860671	7071908	17353663	5855086	17428444	5389623	17278881	6340682
RP_POS_201_00687a15_383	RP	POS	15.38	201.0069			6.17E-01	-0.10	0.60	8.99E-01	0.03	0.28	6.96E-01	-0.08	0.31	6.29E-01	-0.11	0.73	4886767	1746674	4701745	2004504	4676148	2156930	4727341	1861287
RP_NEG_213_91513a15_549	RP	NEG	15.55	213.9151			4.79E-01	-0.17	0.38	9.00E-01	0.02	0.24	5.45E-01	-0.15	0.40	4.77E-01	-0.18	0.45	1391738	407016	1335728	313148	1331752	302372	1339705	326594
RP_POS_120_98109a0_451	RP	POS	0.45	120.9811			1.04E-06	-0.64	1.31	9.00E-01	0.03	1.16	2.35E-04	-0.63	1.39	3.30E-04	-0.65	1.40	4716701	716957	3383354	2270462	3354525	2369716	3412183	2190423

Supplementary table 1: Metabolomics results (in asceding order according to p-value from progressive ALD vs non-progressive ALD comparison, with molecular features with ID_level of 1-2 first)

								all_ALD_vs_control			Prog_ALD_vs_non-prog_ALD			Prog_ALD_vs_control_ALD			Non-prog_ALD_vs_control			Healthy_control		all_ALD		Non-prog_ALD		Progressive_ALD	
								t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA								
Feature_ID	RP_HILIC	POS_NEG	Average.Rt	Average.Mz	Metabolite.name	curated_MSMS	ID_level	p	d	VIP	p	d	VIP	p	d	VIP	p	d	VIP	Mean	SD	Mean	SD	Mean	SD	Mean	SD
HILIC_POS_175_00172a1_384	HILIC	POS	1.384	175.0017				1.80E-12	0.87	1.48	9.00E-01	-0.03	0.61	2.67E-06	0.85	1.47	1.40E-07	0.88	1.95	228569	250422	2284638	2532816	2316774	2395557	2252502	2687087
HILIC_NEG_136_89166a4_671	HILIC	NEG	4.671	136.8917				8.74E-01	0.03	0.61	9.00E-01	-0.02	0.53	9.25E-01	0.02	0.05	8.49E-01	0.05	0.23	7265269	2667027	7349679	2438774	7380589	2670015	7318769	2210359
RP_POS_320_16986a6_254	RP	POS	6.25	320.1699				1.23E-01	-0.31	0.58	9.00E-01	0.03	0.34	1.76E-01	-0.30	0.56	1.61E-01	-0.32	0.51	15279421	1534753	14786513	1599231	14766305	1698709	14806722	1510241
RP_POS_645_49646a10_456	RP	POS	10.46	645.4965				6.28E-01	-0.11	0.33	9.01E-01	0.02	0.08	7.01E-01	-0.09	0.22	6.13E-01	-0.12	0.36	1003233	200387	983972	173702	981784	161467	986161	186759
HILIC_POS_81_9885a2_997	HILIC	POS	2.997	81.9885				7.89E-05	-0.58	1.32	9.01E-01	0.03	0.78	1.22E-03	-0.57	1.39	2.17E-03	-0.60	1.32	1459019	235571	1197298	483125	1191212	518220	1203383	450506
RP_POS_420_25299a11_379	RP	POS	11.38	420.2530				4.03E-04	-0.61	1.21	9.01E-01	0.03	0.94	1.59E-03	-0.60	1.23	3.46E-03	-0.62	1.12	1581976	196469	1416650	280106	1413123	311016	1420178	248524
RP_POS_134_99677a0_451	RP	POS	0.45	134.9968				6.37E-07	-0.64	1.32	9.01E-01	0.03	1.16	1.94E-04	-0.63	1.40	2.90E-04	-0.66	1.41	6808117	945035	4908402	3218635	4868032	3363921	4948771	3100218
RP_NEG_180_97295a14_262	RP	NEG	14.26	180.9730				8.71E-01	-0.03	0.39	9.01E-01	-0.03	0.15	8.42E-01	-0.05	0.14	9.29E-01	-0.02	0.53	2149402	846405	2121140	880110	2132164	863962	2110115	904608
RP_POS_311_21915a10_458	RP	POS	10.46	311.2192				2.78E-01	0.21	0.38	9.01E-01	-0.03	0.18	3.45E-01	-0.20	0.47	3.26E-01	0.23	0.42	5116620	1265559	5403610	1362478	5420642	1492961	5386577	1233198
HILIC_NEG_234_81995a7_394	HILIC	NEG	7.394	234.8200				5.46E-01	-0.12	0.39	9.01E-01	-0.03	0.47	5.63E-01	-0.13	0.21	6.22E-01	-0.11	0.42	495386	25023	492255	26479	492586	24847	491925	28265
HILIC_NEG_228_00932a0_93	HILIC	NEG	0.93	228.0093				3.80E-08	0.78	1.30	9.02E-01	-0.03	1.19	9.19E-05	0.76	1.26	2.48E-06	0.79	1.52	99743	63412	209579	149507	211441	133056	207718	165680
HILIC_POS_158_1541a1_247	HILIC	POS	1.247	158.1541				2.04E-01	-0.27	0.92	9.02E-01	-0.02	0.43	2.08E-01	-0.29	0.83	2.86E-01	-0.26	0.88	1532847	596094	1380285	541893	1387022	604379	1373548	477413
RP_POS_185_11481a13_245	RP	POS	13.25	185.1148				9.31E-01	0.02	0.25	9.02E-01	-0.02	0.30	9.80E-01	0.01	0.37	8.95E-01	0.03	0.55	7996239	1905791	8029594	1826057	8052287	1786115	8006900	1883019
RP_NEG_218_81709a0_757	RP	NEG	0.76	218.8171				2.11E-04	-0.79	1.48	9.02E-01	-0.02	0.14	3.51E-04	-0.80	1.48	9.96E-04	-0.78	1.27	6183019	1657790	4855367	1563033	4874738	1712392	4835996	1415257
RP_POS_320_86957a0_472	RP	POS	0.47	320.8696				6.93E-04	-0.47	1.21	9.02E-01	-0.03	1.23	4.94E-03	-0.49	1.24	1.39E-02	-0.46	1.26	503877	107954	391812	259163	395023	273598	388601	246627
RP_NEG_520_90936a14_241	RP	NEG	14.24	520.9094				9.83E-01	0.00	0.63	9.02E-01	-0.03	0.33	9.40E-01	-0.02	0.38	9.62E-01	0.01	0.62	1172240	528925	1169739	671878	1178060	564282	1161418	770388
HILIC_NEG_352_75458a2_934	HILIC	NEG	2.934	352.7546				2.03E-06	-0.62	1.33	9.03E-01	0.03	0.76	2.34E-04	-0.61	1.47	6.59E-04	-0.63	1.48	496202	63895	379950	204588	377440	219848	382461	190318
HILIC_NEG_229_06918a0_93	HILIC	NEG	0.93	229.0692				7.07E-09	0.79	1.28	9.03E-01	-0.03	1.09	3.51E-05	0.78	1.31	2.66E-06	0.80	1.49	55296	49712	153774	132077	155390	123718	152157	141185
RP_POS_133_03453a13_108	RP	POS	13.11	133.0345				1.57E-01	-0.30	0.52	9.03E-01	-0.02	0.18	1.90E-01	-0.32	0.55	2.04E-01	-0.29	0.61	4800346	2103943	4197714	1927239	4221299	1802778	4174128	2062319
HILIC_POS_126_10269a4_556	HILIC	POS	4.556	126.1027				9.84E-11	0.81	1.29	9.03E-01	0.03	0.74	2.11E-06	0.82	1.52	6.53E-06	0.79	1.44	284071	94651	639822	472513	634047	481902	645598	467757
HILIC_POS_64_0167a4_326	HILIC	POS	4.326	64.0167				4.35E-01	0.14	0.98	9.04E-01	-0.03	0.82	5.40E-01	0.13	0.33	4.69E-01	0.15	0.66	247559902	45598300	255443196	59901286	256173649	61238780	254712743	59146250
HILIC_NEG_566_34772a1_07	HILIC	NEG	1.07	566.3477				2.83E-05	0.78	1.28	9.04E-01	-0.02	0.65	6.62E-04	0.77	1.22	4.36E-05	0.79	1.62	469908	192770	657216	236972	660105	190192	654328	277971
RP_POS_410_32654a9_934	RP	POS	9.93	410.3265				6.54E-02	0.28	1.12	9.04E-01	-0.03	0.36	1.23E-01	0.27	0.68	1.45E-01	0.30	1.22	647365	597316	930800	1094663	944137	1214905	917462	971943
HILIC_POS_364_77948a3_008	HILIC	POS	3.008	364.7795				4.49E-05	-0.54	1.36	9.04E-01	0.03	0.77	1.74E-03	-0.53	1.47	2.66E-03	-0.55	1.50	1102724	168531	856333	501489	850224	530550	862441	475978
RP_NEG_192_92888a15_361	RP	NEG	15.36	192.9289				6.51E-01	0.09	0.58	9.04E-01	0.03	0.37	6.51E-01	0.10	0.42	7.31E-01	0.07	0.37	3671795	1149312	3781535	1298151	3765732	1284874	3797337	1324151
RP_POS_199_13049a13_242	RP	POS	13.24	199.1305				7.11E-01	0.09	0.33	9.04E-01	-0.02	0.25	7.61E-01	0.08	0.20	6.99E-01	0.10	0.56	26867959	5075527	27231855	3978100	27277941	3908901	27185769	3723128
HILIC_NEG_566_34814a1_193	HILIC	NEG	1.193	566.3481				2.26E-05	0.80	1.29	9.04E-01	0.02	0.63	3.69E-04	0.81	1.26	5.15E-05	0.79	1.61	3103342	1190679	4269609	1429658	4252256	1133988	4286962	1686123
RP_POS_310_31015a11_247	RP	POS	11.25	310.3102				1.53E-11	0.97	1.50	9.04E-01	0.02	0.82	3.23E-06	0.98	1.50	2.57E-10	0.95	1.90	146059397	63887519	282847841	143937542	281103536	105174581	284592146	175473493
RP_POS_352_24551a10_98	RP	POS	10.98	352.2455				1.69E-01	0.27	1.15	9.05E-01	0.02	1.41	1.93E-01	0.29	1.00	2.49E-01	0.26	1.07	1847317	414370	1966283	438092	1960995	457563	1971572	422310
RP_POS_177_09097a6_349	RP	POS	6.35	177.0910				1.82E-01	-0.23	0.76	9.05E-01	-0.03	0.82	2.40E-01	-0.24	0.59	2.82E-01	-0.21	0.79	1025699	252203	948026	365997	952434	360021	943617	375482
HILIC_POS_87_09226a0_546	HILIC	POS	0.546	87.0923				1.15E-03	-0.59	1.02	9.05E-01	-0.02	0.71	4.73E-03	-0.60	1.03	4.48E-03	-0.58	1.01	4429409	947865	3724298	1225282	3739048	1171397	3709548	1288665
HILIC_NEG_130_98364a7_352	HILIC	NEG	7.352	130.9836				8.23E-04	-0.59	1.12	9.05E-01	-0.02	0.69	2.07E-03	-0.60	1.14	6.50E-03	-0.58	1.03	2306433	154476	2186319	208481	2188814	226385	2183824	191188
RP_POS_278_24539a11_166	RP	POS	11.17	278.2454				4.73E-05	0.73	1.14	9.06E-01	0.02	0.31	3.07E-04	0.74	1.27	4.57E-04	0.72	1.30	1309998	270752	1569451	357026	1565184	358423	1573718	359210
HILIC_POS_163_12299a1_306	HILIC	POS	1.306	163.1230				1.45E-04	0.54	1.08	9.06E-01	0.03	0.73	3.42E-03	0.56	1.09	2.46E-03	0.53	1.01	949657	858351	1913658	1928826	1890606	1831548	1936711	2039857
RP_NEG_437_29175a9_933	RP	NEG	9.93	437.2918				7.21E-02	0.28	1.05	9.06E-01	-0.03	0.36	1.33E-01	0.27	0.63	1.48E-01	0.29	1.23	2103521	1951089	2984810	3402109	3025411	3736024	2944210	3069799
RP_NEG_268_98416a8_483	RP	NEG	8.48	268.9842				9.73E-01	-0.01	0.76	9.06E-01	-0.02	0.29	9.36E-01	-0.02	0.99	9.83E-01	0.00	0.27	2435183	165574	2434071	157921	2435954	158128	2432188	159296
RP_POS_886_75903a0_497	RP	POS	0.50	886.7590				3.10E-06	-0.58	1.31	9.06E-01	0.03	1.20	6.26E-04	-0.56	1.38	9.97E-04	-0.59	1.38	4499220	421140	3411170	2094216	3386199	2199878	3436140	2005057
HILIC_POS_183_11253a0_753	HILIC	POS	0.753	183.1125				1.76E-03	0.51	1.04	9.06E-01	0.03	0.64	1.08E-02	0.52	1.06	7.55E-03	0.50	0.92	2144717	740359	2716910	1194476	2702708	1102186	2731112	1291292
HILIC_POS_203_10271a7_689	HILIC	POS	7.689	203.1027				2.70E-01	0.20	0.62	9.06E-01	0.02	0.52	3.29E-01	0.22	0.50	3.46E-01	0.19	0.51	657036	51777	669375	62760	668629	57337	670121	68333
HILIC_NEG_406_62949a2_947	HILIC	NEG	2.947	406.6295				2.72E-05	-0.57	1.32	9.06E-01	0.03	0.76	9.44E-04	-0.56	1.44	1.98E-03	-0.58	1.45	424091	67030	330072	180526	327926	193614	332218	168372
RP_POS_186_11221a0_704	RP	POS	0.70	186.1122				7.65E-03	0.51	0.78	9.06E-01	-0.02	0.12	1.99E-02	0.49	0.93	1.72E-02	0.52	0.88	1163468	492730	1452110	579434	1458980	597216	1445241	567077
RP_POS_524_2691a6_992	RP	POS	6.99	524.2691				2.01E-02	-0.40	0.86	9.06E-01	-0.03	0.75	3.29E-02	-0.41	0.84	6.69E-02	-0.39	0.85	778172	46891	752832	67097	753627	72770	752036	61636
RP_NEG_197_06781a0_709	RP	NEG	0.71	197.0678				1.17E-02	-0.51	1.08	9.06E-01	0.02	0.35	4.08E-02	-0.49	1.05	1.12E-02	-0.52	1.15	709737	499728	441876	523944	435666	392866	448087	632625
HILIC_NEG_150_88956a2_989	HILIC	NEG	2.989	150.8896				8.61E-01	-0.03	0.87	9.07E-01	0.02	0.56	9.21E-01	-0.02	0.55	8.32E-01	-0.05	0.67	786414	282823	776061	308450	772411	302740	779710	317090
RP_POS_223_09392a13_632	RP	POS	13.63	223.0939				1.19E-01	0.32	0.78	9.07E-01	0.02	0.15	1.38E-01	0.33	0.65	1.83E-01	0.31	0.58	12866275	7243561	15199465	7229429	15113957	7592940	15284973	6923024
RP_POS_424_2818a11_127	RP	POS	11.13	424.2818				1.16E-01	0.31	0.68	9.07E-01	-0.02	0.24	1.82E-01	0.30	0.59	1.46E-01	0.32	0.59	1080383	1993897	1740498	2168917	1766151	2154026	1714846	2205276
RP_POS_173_02884a15_646	RP	POS	15.65	173.0288				6.15E-01	-0.11	0.34	9.07E-01	0.02	0.11	6.78E-01	-0.10	0.22	6.19E-01	-0.12	0.46	95323810	37374892	91552492	34259518	91147591	36089295	91957392	32689611
RP_POS_216_95068a0_453	RP	POS	0.45	216.9507				1.73E-04	-0.54	1.20	9.07E-01	-0.03	1.07	1.79E-03	-0.55	1.22	5.40E-03	-0.53	1.27	1370573	333690	1002545	742107	1011254	781006	993835	708915
RP_POS_148_97328a15_454	RP	POS	15.45	148.9733				6.39E-02	-0.34	0.63	9.07E-01	0.02	0.32	1.43E-01	-0.33	0.57	7.52E-02	-0.35	0.76	3115446	543309	2893779	678563	2885822	588936	2901736	763753
RP_NEG_149_02361a9_441	RP	POS	9.44	149.0236	Unknown	149.0228(100), 121.0287(8)	4	5.89E-01	0.10	0.48	9.08E-01	0.02	0.73	6.13E-01	0.11	0.33	6.68E-01	0.09	0.52	3824037	216923	3849449	268457	3846306	246153	3852592	291544
RP_NEG_539_27667a10_326	RP	POS	10.33	539.2767				9.15E-08	1.01	1.61	9.08E-01	0.02	0.40	4.54E-07	1.02	1.74	3.92E-06	0.99	1.59	307505	183307	544973	222579	542385	243399	547561	202081
RP_POS_368_27951a8_181	RP	POS	8.18	368.2795				3.46E-02	0.35	1.00	9.08E-01	-0.02	0.99	6.94E-02	0.36	0.85	8.77E-02	0.33	1.02	969277	419836	1182410	658141	1174769	656430	1190051	666422
HILIC_POS_199_99051a4_327	HILIC	POS	4.327	199.9905				2.00E-01	0.22	0.99	9.08E-01	-0.02	0.84	2.98E-01	0.21	0.52	2.61E-01	0.23	0.80	3344872	637345	3533307	922951	3544022	956235	3522593	898022
RP_POS_249_18294a8_904	RP	POS	8.90	249.1829				8.08E-01	0.04	0.42	9.09E-01	-0.02	0.39	8.78E-01	0.03	0.32	7.92E-01	0.06	0.41	1972868	827637	2016615	1043028	2028687	1069752	2004543	1026328
RP_POS_163_97708a0_677	RP	POS	0.68	163.9771				4.76E-06	0.63	1.28	9.09E-01	-0.03	1.15	4.95E-04	0.62	1.32	4.09E-04	0.64	1.36	4145148	708220	5191098	1791946	5211832	1826618	5170364	1774897
RP_POS_232_92776a0_453	RP	POS	0.45	232.9278				4.50E-04	-0.53	1.18	9.09E-01	-0.02	1.07	4.74E-03	-0.51	1.19	4.87E-03	-0.54	1.25	5113572	1440792	3741207	2801594	3708798	2912776	3773617	2715075
HILIC_NEG_144_92345a4_164	HILIC	NEG	4.164	144.9235				1.12E-01	-0.33	0.73	9.09E-01	-0.02	0.80	1.45E-01	-0.34	0.56	1.56E-01	-0.32	0.53	43023111	9370794	39967845	9075675	40072676	8617286	39863015	9598786
RP_POS_359_20868a11_379	RP	POS	11.38	359.2087				1.41E-03	-0.56	1.10	9.09E-01	-0.02	0.94	2.27E-03	-0.57	1.17	1.29E-02	-0.54	1.05	1034397	134495	933859	187421	936023	215757	931695	156237
HILIC_NEG_132_92368a2_946	HILIC	NEG	2.946	132.9237				5.85E-02	-0.41	1.02	9.09E-01	-0.02	0.73	8.06E-02	-0.42	0.82	8.81E-02	-0.39	0.66	25439289	5990855	23125131	5533129	23188787	5308723	23061475	5802158
RP_POS_281_17184a9_303	RP	POS	9.30	281.1718				1.31E-05	-0.65	1.15	9.09E-01	0.02	0.98	8.69E-04	-0.63	1.22	2.74E-04	-0.66	1.24	3779797	382465	3310000	774871	3301104	747701	3318896	808631
HILIC_POS_440_70877a3_013	HILIC	POS	3.013	440.7088				2.05E-05	-0.61	1.33	9.09E-01	0.02	0.76	7.40E-04	-0.59	1.45	1.02E-03	-0.62	1.43	386671	76026	289461	172930	287476	181318	291446	165939
HILIC_POS_338_23248a0_759	HILIC	POS	0.759	338.2325				4.39E-01	-0.15	0.44	9.09E-01	-0.02	0.49	4.88E-01	-0.16	0.29	5.07E-01	-0.14	0.31	582312	277553	536743	319005	540402	277166	533085	358827
HILIC_NEG_115_92065a1_049	HILIC	NEG	1.049	115.9207				1.03E-01	0.31	0.91	9.10E-01	0.02	0.50	1.33E-01	0.32	0.67	1.73E-01	0.30	0.57	28335843	7801372	31065098	9050898	30961475	9315375	31168721	8871933
HILIC_POS_356_00937a7_391	HILIC	POS	7.391	356.0094				8.23E-01	0.04	0.43	9.10E-01	0.02	0.44	8.00E-01	0.05	0.48	8.90E-01	0.03	0.24	1067381	41807	1069394	50492	1068817	51593	1069972	49884
RP_NEG_764_80872a0_496	RP	NEG	0.50	764.8087				6.27E-06	-0.57	1.28	9.10E-01	-0.03	1.19	5.87E-04	-0.58	1.36	1.60E-03	-0.56	1.34	1841602	182800	1470486	717678	1478674	740243	1462298	701812
HILIC_NEG_185_96243a0_699	HILIC	NEG	0.699	185.9624				4.93E-05	0.78	1.30	9.10E-01	-0.02	0.83	2.62E-04	0.77	1.48	2.64E-04	0.79	1.31	722935	387015	1079983	443825	1085039	460736	1074927	430872
HILIC_NEG_454_77625a2_923	HILIC	NEG	2.923	454.7763				6.71E-07	-0.62	1.35	9.10E-01	0.03	0.76	1.76E-04	-0.61	1.49	5.50E-04	-0.63	1.52	1285180	117070	990387	522945	984431	561034	996342	487537
RP_POS_916_52686a13_165	RP	POS	13.17	916.5269				9.40E-01	0.02	0.55	9.10E-01	-0.02	0.30	9.83E-01	0.01	0.57	9.08E-01	0.03	0.44	943533	571044	952057	512358	957870	496412	946245	532808
RP_POS_279_1088a8_874	RP	POS	8.87	279.1088				8.20E-01	0.05	0.45	9.11E-01	-0.02	0.20	8.80E-01	0.03	0.30	7.97E-01	0.06	0.33	1025323	179473	1033730	185193	1035827	180791	1031633	191307
RP_NEG_179_05704a3_266	RP	NEG	3.27	179.0570				7.51E-01	-0.06	0.38	9.11E-01	-0.02	0.09	7.45E-01	-0.07	0.25	8.20E-01	-0.05	0.54	1505484	1485771	1405280	1738184	1424902	1672082	1385658	1818676
RP_POS_235_092a0_629	RP	POS	0.63	235.0920				3.20E-05	-0.59	1.24	9.11E-01	0.02	1.11	1.04E-03	-0.58	1.29	1.32E-03	-0.60	1.30	9991588	2245965	7178917	5150132	7120830	5382015	7237005	4961456
HILIC_NEG_195_81091a3_955	HILIC	NEG	3.955	195.8109				1.53E-01	0.22	0.82	9.11E-01	-0.02	0.45	3.25E-01	0.20	0.37	1.71E-01	0.23	0.95	364687	416723	519607	785291	528463	656284	510752	902818
RP_NEG_872_565a13_73	RP	NEG	13.73	872.5650				3.83E-04	0.66	1.15	9.11E-01	0.02	0.38	1.71E-03	0.67	1.15	1.76E-03	0.65	1.11	7726445	3099200	10230862	3817891	10187940	3709829	10273784	3960235
HILIC_POS_162_14861a1_047	HILIC	POS	1.047	162.1486				6.54E-04	-0.66	1.27	9.12E-01	0.02	0.73	2.26E-03	-0.64	1.30	2.42E-03	-0.67	1.24	727385	278420	516289	319238	512719	335501	519859	305481
HILIC_NEG_103_03988a0_928	HILIC	NEG	0.928	103.0399				2.21E-06	0.66	1.14	9.12E-01	-0.02	1.26	1.44E-03	0.65	1.02	1.08E-05	0.68	1.43	16897165	9488159	30872499	22554166	31124064	17791731	30620934	26666222
RP_POS_215_96272a15_558	RP	POS	15.56	215.9627				3.99E-01	-0.17	0.41	9.12E-01	-0.02	0.16	4.29E-01	-0.18	0.38	4.78E-01	-0.16	0.32	4799796	128314	4777352	135148	4778859	131492	4775845	140029
RP_NEG_1003_67517a10_932	RP	NEG	10.93	1003.6752				3.59E-01	0.17	1.00	9.12E-01	-0.02	0.98	4.89E-01	0.16	0.69	3.58E-01	0.18	0.87	862158	336105	929305	417596	933949	352880	924660	477246
RP_POS_531_47534a15_099	RP	POS	15.10	531.4753				9.69E-01	-0.01	0.37	9.12E-01	0.02	0.07	9.85E-01	0.00	0.39	9.31E-01	-0.02	0.40	11120962	1002008	11112819	1152409	11100051	1156189	11125587	1160212
RP_POS_528_30829a10_551	RP	POS	10.55	528.3083				2.88E-06	0.84	1.56	9.12E-01	0.02	0.12	6.47E-05	0.85	1.51	2.10E-05	0.83	1.54	1759594	973702	2854697	1282635	2840485	1160897	2868908	1405625
HILIC_NEG_219_84549a3_021	HILIC	NEG	3.021	219.8455				5.26E-02	-0.38	1.04	9.13E-01	0.02	0.77	9.61E-02	-0.37	0.74	7.42E-02	-0.39	0.66	1053628	205857	968927	224847	966439	222425	971414	229476
RP_NEG_564_83026a0_448	RP	NEG	0.45	564.8303				2.82E-02	-0.38	0.98	9.13E-01	0.02	0.95	6.60E-02	-0.37	0.92	5.85E-02	-0.39	1.02	1267723	461735	1033592	654358	1026378	676287	1040806	638465
RP_POS_320_23502a10_849	RP	POS	10.85	320.2350				1.23E-06	0.80	1.25	9.13E-01	0.02	0.13	1.12E-04	0.81	1.24	1.14E-05	0.79	1.51	18439480	5267396	24979006	8346969	24886989	7154979	25071022	9463333
RP_NEG_452_92499a13_622	RP	NEG	13.62	452.9250				1.57E-01	0.27	0.49	9.13E-01	-0.02	0.33	2.12E-01	0.26	0.53	2.15E-01	0.28	0.66	1489572	578953	1665087	673321	1672496	740642	1657678	606062
RP_POS_348_202a6_254	RP	POS	6.25	348.2020				5.61E-01	-0.12	0.39	9.13E-01	-0.02	0.27	5.55E-01	-0.13	0.38	6.40E-01	-0.11	0.28	573880	72009	565453	67095	566190	72556	564715	61886
HILIC_POS_227_17558a0_505	HILIC	POS	0.505	227.1756				1.06E-04	-0.68	1.23	9.13E-01	0.02	0.72	6.87E-04	-0.66	1.35	9.92E-04	-0.69	1.29	20361493	6734193	14139079	9414757	14035595	10013654	14242563	8876323
HILIC_POS_618_66107a3_005	HILIC	POS	3.005	618.6611				3.88E-05	-0.56	1.35	9.13E-01	-0.02	0.76	8.73E-04	-0.57	1.47	2.98E-03	-0.55	1.44	456606	81004	347399	212227	349725	223253	345073	202848
RP_NEG_128_95856a0_499	RP	NEG	0.50	128.9586				4.10E-05	-0.52	1.26	9.13E-01	0.02	1.21	1.84E-03	-0.50	1.31	3.92E-03	-0.53	1.32	2291985	256785	1809095	1041019	1797687	1116886	1820503	970493
RP_NEG_395_19012a11_987	RP	NEG	11.99	395.1901				5.41E-02	0.36	0.73	9.13E-01	0.02	0.47	7.25E-02	0.37	0.69	1.11E-01	0.35	0.76	91437	168714	161928	199613	159742	213263	164113	187118

Supplementary table 1: Metabolomics results (in asceding order according to p-value from progressive ALD vs non-progressive ALD comparison, with molecular features with ID_level of 1-2 first)

								all_ALD_vs_control			Prog_ALD_vs_non-prog_ALD			Prog_ALD_vs_control_ALD			Non-prog_ALD_vs_control			Healthy_control		all_ALD		Non-prog_ALD		Progressive_ALD	
								t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA								
Feature_ID	RP_HILIC	POS_NEG	Average.Rt	Average.Mz	Metabolite.name	curated_MSMS	ID_level	p	d	VIP	p	d	VIP	p	d	VIP	p	d	VIP	Mean	SD	Mean	SD	Mean	SD	Mean	SD
HILIC_POS_344_72208a3_019	HILIC	POS	3.019	344.7221				1.37E-04	-0.53	1.33	9.14E-01	-0.02	0.76	1.65E-03	-0.54	1.43	5.95E-03	-0.52	1.44	254416	47751	197237	118203	198530	125723	195944	111443
RP_NEG_840_7829a0_496	RP	NEG	0.50	840.7829				1.10E-06	-0.61	1.31	9.14E-01	0.02	1.20	3.02E-04	-0.59	1.40	6.21E-04	-0.62	1.38	5042641	493159	3779994	2300729	3754942	2431292	3805046	2186840
RP_POS_162_96411a11_247	RP	POS	11.25	162.9641				1.02E-11	0.98	1.51	9.14E-01	0.02	0.80	2.60E-06	0.99	1.51	1.64E-10	0.97	1.92	875846	393320	1723010	878814	1713439	641046	1732580	1072038
HILIC_NEG_482_55823a2_946	HILIC	NEG	2.946	482.5582				2.83E-05	-0.58	1.30	9.14E-01	-0.02	0.75	4.99E-04	-0.59	1.43	2.66E-03	-0.57	1.42	303366	52034	234667	128379	236064	137988	233270	119391
HILIC_NEG_234_82014a4_68	HILIC	NEG	4.68	234.8201				3.49E-01	0.17	0.53	9.14E-01	0.02	0.41	3.74E-01	0.19	0.35	4.55E-01	0.16	0.75	675330	301212	736084	361100	732157	379798	740010	345208
RP_POS_185_11507a12_894	RP	POS	12.89	185.1151				6.90E-01	-0.08	0.34	9.15E-01	0.02	0.28	7.77E-01	-0.07	0.18	6.63E-01	-0.09	0.40	6333405	2669203	6111305	2906438	6079884	2370535	6142726	3383151
RP_NEG_348_89621a0_499	RP	NEG	0.50	348.8962				7.48E-05	-0.51	1.25	9.15E-01	-0.02	1.22	1.45E-03	-0.52	1.32	6.64E-03	-0.50	1.30	6579386	960131	5086414	3230227	5121307	3464381	5051522	3012849
RP_POS_468_29883a10_454	RP	POS	10.45	468.2988				8.84E-01	0.03	0.72	9.15E-01	0.02	0.18	8.57E-01	0.04	0.69	9.44E-01	0.01	0.54	664846	160434	670034	211124	667754	211129	672313	213238
HILIC_NEG_134_89478a7_391	HILIC	NEG	7.391	134.8948				8.09E-01	0.05	0.33	9.15E-01	0.02	1.15	7.94E-01	0.06	0.10	8.62E-01	0.04	0.63	11674559	520025	11699939	498772	11694554	487246	11705323	514934
HILIC_NEG_136_89168a0_936	HILIC	NEG	0.936	136.8917				3.87E-02	0.38	1.21	9.15E-01	-0.02	0.79	6.73E-02	0.37	0.91	7.59E-02	0.39	1.09	9757555	1958501	10651019	2434900	10677229	2659750	10624809	2214227
HILIC_POS_228_02203a4_865	HILIC	POS	4.865	228.0220				9.60E-01	0.01	0.63	9.15E-01	-0.02	0.22	9.97E-01	0.00	0.57	9.33E-01	0.02	0.29	613445	382247	617178	319343	620610	367884	613746	265856
RP_POS_685_43457a13_57	RP	POS	13.57	685.4346				2.56E-01	0.21	0.93	9.15E-01	-0.02	0.22	3.27E-01	0.19	0.65	3.25E-01	0.22	0.70	97539709	6060561	99053686	7716602	99136288	8512604	98971084	6915835
RP_POS_441_29599a14_018	RP	POS	14.02	441.2960				5.44E-01	0.11	0.55	9.15E-01	-0.02	0.33	6.30E-01	0.10	0.46	5.71E-01	0.12	0.38	13883652	5871416	14654986	7245710	14732454	7563741	14577518	6989251
HILIC_NEG_115_92067a7_422	HILIC	NEG	7.422	115.9207				8.98E-01	-0.03	0.39	9.16E-01	0.02	0.42	9.40E-01	-0.02	0.42	8.72E-01	-0.04	0.21	53441552	8744769	53220737	7264275	53143136	7032095	53298339	7560004
RP_POS_229_18031a7_809	RP	POS	7.81	229.1803				6.83E-01	0.09	0.42	9.16E-01	-0.02	0.46	7.44E-01	0.08	0.48	6.73E-01	0.10	0.43	1406630	196882	1422604	171944	1424437	165364	1420771	179947
HILIC_POS_246_10959a5_463	HILIC	POS	5.463	246.1096				3.75E-01	-0.16	0.44	9.16E-01	-0.02	0.32	4.57E-01	-0.15	0.58	4.35E-01	-0.17	0.29	1492682	54597	1481974	71089	1481220	77599	1482729	64712
HILIC_POS_394_31653a7_325	HILIC	POS	7.325	394.3165				9.45E-01	-0.01	0.54	9.16E-01	0.02	0.30	9.92E-01	0.00	0.41	9.14E-01	-0.02	0.23	3059577	509518	3052238	573681	3046155	605484	3058320	546123
HILIC_NEG_215_06737a6_522	HILIC	NEG	6.522	215.0674				4.34E-05	-0.57	1.10	9.16E-01	-0.02	0.68	2.93E-03	-0.58	1.14	6.27E-04	-0.56	1.21	3258186	186546	3022410	447300	3027146	393714	3017674	499181
RP_POS_264_95483a0_454	RP	POS	0.45	264.9548				1.77E-04	-0.55	1.19	9.17E-01	0.02	1.08	2.70E-03	-0.53	1.23	3.38E-03	-0.56	1.26	730971	184830	532665	393141	528534	412018	536795	377466
RP_POS_177_08653a0_63	RP	POS	0.63	177.0865				1.72E-06	-0.70	1.33	9.17E-01	0.02	1.12	1.38E-04	-0.69	1.40	1.70E-04	-0.71	1.37	3252912	736423	2223710	1567573	2207261	1623007	2240159	1526438
RP_NEG_128_03394a1_128	RP	NEG	1.13	128.0339				1.55E-09	0.82	1.40	9.17E-01	0.02	0.88	1.73E-05	0.84	1.43	6.61E-07	0.81	1.56	1104775	190439	1499752	504182	1494481	445517	1505022	561288
RP_POS_271_90927a15_67	RP	POS	15.67	271.9093				2.02E-01	-0.23	1.00	9.18E-01	0.02	0.49	3.23E-01	-0.21	1.10	2.27E-01	-0.24	0.64	4338566	1380497	3944015	1851795	3924689	1673266	3963341	2031672
RP_NEG_434_87195a0_449	RP	NEG	0.45	434.8720				3.77E-04	-0.53	1.17	9.18E-01	0.02	1.08	4.55E-03	-0.52	1.19	4.38E-03	-0.54	1.23	3731206	1017331	2735305	2028962	2714142	2091400	2756468	1985579
HILIC_POS_160_03464a4_868	HILIC	POS	4.868	160.0346				7.87E-01	0.05	0.33	9.18E-01	0.02	0.22	7.45E-01	0.07	0.49	8.59E-01	0.04	0.09	7458395	5293226	7751816	5372825	7695994	6710079	7807637	3645834
RP_NEG_888_50806a10_328	RP	NEG	10.33	888.5081				7.32E-01	-0.08	0.36	9.18E-01	0.02	0.26	7.83E-01	-0.07	0.25	7.11E-01	-0.09	0.35	842545	1088060	771045	767855	763089	644424	779002	880809
RP_POS_800_07922a13_711	RP	POS	13.71	800.0792				1.95E-03	-0.59	1.00	9.19E-01	-0.02	0.59	4.57E-03	-0.60	1.07	7.88E-03	-0.58	0.94	1766689	675936	1301921	794674	1310094	827431	1293748	768846
HILIC_NEG_202_92915a7_353	HILIC	NEG	7.353	202.9292				1.74E-02	-0.41	0.87	9.19E-01	-0.02	0.75	4.80E-02	-0.42	0.85	3.75E-02	-0.40	1.01	621254	49290	594120	69685	594836	63147	593403	76305
HILIC_NEG_144_92336a3_015	HILIC	NEG	3.015	144.9234				5.61E-01	-0.16	0.93	9.19E-01	0.02	0.48	5.90E-01	-0.15	0.55	5.62E-01	-0.17	0.50	10757231	2166260	10522393	1147583	10510601	1258550	10534185	1037563
HILIC_NEG_187_9781a0_93	HILIC	NEG	0.93	187.9781				2.72E-08	0.79	1.32	9.19E-01	-0.02	1.17	8.58E-05	0.78	1.26	1.19E-06	0.80	1.57	459018	256401	902939	591898	909007	510829	896872	668442
HILIC_NEG_241_01044a0_577	HILIC	NEG	0.577	241.0104				4.86E-02	-0.55	1.36	9.19E-01	-0.02	0.70	5.05E-02	-0.56	0.90	6.28E-02	-0.54	1.02	939203	356700	805044	186180	806946	202912	803142	169861
HILIC_POS_144_17468a0_542	HILIC	POS	0.542	144.1747				7.99E-05	-0.65	1.38	9.19E-01	-0.02	0.61	7.93E-04	-0.66	1.16	1.05E-03	-0.64	1.08	1539833	142983	1399424	224922	1401716	224681	1397132	227421
HILIC_POS_272_78702a3_016	HILIC	POS	3.016	272.7870				3.36E-05	-0.55	1.35	9.20E-01	-0.02	0.76	1.30E-03	-0.54	1.47	2.30E-03	-0.56	1.48	1260010	199515	970588	573607	964753	608331	976423	542797
RP_POS_166_98494a10_261	RP	POS	10.26	166.9849				7.17E-01	0.08	0.63	9.20E-01	0.02	0.09	7.24E-01	0.09	0.39	7.63E-01	0.07	0.52	10741652	4048730	11036988	3792131	10998537	3227196	11075439	4316965
RP_NEG_267_16104a8_332	RP	NEG	8.33	267.1610				8.04E-02	-0.31	0.59	9.20E-01	-0.02	0.17	1.20E-01	-0.32	0.60	1.50E-01	-0.30	0.52	1339093	78246	1308253	105328	1309317	106610	1307190	105102
RP_POS_185_58588a0_622	RP	POS	0.62	185.5859				2.05E-04	-0.53	1.19	9.20E-01	-0.02	1.08	3.10E-03	-0.52	1.21	4.23E-03	-0.54	1.25	1577023	349683	1193743	785820	1185815	827627	1201671	750023
HILIC_POS_188_12811a4_027	HILIC	POS	4.027	188.1281				2.50E-01	0.20	0.46	9.21E-01	-0.02	0.29	2.85E-01	0.19	0.43	3.50E-01	0.22	0.32	1884698	1008653	2142689	1328303	2156034	1604833	2129344	994452
RP_NEG_203_00168a4_112	RP	NEG	4.11	203.0017				9.62E-01	-0.01	0.60	9.21E-01	-0.02	0.46	9.37E-01	-0.02	0.52	9.98E-01	0.00	0.29	3689667	5427244	3638675	4859945	3687444	3939192	3589905	5674334
HILIC_NEG_78_91827a1_363	HILIC	NEG	1.363	78.9183				1.44E-05	0.58	1.03	9.21E-01	-0.02	0.69	3.05E-03	0.60	0.93	1.51E-04	0.57	1.19	1468739	415965	2084503	1150042	2072995	933664	2096011	1341710
HILIC_NEG_614_66974a2_927	HILIC	NEG	2.927	614.6697				1.45E-05	-0.57	1.33	9.21E-01	-0.02	0.76	7.56E-04	-0.56	1.46	1.59E-03	-0.59	1.48	218395	32357	168082	95842	167125	102115	169039	90164
RP_POS_249_18303a8_812	RP	POS	8.81	249.1830	Matrin	249.1816(100)	3	9.76E-01	0.01	0.37	9.21E-01	-0.02	0.41	9.82E-01	0.00	0.30	9.41E-01	0.02	0.32	1414639	588187	1418405	701862	1425411	713069	1411399	697643
HILIC_NEG_622_70093a2_921	HILIC	NEG	2.921	622.7009				5.78E-07	-0.64	1.35	9.23E-01	-0.02	0.76	1.40E-04	-0.63	1.51	4.10E-04	-0.65	1.52	542716	61632	410043	227306	407823	242520	412263	213458
RP_POS_362_88556a0_456	RP	POS	0.46	362.8856				6.64E-02	-0.33	0.93	9.23E-01	-0.02	0.89	9.61E-02	-0.34	0.85	1.33E-01	-0.32	0.95	582061	214898	494005	280018	496737	292175	491272	270256
HILIC_POS_118_12289a1_071	HILIC	POS	1.071	118.1229				4.18E-02	-0.48	1.04	9.23E-01	-0.02	0.65	5.75E-02	-0.47	0.96	5.66E-02	-0.49	0.87	773991	497792	572628	384345	568884	410133	576372	360858
RP_POS_443_33423a13_24	RP	POS	13.24	443.3342				1.38E-01	-0.32	0.58	9.23E-01	-0.02	0.32	1.50E-01	-0.32	0.63	2.06E-01	-0.31	0.57	5226796	2021102	4617240	1890349	4635650	2081197	4598830	1699322
HILIC_POS_145_13358a2_668	HILIC	POS	2.668	145.1336				6.35E-05	0.49	0.83	9.23E-01	0.02	0.98	1.12E-02	0.50	0.78	4.92E-04	0.48	1.18	327912	389757	1176625	1927625	1157920	1513955	1195331	2283535
RP_POS_145_06491a6_163	RP	POS	6.16	145.0649				6.29E-01	-0.10	0.30	9.24E-01	0.02	0.26	7.08E-01	-0.09	0.26	6.28E-01	-0.10	0.19	1154076	179686	1136014	193663	1134162	182160	1137866	206365
RP_POS_600_46826a10_547	RP	POS	10.55	600.4683				1.57E-01	0.36	0.97	9.25E-01	0.02	0.36	1.69E-01	0.37	0.79	1.89E-01	0.35	0.91	1200092	360896	1298107	231481	1295913	233946	1300301	231343
RP_NEG_220_814a0_757	RP	NEG	0.76	220.8140				1.62E-04	-0.80	1.52	9.25E-01	0.02	0.13	3.42E-04	-0.79	1.48	6.83E-04	-0.81	1.31	6000700	1614690	4676773	1550021	4662100	1736248	4691445	1356159
HILIC_NEG_634_7251a2_91	HILIC	NEG	2.91	634.7251				6.04E-07	-0.63	1.35	9.25E-01	0.02	0.77	1.63E-04	-0.62	1.51	4.66E-04	-0.64	1.52	883329	90233	671856	369101	668371	393301	675342	347190
RP_POS_159_96886a0_254	RP	POS	0.25	159.9689				7.89E-01	-0.06	0.36	9.25E-01	-0.02	0.25	7.79E-01	-0.07	0.24	8.41E-01	-0.05	0.39	2493696	271065	2479010	262203	2481481	261511	2476538	265526
HILIC_NEG_468_80127a2_911	HILIC	NEG	2.911	468.8013				5.39E-05	-0.58	1.37	9.25E-01	-0.02	0.77	1.08E-03	-0.57	1.50	2.02E-03	-0.59	1.49	252377	49502	193634	109334	192603	116504	194664	102841
RP_NEG_251_82169a15_599	RP	NEG	15.60	251.8217				2.29E-01	-0.25	0.72	9.26E-01	-0.02	0.25	2.65E-01	-0.26	0.62	2.87E-01	-0.24	0.52	1657642	62731	1642287	59851	1642849	57847	1641724	62373
HILIC_NEG_484_55756a2_946	HILIC	NEG	2.946	484.5576				1.12E-05	-0.64	1.32	9.26E-01	-0.02	0.75	2.09E-04	-0.65	1.44	1.14E-03	-0.63	1.43	202613	39775	151644	85716	152449	92107	150839	79746
RP_POS_352_24548a10_568	RP	POS	10.57	352.2455				9.98E-02	-0.33	0.58	9.26E-01	-0.02	0.24	1.45E-01	-0.34	0.61	1.34E-01	-0.32	0.64	1819647	447605	1666532	457693	1670827	407655	1662238	506973
HILIC_POS_139_12311a3_027	HILIC	POS	3.027	139.1231				7.36E-03	0.41	1.01	9.26E-01	-0.02	0.74	2.31E-02	0.40	0.84	3.56E-02	0.42	0.96	10275192	1008571	10975361	1833500	10992543	2007762	10958180	1661429
RP_NEG_369_20526a10_703	RP	NEG	10.70	369.2053				1.08E-07	0.72	1.58	9.26E-01	-0.02	0.50	6.30E-05	0.71	1.46	5.80E-05	0.73	1.58	371711	200910	744589	558977	749793	569070	739385	554429
RP_NEG_338_87787a15_473	RP	NEG	15.47	338.8779				4.93E-01	0.14	0.33	9.27E-01	0.02	0.37	5.02E-01	0.15	0.30	5.77E-01	0.13	0.30	5537264	462830	5602406	471067	5598035	503230	5606777	441652
RP_NEG_285_20847a9_593	RP	NEG	9.59	285.2085	FA 16:1;2O	285.2063(100), 223.2058(60), 267.1978(45)	3	7.94E-02	0.33	0.68	9.27E-01	0.02	0.31	1.22E-01	0.34	0.63	1.26E-01	0.32	0.63	2339593	328543	2464097	386933	2460515	369665	2467678	407200
RP_POS_777_54163a13_156	RP	POS	13.16	777.5416				8.99E-01	0.03	0.19	9.27E-01	-0.02	0.33	9.42E-01	0.02	0.29	8.72E-01	0.04	0.14	958262	362697	967485	337930	970613	293524	964357	380194
RP_POS_485_80945a0_407	RP	POS	0.41	485.8095				5.17E-01	-0.15	0.55	9.27E-01	-0.02	0.33	5.28E-01	-0.16	0.34	5.64E-01	-0.15	0.84	616149	732889	524361	544388	529368	526932	519354	566618
HILIC_NEG_136_89166a1_69	HILIC	NEG	1.69	136.8917				2.26E-02	-0.43	0.67	9.28E-01	-0.02	0.51	4.64E-02	-0.42	0.75	4.34E-02	-0.44	0.75	6876242	2441011	5662718	2879978	5636393	2982834	5689043	2803409
HILIC_NEG_195_81113a3_033	HILIC	NEG	3.033	195.8111				5.97E-02	0.28	1.02	9.28E-01	-0.02	0.80	1.13E-01	0.29	0.72	1.54E-01	0.27	0.83	112650547	16705212	121088513	33070517	120787952	34108956	121389073	32342427
RP_POS_332_28049a9_906	RP	POS	9.91	332.2805				8.90E-01	-0.03	0.88	9.28E-01	-0.02	0.15	8.68E-01	-0.04	0.53	9.37E-01	-0.02	0.60	640866	193127	635335	208098	637222	217149	633449	200829
RP_POS_465_37732a11_158	RP	POS	11.16	465.3773				9.25E-01	0.02	0.74	9.28E-01	-0.02	0.19	9.66E-01	0.01	0.53	9.01E-01	0.03	0.59	1333390	405902	1341288	426865	1345157	429990	1337419	428048
RP_POS_199_13048a13_807	RP	POS	13.81	199.1305				3.90E-01	0.16	0.73	9.28E-01	-0.02	0.83	4.91E-01	0.15	0.31	4.08E-01	0.17	0.61	27705291	12973782	30073324	14892280	30208086	13775594	29938561	16071156
RP_POS_223_09421a11_209	RP	POS	11.21	223.0942				7.05E-01	-0.08	0.33	9.29E-01	-0.02	0.43	6.91E-01	-0.09	0.38	7.74E-01	-0.07	0.47	8534452	2993355	8303601	2968541	8330437	3312696	8276764	2613215
HILIC_NEG_158_97836a7_353	HILIC	NEG	7.353	158.9784				9.43E-05	-0.63	1.18	9.29E-01	0.02	0.78	1.15E-03	-0.62	1.24	1.22E-03	-0.64	1.24	20084260	980751	19109590	1633785	19094860	1686588	19124319	1596234
RP_POS_513_84296a11_952	RP	POS	11.95	513.8430				9.25E-01	0.02	0.34	9.29E-01	0.02	0.30	8.98E-01	0.03	0.29	9.70E-01	0.01	0.31	209619	398138	217531	462849	213366	488523	221695	440613
RP_POS_167_97151a0_253	RP	POS	0.25	167.9715				6.47E-01	-0.09	0.41	9.29E-01	-0.02	0.26	6.42E-01	-0.10	0.34	7.21E-01	-0.08	0.35	2797953	1671496	2639977	1738377	2655570	1883979	2624384	1598658
RP_POS_640_81689a0_499	RP	POS	0.50	640.8169				1.86E-08	-0.69	1.37	9.29E-01	0.02	1.19	2.80E-05	-0.68	1.50	1.15E-04	-0.70	1.44	2125859	150903	1574888	871080	1567076	929614	1582699	817764
RP_POS_296_25836a9_592	RP	POS	9.59	296.2584	Hexadecanedioic acid [M+Na]+	296.2584(30), 81.0705(100), 261.2233(70)	3	5.76E-01	-0.15	0.71	9.29E-01	0.01	0.54	6.24E-01	-0.15	0.61	5.57E-01	-0.16	0.61	4957836	8048303	4117730	4430437	4077995	3031888	4157465	5519291
RP_NEG_238_84509a15_583	RP	NEG	15.58	238.8451				2.43E-01	0.22	0.83	9.29E-01	0.02	0.33	2.94E-01	0.23	0.69	3.13E-01	0.22	0.83	469433	28178	476416	31904	476131	30524	476700	33536
HILIC_NEG_209_83401a3_059	HILIC	NEG	3.059	209.8340				4.27E-03	0.37	1.25	9.30E-01	0.02	0.75	1.65E-02	0.38	1.34	5.74E-02	0.36	1.40	1280241	71659	1359989	243162	1357829	268543	1362148	217571
RP_NEG_353_16406a11_162	RP	NEG	11.16	353.1641				3.73E-02	0.36	1.11	9.30E-01	-0.02	1.04	7.94E-02	0.35	1.00	7.49E-02	0.37	1.03	916913	71276	951234	101600	952132	105405	950336	98712
HILIC_NEG_199_80508a3_033	HILIC	NEG	3.033	199.8051				2.44E-02	0.40	1.07	9.30E-01	-0.02	0.80	4.77E-02	0.39	0.80	5.79E-02	0.41	0.93	71432490	13257171	78200772	17768126	78357273	19307890	78044270	16279157
HILIC_NEG_253_79361a3_137	HILIC	NEG	3.137	253.7936				2.21E-05	0.52	1.25	9.30E-01	-0.02	0.74	2.53E-03	0.51	1.39	2.38E-03	0.53	1.39	314489	159721	750374	943830	758683	963981	742066	932959
RP_NEG_253_14417a7_723	RP	NEG	7.72	253.1442				1.75E-01	-0.23	0.65	9.31E-01	-0.02	0.21	2.04E-01	-0.24	0.59	2.95E-01	-0.23	0.54	12634647	470048	12489493	658170	12495265	726527	12483721	589327
RP_POS_282_27792a10_848	RP	POS	10.85	282.2779				4.75E-06	0.76	1.20	9.31E-01	-0.02	0.69	3.58E-04	0.77	1.24	1.91E-05	0.75	1.48	1217452071	366404542	#########	570076061	1635207843	457580860	1645199927	668711170
RP_POS_234_96066a0_453	RP	POS	0.45	234.9607				7.56E-05	-0.56	1.22	9.31E-01	-0.02	1.08	1.04E-03	-0.57	1.25	3.42E-03	-0.55	1.28	2065303	456426	1527249	1033716	1536303	1095045	1518194	979620
RP_POS_846_52124a12_756	RP	POS	12.76	846.5212				5.60E-03	0.52	0.93	9.31E-01	-0.02	0.34	1.48E-02	0.51	0.90	1.44E-02	0.53	0.90	1257682	830384	1765730	988226	1774385	1024751	1757074	960648
RP_POS_122_92456a0_499	RP	POS	0.50	122.9246				5.66E-05	-0.51	1.26	9.31E-01	-0.02	1.21	1.42E-03	-0.52	1.34	6.31E-03	-0.50	1.32	8531691	1053614	6657102	4094370	6692943	4392582	6621260	3817390
RP_POS_253_14149a8_847	RP	POS	8.85	253.1415				6.60E-01	0.08	0.29	9.31E-01	0.02	0.43	6.71E-01	0.09	0.41	7.41E-01	0.07	0.59	514501	268625	540544	350616	537481	357613	543608	347081
RP_POS_166_98502a11_345	RP	POS	11.35	166.9850				1.92E-01	0.26	0.58	9.31E-01	0.02	0.24	2.13E-01	0.27	0.62	2.73E-01	0.26	0.61	13147278	5387565	14602832	5530036	14554617	5984703	14651047	5095616
HILIC_NEG_134_89471a5_381	HILIC	NEG	5.381	134.8947				6.63E-01	0.09	0.83	9.31E-01	-0.02	0.54	7.24E-01	0.08	0.48	6.68E-01	0.10	0.32	14355448	6322766	14917655	6289938	14972481	6336914	14862829	6306461
HILIC_POS_332_24283a1_204	HILIC	POS	1.204	332.2428				4.38E-01	0.14	0.63	9.31E-01	-0.02	0.71	5.52E-01	0.13	0.30	4.52E-01	0.15	0.41	3178081	1639675	3456110	2078613	3474223	1859945	3437996	2295511
RP_POS_554_46216a13_931	RP	POS	13.93	554.4622				2.36E-01	-0.25	0.52	9.31E-01	0.02	0.55	2.78E-01	-0.25	0.46	2.83E-01	-0.26	0.62	4733514	1384423	4402681	1270757	4391624	1415885	4413738	1121437
RP_NEG_339_20209a11_182	RP	NEG	11.18	339.2021				6.06E-01	0.10	0.49	9.31E-01	0.02	0.19	6.19E-01	0.11	0.36	6.71E-01	0.10	0.69	889242	419696	933748	430678	930009	427004	937486	438625
RP_POS_369_33496a11_038	RP	POS	11.04	369.3350				1.47E-02	-0.48	1.06	9.31E-01	0.02	0.89	2.28E-02	-0.48	1.05	3.49E-02	-0.49	0.99	681279	149662	603378	160192	601988	182036	604768	136768

Supplementary table 1: Metabolomics results (in asceding order according to p-value from progressive ALD vs non-progressive ALD comparison, with molecular features with ID_level of 1-2 first)

							all_ALD_vs_control			Prog_ALD_vs_non-prog_ALD			Prog_ALD_vs_control_ALD			Non-prog_ALD_vs_control			Healthy_control		all_ALD		Non-prog_ALD		Progressive_ALD	
							t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA								
Feature_ID	RP_HILIC	POS_NEG	Average.Rt	Average.Mz	Metabolite.name	curated_MSMS	ID_level	p	d	VIP	p	d	VIP	p	d	VIP	p	d	VIP	Mean	SD	Mean	SD	Mean	SD	Mean	SD
HILIC_POS_334_69373a3_023	HILIC	POS	3.023	334.6937				7.29E-04	-0.49	1.31	9.31E-01	-0.02	0.75	5.00E-03	-0.49	1.39	1.20E-02	-0.48	1.41	463668	102616	363091	225885	365051	238101	361132	215382
RP_POS_750_78333a0_498	RP	POS	0.50	750.7833				3.87E-05	-0.52	1.27	9.31E-01	-0.02	1.21	1.32E-03	-0.53	1.34	4.49E-03	-0.51	1.33	6669530	854890	5162746	3194348	5190438	3372864	5135055	3039439
HILIC_POS_114_0666a1_232	HILIC	POS	1.232	114.0666				4.95E-02	-0.39	1.02	9.32E-01	-0.02	0.77	7.99E-02	-0.40	0.64	7.93E-02	-0.38	0.84	988070159	214702594	898908528	230417550	900888120	218269252	896928936	244160902
RP_POS_250_86765a0_515	RP	POS	0.52	250.8677				1.13E-05	-0.69	1.24	9.32E-01	-0.02	1.01	1.64E-04	-0.70	1.31	5.04E-04	-0.68	1.28	461544	117166	326471	204343	328223	214518	324719	195807
RP_POS_475_41397a10_975	RP	POS	10.98	475.4140				3.18E-02	0.38	1.17	9.33E-01	0.02	0.94	6.58E-02	0.39	1.10	6.24E-02	0.37	1.03	1517754	399128	1710656	525682	1706173	497463	1715139	557505
RP_NEG_344_98062a8_89	RP	NEG	8.89	344.9806				2.91E-01	0.22	0.60	9.33E-01	-0.02	0.37	3.63E-01	0.21	0.55	3.23E-01	0.22	0.50	5759404	246417	5812921	248111	5815035	248040	5810806	250682
RP_POS_464_37329a11_978	RP	POS	11.98	464.3733				2.84E-01	-0.18	1.02	9.33E-01	0.02	0.48	3.80E-01	-0.17	0.58	3.49E-01	-0.19	0.87	11221172	822624	11019780	1168025	11009849	1208810	11029710	1137974
RP_POS_245_11447a8_597	RP	POS	8.60	245.1145	Unknown	245.1135(100)	4	1.16E-03	-0.56	0.97	9.33E-01	-0.02	0.44	7.11E-03	-0.56	0.98	4.30E-03	-0.55	0.99	14461618	708799	13915125	1024528	13923825	941534	13906425	1110899
RP_POS_160_0369a0_59	RP	POS	0.59	160.0369				4.71E-02	0.29	0.79	9.33E-01	0.02	0.69	1.18E-01	0.30	0.87	1.10E-01	0.28	0.87	478464	241139	609434	493588	605266	466294	613602	524179
RP_POS_189_08682a0_625	RP	POS	0.63	189.0868				1.81E-05	-0.67	1.29	9.33E-01	-0.02	1.10	2.29E-04	-0.67	1.39	8.29E-04	-0.66	1.31	4626349	1268571	3180143	2289136	3199464	2428103	3160823	2165822
RP_POS_318_24042a9_59	RP	POS	9.59	318.2404		318.2414(100)	4	5.39E-01	-0.15	0.68	9.33E-01	0.02	0.59	6.09E-01	-0.14	0.63	5.13E-01	-0.16	0.60	4338626	5865935	3647792	4102956	3613143	2547534	3682440	5245920
RP_NEG_352_85284a15_665	RP	NEG	15.67	352.8528				3.21E-01	-0.21	0.38	9.34E-01	0.02	0.24	3.91E-01	-0.20	0.39	3.48E-01	-0.22	0.38	12742543	3451926	12049008	3264507	12021575	3231906	12076442	3329377
RP_POS_266_17236a11_133	RP	POS	11.13	266.1724				2.55E-02	0.37	0.82	9.34E-01	-0.02	0.34	5.18E-02	0.36	0.75	7.06E-02	0.38	0.76	1261222	713286	1642025	1100069	1651253	1212179	1632798	987648
RP_NEG_473_28503a13_276	RP	NEG	13.28	473.2850				8.99E-01	0.03	0.38	9.34E-01	0.02	0.17	8.80E-01	0.03	0.38	9.39E-01	0.02	0.33	132665	80230	134771	83413	134073	82981	135469	84679
RP_NEG_325_27414a10_642	RP	NEG	10.64	325.2741				2.30E-02	-0.38	0.90	9.34E-01	-0.02	0.79	4.15E-02	-0.39	0.91	7.31E-02	-0.37	0.87	705088	113474	643886	171712	645322	184460	642450	159819
RP_POS_545_40173a10_933	RP	POS	10.93	545.4017				4.96E-01	-0.13	0.54	9.34E-01	0.02	0.57	5.80E-01	-0.12	0.49	5.14E-01	-0.14	0.64	19774666	2988905	19349847	3256056	19322701	3126622	19376993	3412169
RP_POS_138_95358a0_253	RP	POS	0.25	138.9536				2.78E-01	0.20	0.73	9.34E-01	0.02	0.20	3.19E-01	0.21	0.40	3.67E-01	0.20	0.75	1750912	583989	1887034	692210	1881276	706461	1892792	684787
RP_NEG_187_94193a15_415	RP	NEG	15.42	187.9419				4.66E-01	-0.14	0.66	9.34E-01	0.02	0.07	5.33E-01	-0.13	0.71	5.17E-01	-0.15	0.35	3819038	452047	3748658	532581	3744228	582689	3753088	483225
RP_NEG_152_88289a0_524	RP	NEG	0.52	152.8829				3.49E-02	0.30	0.89	9.34E-01	-0.02	0.93	1.22E-01	0.29	0.89	7.49E-02	0.31	0.89	2014818	566682	2355624	1243111	2365939	1178147	2345310	1316791
HILIC_NEG_129_05566a0_83	HILIC	NEG	0.83	129.0557				2.51E-01	0.19	0.92	9.34E-01	0.02	0.91	3.56E-01	0.20	0.39	3.07E-01	0.18	0.47	50953156	16153762	55271351	24097944	55071401	19884058	55471300	27889348
RP_POS_163_07553a6_163	RP	POS	6.16	163.0755				4.78E-01	-0.14	0.42	9.34E-01	0.02	0.18	5.52E-01	-0.14	0.38	5.01E-01	-0.15	0.30	7354823	1067392	7199142	1093671	7190079	1087139	7208206	1111126
HILIC_POS_227_12563a1_232	HILIC	POS	1.232	227.1256				3.10E-02	-0.42	1.00	9.35E-01	0.02	0.77	7.01E-02	-0.41	0.66	4.38E-02	-0.42	0.98	165088327	37893882	147503325	42922685	147148548	39616310	147858103	46396163
HILIC_POS_302_19592a1_54	HILIC	POS	1.54	302.1959				3.31E-05	0.56	0.95	9.35E-01	0.02	0.52	2.24E-03	0.57	1.04	1.13E-03	0.55	1.13	372006	244817	715443	670442	709912	632775	720973	712525
HILIC_POS_170_15401a0_687	HILIC	POS	0.687	170.1540				3.06E-01	-0.20	0.91	9.35E-01	-0.02	0.87	3.28E-01	-0.20	0.46	4.06E-01	-0.19	0.32	3481538	448469	3384254	508971	3388444	554128	3380065	465076
HILIC_POS_554_39386a1_321	HILIC	POS	1.321	554.3939				1.17E-02	0.40	1.02	9.35E-01	-0.02	0.53	4.46E-02	0.39	0.72	3.16E-02	0.41	1.07	495716	119747	570771	200637	572417	197588	569124	205634
HILIC_POS_200_06842a4_856	HILIC	POS	4.856	200.0684				2.10E-01	0.22	0.79	9.35E-01	0.02	0.65	2.87E-01	0.23	0.38	2.81E-01	0.21	0.41	3707831	897477	3961839	1228147	3951766	1125693	3971913	1334197
RP_POS_170_97743a15_392	RP	POS	15.39	170.9774				4.11E-02	0.36	0.60	9.35E-01	-0.02	0.42	8.99E-02	0.35	0.59	6.99E-02	0.37	0.66	5163868	2717306	6417393	3635758	6447116	3583931	6387669	3723021
RP_NEG_347_79639a15_613	RP	NEG	15.61	347.7964				3.07E-01	-0.22	0.66	9.35E-01	-0.02	0.52	3.31E-01	-0.23	0.66	3.77E-01	-0.21	0.72	847265	56821	835531	53049	835964	55049	835098	51527
HILIC_NEG_136_89168a1_488	HILIC	NEG	1.488	136.8917				2.09E-01	0.23	0.59	9.36E-01	-0.02	0.90	3.26E-01	0.22	0.35	2.24E-01	0.24	0.51	5434425	1329221	5799781	1663230	5813337	1420071	5786225	1890011
RP_POS_299_25797a10_25	RP	POS	10.25	299.2580				6.93E-01	0.08	0.42	9.36E-01	-0.02	0.16	7.54E-01	0.07	0.53	6.99E-01	0.09	0.56	3756704	578307	3804007	614982	3809013	620577	3799001	615596
RP_POS_326_88602a0_498	RP	POS	0.50	326.8860				5.91E-06	-0.56	1.30	9.36E-01	0.02	1.20	6.54E-04	-0.55	1.38	1.73E-03	-0.57	1.37	14402177	1336862	11105265	6540565	11052025	6989573	11158504	6129527
RP_POS_243_19559a8_339	RP	POS	8.34	243.1956				7.73E-01	0.07	0.52	9.36E-01	0.02	0.43	7.71E-01	0.07	0.49	8.11E-01	0.06	0.35	1904149	247389	1918129	202676	1916485	188169	1919773	218129
HILIC_POS_158_11752a3_102	HILIC	POS	3.102	158.1175				8.28E-01	0.04	0.62	9.36E-01	0.02	0.45	8.24E-01	0.05	0.22	8.69E-01	0.04	0.59	7376692	8839754	7770490	8992590	7697542	8112111	7843437	9877575
HILIC_POS_132_06575a5_65	HILIC	POS	5.65	132.0658				5.33E-01	0.10	0.72	9.36E-01	0.02	0.70	5.96E-01	0.11	0.78	6.09E-01	0.09	0.41	4628137	1548961	4853781	2348061	4834828	2084875	4872733	2606120
RP_POS_563_42761a11_158	RP	POS	11.16	563.4276				9.82E-01	0.00	0.38	9.36E-01	0.02	0.58	9.52E-01	0.01	0.40	9.80E-01	0.00	0.37	550440	392218	552510	586812	547774	552344	557245	624975
RP_POS_143_99864a15_465	RP	POS	15.47	143.9986				3.38E-01	-0.20	0.52	9.36E-01	0.02	0.30	4.08E-01	-0.19	0.43	3.68E-01	-0.21	0.68	2992321	868153	2823360	838059	2816599	836896	2830122	847663
RP_NEG_526_29468a10_551	RP	NEG	10.55	526.2947				1.70E-06	0.86	1.53	9.36E-01	-0.02	0.23	5.49E-05	0.85	1.52	1.18E-05	0.86	1.54	1098452	584845	1776361	781848	1782659	727289	1770063	840248
HILIC_NEG_173_96242a1_299	HILIC	NEG	1.299	173.9624				7.21E-04	0.51	0.88	9.36E-01	0.02	0.83	2.05E-02	0.52	0.84	4.84E-04	0.50	1.45	1370265	171909	1527612	333830	1524929	208886	1530295	426041
HILIC_NEG_334_69348a2_947	HILIC	NEG	2.947	334.6935				7.37E-06	-0.61	1.32	9.37E-01	0.02	0.76	4.16E-04	-0.60	1.45	1.02E-03	-0.61	1.47	1254191	184431	972866	505891	968838	539351	976893	475544
RP_NEG_299_2597a10_775	RP	NEG	10.78	299.2597				1.23E-01	-0.28	0.85	9.37E-01	0.02	0.86	1.81E-01	-0.27	0.69	1.86E-01	-0.29	0.94	4964321	543547	4778446	703233	4772863	753455	4784028	656817
HILIC_POS_126_09161a0_548	HILIC	POS	0.548	126.0916				1.60E-01	0.16	0.68	9.37E-01	-0.02	0.35	3.24E-01	0.15	0.58	3.23E-01	0.17	0.42	424071	335239	16760474	115391565	17675412	122116945	15845536	109489310
RP_POS_313_27365a10_663	RP	POS	10.66	313.2737				2.72E-01	-0.22	0.58	9.37E-01	0.02	0.59	3.30E-01	-0.21	0.58	3.21E-01	-0.23	0.68	1591284	263212	1531707	268318	1529581	287299	1533834	250815
HILIC_NEG_330_69919a2_946	HILIC	NEG	2.946	330.6992				5.99E-06	-0.60	1.33	9.37E-01	0.02	0.76	3.96E-04	-0.59	1.47	1.10E-03	-0.61	1.47	871617	118679	676499	356059	673682	381353	679316	332712
HILIC_POS_346_7193a3_018	HILIC	POS	3.018	346.7193				2.52E-04	-0.53	1.32	9.37E-01	-0.02	0.75	2.42E-03	-0.54	1.40	5.99E-03	-0.52	1.43	317240	65848	247760	142278	248885	149556	246635	136123
RP_POS_626_29712a10_932	RP	POS	10.93	626.2971				3.70E-04	-0.82	1.42	9.38E-01	-0.01	1.11	7.25E-04	-0.83	1.53	8.23E-04	-0.82	1.25	567711	224953	399369	180604	400795	179545	397943	183469
RP_POS_806_05994a13_202	RP	POS	13.20	806.0599				6.66E-04	0.69	1.16	9.38E-01	0.02	0.32	3.22E-03	0.70	1.13	1.11E-03	0.68	1.24	5250051	800951	5843155	831470	5836656	677404	5849654	968417
HILIC_NEG_184_83141a2_949	HILIC	NEG	2.949	184.8314				1.20E-05	-0.56	1.33	9.38E-01	0.02	0.77	7.64E-04	-0.55	1.45	2.16E-03	-0.56	1.49	1827393	176423	1489156	673339	1483899	723564	1494414	626435
RP_NEG_486_86917a0_498	RP	NEG	0.50	486.8692				5.29E-06	-0.57	1.30	9.39E-01	-0.02	1.22	5.34E-04	-0.58	1.38	1.67E-03	-0.56	1.36	1945691	192688	1515406	837187	1521878	875010	1508934	806437
RP_NEG_922_58124a13_876	RP	NEG	13.88	922.5812				3.95E-01	-0.19	0.54	9.39E-01	0.01	0.64	4.78E-01	-0.18	0.55	3.90E-01	-0.20	0.43	5714177	1403583	5477537	1204213	5468229	967134	5486844	1412206
RP_POS_223_09438a13_807	RP	POS	13.81	223.0944				4.78E-01	0.15	0.59	9.39E-01	-0.02	0.23	5.59E-01	0.14	0.36	4.88E-01	0.15	0.38	13140349	5487383	13937375	5493083	13979804	5029498	13894945	5971950
RP_POS_133_03452a15_301	RP	POS	15.30	133.0345				5.43E-01	-0.14	0.51	9.39E-01	0.01	0.71	5.95E-01	-0.13	0.57	5.57E-01	-0.14	0.33	114964928	17646093	112857433	14562842	112744960	14768053	112969905	14503779
HILIC_NEG_434_71805a2_933	HILIC	NEG	2.933	434.7181				2.54E-06	-0.64	1.33	9.39E-01	-0.02	0.76	1.04E-04	-0.64	1.48	9.53E-04	-0.63	1.47	188596	29232	141614	80150	142233	87322	140995	73165
HILIC_NEG_624_69891a2_921	HILIC	NEG	2.921	624.6989				1.47E-06	-0.61	1.34	9.39E-01	0.02	0.76	2.40E-04	-0.60	1.49	7.32E-04	-0.62	1.51	437486	47875	334205	185958	332770	198680	335641	174324
HILIC_POS_522_3562a1_113	HILIC	POS	1.113	522.3562				7.83E-04	0.61	1.15	9.39E-01	0.02	0.71	5.66E-03	0.62	1.05	1.67E-03	0.60	1.28	16564837	8073811	22769754	10335637	22690057	8572743	22849451	11930047
RP_POS_399_30847a10_651	RP	POS	10.65	399.3085				9.96E-01	0.00	0.55	9.39E-01	0.02	0.32	9.70E-01	0.01	0.61	9.78E-01	-0.01	0.53	32437716	3578338	32441204	3428286	32414888	3590378	32467519	3294529
RP_POS_374_26251a11_167	RP	POS	11.17	374.2625				1.50E-08	1.02	1.87	9.39E-01	-0.01	0.85	2.70E-06	1.01	1.66	6.85E-08	1.02	1.99	369733	126466	549296	168636	550589	142093	548004	193036
RP_NEG_333_87619a15_715	RP	NEG	15.72	333.8762				8.57E-01	-0.04	0.72	9.39E-01	-0.02	0.47	8.49E-01	-0.04	0.52	8.99E-01	-0.03	0.43	762006	240190	753015	259131	754998	246992	751032	273230
RP_POS_463_20038a11_254	RP	POS	11.25	463.2004				6.47E-03	0.47	1.40	9.40E-01	-0.02	0.82	2.87E-02	0.47	1.21	1.26E-02	0.48	1.45	566958	246234	722215	342063	724817	310227	719613	374363
RP_POS_383_96194a0_638	RP	POS	0.64	383.9619				6.65E-07	-0.62	1.30	9.40E-01	-0.02	1.16	1.15E-04	-0.63	1.41	7.56E-04	-0.61	1.35	1730065	148224	1364241	646798	1369153	691646	1359328	605647
RP_POS_255_15912a7_727	RP	POS	7.73	255.1591				7.24E-01	-0.07	0.26	9.40E-01	0.02	0.19	7.93E-01	-0.06	0.21	7.15E-01	-0.08	0.41	29659518	1428287	29552881	1623483	29540627	1442428	29565134	1801188
RP_POS_369_1521a6_444	RP	POS	6.44	369.1521		369.1526(100)	4	2.33E-01	-0.23	0.45	9.40E-01	-0.02	0.32	2.81E-01	-0.24	0.43	3.03E-01	-0.22	0.40	8901924	776482	8706261	863678	8712760	848872	8699762	886811
RP_NEG_257_2132a10_235	RP	NEG	10.24	257.2132				2.65E-02	-0.43	0.92	9.41E-01	-0.02	0.79	3.91E-02	-0.43	0.89	6.19E-02	-0.42	0.87	1078333	131314	1015431	150232	1016560	161860	1014302	139279
HILIC_POS_86_07201a1_232	HILIC	POS	1.232	86.0720				1.58E-02	-0.45	1.10	9.41E-01	-0.02	0.75	3.74E-02	-0.46	0.75	3.13E-02	-0.44	1.05	4269824	761192	3865333	921306	3872256	855967	3858410	991037
RP_POS_229_14093a5_601	RP	POS	5.60	229.1409				9.49E-01	0.01	0.38	9.41E-01	-0.02	0.28	9.85E-01	0.00	0.23	9.28E-01	0.02	0.28	1090654	476639	1097197	581394	1101551	602177	1092843	565934
RP_POS_731_60516a13_489	RP	POS	13.49	731.6052				7.29E-02	-0.40	0.71	9.41E-01	-0.01	0.54	8.60E-02	-0.40	0.75	1.13E-01	-0.39	0.67	2358133	1589582	1783562	1383731	1793898	1488855	1773227	1285142
HILIC_POS_132_00327a4_323	HILIC	POS	4.323	132.0033				3.62E-01	0.16	1.00	9.41E-01	-0.02	0.83	4.56E-01	0.15	0.42	4.21E-01	0.17	0.75	29892635	5568047	31038547	7674323	31095832	7878053	30981261	7544667
RP_NEG_224_06204a6_61	RP	NEG	6.61	224.0620				2.62E-01	-0.30	0.76	9.41E-01	0.01	0.42	3.15E-01	-0.29	0.58	2.50E-01	-0.31	0.59	97020869	171848732	60580175	99988124	59835585	66301133	61324765	125707245
RP_POS_269_20935a9_74	RP	POS	9.74	269.2094				5.10E-01	-0.13	0.51	9.42E-01	0.02	0.43	5.73E-01	-0.12	0.34	5.48E-01	-0.14	0.56	1365754	86499	1353858	94181	1353162	100292	1354553	88667
RP_POS_824_57849a11_766	RP	POS	11.77	824.5785				3.85E-02	0.26	0.60	9.42E-01	0.02	0.31	1.48E-01	0.26	0.54	1.12E-01	0.25	0.64	1189883	1355385	2504921	5811449	2462114	5308570	2547728	6328543
RP_POS_318_24023a9_44	RP	POS	9.44	318.2402				7.16E-01	-0.10	0.66	9.42E-01	-0.01	0.36	7.20E-01	-0.11	0.52	7.34E-01	-0.09	0.46	3500683	4899942	3169008	2636539	3188422	2030162	3149594	3149954
RP_NEG_336_785a15_4	RP	NEG	15.40	336.7850				4.70E-01	0.20	0.69	9.42E-01	-0.01	0.40	4.79E-01	0.19	0.62	4.97E-01	0.20	0.42	1253092	165184	1275450	93043	1276134	118922	1274765	57854
HILIC_NEG_158_93895a4_275	HILIC	NEG	4.275	158.9390				5.99E-01	0.10	0.89	9.42E-01	-0.02	0.77	6.73E-01	0.09	0.20	6.26E-01	0.10	0.38	6603429	1247510	6746289	1560406	6757708	1593573	6734870	1542623
RP_POS_726_54169a13_644	RP	POS	13.64	726.5417				1.68E-02	-0.55	0.98	9.42E-01	0.01	0.25	2.96E-02	-0.55	0.95	2.17E-02	-0.56	0.97	1764845	1124559	1222599	897624	1216036	847117	1229162	954048
RP_NEG_294_9538a0_464	RP	NEG	0.46	294.9538				1.17E-06	-0.68	1.31	9.42E-01	-0.02	1.13	1.19E-04	-0.69	1.38	2.50E-04	-0.67	1.38	791293	115774	613487	280779	615530	287654	611445	276639
HILIC_POS_139_12294a1_385	HILIC	POS	1.385	139.1229				3.27E-03	0.58	1.22	9.42E-01	-0.01	0.54	8.61E-03	0.58	1.03	7.85E-03	0.59	1.20	10237668	5289308	13602248	5696905	13643675	5810313	13560822	5639908
RP_POS_283_26303a10_386	RP	POS	10.39	283.2630				7.05E-01	0.06	0.77	9.43E-01	0.02	0.04	7.53E-01	0.06	0.58	7.69E-01	0.05	0.59	2034403	283551	2062513	545342	2058568	460226	2066459	623720
HILIC_NEG_132_92348a2_998	HILIC	NEG	2.998	132.9235				8.78E-01	0.03	0.93	9.43E-01	0.01	0.83	8.65E-01	0.04	0.43	9.14E-01	0.03	0.22	12891589	3117030	12987832	2903197	12966876	2949038	13008788	2886416
RP_POS_388_1694a10_703	RP	POS	10.70	388.1694				1.89E-06	0.70	1.53	9.43E-01	-0.02	0.60	4.98E-05	0.70	1.50	3.33E-04	0.71	1.47	165223	117447	325536	241274	327276	266433	323795	215920
RP_NEG_286_77243a0_522	RP	NEG	0.52	286.7724				1.62E-08	-0.79	1.39	9.43E-01	0.02	1.13	6.41E-06	-0.78	1.51	2.56E-05	-0.79	1.44	1475494	192450	1123429	472173	1120027	501946	1126831	445500
RP_POS_546_245a7_847	RP	POS	7.85	546.2450				8.09E-02	-0.39	0.85	9.43E-01	0.01	0.81	1.16E-01	-0.38	0.72	9.99E-02	-0.40	0.80	633995	61246	612544	52279	612167	51552	612920	53517
RP_POS_217_08084a0_618	RP	POS	0.62	217.0808				3.20E-05	-0.55	1.24	9.43E-01	0.02	1.14	1.34E-03	-0.54	1.30	2.33E-03	-0.56	1.32	5440694	868536	4145421	2583188	4126906	2720000	4163935	2466334
RP_POS_377_21988a11_161	RP	POS	11.16	377.2199				6.33E-01	-0.08	0.71	9.43E-01	-0.02	0.68	6.48E-01	-0.09	0.57	7.23E-01	-0.07	0.67	18094036	1005793	17984243	1437994	17994534	1527475	17973953	1358109
RP_NEG_602_28308a10_5	RP	POS	10.50	602.2831				4.11E-01	0.20	0.80	9.43E-01	0.01	0.11	4.39E-01	0.21	0.60	4.45E-01	0.19	0.63	478989	345391	533715	249695	531928	222899	535501	276184
HILIC_NEG_115_92075a1_415	HILIC	NEG	1.415	115.9208				2.66E-02	-0.36	0.94	9.44E-01	-0.02	0.68	5.83E-02	-0.36	0.70	7.65E-02	-0.35	0.63	19093452	1594996	18224048	2629545	18242795	2693827	18205300	2590888
RP_POS_818_77045a0_498	RP	POS	0.50	818.7705				1.58E-05	-0.54	1.28	9.44E-01	0.02	1.21	1.28E-03	-0.53	1.35	2.22E-03	-0.55	1.35	5650497	631952	4356419	2654423	4337564	2786308	4375274	2543910
RP_POS_476_29556a11_144	RP	POS	11.14	476.2956				1.49E-02	0.39	0.93	9.44E-01	-0.02	0.29	3.43E-02	0.39	0.83	5.26E-02	0.40	0.78	152733	186709	264288	304268	266434	335298	262141	273154
HILIC_NEG_122_92595a2_933	HILIC	NEG	2.933	122.9260				4.11E-07	-0.65	1.34	9.44E-01	0.02	0.77	7.86E-05	-0.64	1.51	4.24E-04	-0.66	1.49	375332	36312	297620	130662	296699	141666	298541	120095
RP_POS_334_14359a9_318	RP	POS	9.32	334.1436				1.14E-01	0.23	0.98	9.44E-01	-0.02	0.44	3.20E-01	0.22	0.74	8.68E-02	0.23	0.79	352860	165571	428117	371293	430730	240848	425504	469583

Supplementary table 1: Metabolomics results (in asceding order according to p-value from progressive ALD vs non-progressive ALD comparison, with molecular features with ID_level of 1-2 first)

								all_ALD_vs_control			Prog_ALD_vs_non-prog_ALD			Prog_ALD_vs_control_ALD			Non-prog_ALD_vs_control			Healthy_control		all_ALD		Non-prog_ALD		Progressive_ALD	
								t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA								
Feature_ID	RP_HILIC	POS_NEG	Average.Rt	Average.Mz	Metabolite.name	curated_MSMS	ID_level	p	d	VIP	p	d	VIP	p	d	VIP	p	d	VIP	Mean	SD	Mean	SD	Mean	SD	Mean	SD
RP_POS_357_19379a11_258	RP	POS	11.26	357.1938				4.35E-05	0.81	1.52	9.45E-01	0.01	0.90	2.59E-04	0.82	1.45	1.55E-04	0.81	1.48	1123127	249302	1352315	270071	1350425	251824	1354204	289728
RP_NEG_284_7753a0_522	RP	NEG	0.52	284.7753				1.90E-08	-0.77	1.39	9.45E-01	0.01	1.14	7.79E-06	-0.76	1.51	3.78E-05	-0.78	1.43	2172952	265548	1669347	694975	1664494	743187	1674200	650740
RP_POS_375_16388a6_593	RP	POS	6.59	375.1639				2.14E-01	-0.24	0.45	9.45E-01	-0.01	0.33	2.55E-01	-0.25	0.45	2.93E-01	-0.23	0.47	1640124	182216	1592088	205910	1593518	211560	1590657	202241
RP_NEG_378_98596a6_755	RP	NEG	6.76	378.9860				8.04E-01	-0.05	0.48	9.46E-01	-0.01	0.35	8.04E-01	-0.06	0.29	8.44E-01	-0.04	0.44	2703241	843272	2660916	813633	2666489	779735	2655342	854083
RP_NEG_564_34491a11_625	RP	NEG	11.63	564.3449				1.39E-01	0.23	0.66	9.46E-01	0.01	0.38	2.40E-01	0.24	0.65	2.10E-01	0.23	0.83	4628617	816161	4930082	1412217	4920407	1274672	4939757	1550624
RP_POS_155_02971a15_449	RP	POS	15.45	155.0297				6.26E-01	-0.11	0.59	9.46E-01	0.01	0.30	6.73E-01	-0.11	0.36	6.33E-01	-0.12	0.64	16064855	701745	15998126	561391	15994302	554149	16001950	574142
RP_POS_304_26099a10_847	RP	POS	10.85	304.2610				5.38E-06	0.86	1.35	9.46E-01	-0.01	0.24	7.59E-05	0.85	1.36	2.69E-05	0.86	1.57	525115769	132986682	666688280	160033711	667777152	151571566	665599408	169610988
HILIC_NEG_518_67914a2_932	HILIC	NEG	2.932	518.6791				7.68E-07	-0.66	1.32	9.46E-01	0.01	0.75	1.13E-04	-0.65	1.46	3.58E-04	-0.66	1.48	167612	24159	124280	71618	123796	76349	124764	67330
HILIC_POS_154_0864a0_546	HILIC	POS	0.546	154.0864				1.57E-01	0.16	0.69	9.47E-01	-0.02	0.35	3.20E-01	0.16	0.58	3.19E-01	0.17	0.42	171922	113896	7091917	48468142	7418540	50944511	6765294	46375670
RP_POS_273_10992a8_624	RP	POS	8.62	273.1099				7.50E-01	-0.06	0.31	9.47E-01	-0.01	0.40	7.66E-01	-0.07	0.33	7.90E-01	-0.06	0.36	3043253	208720	3029406	225716	3030925	196255	3027886	253800
RP_POS_780_55298a12_465	RP	POS	12.47	780.5530				5.42E-03	-0.64	1.08	9.47E-01	-0.01	0.58	1.03E-02	-0.64	1.12	8.31E-03	-0.63	1.02	8810069	5034252	5947898	4083449	5975327	3713749	5920469	4460486
RP_POS_569_43268a11_608	RP	POS	11.61	569.4327				9.51E-01	0.01	0.84	9.47E-01	0.01	0.67	9.29E-01	0.02	0.51	9.82E-01	0.01	0.72	4577811	1110052	4592053	1193305	4584055	1314680	4600052	1071681
HILIC_NEG_266_79578a2_936	HILIC	NEG	2.936	266.7958				1.00E-06	-0.63	1.34	9.47E-01	0.01	0.76	1.44E-04	-0.62	1.49	5.83E-04	-0.64	1.50	656150	75558	505569	260925	503824	280936	507315	242119
RP_POS_163_97723a7_1	RP	POS	7.10	163.9772				9.13E-01	-0.02	0.37	9.47E-01	-0.01	0.14	8.97E-01	-0.03	0.44	9.46E-01	-0.02	0.67	28387358	6793591	28237057	6591851	28280956	6960867	28193158	6271697
RP_POS_890_78992a11_672	RP	POS	11.67	890.7899				6.70E-02	-0.48	0.86	9.47E-01	0.01	0.46	8.56E-02	-0.47	0.77	7.46E-02	-0.48	0.84	666808	727961	410249	443619	407305	426786	413193	464163
RP_NEG_893_19391a9_868	RP	NEG	9.87	893.1939				2.08E-01	-0.27	0.70	9.48E-01	-0.01	0.45	2.39E-01	-0.28	0.54	2.62E-01	-0.27	0.61	4749487	341251	4662965	308696	4665012	311132	4660917	309385
RP_POS_282_27994a11_254	RP	POS	11.25	282.2799				4.28E-08	0.81	1.23	9.48E-01	-0.01	0.43	9.12E-05	0.80	1.26	5.50E-07	0.82	1.59	7831501	2812743	12325290	5780982	12363580	4715011	12287001	6729579
RP_NEG_556_3266a8_911	RP	NEG	8.91	556.3266				9.40E-04	-0.52	1.34	9.48E-01	-0.01	0.52	2.18E-02	-0.51	1.27	6.53E-04	-0.53	1.29	3596400	1031271	2718829	1809526	2706850	1207723	2730809	2270837
RP_POS_223_13063a7_184	RP	POS	7.18	223.1306				8.29E-01	0.05	0.57	9.48E-01	-0.01	0.63	8.68E-01	0.04	0.41	8.17E-01	0.05	0.59	1633155	221649	1642678	195399	1643970	177500	1641386	213614
HILIC_NEG_205_83936a3_059	HILIC	NEG	3.059	205.8394				2.01E-01	0.21	1.05	9.48E-01	-0.01	0.82	2.93E-01	0.20	0.61	2.79E-01	0.22	0.95	3941947	747297	4167112	1145310	4174626	1186528	4159598	1114574
HILIC_NEG_100_93327a2_941	HILIC	NEG	2.941	100.9333				3.35E-03	0.44	1.13	9.49E-01	-0.01	0.79	1.52E-02	0.43	1.01	2.31E-02	0.44	1.11	15869858	1512956	17081302	3023184	17100970	3241969	17061635	2820400
RP_POS_851_55768a13_718	RP	POS	13.72	851.5577				2.32E-01	0.24	0.45	9.49E-01	-0.01	0.61	2.80E-01	0.24	0.52	2.98E-01	0.23	0.64	2970289	1293267	3294477	1400706	3285505	1378472	3303449	1436539
HILIC_NEG_250_95161a1_203	HILIC	NEG	1.203	250.9516				7.17E-08	0.79	1.44	9.49E-01	-0.01	0.69	8.08E-06	0.80	1.43	4.04E-05	0.78	1.35	904792	810718	2190115	1703757	2179229	1796466	2201002	1623972
HILIC_POS_224_12802a5_648	HILIC	POS	5.648	224.1280				8.86E-01	-0.03	0.63	9.49E-01	-0.01	0.64	9.24E-01	-0.02	0.03	8.73E-01	-0.03	0.10	6281780	1090906	6249441	1160690	6242030	1095683	6256852	1233395
RP_POS_279_19238a9_193	RP	POS	9.19	279.1924	Unknown	279.1907(100)	4	5.76E-01	-0.11	0.51	9.50E-01	-0.01	0.67	6.40E-01	-0.10	0.33	6.07E-01	-0.11	0.66	3647778	372753	3603773	422737	3601096	436628	3606449	412797
RP_POS_499_82739a5_296	RP	POS	5.30	499.8274				6.57E-02	0.28	0.80	9.50E-01	-0.01	0.62	1.65E-01	0.28	0.49	1.10E-01	0.27	0.79	1587808	1525868	2331310	2948963	2312641	2536807	2349979	3336786
HILIC_POS_195_11623a0_846	HILIC	POS	0.846	195.1162				5.00E-01	0.13	0.59	9.50E-01	-0.01	0.60	5.77E-01	0.12	0.25	5.35E-01	0.13	0.24	1242000	342255	1291542	407745	1294122	409192	1288962	410430
RP_POS_167_05643a0_727	RP	POS	0.73	167.0564				4.76E-04	-0.95	1.72	9.50E-01	-0.01	0.41	7.81E-04	-0.94	1.47	5.68E-04	-0.95	1.69	1349957	1117073	557413	618431	553523	570279	561304	668932
RP_POS_392_1918a6_593	RP	POS	6.59	392.1918				9.69E-02	-0.32	0.65	9.50E-01	-0.01	0.56	1.24E-01	-0.32	0.65	1.64E-01	-0.31	0.65	3726086	415964	3578340	476098	3581330	509000	3575350	445943
HILIC_NEG_115_92074a5_742	HILIC	NEG	5.742	115.9207				5.51E-01	-0.11	0.49	9.51E-01	-0.01	0.48	6.49E-01	-0.10	0.28	5.61E-01	-0.11	0.41	38546348	5887877	37779216	7470965	37732777	6545924	37825655	8361590
RP_POS_772_58411a13_557	RP	POS	13.56	772.5841				1.02E-06	-1.36	2.20	9.51E-01	0.01	0.77	1.31E-06	-1.35	2.03	1.21E-06	-1.36	1.92	18093793	7552710	9947229	3672301	9924481	3730038	9969977	3651379
RP_POS_223_09416a12_89	RP	POS	12.89	223.0942				9.80E-01	0.00	0.35	9.51E-01	0.01	0.54	9.60E-01	0.01	0.22	9.93E-01	0.00	0.17	12336300	4636317	12360831	5579098	12326344	5217791	12395318	5971611
HILIC_NEG_186_93375a1_687	HILIC	NEG	1.687	186.9338				2.54E-02	-0.47	1.05	9.51E-01	0.01	0.62	3.91E-02	-0.47	0.82	4.43E-02	-0.48	1.06	3021863	1772249	2201934	1688297	2191559	1815498	2212310	1569270
RP_NEG_966_56793a13_977	RP	NEG	13.98	966.5679				1.43E-02	0.43	1.12	9.51E-01	-0.01	0.63	3.00E-02	0.44	0.97	4.19E-02	0.42	1.10	2308770	1481707	3140221	2022931	3127803	2099941	3152639	1964166
RP_POS_141_95854a0_25	RP	POS	0.25	141.9585				6.01E-01	-0.11	0.43	9.52E-01	-0.01	0.24	6.17E-01	-0.12	0.34	6.56E-01	-0.10	0.33	4492559	486269	4441118	464682	4443962	470784	4438273	463261
HILIC_NEG_174_95631a7_95	HILIC	NEG	7.95	174.9563				3.17E-04	-0.48	0.86	9.52E-01	-0.01	0.58	7.81E-03	-0.48	1.06	5.19E-03	-0.49	0.91	63431015	9425078	51918764	26264163	51758405	26012024	52079124	26777085
HILIC_NEG_332_69598a2_946	HILIC	NEG	2.946	332.6960				1.20E-05	-0.58	1.33	9.52E-01	0.01	0.76	5.79E-04	-0.57	1.45	1.66E-03	-0.59	1.46	1618089	220137	1269428	659504	1265411	707153	1273446	615362
RP_NEG_188_98595a2_662	RP	NEG	2.66	188.9860				1.09E-01	-0.37	0.80	9.52E-01	-0.01	0.67	1.52E-01	-0.36	0.77	1.22E-01	-0.37	0.79	3773333	3081452	2793458	2481027	2778373	2282836	2808544	2687901
RP_POS_159_96918a0_88	RP	POS	0.88	159.9692				2.61E-01	-0.25	0.49	9.52E-01	-0.01	0.26	2.88E-01	-0.25	0.51	3.18E-01	-0.24	0.55	6504952	3170698	5794915	2746646	5811527	2834925	5778302	2684162
RP_NEG_282_98325a7_564	RP	NEG	7.56	282.9833				7.55E-01	-0.07	0.66	9.52E-01	-0.01	0.27	7.62E-01	-0.07	0.60	7.94E-01	-0.06	0.44	4260721	988860	4198285	942438	4203960	902505	4192609	989911
RP_POS_497_39612a10_981	RP	POS	10.98	497.3961				1.31E-01	0.31	0.93	9.52E-01	0.01	1.05	1.87E-01	0.31	0.86	1.62E-01	0.30	0.85	1174452	397474	1298592	402402	1296176	351582	1301008	451152
RP_POS_424_28171a11_038	RP	POS	11.04	424.2817				7.82E-02	0.33	0.68	9.52E-01	-0.01	0.29	1.30E-01	0.33	0.61	1.15E-01	0.34	0.63	1249683	2024546	2019381	2376240	2033644	2379444	2005117	2397103
RP_POS_246_8624a0_246	RP	POS	0.25	246.8624				9.73E-01	0.01	0.30	9.53E-01	0.01	0.44	9.52E-01	0.01	0.25	9.99E-01	0.00	0.53	3721339	470991	3724649	539231	3721418	589365	3727879	490001
HILIC_POS_356_7482a3_014	HILIC	POS	3.014	356.7482				4.74E-05	-0.56	1.34	9.53E-01	-0.01	0.77	1.23E-03	-0.56	1.46	2.31E-03	-0.57	1.44	355214	65235	271649	161109	270686	170279	272611	153118
HILIC_NEG_160_842a2_961	HILIC	NEG	2.961	160.8420				6.64E-01	0.08	1.03	9.53E-01	-0.01	0.79	7.11E-01	0.08	0.70	6.95E-01	0.09	0.93	39132139	8830973	39943141	10047423	40003181	11080131	39883101	9010272
HILIC_POS_330_22736a0_901	HILIC	POS	0.901	330.2274				6.47E-01	0.08	0.60	9.53E-01	-0.01	0.87	7.25E-01	0.08	0.39	6.54E-01	0.09	0.34	377228	167589	393894	207890	395136	188333	392652	227697
RP_POS_1005_68726a10_931	RP	POS	10.93	1005.6873				8.16E-01	0.05	0.98	9.53E-01	0.01	1.13	8.26E-01	0.05	0.66	8.45E-01	0.04	0.85	1015435	604958	1044382	620158	1040681	503524	1048084	723517
HILIC_POS_116_89114a3_019	HILIC	POS	3.019	116.8911				3.20E-06	-0.62	1.37	9.53E-01	-0.01	0.78	2.47E-04	-0.61	1.52	7.69E-04	-0.63	1.49	1866747	255387	1444295	740728	1439878	792158	1448711	693542
RP_POS_423_32294a11_416	RP	POS	11.42	423.3229				5.12E-01	0.11	0.78	9.53E-01	-0.01	0.78	6.04E-01	0.10	0.63	5.60E-01	0.12	0.63	807068	667747	908491	987471	914308	991896	902674	993061
RP_POS_523_42212a10_881	RP	POS	10.88	523.4221				4.98E-01	-0.12	0.46	9.53E-01	-0.01	0.11	5.02E-01	-0.13	0.50	6.14E-01	-0.11	0.39	2548200	286454	2504722	387853	2507004	449524	2502440	319135
RP_POS_389_23569a11_379	RP	POS	11.38	389.2357				7.24E-04	-0.60	1.11	9.54E-01	-0.01	0.89	1.31E-03	-0.60	1.20	7.43E-03	-0.59	1.05	914654	130291	811838	177700	812874	205254	810801	147198
RP_NEG_244_98633a6_179	RP	NEG	6.18	244.9863				9.54E-01	-0.01	1.05	9.54E-01	-0.01	0.52	9.41E-01	-0.02	1.16	9.75E-01	-0.01	0.67	3840908	1896159	3819705	1513127	3828521	1471252	3810890	1568787
RP_NEG_164_07065a1_452	RP	NEG	1.45	164.0707				4.62E-02	-0.47	0.97	9.54E-01	-0.01	0.52	6.46E-02	-0.48	0.80	5.94E-02	-0.47	1.03	834601	474290	647161	361883	649266	331623	645055	393202
HILIC_POS_630_68988a2_992	HILIC	POS	2.992	630.6899				5.81E-06	-0.61	1.35	9.54E-01	-0.01	0.76	2.35E-04	-0.62	1.48	1.26E-03	-0.61	1.47	437871	63661	339329	175263	340339	188390	338319	162998
RP_POS_261_13071a13_014	RP	POS	13.01	261.1307				6.66E-02	-0.34	0.65	9.55E-01	0.01	0.25	1.38E-01	-0.33	0.68	8.56E-02	-0.34	0.88	2510855	439201	2333215	551134	2330057	486157	2336373	614270
RP_POS_353_03558a0_617	RP	POS	0.62	353.0356				4.40E-10	-0.79	1.40	9.55E-01	-0.01	1.14	1.28E-06	-0.80	1.59	2.12E-05	-0.79	1.44	1334960	140000	923194	555840	926375	598343	920012	515933
RP_POS_377_30374a11_038	RP	POS	11.04	377.3037				1.42E-02	-0.46	1.03	9.56E-01	-0.01	0.94	2.12E-02	-0.46	1.04	4.33E-02	-0.45	0.98	1701902	322426	1528009	387467	1530179	432400	1525840	341095
HILIC_NEG_181_83746a3_043	HILIC	NEG	3.043	181.8375				4.35E-06	0.72	1.19	9.56E-01	-0.01	0.69	1.43E-04	0.72	1.28	1.85E-04	0.71	1.28	324342	140642	496522	250920	495119	252604	497925	251781
RP_POS_190_99968a0_257	RP	POS	0.26	190.9997				9.73E-01	-0.01	0.32	9.56E-01	-0.01	0.42	9.51E-01	-0.01	0.44	9.98E-01	0.00	0.26	1326287	144762	1325219	178434	1326215	200796	1324222	154940
RP_POS_203_62335a10_849	RP	POS	10.85	203.6234				3.73E-06	0.72	1.18	9.56E-01	-0.01	0.69	6.64E-04	0.72	1.17	1.42E-05	0.71	1.39	5673843	1704869	7790496	3085103	7773261	2397257	7807730	3671854
RP_POS_229_14133a5_663	RP	POS	5.66	229.1413				8.63E-01	0.03	0.44	9.56E-01	-0.01	0.31	8.59E-01	0.04	0.30	8.99E-01	0.03	0.41	924967	381245	938813	424037	936452	422753	941174	429597
RP_POS_263_20062a9_307	RP	POS	9.31	263.2006				1.78E-03	0.36	0.76	9.56E-01	-0.01	0.77	3.78E-03	0.37	1.13	6.92E-02	0.36	0.71	66349	30869	1215872	3578855	1196110	4299510	1235634	2718679
RP_NEG_774_79639a0_496	RP	NEG	0.50	774.7964				3.83E-06	-0.58	1.29	9.57E-01	0.01	1.20	6.66E-04	-0.58	1.35	8.74E-04	-0.59	1.35	1305966	144097	1002708	573456	999576	590204	1005840	562187
HILIC_NEG_556_49017a2_945	HILIC	NEG	2.945	556.4902				1.57E-04	-0.57	1.28	9.57E-01	-0.01	0.75	1.25E-03	-0.57	1.39	4.06E-03	-0.56	1.38	134968	30654	103392	59516	103716	63945	103069	55384
RP_POS_188_12798a0_619	RP	POS	0.62	188.1280				6.58E-01	0.09	0.21	9.57E-01	-0.01	0.10	7.04E-01	0.09	0.20	6.73E-01	0.10	0.19	268724	219449	288203	203035	289302	206769	287104	201325
RP_NEG_312_97357a8_477	RP	NEG	8.48	312.9736				1.97E-01	-0.25	0.52	9.57E-01	-0.01	0.13	2.39E-01	-0.26	0.51	2.66E-01	-0.25	0.53	1754532	105536	1726028	113840	1726641	116295	1725414	112509
RP_POS_902_58533a14_328	RP	POS	14.33	902.5853				7.71E-01	-0.07	0.92	9.57E-01	-0.01	0.19	7.76E-01	-0.07	0.64	8.00E-01	-0.06	0.72	1259483	938262	1205888	765351	1210003	719733	1201773	815739
RP_POS_191_10657a6_585	RP	POS	6.59	191.1066				8.24E-01	0.04	0.44	9.57E-01	0.01	0.45	8.24E-01	0.05	0.24	8.68E-01	0.04	0.32	349738	213338	359863	252309	358507	258813	361219	248256
RP_POS_262_91586a15_43	RP	POS	15.43	262.9159				6.41E-01	0.11	0.26	9.58E-01	0.01	0.13	6.36E-01	0.11	0.24	6.91E-01	0.10	0.28	16701248	1963444	16878675	1497329	16870653	1722020	16886698	1250702
HILIC_POS_260_18558a1_087	HILIC	POS	1.087	260.1856				2.31E-01	0.17	0.33	9.58E-01	-0.01	0.59	3.90E-01	0.16	0.43	3.12E-01	0.17	0.36	9351553	7368161	11956012	17283358	12048543	16319471	11863480	18362532
RP_NEG_459_11221a0_707	RP	NEG	0.71	459.1122				7.02E-03	-0.41	1.07	9.58E-01	-0.01	1.05	2.09E-02	-0.42	1.07	3.92E-02	-0.41	1.12	1882133	500470	1527821	934794	1532816	997488	1522826	877770
HILIC_POS_114_09164a0_505	HILIC	POS	0.505	114.0916				1.17E-04	-0.64	1.25	9.58E-01	-0.01	0.73	7.27E-04	-0.64	1.36	1.79E-03	-0.63	1.31	318186070	86956286	235345726	135150859	236065908	143074384	234625545	128191038
HILIC_POS_339_0376a5_461	HILIC	POS	5.461	339.0376				4.61E-02	-0.40	0.83	9.58E-01	-0.01	0.29	6.67E-02	-0.39	0.78	8.19E-02	-0.40	0.88	1100370	128984	1046139	136574	1045411	150161	1046867	123027
RP_POS_156_95285a15_566	RP	POS	15.57	156.9529				6.51E-01	0.09	0.58	9.58E-01	-0.01	0.23	7.10E-01	0.09	0.45	6.60E-01	0.10	0.59	11003270	1125429	11107195	1125178	11113178	1052749	11101212	1203966
RP_POS_185_05739a6_163	RP	POS	6.16	185.0574				3.93E-01	-0.17	0.36	9.58E-01	-0.01	0.16	4.73E-01	-0.16	0.33	4.27E-01	-0.17	0.29	2820773	425609	2744633	466145	2742171	447102	2747094	488982
HILIC_NEG_134_89481a7_675	HILIC	NEG	7.675	134.8948				1.57E-03	-0.57	0.95	9.58E-01	-0.01	0.27	3.72E-03	-0.58	1.09	8.94E-03	-0.56	0.92	40324318	4703700	36925768	6103619	36957987	6655215	36893549	5565485
HILIC_POS_616_66266a3_005	HILIC	POS	3.005	616.6627				7.51E-05	-0.54	1.35	9.58E-01	0.01	0.76	1.79E-03	-0.54	1.46	3.11E-03	-0.55	1.43	528239	96241	405910	245497	404621	258394	407199	234514
RP_POS_576_67114a10_876	RP	POS	10.88	576.6711				4.62E-01	-0.09	0.37	9.59E-01	-0.01	0.22	6.33E-01	-0.10	0.47	4.89E-01	-0.09	0.35	1172240	146803	1127715	544150	1130555	381975	1124874	672548
RP_POS_619_47931a11_387	RP	POS	11.39	619.4793				2.07E-01	-0.23	0.84	9.59E-01	0.01	0.23	2.88E-01	-0.23	0.61	2.56E-01	-0.24	0.63	848951	378302	745355	460880	742963	453652	747746	472593
RP_NEG_765_16821a9_606	RP	NEG	9.61	765.1682				1.17E-01	-0.30	0.49	9.59E-01	-0.01	0.57	1.60E-01	-0.30	0.54	1.76E-01	-0.29	0.49	10934245	932987	10621149	1074833	10626706	1081775	10615593	1078799
RP_NEG_299_25943a11_158	RP	NEG	11.16	299.2594				5.31E-01	0.11	0.97	9.59E-01	-0.01	0.92	5.95E-01	0.11	0.84	5.87E-01	0.12	0.97	12797287	3547133	13289862	4674779	13313921	5029225	13265802	4342676
RP_POS_530_32129a10_388	RP	POS	10.39	530.3213				1.41E-02	0.45	1.11	9.59E-01	0.01	0.84	4.08E-02	0.46	0.93	2.31E-02	0.45	1.04	1626424	598991	1951852	734137	1948086	629803	1955618	832005
HILIC_POS_534_69897a3_006	HILIC	POS	3.006	534.6990				5.40E-05	-0.55	1.35	9.59E-01	0.01	0.77	1.53E-03	-0.54	1.47	2.73E-03	-0.56	1.46	810381	143090	619940	378942	617998	398745	621883	362104
RP_POS_164_02917a0_529	RP	POS	0.53	164.0292				2.36E-01	0.18	1.14	9.59E-01	0.01	0.98	3.64E-01	0.19	1.07	2.95E-01	0.18	1.06	433282	134331	473229	236000	472021	198239	474437	270605
RP_POS_223_20541a8_904	RP	POS	8.90	223.2054	Unknown	223.0948(100), 135.1169(35), 73.0653(25)	4	7.78E-01	0.05	0.42	9.60E-01	0.01	0.44	7.87E-01	0.06	0.32	8.27E-01	0.05	0.39	654353	307462	673039	374138	671127	378601	674951	373456
HILIC_POS_260_76056a3_023	HILIC	POS	3.023	260.7606				3.14E-04	-0.51	1.33	9.60E-01	0.01	0.76	4.28E-03	-0.50	1.42	6.02E-03	-0.51	1.43	1041283	207885	814452	488427	811962	510070	816943	470965
HILIC_POS_130_15916a0_576	HILIC	POS	0.576	130.1592				2.07E-01	-0.20	0.69	9.60E-01	0.01	0.46	2.85E-01	-0.19	0.37	3.20E-01	-0.20	0.38	5675973	762281	5435228	1334062	5428459	1464235	5441996	1204859
RP_POS_160_05946a0_622	RP	POS	0.62	160.0595				1.02E-04	-0.56	1.21	9.60E-01	0.01	1.09	1.73E-03	-0.55	1.26	3.03E-03	-0.56	1.28	2432339	578612	1769466	1291548	1762969	1361925	1775963	1230980

Supplementary table 1: Metabolomics results (in asceding order according to p-value from progressive ALD vs non-progressive ALD comparison, with molecular features with ID_level of 1-2 first)

								all_ALD_vs_control			Prog_ALD_vs_non-prog_ALD			Prog_ALD_vs_control_ALD			Non-prog_ALD_vs_control			Healthy_control		all_ALD		Non-prog_ALD		Progressive_ALD	
								t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA								
Feature_ID	RP_HILIC	POS_NEG	Average.Rt	Average.Mz	Metabolite.name	curated_MSMS	ID_level	p	d	VIP	p	d	VIP	p	d	VIP	p	d	VIP	Mean	SD	Mean	SD	Mean	SD	Mean	SD
RP_NEG_850_59747a10_918	RP	NEG	10.92	850.5975				5.48E-03	0.40	1.41	9.60E-01	-0.01	0.35	3.86E-02	0.40	1.00	1.96E-02	0.41	1.33	1176658	497150	1566120	1057695	1571436	991842	1560805	1129806
RP_NEG_280_98236a9_007	RP	NEG	9.01	280.9824				1.97E-01	-0.18	0.41	9.60E-01	-0.01	0.30	8.79E-02	-0.19	0.77	4.45E-01	-0.18	0.66	4064893	183128	3996651	414665	3998737	563444	3994566	172989
RP_POS_539_3540fa9_527	RP	POS	9.53	539.3541				1.73E-02	-0.44	0.86	9.61E-01	0.01	0.58	3.43E-02	-0.43	0.81	4.09E-02	-0.44	0.88	518762	25574	505272	31635	505115	33647	505429	29829
RP_POS_190_91154a0_499	RP	POS	0.50	190.9115				5.91E-05	-0.50	1.26	9.61E-01	-0.01	1.21	1.65E-03	-0.51	1.33	6.16E-03	-0.50	1.32	7917946	942463	6190279	3807291	6209181	4080442	6171376	3554719
RP_NEG_377_20117a10_157	RP	NEG	10.16	377.2012				6.06E-01	-0.13	0.70	9.61E-01	0.01	0.93	6.24E-01	-0.13	0.26	6.24E-01	-0.14	0.78	7032262	6225425	6427477	3793217	6408705	4387511	6446248	3133633
RP_NEG_369_00562a1_093	RP	NEG	1.09	369.0056				2.03E-01	-0.27	0.76	9.61E-01	-0.01	0.94	2.31E-01	-0.27	0.74	2.66E-01	-0.26	0.77	1438141	1154486	1138604	1102804	1144059	1165658	1133148	1048024
RP_POS_589_56335a11_166	RP	POS	11.17	589.5634				1.40E-10	0.86	1.38	9.61E-01	0.01	0.80	1.05E-05	0.86	1.44	7.71E-08	0.85	1.57	740466	519832	1963209	1491985	1955833	1276001	1970584	1693864
RP_NEG_349_90378a15_451	RP	NEG	15.45	349.9038				2.88E-01	-0.18	0.38	9.61E-01	0.01	0.47	3.69E-01	-0.18	0.60	3.64E-01	-0.19	0.47	2684483	247535	2625001	342989	2623324	358960	2626678	329888
RP_POS_1067_69702a10_617	RP	POS	10.62	1067.6970				1.24E-03	0.63	1.40	9.62E-01	0.01	0.98	7.81E-03	0.63	1.21	1.46E-03	0.62	1.44	1113500	588105	1531655	659572	1528458	477866	1534852	806581
RP_POS_232_92702a15_334	RP	POS	15.33	232.9270				5.41E-01	0.14	0.72	9.62E-01	-0.01	0.32	5.75E-01	0.13	0.59	5.73E-01	0.14	0.97	1165279	82632	1175255	69728	1175592	76573	1174918	62925
HILIC_NEG_100_93346a0_745	HILIC	NEG	0.745	100.9335				6.15E-06	0.70	1.26	9.62E-01	0.01	0.27	1.51E-04	0.70	1.42	3.32E-04	0.69	1.21	6967797	2058153	9475112	3777733	9457105	3916593	9493120	3673340
HILIC_POS_375_32132a0_892	HILIC	POS	0.892	375.3213				9.03E-01	0.02	0.37	9.62E-01	0.01	0.77	9.03E-01	0.03	0.08	9.29E-01	0.02	0.35	5306213	601418	5322063	729094	5318598	624649	5325529	826919
RP_NEG_351_02167a0_619	RP	NEG	0.62	351.0217				8.19E-08	-0.74	1.34	9.63E-01	0.01	1.13	1.62E-05	-0.73	1.48	8.65E-05	-0.74	1.37	1924883	319496	1359062	816519	1355212	876981	1362912	760190
HILIC_NEG_134_89473a7_497	HILIC	NEG	7.497	134.8947				3.21E-02	-0.49	1.00	9.63E-01	-0.01	0.66	4.47E-02	-0.49	0.85	4.84E-02	-0.48	1.07	13936830	5436584	11594222	4456305	11615080	4476172	11573364	4481695
HILIC_POS_90_09194a1_707	HILIC	POS	1.707	90.0919				2.12E-02	-0.40	1.19	9.63E-01	0.01	0.72	5.21E-02	-0.40	1.13	4.51E-02	-0.41	1.01	2046068	398720	1836169	545024	1833642	544028	1838695	551530
RP_POS_589_42773a10_929	RP	POS	10.93	589.4277				7.85E-01	-0.06	1.09	9.63E-01	-0.01	0.05	7.93E-01	-0.06	0.86	8.22E-01	-0.05	1.05	14398381	1972031	14288572	1978778	14297741	1949489	14279402	2027401
RP_POS_339_25104a10_258	RP	POS	10.26	339.2510				5.71E-02	-0.38	0.84	9.64E-01	-0.01	0.76	7.79E-02	-0.38	0.74	1.01E-01	-0.37	0.94	1103232	156038	1040691	165734	1041456	176237	1039927	156319
HILIC_POS_151_03519a7_377	HILIC	POS	7.377	151.0352				5.23E-05	-0.62	1.20	9.64E-01	-0.01	0.80	1.01E-03	-0.62	1.24	9.77E-04	-0.63	1.28	14317902	1526856	12671137	2804107	12658397	2843042	12683876	2793437
RP_POS_221_0696a15_34	RP	POS	15.34	221.0696				1.77E-02	0.47	1.14	9.65E-01	-0.01	0.51	3.74E-02	0.47	1.00	3.06E-02	0.47	1.27	3968500	1429951	4692539	1542478	4699342	1511338	4685736	1588332
HILIC_NEG_128_92854a5_426	HILIC	NEG	5.426	128.9285				1.93E-02	-0.52	0.84	9.66E-01	-0.01	0.55	3.53E-02	-0.51	0.83	2.67E-02	-0.52	0.93	2714127	410018	2518364	357574	2516809	336895	2519918	380557
RP_POS_190_01431a15_422	RP	POS	15.42	190.0143				7.74E-01	-0.06	0.67	9.66E-01	-0.01	0.39	7.79E-01	-0.06	0.37	8.15E-01	-0.05	0.33	2543533	618333	2507144	629406	2509859	656181	2504429	608112
RP_NEG_144_92305a14_262	RP	NEG	14.26	144.9231				2.58E-01	-0.21	0.56	9.66E-01	-0.01	0.43	3.43E-01	-0.22	0.49	2.99E-01	-0.21	0.53	1051900	322086	973646	382420	975291	325908	972001	435033
RP_POS_469_16885a6_836	RP	POS	6.84	469.1689	Unknown	469.1664(100), 325.125(35), 397.1505(33)	4	2.07E-01	-0.23	0.59	9.66E-01	-0.01	0.30	2.65E-01	-0.24	0.50	2.79E-01	-0.23	0.46	1306840	126309	1272298	153429	1272954	152634	1271642	155767
RP_POS_400_22595a11_255	RP	POS	11.26	400.2260				4.54E-05	0.75	1.54	9.66E-01	0.01	1.17	5.28E-04	0.75	1.47	1.77E-04	0.75	1.54	3687957	729564	4379981	918095	4376056	825315	4383905	1010853
RP_POS_872_55444a13_711	RP	POS	13.71	872.5544				3.24E-03	-0.70	1.28	9.67E-01	-0.01	0.59	5.62E-03	-0.71	1.14	5.15E-03	-0.70	1.31	1194190	822451	701686	615544	704290	589366	699083	646649
RP_POS_292_9249a15_444	RP	POS	15.44	292.9249				3.79E-02	-0.47	0.84	9.67E-01	-0.01	0.27	4.51E-02	-0.46	0.86	6.47E-02	-0.47	0.84	2157352	361031	2006228	304519	2004951	353876	2007506	249248
RP_POS_175_10779a0_621	RP	POS	0.62	175.1078				9.42E-03	0.46	0.98	9.67E-01	0.01	0.26	2.70E-02	0.46	0.80	2.41E-02	0.45	1.32	685088	551834	1012858	745387	1009735	721297	1015980	776050
RP_NEG_224_06238a6_09	RP	NEG	6.09	224.0624				2.59E-01	0.15	0.58	9.67E-01	-0.01	0.15	4.85E-01	0.14	0.50	2.72E-01	0.15	0.72	674323	480237	873076	1533327	879490	1165902	866661	1841399
HILIC_NEG_134_89465a7_947	HILIC	NEG	7.947	134.8947				8.74E-01	-0.03	0.43	9.67E-01	-0.01	0.58	8.72E-01	-0.04	0.09	9.03E-01	-0.03	0.72	16095041	10176427	15759270	10859777	15804669	11070512	15713872	10757132
HILIC_NEG_136_89175a3_013	HILIC	NEG	3.013	136.8918				6.04E-01	0.10	0.95	9.67E-01	-0.01	0.81	6.67E-01	0.09	0.19	6.35E-01	0.10	0.27	85136215	13769499	86667729	16399748	86736144	16362248	86599314	16602999
HILIC_NEG_280_76764a1_368	HILIC	NEG	1.368	280.7676				3.65E-17	-1.36	2.38	9.67E-01	-0.01	0.42	8.07E-13	-1.36	2.33	2.72E-13	-1.35	2.50	237845	31930	156785	52794	157002	51704	156568	54387
RP_NEG_196_94653a0_498	RP	NEG	0.50	196.9465				2.36E-05	-0.53	1.26	9.68E-01	-0.01	1.21	1.07E-03	-0.53	1.34	3.87E-03	-0.52	1.33	1873751	200768	1464252	861585	1467778	918829	1460727	809650
HILIC_NEG_612_66968a2_927	HILIC	NEG	2.927	612.6697				8.27E-07	-0.64	1.34	9.68E-01	-0.01	0.77	9.46E-05	-0.64	1.49	6.64E-04	-0.63	1.48	199752	24825	150048	85324	150395	92047	149702	78969
HILIC_NEG_299_73022a3_058	HILIC	NEG	3.058	299.7302				5.42E-03	-0.34	0.58	9.68E-01	-0.01	0.42	4.66E-02	-0.33	0.61	4.66E-02	-0.34	0.62	1102787	72495	975720	429486	973982	437706	977459	425544
HILIC_POS_79_99043a2_995	HILIC	POS	2.995	79.9904				1.35E-04	-0.59	1.33	9.68E-01	-0.01	0.79	1.29E-03	-0.59	1.36	2.41E-03	-0.60	1.31	18056817	3390141	14666671	6058617	14642183	6423599	14691160	5735760
HILIC_NEG_197_04283a0_831	HILIC	NEG	0.831	197.0428				1.44E-01	0.23	0.86	9.68E-01	-0.01	0.97	2.93E-01	0.23	0.44	1.54E-01	0.24	0.54	397843	80589	426527	132851	427064	102434	425991	158636
RP_NEG_303_05084a0_712	RP	NEG	0.71	303.0508				1.62E-02	0.33	0.87	9.68E-01	-0.01	0.32	9.50E-02	0.33	0.80	3.84E-02	0.32	1.05	1301044	570718	1747638	1530358	1741499	1292905	1753777	1749317
HILIC_NEG_96_95986a7_667	HILIC	NEG	7.667	96.9599				6.74E-02	0.33	0.74	9.68E-01	-0.01	0.69	1.07E-01	0.33	0.57	1.23E-01	0.32	0.56	10435319	412275	10603553	536733	10601410	548582	10605695	530181
RP_POS_529_22766a6_992	RP	POS	6.99	529.2277				1.43E-01	-0.25	0.71	9.68E-01	-0.01	0.66	2.00E-01	-0.26	0.60	2.25E-01	-0.25	0.78	2929664	172438	2872413	238089	2873363	244429	2871463	234057
HILIC_NEG_202_92914a5_428	HILIC	NEG	5.428	202.9291				9.76E-01	-0.01	0.10	9.69E-01	0.01	0.29	9.93E-01	0.00	0.07	9.63E-01	-0.01	0.09	2223022	233073	2221595	238122	2220650	219491	2222540	257650
RP_POS_288_13885a10_617	RP	POS	10.62	288.1389				5.31E-01	0.13	0.62	9.69E-01	-0.01	0.36	5.82E-01	0.13	0.63	5.61E-01	0.14	0.68	2554099	489118	2615872	461800	2617703	467124	2614041	461149
RP_POS_562_51727a15_099	RP	POS	15.10	562.5173				5.72E-01	0.12	0.40	9.69E-01	0.01	0.10	6.02E-01	0.12	0.51	6.19E-01	0.11	0.36	6660218	2319592	6925460	2229681	6916631	2187521	6934289	2293252
HILIC_NEG_344_72253a2_938	HILIC	NEG	2.938	344.7225				5.98E-06	-0.59	1.31	9.69E-01	0.01	0.75	3.83E-04	-0.58	1.43	1.43E-03	-0.59	1.50	236966	30701	182588	101578	182188	109366	182988	94263
RP_POS_257_21094a9_193	RP	POS	9.19	257.2109				6.99E-01	-0.08	0.56	9.69E-01	-0.01	0.58	7.14E-01	-0.08	0.38	7.43E-01	-0.08	0.63	984769	103427	976634	101732	977031	103952	976238	100518
RP_POS_129_06596a0_569	RP	POS	0.57	129.0660				2.21E-02	0.41	0.87	9.70E-01	0.01	0.30	3.59E-02	0.42	0.96	5.99E-02	0.41	0.63	1411597	854171	1849246	1097995	1845079	1199412	1853413	998582
HILIC_NEG_207_83685a3_059	HILIC	NEG	3.059	207.8369				1.88E-01	0.22	1.05	9.70E-01	-0.01	0.82	2.71E-01	0.21	0.61	2.71E-01	0.22	0.94	3933990	743858	4164820	1137013	4169124	1177056	4160516	1107466
HILIC_NEG_171_94728a1_403	HILIC	NEG	1.403	171.9473				8.62E-01	0.03	0.51	9.70E-01	-0.01	0.65	8.66E-01	0.04	0.49	8.91E-01	0.03	0.12	2341527	1014224	2378669	1134408	2374387	1105511	2382951	1173811
HILIC_NEG_277_97629a0_972	HILIC	NEG	0.972	277.9763				2.32E-02	-0.50	1.27	9.70E-01	0.01	0.21	4.11E-02	-0.50	0.94	3.17E-02	-0.50	1.30	169313	150087	99849	131178	99356	123544	100343	139652
RP_POS_441_29761a13_01	RP	POS	13.01	441.2976				6.23E-03	-0.59	1.02	9.70E-01	0.01	0.19	1.07E-02	-0.59	1.09	1.30E-02	-0.59	0.99	17806759	2589940	16333239	2364367	16324424	2519908	16342054	2223612
RP_POS_304_89331a15_431	RP	POS	15.43	304.8933				3.64E-01	0.22	0.67	9.71E-01	0.01	0.18	3.74E-01	0.23	0.39	4.12E-01	0.22	0.76	4241770	554382	4338278	382451	4336863	426136	4339692	337530
HILIC_POS_114_89283a3_018	HILIC	POS	3.018	114.8928				4.29E-06	-0.60	1.36	9.71E-01	0.01	0.77	3.48E-04	-0.59	1.51	1.10E-03	-0.60	1.50	12232993	1489894	9576530	4867369	9558557	5193089	9594503	4571347
HILIC_POS_171_11293a0_546	HILIC	POS	0.546	171.1129				1.61E-01	0.16	0.69	9.71E-01	-0.01	0.36	3.25E-01	0.16	0.58	3.25E-01	0.17	0.42	288962	177557	8278632	56583436	8485991	58312893	8071273	55391602
RP_POS_277_11993a9_45	RP	POS	9.45	277.1199				7.01E-01	-0.06	0.36	9.71E-01	0.01	0.38	8.13E-01	-0.05	0.37	6.63E-01	-0.06	0.46	1052774	110157	1041454	220264	1040651	139298	1042256	280387
RP_POS_253_21637a9_843	RP	POS	9.84	253.2164				9.36E-02	0.31	0.91	9.71E-01	0.01	0.62	1.43E-01	0.32	0.68	1.42E-01	0.31	1.04	1087606	109617	1127420	130825	1126946	128005	1127893	134884
RP_POS_456_84372a0_473	RP	POS	0.47	456.8437				3.23E-05	-0.55	1.27	9.72E-01	-0.01	1.21	1.10E-03	-0.55	1.33	3.05E-03	-0.54	1.34	512084	80486	388795	248361	389689	262070	387902	236522
RP_POS_248_03436a3_717	RP	POS	3.72	248.0344				1.19E-01	0.24	0.99	9.72E-01	0.01	0.55	2.35E-01	0.25	0.84	1.68E-01	0.24	0.49	2335960	543969	2549997	962462	2546540	826578	2553454	1090100
RP_POS_304_2489a9_912	RP	POS	9.91	304.2489				8.18E-01	-0.04	0.43	9.72E-01	-0.01	0.54	8.24E-01	-0.05	0.22	8.59E-01	-0.04	0.35	1107045	247650	1094724	305768	1095813	322635	1093635	291205
RP_POS_409_18707a2_893	RP	POS	2.89	409.1871				8.33E-04	-0.67	1.29	9.72E-01	-0.01	1.04	4.05E-03	-0.67	1.21	1.48E-03	-0.66	1.32	1525008	590369	1093523	634172	1095774	535774	1091272	724907
RP_POS_251_16084a8_339	RP	POS	8.34	251.1608				7.30E-01	0.08	0.67	9.73E-01	-0.01	0.53	7.63E-01	0.08	0.46	7.33E-01	0.08	0.62	2783629	340029	2806440	261894	2807340	241090	2805540	283639
HILIC_NEG_216_85336a7_676	HILIC	NEG	7.676	216.8534				5.86E-01	-0.11	0.63	9.73E-01	-0.01	0.72	6.11E-01	-0.11	0.24	6.41E-01	-0.11	0.47	966844	215385	942817	218129	943564	226347	942070	211890
RP_POS_605_38263a14_27	RP	POS	14.27	605.3826				7.53E-01	0.06	0.44	9.73E-01	-0.01	0.14	7.96E-01	0.06	0.29	7.67E-01	0.06	0.69	5749748	1599405	5855000	1762493	5861019	1728950	5848981	1812958
HILIC_NEG_173_92606a0_595	HILIC	NEG	0.595	173.9261				1.17E-01	-0.29	0.89	9.73E-01	-0.01	0.69	1.61E-01	-0.30	0.58	1.78E-01	-0.29	0.67	2258722	391314	2126038	464832	2127625	475043	2124451	459213
RP_POS_361_14664a10_703	RP	POS	10.70	361.1466				4.06E-07	0.73	1.57	9.73E-01	0.01	0.50	3.08E-05	0.73	1.54	1.39E-04	0.72	1.48	185940	126455	378369	279733	377414	296812	379324	264573
HILIC_NEG_352_99701a7_309	HILIC	NEG	7.309	352.9970				2.22E-01	0.26	1.27	9.73E-01	-0.01	0.36	2.71E-01	0.25	0.87	2.68E-01	0.26	0.89	1807692	53404	1821007	51681	1821182	53306	1820831	50546
RP_POS_419_31531a10_978	RP	POS	10.98	419.3153				8.40E-02	0.29	1.28	9.73E-01	0.01	1.15	1.56E-01	0.30	1.17	1.32E-01	0.29	1.07	2474809	421296	2643567	612104	2641488	568787	2645645	658377
RP_POS_660_0816a0_625	RP	POS	0.63	660.0816				3.45E-05	-0.62	1.20	9.73E-01	-0.01	1.03	5.19E-04	-0.62	1.28	1.35E-03	-0.63	1.24	590705	135742	435816	265448	434921	284074	436711	248322
RP_POS_401_34113a11_416	RP	POS	11.42	401.3411				4.05E-01	0.14	0.80	9.73E-01	-0.01	0.77	5.02E-01	0.14	0.65	4.70E-01	0.14	0.68	1087920	875826	1257941	1316751	1262372	1301491	1253510	1345039
RP_POS_378_2428a12_326	RP	POS	12.33	378.2428				1.17E-05	-0.83	1.41	9.73E-01	0.01	0.33	1.67E-04	-0.82	1.37	4.44E-05	-0.83	1.48	3644851	701829	2929192	845738	2926353	769617	2932031	923481
RP_POS_276_10114a8_873	RP	POS	8.87	276.1011				6.59E-01	0.09	0.47	9.73E-01	-0.01	0.10	7.06E-01	0.09	0.34	6.79E-01	0.09	0.28	642169	116848	652682	116473	653073	113952	652292	120099
HILIC_POS_392_27908a0_634	HILIC	POS	0.634	392.2791				3.08E-01	0.17	0.61	9.74E-01	0.01	0.84	4.28E-01	0.17	0.34	3.52E-01	0.16	0.37	535810	249200	595846	385122	594562	316425	597130	446696
RP_POS_315_15613a9_603	RP	POS	9.60	315.1561				2.82E-02	-0.52	0.93	9.74E-01	0.01	0.43	4.03E-02	-0.51	0.96	3.94E-02	-0.52	0.88	2631313	148795	2566205	114222	2565825	116388	2566585	113195
RP_POS_485_19962a6_861	RP	POS	6.86	485.1996				1.55E-01	-0.27	0.57	9.74E-01	-0.01	0.51	2.22E-01	-0.27	0.54	1.97E-01	-0.28	0.60	796431	62654	777517	70429	777285	68174	777749	73307
RP_POS_169_9772a0_774	RP	POS	0.77	169.9772				1.97E-01	0.23	0.74	9.74E-01	-0.01	0.28	2.92E-01	0.23	0.76	2.44E-01	0.23	0.65	1459820	624223	1638714	818696	1641391	765593	1636037	876388
HILIC_POS_300_21713a0_84	HILIC	POS	0.84	300.2171				1.44E-01	-0.25	0.58	9.74E-01	-0.01	0.46	2.32E-01	-0.26	0.42	1.93E-01	-0.25	0.63	1341851	501217	1175491	694247	1177730	622206	1173252	765926
HILIC_POS_189_07329a5_201	HILIC	POS	5.201	189.0733				3.40E-01	0.16	0.73	9.75E-01	-0.01	0.62	4.05E-01	0.16	0.38	4.35E-01	0.17	0.39	5303880	842352	5488430	1218065	5492350	1334786	5484510	1102706
RP_POS_285_98807a0_512	RP	POS	0.51	285.9881				3.20E-05	0.51	1.23	9.75E-01	0.01	1.08	4.49E-03	0.51	1.25	1.80E-03	0.50	1.30	85583	33906	175920	199811	175281	188394	176559	212534
RP_POS_303_19312a9_308	RP	POS	9.31	303.1931				1.66E-03	0.37	0.77	9.75E-01	0.01	0.79	4.27E-03	0.37	1.13	6.38E-02	0.36	0.72	40166	27418	686492	1997787	680174	2386039	692810	1539642
RP_NEG_658_06799a0_626	RP	NEG	0.63	658.0680				1.94E-06	-0.70	1.24	9.75E-01	-0.01	0.96	9.70E-05	-0.70	1.35	2.47E-04	-0.69	1.27	2349011	341133	1879114	714331	1881340	744844	1876889	690035
HILIC_POS_497_06091a3_075	HILIC	POS	3.075	497.0609				3.05E-04	0.49	1.20	9.75E-01	0.01	0.83	2.33E-03	0.50	1.32	1.10E-02	0.49	1.37	538466	42272	587628	109252	587287	120891	587968	97472
HILIC_POS_626_69366a2_992	HILIC	POS	2.992	626.6937				1.68E-05	-0.58	1.35	9.75E-01	0.01	0.76	6.63E-04	-0.58	1.47	1.77E-03	-0.58	1.46	3055299	499920	2317768	1392283	2313454	1481768	2322081	1311790
RP_POS_302_24512a11_608	RP	POS	11.61	302.2451				1.95E-04	0.66	1.06	9.76E-01	-0.01	0.21	2.33E-03	0.66	1.05	5.64E-04	0.66	1.27	1995029	847897	2736492	1143453	2740029	1006416	2732956	1276226
RP_POS_150_96881a0_256	RP	POS	0.26	150.9688				7.78E-01	0.05	0.35	9.76E-01	-0.01	0.52	8.18E-01	0.05	0.21	7.95E-01	0.06	0.15	69251612	5347510	69577163	6520334	69597285	6579945	69557040	6526918
RP_POS_291_06915a0_71	RP	POS	0.71	291.0692				9.19E-03	0.33	0.71	9.76E-01	-0.01	0.31	8.29E-02	0.32	0.72	3.32E-02	0.33	0.94	884502	253290	1176635	1009266	1179729	904109	1173540	1113819
RP_POS_397_31033a11_161	RP	POS	11.16	397.3103				1.91E-02	-0.42	0.80	9.76E-01	0.01	0.61	3.33E-02	-0.41	0.86	5.38E-02	-0.42	0.80	3463628	532351	3181320	705218	3179183	783123	3183458	625717
RP_POS_341_35233a10_861	RP	POS	10.86	341.3523				1.10E-04	-0.78	1.29	9.76E-01	-0.01	0.60	5.94E-04	-0.78	1.26	3.02E-04	-0.77	1.26	2369771	420096	2009114	444358	2010453	408383	2007775	481826
RP_POS_565_4259a10_979	RP	POS	10.98	565.4259				9.23E-01	-0.02	0.71	9.77E-01	0.01	0.51	9.46E-01	-0.02	0.78	9.16E-01	-0.02	0.44	1157333	762112	1141614	880439	1139049	756127	1144180	997209
HILIC_NEG_200_93427a2_944	HILIC	NEG	2.944	200.9343				7.42E-02	-0.35	1.00	9.77E-01	0.01	0.68	1.22E-01	-0.35	0.61	1.02E-01	-0.36	0.63	401113	96545	364731	104137	364428	99365	365034	109712
HILIC_NEG_136_89166a1_329	HILIC	NEG	1.329	136.8917				3.97E-06	-0.85	1.29	9.78E-01	-0.01	0.54	9.16E-05	-0.86	1.32	1.54E-05	-0.85	1.54	4712670	660794	3991908	823132	3994246	716656	3989571	924832

Supplementary table 1: Metabolomics results (in asceding order according to p-value from progressive ALD vs non-progressive ALD comparison, with molecular features with ID_level of 1-2 first)

								all_ALD_vs_control			Prog_ALD_vs_non-prog_ALD			Prog_ALD_vs_control_ALD			Non-prog_ALD_vs_control			Healthy_control		all_ALD		Non-prog_ALD		Progressive_ALD	
								t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA								
Feature_ID	RP_HILIC	POS_NEG	Average.Rt	Average.Mz	Metabolite.name	curated_MSMS	ID_level	p	d	VIP	p	d	VIP	p	d	VIP	p	d	VIP	Mean	SD	Mean	SD	Mean	SD	Mean	SD
HILIC_POS_371_23956a1_439	HILIC	POS	1.439	371.2396				1.52E-01	0.25	0.79	9.78E-01	-0.01	0.69	2.12E-01	0.24	0.50	2.38E-01	0.25	0.42	2328544	332748	2438025	475593	2439370	510789	2436679	442815
RP_NEG_208_78639a15_578	RP	NEG	15.58	208.7864				9.83E-01	0.00	0.85	9.78E-01	-0.01	0.15	9.74E-01	-0.01	0.69	9.95E-01	0.00	0.66	445087	25747	444974	26779	445049	29631	444899	23891
RP_POS_246_94331a0_453	RP	POS	0.45	246.9433				6.48E-04	-0.51	1.16	9.78E-01	0.01	1.06	4.63E-03	-0.51	1.19	7.91E-03	-0.52	1.22	661230	184290	490699	359127	489710	380176	491689	340646
RP_POS_574_48584a14_268	RP	POS	14.27	574.4858				1.66E-01	0.28	0.55	9.79E-01	-0.01	0.15	2.45E-01	0.27	0.59	1.89E-01	0.28	0.64	67249432	15182238	71634787	16036648	71677910	13952776	71591664	18025340
HILIC_NEG_200_85867a5_651	HILIC	NEG	5.651	200.8587				9.00E-01	-0.03	0.51	9.79E-01	-0.01	0.87	9.07E-01	-0.03	0.37	9.15E-01	-0.02	0.04	3883454	881098	3860453	927850	3862906	785682	3858000	1059279
HILIC_POS_262_75803a3_023	HILIC	POS	3.023	262.7580				3.05E-04	-0.52	1.33	9.80E-01	-0.01	0.76	3.38E-03	-0.52	1.39	6.15E-03	-0.51	1.41	1199920	256953	928313	570790	929777	595679	926849	550831
HILIC_NEG_134_89474a1_487	HILIC	NEG	1.487	134.8947				3.97E-01	0.15	0.52	9.80E-01	0.01	0.87	4.79E-01	0.15	0.25	4.55E-01	0.15	0.31	19013610	4383941	19837820	5780649	19822997	5289998	19852643	6287229
RP_POS_419_20367a9_071	RP	POS	9.07	419.2037				5.74E-09	0.70	1.15	9.80E-01	-0.01	0.15	1.22E-04	0.70	1.25	1.08E-05	0.70	1.25	130668	203460	2111952	3092676	2119784	2863254	2104120	3335587
RP_NEG_627_13837a0_621	RP	NEG	0.62	627.1384				2.09E-06	-0.73	1.30	9.80E-01	-0.01	1.02	5.62E-05	-0.74	1.43	1.80E-04	-0.73	1.32	1997540	445784	1427301	809607	1429316	855352	1425285	769851
HILIC_POS_491_4957a1_306	HILIC	POS	1.306	491.4957				7.54E-02	0.29	0.61	9.80E-01	0.01	0.50	1.66E-01	0.30	0.53	1.06E-01	0.29	0.60	232335	208950	320541	321497	319741	273282	321340	366258
RP_POS_143_95935a0_249	RP	POS	0.25	143.9594				8.31E-01	-0.04	0.29	9.80E-01	-0.01	0.18	8.36E-01	-0.05	0.19	8.61E-01	-0.04	0.36	454895	53955	452530	55470	452668	59059	452392	52236
RP_POS_299_25711a10_174	RP	POS	10.17	299.2571				6.14E-01	-0.10	0.67	9.80E-01	0.01	0.67	6.52E-01	-0.10	0.49	6.58E-01	-0.10	0.78	15011695	2184099	14782139	2365551	14776292	2566965	14787985	2171746
RP_POS_301_23651a9_271	RP	POS	9.27	301.2365				4.96E-01	-0.14	0.59	9.80E-01	0.00	0.27	5.30E-01	-0.15	0.30	5.46E-01	-0.14	0.58	1425345	232557	1393459	218109	1393997	220816	1392922	217608
HILIC_NEG_136_89175a4_128	HILIC	NEG	4.128	136.8918				1.18E-01	0.32	0.75	9.81E-01	0.00	0.51	1.61E-01	0.31	0.66	1.61E-01	0.32	0.73	4985446	2879805	5922150	2967218	5929440	3045791	5914860	2917447
RP_POS_352_65912a5_606	RP	POS	5.61	352.6591				5.00E-01	0.12	0.66	9.81E-01	0.01	0.56	5.62E-01	0.12	0.48	5.58E-01	0.12	0.65	1340965	623518	1432987	790181	1431066	752974	1434909	833389
HILIC_POS_260_14896a2_383	HILIC	POS	2.383	260.1490				8.88E-03	0.33	1.22	9.81E-01	0.01	0.84	6.16E-02	0.34	0.92	4.54E-02	0.33	0.73	503202	195848	711142	701793	709459	670614	712825	738477
RP_NEG_429_17966a11_256	RP	NEG	11.26	429.1797				4.63E-02	0.35	0.97	9.81E-01	0.01	1.02	8.95E-02	0.35	0.75	8.70E-02	0.35	1.03	1944850	499752	2171219	681869	2169591	671169	2172848	699220
RP_NEG_416_88354a0_498	RP	NEG	0.50	416.8835				9.07E-06	-0.55	1.28	9.82E-01	0.00	1.21	6.43E-04	-0.55	1.37	2.26E-03	-0.56	1.34	9310550	1015000	7131718	4350012	7121945	4665809	7141492	4057268
HILIC_POS_100_11257a1_071	HILIC	POS	1.071	100.1126				8.45E-02	-0.30	1.07	9.82E-01	0.00	0.61	1.46E-01	-0.29	1.14	1.42E-01	-0.30	0.95	97774868	36957417	83071972	52945373	82953602	53580964	83190343	52845862
RP_NEG_942_76471a0_495	RP	NEG	0.50	942.7647				4.41E-05	-0.58	1.24	9.83E-01	0.00	1.17	1.34E-03	-0.58	1.29	1.59E-03	-0.58	1.31	1172834	151799	985622	350327	986389	354078	984856	350129
RP_POS_860_60785a11_974	RP	POS	11.97	860.6079				5.12E-01	0.12	0.61	9.83E-01	0.00	0.21	5.70E-01	0.12	0.33	5.62E-01	0.13	0.61	5120547	862824	5241110	1007084	5243245	1029712	5238976	994393
RP_POS_343_3382a11_26	RP	POS	11.26	343.3382				3.29E-01	-0.17	0.37	9.83E-01	0.00	0.25	4.02E-01	-0.17	0.34	4.03E-01	-0.18	0.33	20305401	4460991	19337922	5877616	19325605	6062428	19350239	5748428
RP_NEG_979_14014a9_692	RP	NEG	9.69	979.1401				1.63E-01	-0.28	0.62	9.83E-01	0.00	0.46	1.95E-01	-0.28	0.55	2.34E-01	-0.27	0.58	4785640	315732	4693442	338826	4694151	368088	4692732	310579
RP_POS_229_18065a8_339	RP	POS	8.34	229.1807				9.50E-01	-0.01	0.55	9.83E-01	0.00	0.57	9.48E-01	-0.02	0.46	9.60E-01	-0.01	0.39	771097	93659	769960	75180	770117	72881	769803	78152
RP_POS_808_58344a13_375	RP	POS	13.38	808.5834				7.37E-03	0.53	1.13	9.84E-01	0.00	0.29	1.89E-02	0.52	0.96	1.46E-02	0.53	1.01	57486862	18009545	67900672	19761617	67941504	19053498	67859840	20639128
RP_NEG_263_10416a3_746	RP	NEG	3.75	263.1042				9.18E-02	-0.33	0.65	9.84E-01	0.00	0.22	1.71E-01	-0.33	0.58	9.50E-02	-0.34	0.74	8369474	5314873	6481317	5730718	6469474	4293650	6493160	6922194
RP_POS_243_09978a8_492	RP	POS	8.49	243.0998				5.45E-01	0.11	0.42	9.84E-01	0.00	0.43	6.05E-01	0.11	0.24	5.91E-01	0.12	0.31	434496	249662	466851	297195	467458	298304	466245	299109
RP_POS_499_82697a6_697	RP	POS	6.70	499.8270				5.63E-01	0.12	0.68	9.84E-01	0.00	0.29	6.12E-01	0.12	0.31	5.88E-01	0.12	0.90	888958	1289530	1039661	1221020	1037209	1048284	1042114	1383219
RP_POS_355_28217a10_701	RP	POS	10.70	355.2822				8.27E-01	0.04	0.48	9.84E-01	0.00	0.11	8.47E-01	0.05	0.35	8.42E-01	0.04	0.78	29871091	3424219	30025873	3574594	30018834	3001905	30032912	4099351
RP_NEG_213_88892a0_73	RP	NEG	0.73	213.8889				8.53E-01	-0.03	0.69	9.84E-01	0.00	0.52	8.83E-01	-0.03	0.36	8.80E-01	-0.03	0.94	1299933	231630	1288663	447536	1289539	389659	1287786	502822
RP_POS_304_93228a15_367	RP	POS	15.37	304.9323				9.65E-01	-0.01	0.24	9.85E-01	0.00	0.05	9.78E-01	-0.01	0.18	9.63E-01	-0.01	0.21	3925273	500927	3920362	690263	3919062	696547	3921661	690992
HILIC_POS_282_19135a0_578	HILIC	POS	0.578	282.1914				7.65E-04	-0.58	1.13	9.85E-01	0.00	0.66	2.90E-03	-0.58	1.26	5.30E-03	-0.58	1.14	517387	124141	418563	176367	418894	186921	418231	167050
RP_POS_343_33759a0_249	RP	POS	0.25	343.3376				1.83E-01	0.23	0.65	9.85E-01	0.00	0.42	2.48E-01	0.24	0.60	2.62E-01	0.23	0.64	2822530	2064069	3440450	2789149	3435227	2831465	3445674	2774926
RP_POS_287_22269a9_912	RP	POS	9.91	287.2227				4.64E-01	-0.14	0.46	9.85E-01	0.00	0.58	5.20E-01	-0.14	0.30	5.25E-01	-0.14	0.41	709917	143023	687518	169083	687202	176969	687834	162613
RP_POS_589_22803a7_093	RP	POS	7.09	589.2280				1.81E-02	-0.40	1.08	9.86E-01	0.00	0.93	3.25E-02	-0.40	1.04	5.89E-02	-0.40	1.09	2055219	185408	1952570	270233	1952082	301921	1953058	237456
HILIC_POS_264_75504a3_023	HILIC	POS	3.023	264.7550				2.33E-04	-0.52	1.33	9.86E-01	0.00	0.76	2.84E-03	-0.52	1.42	6.24E-03	-0.51	1.43	532398	107008	411968	254863	412420	269378	411517	242221
RP_POS_152_05392a0_709	RP	POS	0.71	152.0539				4.36E-01	0.10	0.42	9.86E-01	0.00	0.66	6.22E-01	0.10	0.28	4.57E-01	0.10	0.88	1069715	157101	1117996	552103	1117042	401937	1118950	674019
RP_POS_181_07205a2_934	RP	POS	2.93	181.0721				5.87E-01	-0.11	0.32	9.86E-01	0.00	0.04	6.32E-01	-0.11	0.24	6.27E-01	-0.11	0.50	6278825	5930845	5610196	6319813	5621052	5982938	5599341	6700701
RP_POS_255_23183a10_018	RP	POS	10.02	255.2318				6.85E-02	-0.37	0.77	9.87E-01	0.00	0.65	9.58E-02	-0.37	0.72	1.09E-01	-0.37	0.78	1977572	189624	1905399	195976	1905729	204257	1905068	189408
RP_POS_226_21611a10_846	RP	POS	10.85	226.2161				9.54E-06	0.81	1.29	9.87E-01	0.00	0.56	3.11E-04	0.81	1.25	1.87E-05	0.81	1.53	579140	245509	835952	313477	836472	248282	835432	369995
RP_POS_814_76312a11_172	RP	POS	11.17	814.7631				5.16E-07	0.74	1.52	9.87E-01	0.00	1.01	1.07E-04	0.73	1.49	3.94E-05	0.74	1.55	217785	104527	370352	218338	370709	210453	369996	228090
HILIC_NEG_234_8203a3_136	HILIC	NEG	3.136	234.8203				9.18E-05	0.48	1.14	9.87E-01	0.00	0.69	4.59E-03	0.48	1.29	5.31E-03	0.48	1.24	996727	354403	1770518	1805140	1767573	1824189	1773463	1804405
RP_NEG_706_8064a0_497	RP	NEG	0.50	706.8064				6.95E-05	-0.52	1.26	9.87E-01	0.00	1.20	2.09E-03	-0.52	1.32	4.38E-03	-0.52	1.32	1361500	181578	1087202	585030	1088140	612559	1086264	562383
RP_POS_413_17972a6_61	RP	POS	6.61	413.1797	Unknown	413.1807(100)	4	1.93E-01	-0.23	0.63	9.87E-01	0.00	0.55	2.64E-01	-0.23	0.52	2.69E-01	-0.23	0.65	864331	51572	849273	69552	849383	69649	849162	70161
RP_POS_629_15143a0_619	RP	POS	0.62	629.1514				6.67E-06	-0.70	1.23	9.88E-01	0.00	0.96	1.73E-04	-0.71	1.31	2.62E-04	-0.70	1.27	418554	101383	297615	179286	297896	183659	297333	176670
HILIC_POS_293_09732a7_451	HILIC	POS	7.451	293.0973				2.26E-01	-0.21	0.85	9.88E-01	0.00	0.59	2.65E-01	-0.21	0.73	3.30E-01	-0.22	1.00	1166017	175460	1118545	234177	1118179	266226	1118912	199802
HILIC_NEG_381_00626a6_639	HILIC	NEG	6.639	381.0063				5.32E-01	-0.11	1.17	9.88E-01	0.00	0.54	5.60E-01	-0.11	0.85	6.13E-01	-0.11	1.20	746883	71346	737111	90803	736971	105195	737251	74782
HILIC_NEG_157_86256a2_949	HILIC	NEG	2.949	157.8626				6.35E-03	0.40	1.10	9.88E-01	0.00	0.79	2.84E-02	0.40	0.92	3.07E-02	0.41	1.13	1360654	271461	1562954	545640	1563786	556928	1562121	539771
RP_POS_303_23175a10_704	RP	POS	10.70	303.2318				3.12E-07	0.72	1.59	9.89E-01	0.00	0.50	7.11E-05	0.71	1.47	8.33E-05	0.72	1.54	1067691	575917	2000420	1389038	2002401	1408843	1998439	1383251
HILIC_POS_295_06619a1_386	HILIC	POS	1.386	295.0662				5.48E-11	0.80	1.38	9.89E-01	0.00	0.66	1.02E-05	0.80	1.39	1.20E-06	0.80	1.82	104858	227083	1829714	2324366	1832983	2198515	1826445	2466196
HILIC_POS_129_06612a5_723	HILIC	POS	5.723	129.0661				6.48E-02	0.33	0.65	9.89E-01	0.00	0.38	1.08E-01	0.33	0.57	1.13E-01	0.33	0.55	16187620	10767842	20610459	13872304	20590950	14013640	20629969	13871775
RP_POS_1043_70276a10_618	RP	POS	10.62	1043.7028				1.11E-03	0.61	1.44	9.89E-01	0.00	0.80	7.78E-03	0.61	1.20	1.58E-03	0.61	1.41	41265780	31352288	64185241	37643859	64133221	29346944	64237261	44741381
RP_NEG_239_12886a8_233	RP	NEG	8.23	239.1289				7.08E-01	-0.06	0.53	9.89E-01	0.00	0.57	7.34E-01	-0.06	0.55	7.68E-01	-0.06	0.50	1088069	77290	1081371	114741	1081216	132198	1081527	95516
HILIC_NEG_117_91909a5_606	HILIC	NEG	5.606	117.9191				4.79E-01	-0.14	0.83	9.89E-01	0.00	0.64	5.28E-01	-0.14	0.26	5.27E-01	-0.14	0.39	1526715	264213	1488252	271101	1488618	265412	1487885	279369
RP_POS_379_21448a11_161	RP	POS	11.16	379.2145				4.42E-01	-0.13	0.71	9.89E-01	0.00	0.66	5.10E-01	-0.13	0.53	5.21E-01	-0.13	0.69	6546278	369163	6481315	528209	6480612	553326	6482017	507478
RP_POS_816_58661a13_708	RP	POS	13.71	816.5866				7.78E-07	-1.02	1.60	9.90E-01	0.00	0.46	3.33E-06	-1.02	1.64	5.30E-06	-1.02	1.60	11970287	2799832	8776990	2823525	8780720	2931514	8773260	2741074
RP_NEG_163_03865a9_442	RP	POS	9.44	163.0387	4-hydroxycoumarin	163.038(100)	3	7.63E-01	-0.07	0.33	9.90E-01	0.00	0.73	7.92E-01	-0.06	0.60	7.75E-01	-0.07	0.20	1375320	123498	1367928	108952	1367785	102422	1368071	116159
RP_NEG_439_80557a15_501	RP	NEG	15.50	439.8056				9.87E-01	0.00	0.55	9.90E-01	0.00	0.50	9.83E-01	0.00	0.32	9.93E-01	0.00	0.39	1364075	62929	1363866	60958	1363946	66374	1363786	55698
HILIC_NEG_258_7644a2_945	HILIC	NEG	2.945	258.7644				3.79E-06	-0.59	1.33	9.90E-01	0.00	0.76	2.98E-04	-0.59	1.47	1.30E-03	-0.59	1.48	1816917	203237	1426757	723318	1425816	778455	1427698	671611
HILIC_POS_297_07977a4_868	HILIC	POS	4.868	297.0798				9.49E-01	0.01	0.32	9.90E-01	0.00	0.23	9.43E-01	0.01	0.47	9.63E-01	0.01	0.04	497452	568672	504836	560797	504144	715935	505528	350487
RP_POS_805_54333a12_701	RP	POS	12.70	805.5433				8.21E-02	0.33	0.66	9.90E-01	0.00	0.27	9.83E-02	0.33	0.81	1.53E-01	0.33	0.55	1087856	568249	1300055	656412	1299246	754146	1300863	549372
HILIC_POS_387_21371a2_925	HILIC	POS	2.925	387.2137				7.81E-01	-0.05	0.90	9.90E-01	0.00	0.84	8.07E-01	-0.05	0.43	8.12E-01	-0.05	0.30	1510759	261112	1495158	316611	1495541	309500	1494775	326711
RP_POS_499_82724a5_457	RP	POS	5.46	499.8272				2.57E-01	-0.25	1.43	9.90E-01	0.00	0.68	3.21E-01	-0.24	1.20	2.81E-01	-0.25	1.11	1752168	1537474	1402529	1385201	1400866	1233893	1404192	1534349
RP_POS_293_20862a10_121	RP	POS	10.12	293.2086				5.08E-02	-0.32	0.91	9.91E-01	0.00	0.78	1.45E-01	-0.32	0.77	6.18E-02	-0.32	0.97	5629547	582872	5356305	915604	5355217	718168	5357393	1085358
RP_POS_239_16162a8_616	RP	POS	8.62	239.1616				2.54E-01	0.21	0.65	9.91E-01	0.00	0.52	3.41E-01	0.22	0.37	2.93E-01	0.21	0.63	4787997	594608	4933346	699811	4932548	614527	4934144	782191
RP_POS_391_28409a11_573	RP	POS	11.57	391.2841				5.10E-02	-0.41	1.03	9.92E-01	0.00	0.51	7.66E-02	-0.41	0.74	7.78E-02	-0.41	1.08	3104452	228319	3012327	222887	3012088	226792	3012566	221216
HILIC_POS_79_05497a0_505	HILIC	POS	0.505	79.0550				5.25E-05	-0.67	1.26	9.92E-01	0.00	0.74	4.30E-04	-0.68	1.38	8.64E-04	-0.67	1.33	582257	162323	420105	248386	420369	261093	419841	237657
RP_POS_431_75708a13_369	RP	POS	13.37	431.7571				1.25E-02	0.52	1.09	9.92E-01	0.00	0.25	2.12E-02	0.53	0.94	2.45E-02	0.52	0.96	1818533	765222	2217747	737645	2216967	763161	2218526	718978
HILIC_POS_189_07352a4_923	HILIC	POS	4.923	189.0735				7.64E-01	-0.06	0.46	9.92E-01	0.00	0.64	7.80E-01	-0.07	0.11	7.89E-01	-0.06	0.29	7927622	3352268	7726243	3036228	7729330	3095597	7723156	3007117
RP_NEG_373_00531a0_708	RP	NEG	0.71	373.0053				1.83E-03	-0.50	1.08	9.92E-01	0.00	1.03	1.02E-02	-0.50	1.10	9.99E-03	-0.50	1.13	1135725	292672	906094	493070	905609	496172	906578	494985
HILIC_POS_499_0563a3_075	HILIC	POS	3.075	499.0563				3.70E-04	0.50	1.21	9.93E-01	0.00	0.84	2.31E-03	0.50	1.33	1.08E-02	0.50	1.37	704019	60774	769449	142574	769314	158876	769583	125809
HILIC_NEG_234_82027a7_68	HILIC	NEG	7.68	234.8203				2.23E-01	-0.25	0.59	9.93E-01	0.00	0.60	2.67E-01	-0.25	0.60	2.80E-01	-0.25	0.48	4875609	892148	4652275	890374	4653060	918507	4651491	870663
RP_NEG_291_08362a0_622	RP	NEG	0.62	291.0836				7.53E-06	-0.64	1.27	9.93E-01	0.00	1.09	2.95E-04	-0.64	1.34	6.51E-04	-0.64	1.30	197133276	45555617	136336515	101595873	136422581	106089790	136250448	97974648
HILIC_NEG_132_92365a7_354	HILIC	NEG	7.354	132.9237				2.44E-01	-0.18	0.68	9.93E-01	0.00	0.59	3.65E-01	-0.18	0.30	3.16E-01	-0.18	1.11	2745350	128678	2707927	223791	2707740	208961	2708114	239837
RP_NEG_201_02246a5_964	RP	NEG	5.96	201.0225				2.13E-01	-0.44	0.99	9.94E-01	0.00	0.52	2.15E-01	-0.44	0.76	2.13E-01	-0.44	0.69	3425290	9137910	1364593	1251637	1363568	1071559	1365619	1420184
RP_NEG_395_20816a9_14	RP	NEG	9.14	395.2082				4.02E-07	0.64	1.18	9.94E-01	0.00	0.25	1.89E-04	0.64	1.27	2.81E-04	0.64	1.10	1118964	1534537	4735093	6191762	4730063	6315960	4740123	6129179
RP_NEG_609_55774a15_218	RP	NEG	15.22	609.5577				5.64E-01	0.11	0.40	9.94E-01	0.00	0.52	6.13E-01	0.11	0.25	6.17E-01	0.11	0.61	5300218	286861	5335621	340756	5335348	341162	5335894	343813
RP_POS_214_91718a15_334	RP	POS	15.33	214.9172				5.40E-01	-0.12	0.37	9.94E-01	0.00	0.20	5.75E-01	-0.12	0.35	6.05E-01	-0.12	0.54	2062105	83860	2051207	96417	2051133	106504	2051281	86251
HILIC_NEG_113_92621a2_939	HILIC	NEG	2.939	113.9262				1.34E-01	0.22	0.64	9.94E-01	0.00	0.55	2.05E-01	0.22	0.43	2.62E-01	0.22	0.56	1054494	107587	1098422	220586	1098257	238487	1098586	203551
HILIC_NEG_180_85939a2_98	HILIC	NEG	2.98	180.8594				7.29E-01	0.06	0.31	9.94E-01	0.00	0.42	7.60E-01	0.06	0.34	7.67E-01	0.06	0.63	1117785	298905	1140155	365614	1140410	387676	1139901	346095
HILIC_NEG_256_76682a2_946	HILIC	NEG	2.946	256.7668				3.41E-06	-0.61	1.34	9.95E-01	0.00	0.76	2.39E-04	-0.61	1.47	1.03E-03	-0.61	1.48	1259696	159680	982477	496447	982816	532021	982139	463576
HILIC_POS_161_1284a6_821	HILIC	POS	6.821	161.1284				5.14E-01	0.12	0.70	9.95E-01	0.00	0.38	5.73E-01	0.12	0.54	5.79E-01	0.12	0.58	6132524	4444728	6773631	5817380	6769806	5867690	6777456	5826204
HILIC_NEG_520_67883a2_932	HILIC	NEG	2.932	520.6788				1.25E-05	-0.56	1.32	9.96E-01	0.00	0.76	6.56E-04	-0.56	1.44	2.28E-03	-0.56	1.48	220751	27814	170598	98781	170544	105737	170652	92381
HILIC_POS_252_04523a2_995	HILIC	POS	2.995	252.0452				4.82E-04	-0.52	1.30	9.96E-01	0.00	0.75	4.71E-03	-0.52	1.27	5.94E-03	-0.52	1.34	2398993	393169	2020441	788491	2020871	806501	2020011	778254
HILIC_POS_128_10715a1_104	HILIC	POS	1.104	128.1072				8.68E-01	-0.04	0.61	9.96E-01	0.00	0.95	8.75E-01	-0.05	0.12	8.71E-01	-0.04	0.13	513872	954497	484076	548327	484365	456883	483787	631441
HILIC_NEG_100_93347a4_301	HILIC	NEG	4.301	100.9335				3.96E-01	0.14	0.89	9.96E-01	0.00	0.76	4.87E-01	0.14	0.25	4.79E-01	0.14	0.45	29919318	2759487	30482830	4458222	30485039	4449948	30480621	4511659
RP_POS_191_17972a8_904	RP	POS	8.90	191.1797				8.43E-01	0.04	0.42	9.96E-01	0.00	0.41	8.64E-01	0.04	0.32	8.62E-01	0.04	0.37	760760	361981	775986	424323	776188	434603	775784	418205
RP_POS_223_09419a0_672	RP	POS	0.67	223.0942				5.22E-05	0.61	1.23	9.96E-01	0.00	1.08	1.29E-03	0.61	1.27	8.77E-04	0.62	1.26	1281810	320627	1632923	607492	1633211	595804	1632636	625014

Supplementary table 1: Metabolomics results (in asceding order according to p-value from progressive ALD vs non-progressive ALD comparison, with molecular features with ID_level of 1-2 first)

								all_ALD_vs_control			Prog_ALD_vs_non-prog_ALD			Prog_ALD_vs_control_ALD			Non-prog_ALD_vs_control			Healthy_control		all_ALD		Non-prog_ALD		Progressive_ALD	
								t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA	t-test	Cohen's	PLS-DA								
Feature_ID	RP_HILIC	POS_NEG	Average.Rt	Average.Mz	Metabolite.name	curated_MSMS	ID_level	p	d	VIP	p	d	VIP	p	d	VIP	p	d	VIP	Mean	SD	Mean	SD	Mean	SD	Mean	SD
RP_NEG_418_16086a11_615	RP	NEG	11.62	418.1609				4.78E-02	0.38	0.64	9.96E-01	0.00	0.38	8.93E-02	0.38	0.62	7.35E-02	0.38	0.65	557300	197411	641615	228934	641510	215657	641719	243686
RP_POS_310_2012a5_931	RP	POS	5.93	310.2012	Unknown	85.0292(100), 310.2007(45)	4	5.64E-01	-0.12	0.56	9.96E-01	0.00	0.25	6.13E-01	-0.12	0.60	5.99E-01	-0.12	0.26	2583146	1631462	2389660	1671431	2388911	1615891	2390409	1741629
RP_POS_438_29779a10_706	RP	POS	10.71	438.2978				2.18E-01	0.22	0.75	9.96E-01	0.00	0.98	2.87E-01	0.22	0.96	2.86E-01	0.22	0.67	3099329	1022873	3375737	1292022	3376309	1301495	3375165	1295692
RP_POS_331_18817a9_072	RP	POS	9.07	331.1882				2.85E-03	-0.59	1.07	9.97E-01	0.00	0.33	8.40E-03	-0.59	1.05	6.32E-03	-0.59	1.02	1477890	95394	1416266	102707	1416225	98593	1416307	107666
RP_POS_383_29657a11_608	RP	POS	11.61	383.2966				5.70E-02	-0.36	0.65	9.98E-01	0.00	0.39	7.62E-02	-0.36	0.68	1.15E-01	-0.36	0.53	1950296	311129	1821448	372717	1821565	418840	1821330	324412
RP_POS_606_82281a0_498	RP	POS	0.50	606.8228				1.16E-04	-0.51	1.25	9.98E-01	0.00	1.18	2.54E-03	-0.51	1.31	5.68E-03	-0.51	1.31	1058003	153800	842070	470271	841947	497539	842192	446406
RP_POS_379_215a10_142	RP	POS	10.14	379.2150				3.95E-01	-0.24	0.95	9.99E-01	0.00	0.87	4.05E-01	-0.24	0.52	4.17E-01	-0.24	0.93	5680454	7941850	4421770	4039662	4422529	4415488	4421010	3670727
RP_POS_756_55353a12_817	RP	POS	12.82	756.5535				4.56E-02	0.35	0.78	9.99E-01	0.00	0.22	7.73E-02	0.35	0.70	9.52E-02	0.35	0.68	47143237	25851907	58811415	34616901	58816871	36673786	58805960	32804705
HILIC_NEG_444_74869a2_929	HILIC	NEG	2.929	444.7487				3.18E-06	-0.61	1.33	9.99E-01	0.00	0.76	2.22E-04	-0.61	1.48	1.15E-03	-0.61	1.48	448170	56927	344608	187321	344586	202447	344630	172943
HILIC_NEG_142_94432a1_687	HILIC	NEG	1.687	142.9443				2.78E-02	-0.46	1.04	9.99E-01	0.00	0.62	3.98E-02	-0.46	0.85	5.31E-02	-0.46	1.04	871884	472408	655409	466173	655366	506638	655452	427069
RP_NEG_704_8075a0_498	RP	NEG	0.50	704.8075				2.12E-05	-0.54	1.27	9.99E-01	0.00	1.21	1.14E-03	-0.54	1.34	2.65E-03	-0.54	1.33	6157136	796139	4738919	2887713	4739157	3035859	4738681	2762519
RP_NEG_390_12875a11_16	RP	NEG	11.16	390.1288				1.89E-02	0.45	0.91	9.99E-01	0.00	0.78	4.55E-02	0.45	0.82	3.14E-02	0.45	1.13	554444	51862	580931	60313	580936	55379	580926	65441
HILIC_POS_501_05304a3_077	HILIC	POS	3.077	501.0530				2.82E-04	0.50	1.18	1.00E+00	0.00	0.80	2.39E-03	0.50	1.28	9.53E-03	0.50	1.36	531090	42644	580210	107673	580213	118675	580207	96641
RP_POS_166_98497a10_575	RP	POS	10.58	166.9850				1.73E-01	-0.28	0.51	1.00E+00	0.00	0.30	2.12E-01	-0.28	0.59	2.24E-01	-0.28	0.74	15020383	4269496	13830989	4127457	13831061	4288756	13830917	4003254
RP_POS_674_81097a0_497	RP	POS	0.50	674.8110				4.09E-07	-0.62	1.33	1.00E+00	0.00	1.19	2.08E-04	-0.62	1.42	4.31E-04	-0.62	1.41	2277676	164208	1738320	960806	1738334	994581	1738305	935919