

Supplementary file

Table (1S): Tentatively identified metabolites in ET & ETM extracts of *Z. decumbens* using LC-ESI-TOF-MS/MS (Negative/ Positive Modes):

No.	Rt (min.)	Identified metabolite	Exact Formula	[M-H] ⁻	[M+H] ⁺	Ms/Ms	Compounds detected in ET	Compounds detected in ETM
Flavonoid derivatives								
1	4.23	kaempferol-O-deoxyhexoyl-hexoside-O-deoxyhexoside	C ₃₃ H ₄₀ O ₁₉	739.0338		285		✓
2	4.43	Hesperidin	C ₂₈ H ₃₄ O ₁₅	609.1427	611.1586	563, 301	✓	✓
3	4.48	Kaempferol-O-pentoside	C ₂₀ H ₁₈ O ₁₀	417.1555		399, 285		✓
4	4.64	Quercetin-O- hexuronide	C ₂₁ H ₁₈ O ₁₃	477.1536		393, 301, 179, 273, 151	✓	✓
5	4.73	Rutin	C ₂₇ H ₃₀ O ₁₆	609.1418		301		✓
6	4.77	Taxifolin	C ₁₅ H ₁₂ O ₇	303.1809		285, 257, 195		✓
7	4.85	Acacetin-O-deoxyhexosyl-hexoside	C ₂₈ H ₃₂ O ₁₄	591.9002		283, 445		✓
8	5.33	Kaempferol-O- deoxyhexoside	C ₂₁ H ₂₀ O ₁₀	431.1454		385, 285		✓
9	5.53	Rhoifolin	C ₂₇ H ₃₀ O ₁₄	577.1207		531, 269	✓	✓
10	5.54	Quercetin-O-di-hexoside	C ₂₇ H ₃₀ O ₁₇	625.143		607, 301	✓	
11	5.56	Baicalein-O- hexuronide	C ₂₁ H ₁₈ O ₁₁	445.1728		399, 269, 205, 195	✓	✓
12	5.64	Kaempferol-O- deoxyhexosyl-hexoside	C ₂₇ H ₃₀ O ₁₅	593.1508		285	✓	
13	5.84	Eriodictyol-O- hexoside	C ₂₁ H ₂₂ O ₁₁	449.0987	451.1963	403, 287, 179	✓	✓
14	5.91	Isorhamnetin-O- deoxyhexosyl-hexoside	C ₂₈ H ₃₂ O ₁₆	623.1595	625.1817	315, 300	✓	✓
15	5.95	Isorhamnetin-O-hexoside	C ₂₂ H ₂₂ O ₁₂	477.1029	479.1166	315, 300, 271	✓	✓
16	6.01	Gossypin	C ₂₁ H ₂₀ O ₁₃	479.1079		317, 271, 243	✓	✓
17	6.02	Isoquercitrin	C ₂₁ H ₂₀ O ₁₂	463.0862	465.2480	417, 301, 287, 283	✓	✓
18	6.71	Phlorizin	C ₂₁ H ₂₄ O ₁₀	435.2259	437.1428	389, 273	✓	✓
19	6.72	Luteolin-O- hexoside	C ₂₁ H ₂₀ O ₁₁	447.0929		401, 314, 285	✓	
20	6.88	Syringetin-O- hexoside	C ₂₃ H ₂₄ O ₁₃	507.1491		463, 355, 345, 327, 303, 85	✓	✓
21	7.15	Quercetin-O-pentoside	C ₂₀ H ₁₈ O ₁₁	433.2085		387, 301	✓	✓
22	7.21	Kaempferol-O-hexuronide	C ₂₁ H ₁₈ O ₁₂	461.1099		415, 285	✓	✓
23	7.54	Quercitrin	C ₂₁ H ₂₀ O ₁₁	447.1337		401, 301	✓	
24	8.31	Naringenin-O- hexoside	C ₂₁ H ₂₂ O ₁₀	433.2072		271, 151	✓	✓
25	8.58	Myricetin	C ₁₅ H ₁₀ O ₈	317.1109		209, 181		✓
26	8.64	Hyperoside	C ₂₁ H ₂₀ O ₁₂		465.2805	301	✓	

Continuing: Table (1S): Tentatively identified metabolites in ET & ETM extracts of *Z. decumbens* using LC-ESI-TOF-MS/MS
(Negative/ Positive Modes):

No.	Rt (min.)	Identified metabolite	Exact Formula	[M-H] ⁻	[M+H] ⁺	Ms/Ms	Compounds detected in ET	Compounds detected in ETM
27	8.69	Quercetin	C ₁₅ H ₁₀ O ₇	301.1175	303.0505	283, 273, 259, 255, 229, 227, 193, 151	√	√
28	9.33	Luteolin	C ₁₅ H ₁₀ O ₆	285.1237	287.0553	267, 243, 239, 229, 176, 161	√	√
29	9.37	Isorhamnetin	C ₁₆ H ₁₂ O ₇	315.0549	317.0659	300, 271, 164	√	√
30	9.44	Naringenin	C ₁₅ H ₁₂ O ₅	271.1072		253, 243, 197	√	√
31	9.69	Hesperetin	C ₁₆ H ₁₄ O ₆	301.1172		283, 255, 193, 179, 151	√	√
32	10.10	Tetrahydroxy flavanone	C ₁₅ H ₁₂ O ₆	286.9382	289.1335	259, 241, 180	√	√
33	10.36	Acacetin	C ₁₆ H ₁₂ O ₅	283.1068	285.1133	268, 265, 237	√	√
34	11.07	Apigenin	C ₁₅ H ₁₀ O ₅	269.2096		223, 93	√	√
35	11.68	Dihydroxy methoxy flavone	C ₁₆ H ₁₄ O ₅		287.0547	269, 193	√	
36	12.68	Pentahydroxy flavan	C ₁₅ H ₁₄ O ₆	288.955		181	√	√
37	12.90	Kaempferide	C ₁₆ H ₁₂ O ₆	299.2022	301.1413	281, 253, 193	√	√
38	16.59	Tetrahydroxy methoxy flavone	C ₁₆ H ₁₂ O ₇		317.1749	299, 150, 123, 109		√
Phenolic acids								
No.	Rt (min.)	Identified metabolite	Exact Formula	[M-H] ⁻	[M+H] ⁺	Ms/Ms	Compounds detected in ET	Compounds detected in ETM
39	0.95	Gentisic acid	C ₇ H ₆ O ₄	153.0209		109	√	√
40	1.02	Sinapic acid	C ₁₁ H ₁₂ O ₅	223.0648	225.0849	205, 179, 163, 91	√	
41	1.06	Hydroxybenzoic acid	C ₇ H ₆ O ₃	137.0246		93	√	
42	1.07	Homogentisic acid	C ₈ H ₈ O ₄	167.0357		123, 108	√	√
43	1.10	Vanillic acid	C ₈ H ₈ O ₄	167.0332		108, 123, 152	√	√
44	1.26	Coumaric acid	C ₉ H ₈ O ₃	163.0407	165.0538	119, 93	√	√
45	1.27	Quinic acid	C ₇ H ₁₂ O ₆	191.0675		173, 101		√
46	1.31	Ferulic acid	C ₁₀ H ₁₀ O ₄	193.0493	195.0647	162, 149	√	√
47	1.42	Caffeic acid	C ₉ H ₈ O ₄	179.0034		135, 71	√	√
48	1.52	Salicylic acid	C ₇ H ₆ O ₃	137.0377		119, 93	√	
49	1.93	Sinapoyl malate	C ₁₅ H ₁₆ O ₉	339.0857		321, 303, 295, 279, 207	√	√
50	1.98	Benzoic acid	C ₇ H ₆ O ₂		123.0544	105, 78		√
51	2.18	Shikimic acid	C ₇ H ₁₀ O ₅	173.0073		155, 131	√	√

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(Negative/ Positive Modes):

No.	Rt (min.)	Identified metabolite	Exact Formula	[M-H] ⁻	[M+H] ⁺	Ms/Ms	Compounds detected in ET	Compounds detected in ETM
52	2.64	Hydroxy phenylacetic acid	C ₈ H ₈ O ₃	151.0370		107, 106, 93		✓
53	3.92	Methoxy cinnamic acid	C ₁₀ H ₁₀ O ₃		179.0779	161, 134, 107		✓
Fatty acids								
No.	Rt (min.)	Identified metabolite	Exact Formula	[M-H] ⁻	[M+H] ⁺	Ms/Ms	Compounds detected in ET	Compounds detected in ETM
54	4.10	Chlorogenic acid	C ₁₆ H ₁₈ O ₉	353.0921		179, 175	✓	✓
55	5.81	Cinnamate	C ₉ H ₈ O ₂	146.9949	149.0313	103		✓
56	6.43	Sinapoyl hexoside	C ₁₇ H ₂₂ O ₁₀		387.1639	225, 207	✓	✓
57	0.80	Methyl glutaric acid	C ₆ H ₁₀ O ₄	145.0493		127, 101		✓
58	0.81	Hydroxy methyl pentanoate	C ₆ H ₁₂ O ₃	131.0337		113, 87		✓
59	1.05	Citraconic acid	C ₅ H ₆ O ₄	129.0006		85		✓
60	1.18	Aconitate	C ₆ H ₆ O ₆	173.0809		155, 137, 129, 83		✓
61	1.56	Isopropyl malic acid	C ₇ H ₁₂ O ₅	175.0702		157, 139, 85		✓
62	2.69	Arachidonic acid	C ₂₀ H ₃₂ O ₂	303.1335		258	✓	
63	5.22	Sebacate	C ₁₀ H ₁₈ O ₄	201.1128		183, 157, 156, 113		✓
64	9.78	Linolenic acid	C ₁₈ H ₃₀ O ₂	277.1442		233	✓	✓
65	18.42	Linoleic acid	C ₁₈ H ₃₂ O ₂		281.1939	263	✓	✓
Organic acids derivatives								
No.	Rt (min.)	Identified metabolite	Exact Formula	[M-H] ⁻	[M+H] ⁺	Ms/Ms	Compounds detected in ET	Compounds detected in ETM
66	0.82	Succinic acid	C ₄ H ₆ O ₄	117.0192		99, 73	✓	✓
67	0.90	Lactic acid	C ₃ H ₆ O ₃	89.026		71		✓
68	0.95	Methyl lactic acid	C ₄ H ₈ O ₃	103.0399		73, 59, 57	✓	✓
69	0.96	Maleic acid	C ₄ H ₄ O ₄	115.0399		97, 71		✓
70	0.98	Methylmalonic acid	C ₄ H ₆ O ₄	117.0572		99, 73		✓
71	1.01	Hydroxybutyric acid	C ₄ H ₈ O ₃	103.0398		73, 59		✓
72	1.015	Mucate	C ₆ H ₁₀ O ₈	209.079		191, 165, 137, 121		✓
73	2.90	Phenyl lactic acid	C ₉ H ₁₀ O ₃	165.0211		147, 121	✓	✓
Miscellaneous metabolites								
No.	Rt. (min.)	Identified metabolite	Exact Formula	[M-H] ⁻	[M+H] ⁺	Ms/Ms	Compounds detected in ET	Compounds detected in ETM
74	1.23	Citramalate	C ₅ H ₈ O ₅	147.0298		129, 59, 57	✓	✓
75	1.23	Ketoisoleucine	C ₆ H ₁₀ O ₃	129.0282		85, 69, 55	✓	✓

Continuing: Table (1S): Tentatively identified metabolites in ET & ETM extracts of *Z. decumbens* using LC-ESI-TOF-MS/MS (Negative/ Positive Modes):

No.	Rt (min.)	Identified metabolite	Exact Formula	[M-H] ⁻	[M+H] ⁺	Ms/Ms	Compounds detected in ET	Compounds detected in ETM
76	1.27	Hydroxy methyl glutaric acid	C ₆ H ₁₀ O ₅	161.0831		143, 117, 99	✓	✓
77	1.72	Syringaldehyde	C ₉ H ₁₀ O ₄		183.0946	165, 153, 123	✓	✓
78	2.18	Suberic acid	C ₈ H ₁₄ O ₄	173.0073		155, 129, 85	✓	✓
79	2.31	Dihydroxy mandelate	C ₈ H ₈ O ₅	183.0482		138	✓	✓
80	2.68	Hydroxy methoxy phenylacetic acid	C ₉ H ₁₀ O ₄	181.0531		163, 151, 137		✓
81	4.25	Hydroxy methoxy cinnamaldehyde	C ₁₀ H ₁₀ O ₃		179.0827	161, 135, 124		✓
82	5.49	Hydroxy methoxy mandelate	C ₉ H ₁₀ O ₅	197.096		167, 153, 122		✓
83	5.72	Esculin	C ₁₅ H ₁₆ O ₉	339.1081		311, 293, 177	✓	✓
84	7.02	Sinapyl aldehyde	C ₁₁ H ₁₂ O ₄	207.071		189, 178	✓	✓
85	7.26	Dihydroxy coumarin	C ₉ H ₆ O ₄	177.0262		133	✓	
86	8.30	Cinnamaldehyde	C ₉ H ₈ O		133.101	103, 77	✓	

All fragmentation was firstly applied according to ESI negative mode if available, the error in metabolites identification was within ± 10 ppm & highlighted compounds represent changed compounds appearing after microbial biotransformation (ETM)



Figure (1S): Venn Diagram of the number of compounds detected in ET & ETM extracts of *Z. decumbens*

Spectrum from IDA-NEG-240116-SM0289-4.wiff (sampl...xperiment 6, -TOF MS² (50 - 1000) from 4.230 min
Precursor: 738.8 Da, Gaussian smoothed, Gaussian smoothed

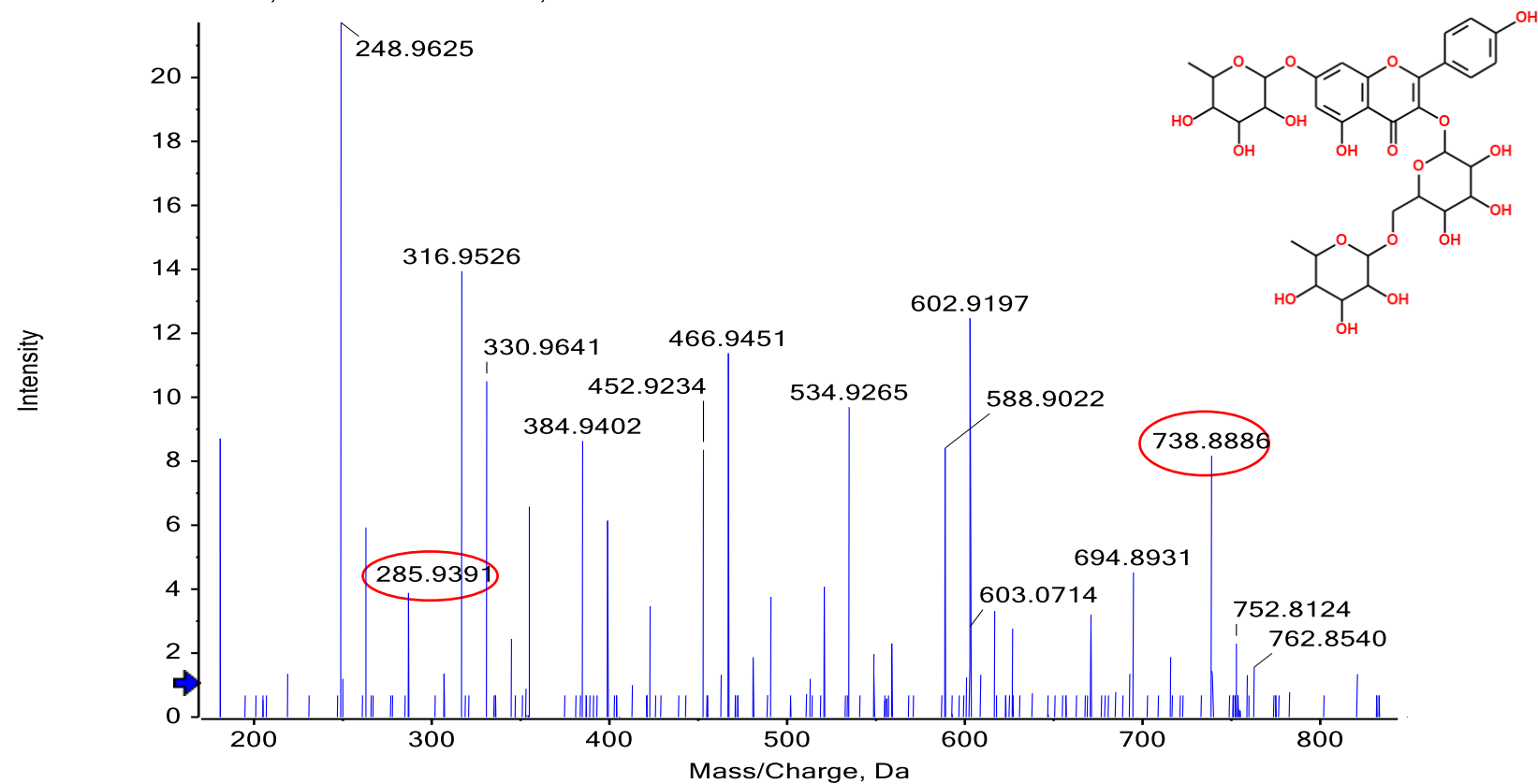


Figure (2S): LC/Ms-Ms of kaempferol-*O*-deoxyhexoyl-hexosyl-*O*-deoxyhexoside of ETM in ESI negative mode

Spectrum from IDA-NEG-240116-SM0289-4.wiff (sample experiment 14, -TOF MS² (50 - 1000) from 4.737 min
cursor: 609.1 Da, Gaussian smoothed

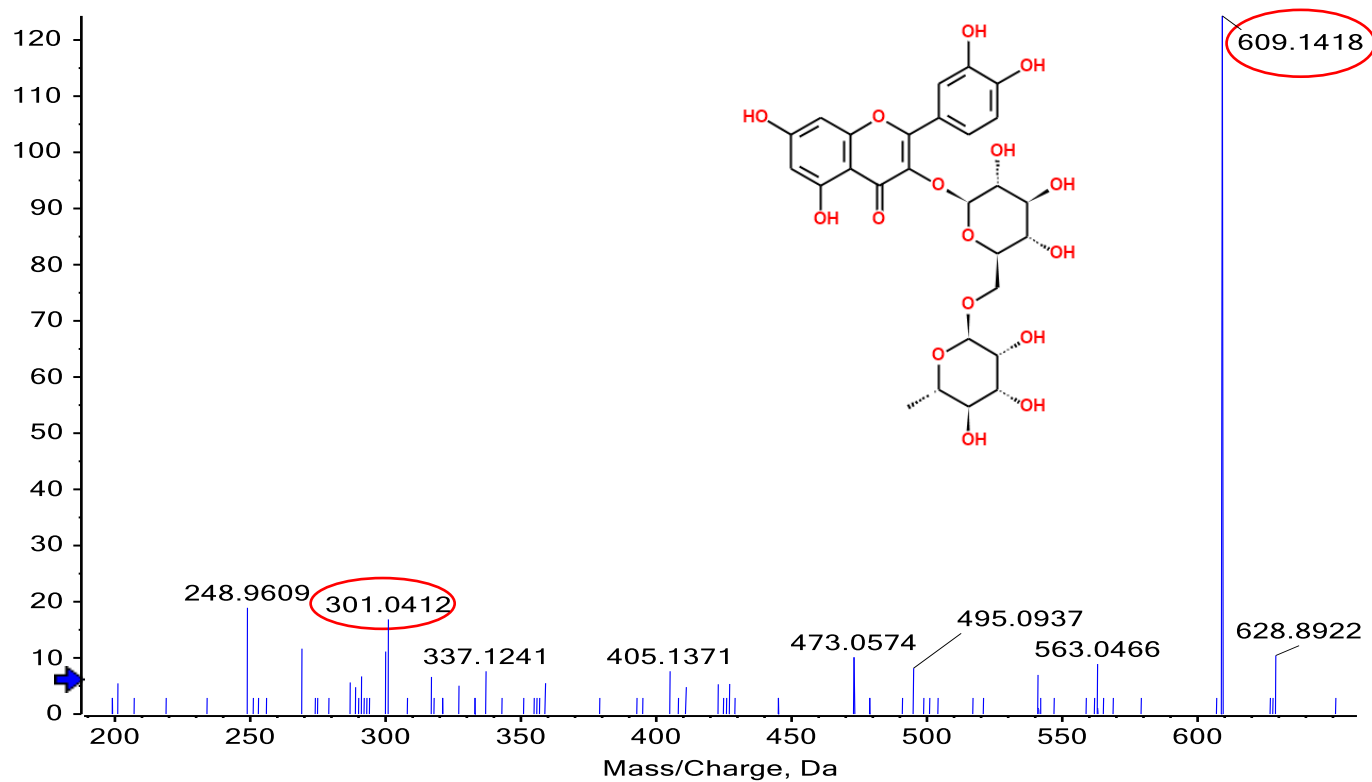


Figure (3S): LC/Ms-Ms of rutin of ETM in ESI negative mode

Spectrum from IDA-NEG-240116-SM0289-4.wiff (sampl...periment 13, -TOF MS² (50 - 1000) from 4.853 min
Precursor: 591.9 Da, Gaussian smoothed, Gaussian ...n smoothed, Gaussian smoothed, Gaussian smoothed

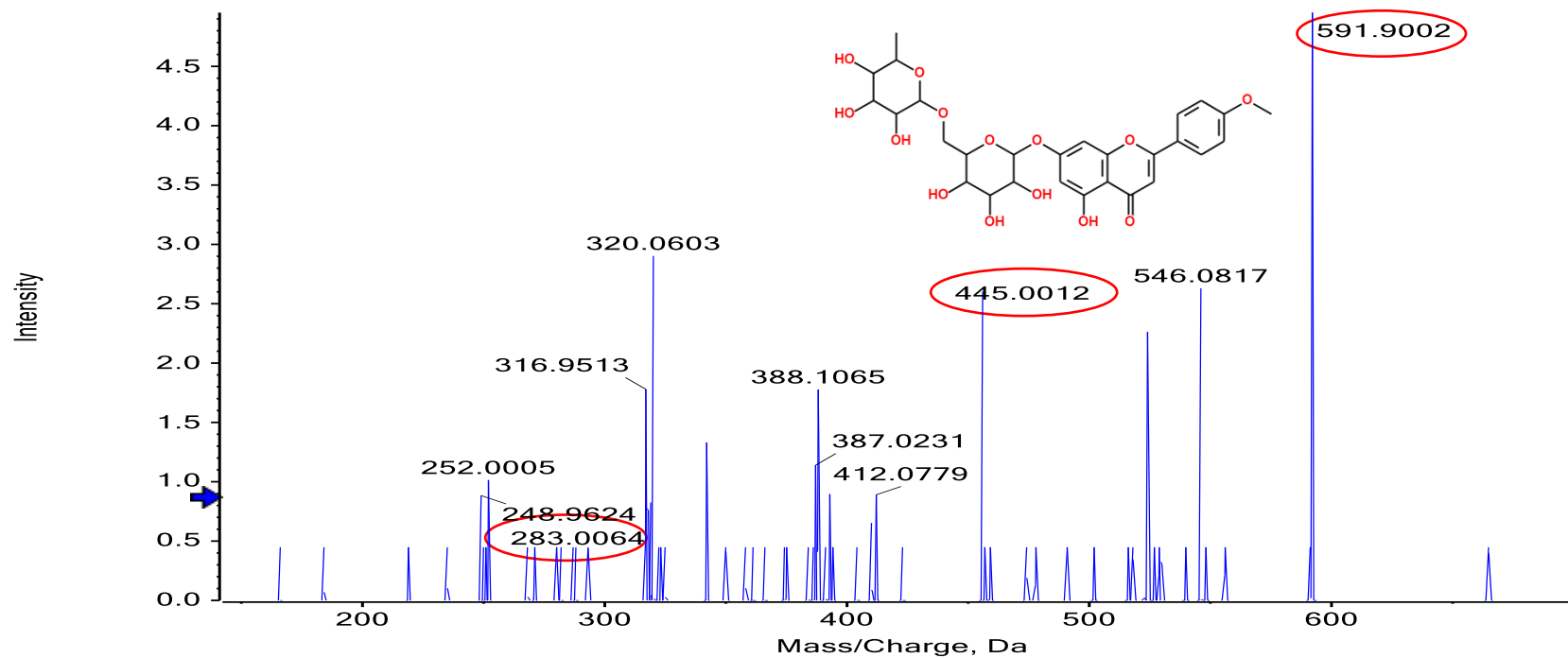


Figure (4S): LC/Ms-Ms of Acacetin-*O*-deoxyhexosyl-hexoside of ETM in ESI negative mode

Spectrum from IDA-NEG-240116-SM0289-4.wiff (sampl...xperiment 5, -TOF MS² (50 - 1000) from 4.488 min
Precursor: 417.1 Da, Gaussian smoothed

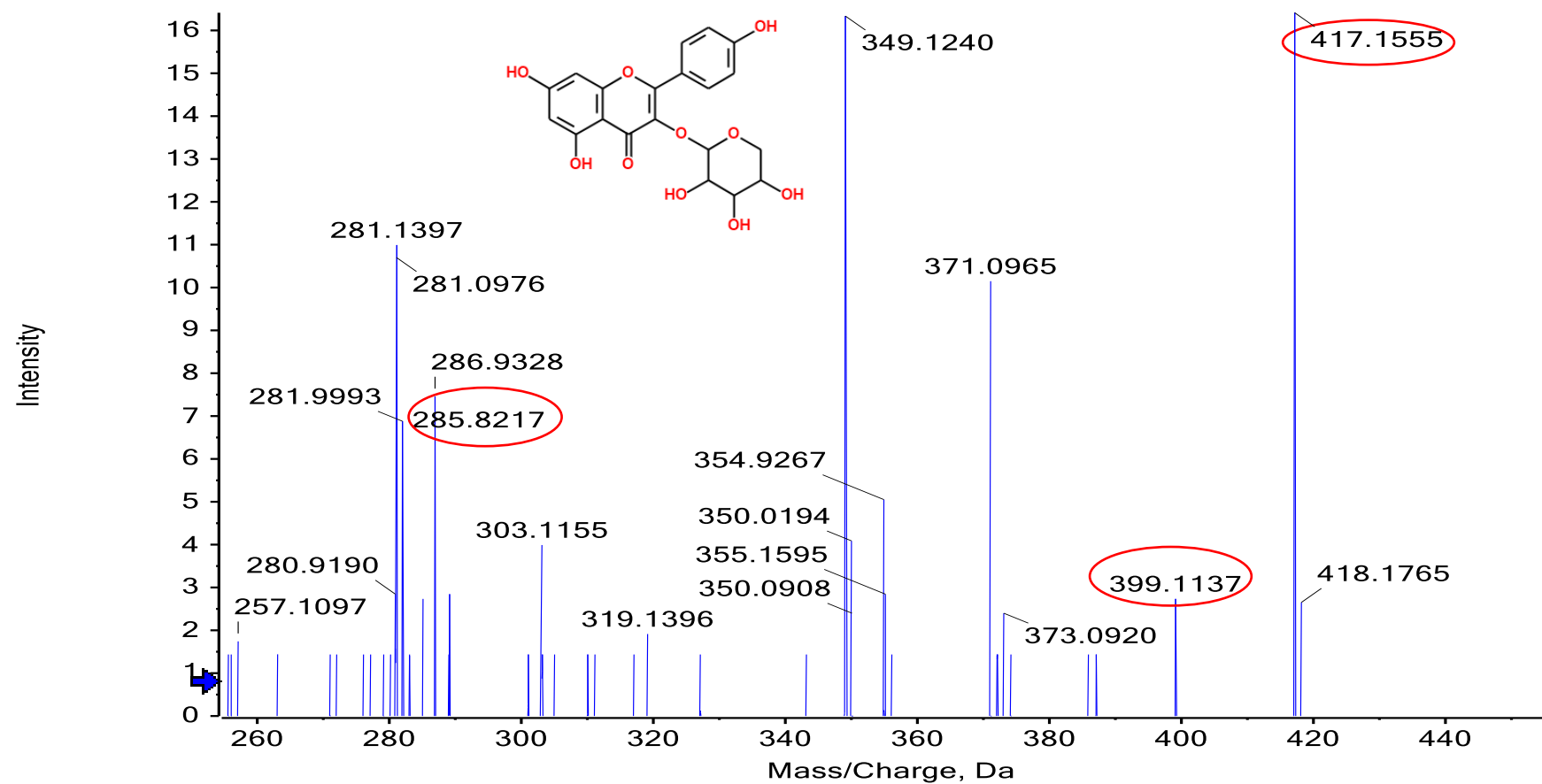


Figure (5S): LC/Ms-Ms of kaempferol-*O*-pentoside of ETM in ESI negative mode

Spectrum from IDA-NEG-240116-SM0289-4.wiff (sampl...xperiment 7, -TOF MS² (50 - 1000) from 5.334 min
Precursor: 431.1 Da, Gaussian smoothed, Gaussian smoothed, Gaussian smoothed

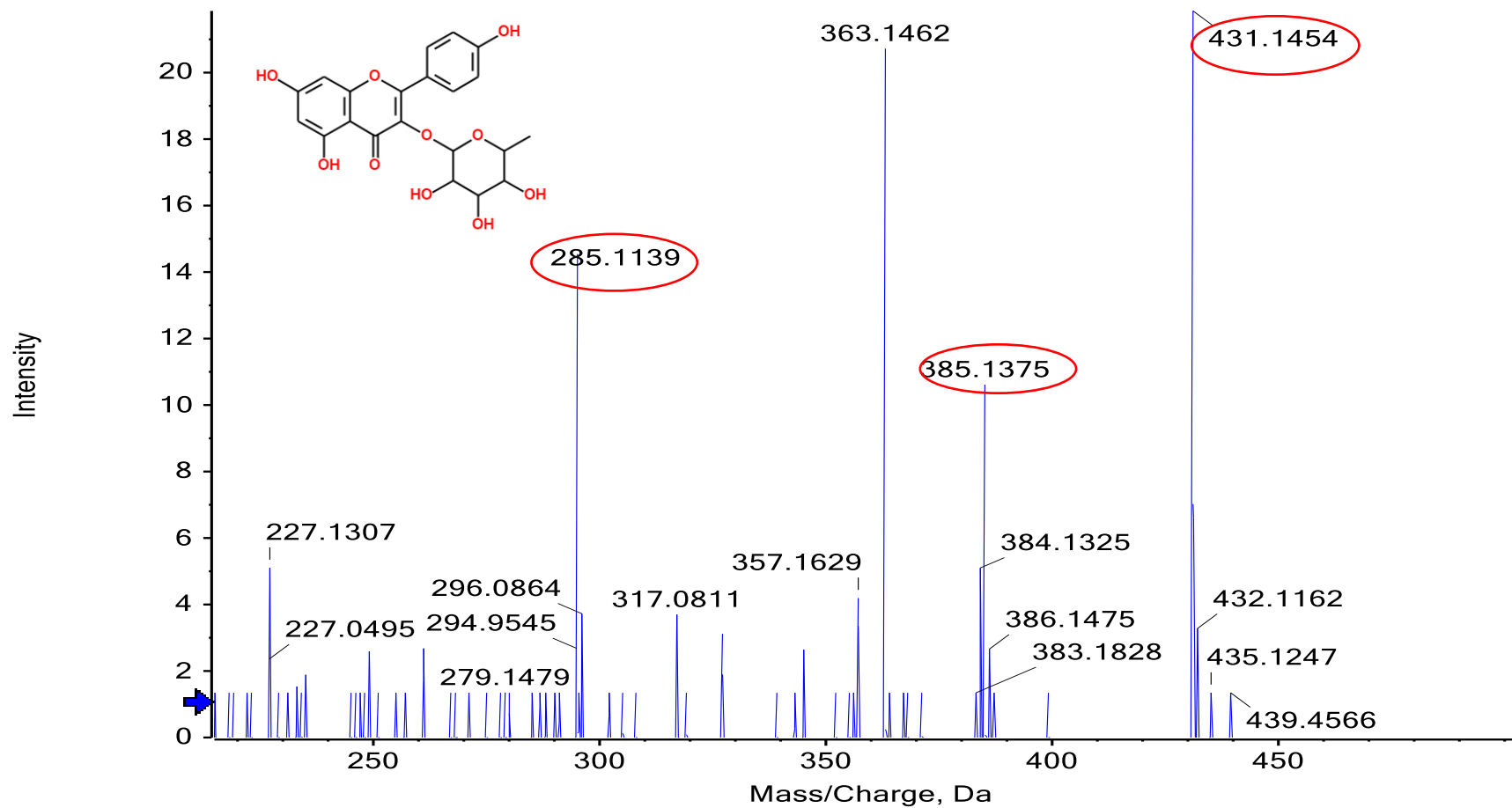


Figure (6S): LC/Ms-Ms of Kaempferol-O- deoxyhexoside of ETM in ESI negative mode

Spectrum from IDA-NEG-240116-SM0289-4.wiff (sampl...xperiment 4, -TOF MS² (50 - 1000) from 4.771 min
Precursor: 303.1 Da, Gaussian smoothed

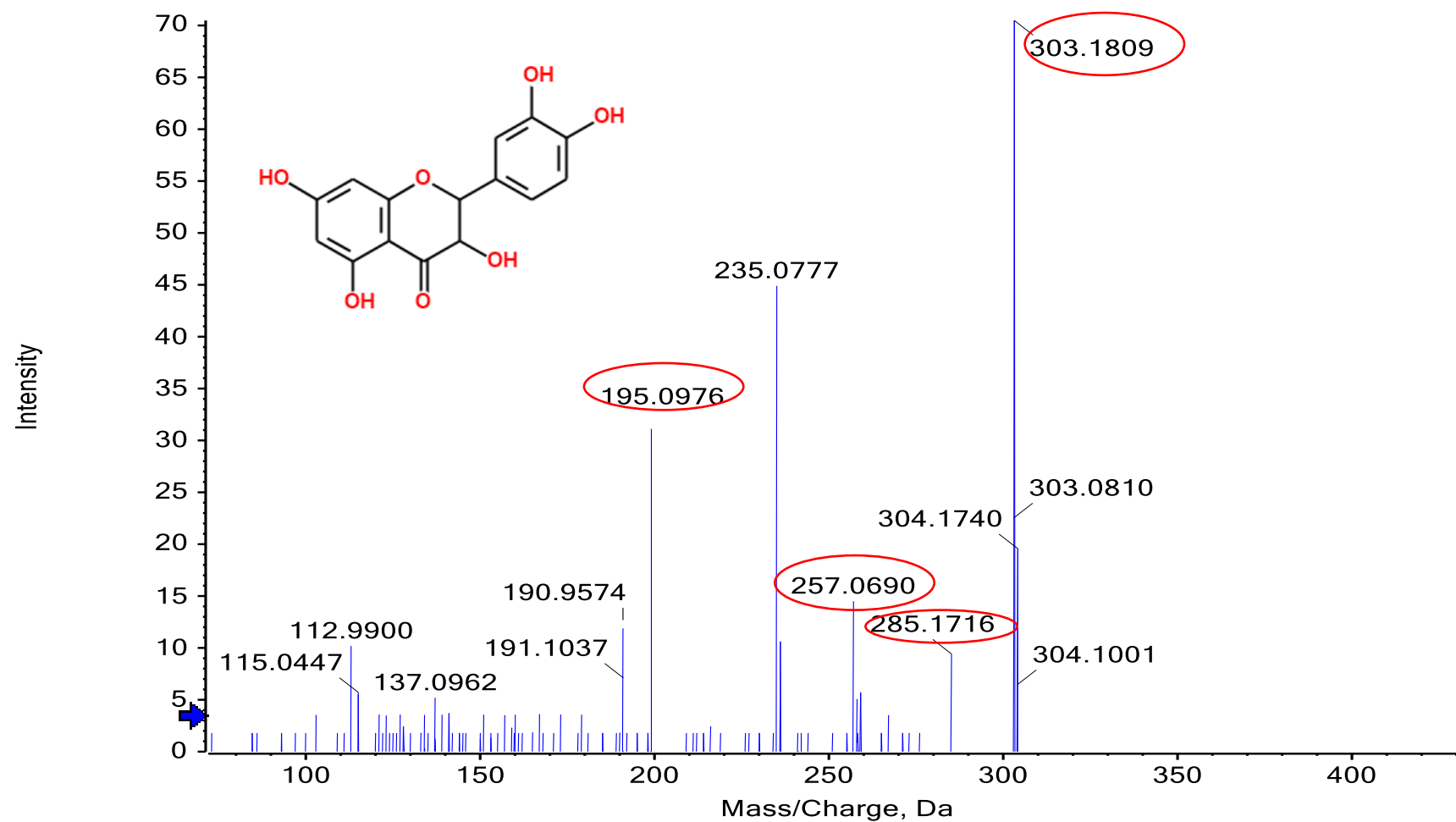


Figure (7S): LC/Ms-Ms of taxifolin of ETM in ESI negative mode

Spectrum from IDA-NEG-240116-SM0289-4.wiff (sample 1) - ...9-4, Experiment 2, -TOF MS² (50 - 1000) from 8.580 min
Precursor: 317.1 Da

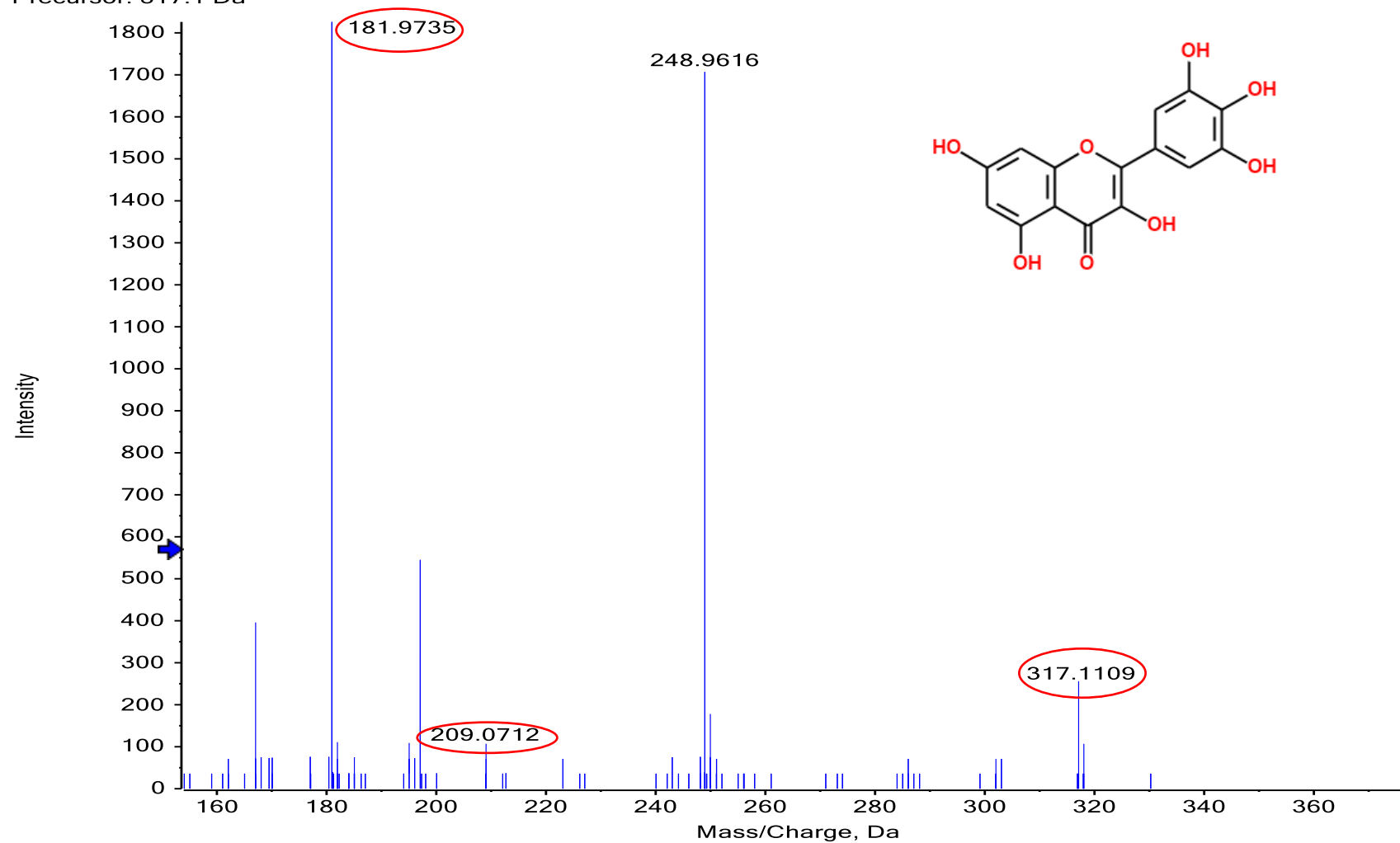


Figure (8S): LC/Ms-Ms of myrecetin of ETM in ESI negative mode

Spectrum from IDA-POS-240115-SM0289-4.wiff (sampl...periment 3, +TOF MS² (50 - 1000) from 16.591 min
Precursor: 317.3 Da, CE: 35.0, Gaussian smoothed

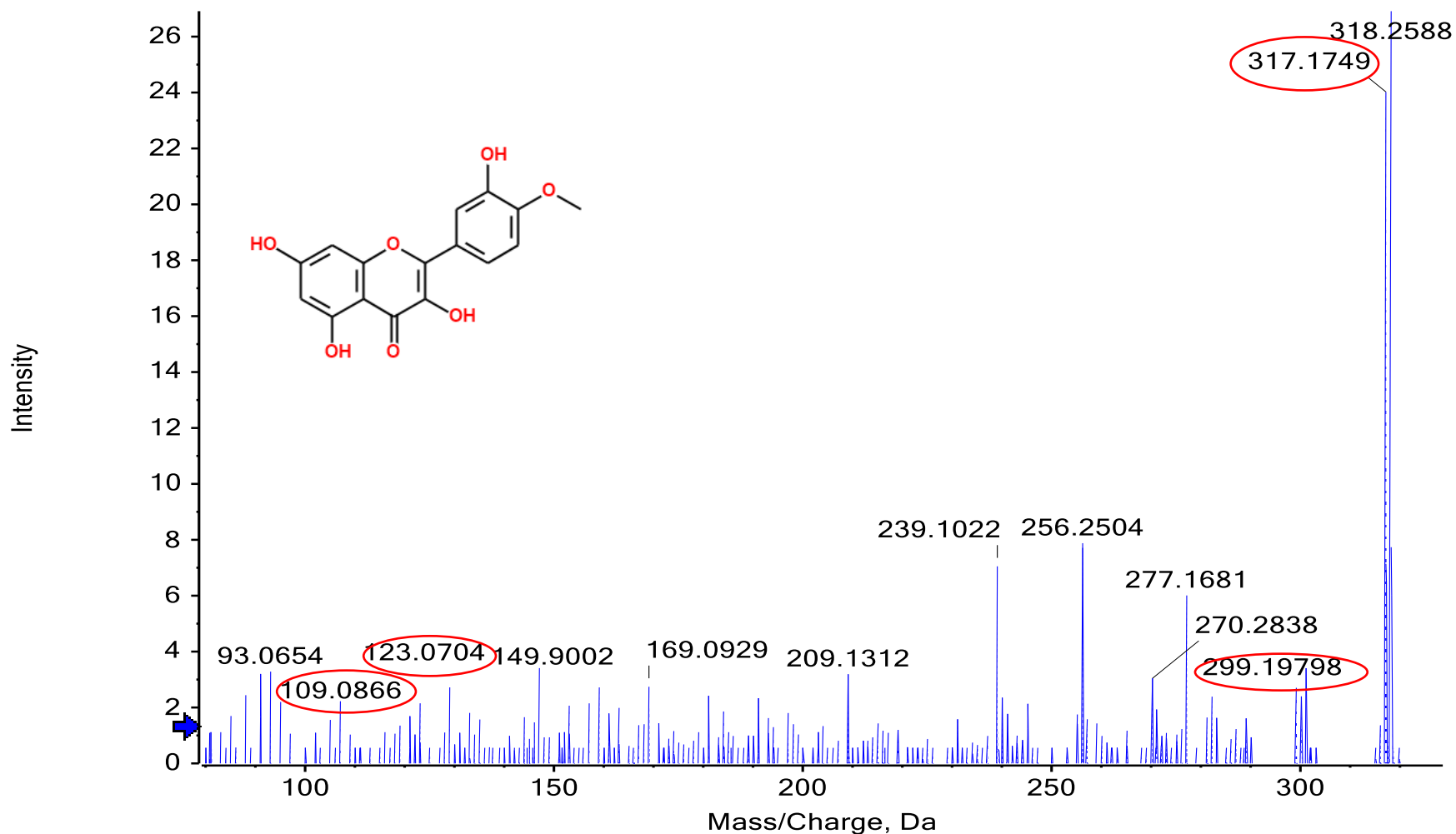


Figure (9S): LC/Ms-Ms of tetrahydroxy methoxy flavone of ETM in ESI positive mode

Spectrum from IDA-NEG-240116-SM0289-4.wiff (sampl...xperiment 3, -TOF MS² (50 - 1000) from 2.643 min
Precursor: 151.0 Da

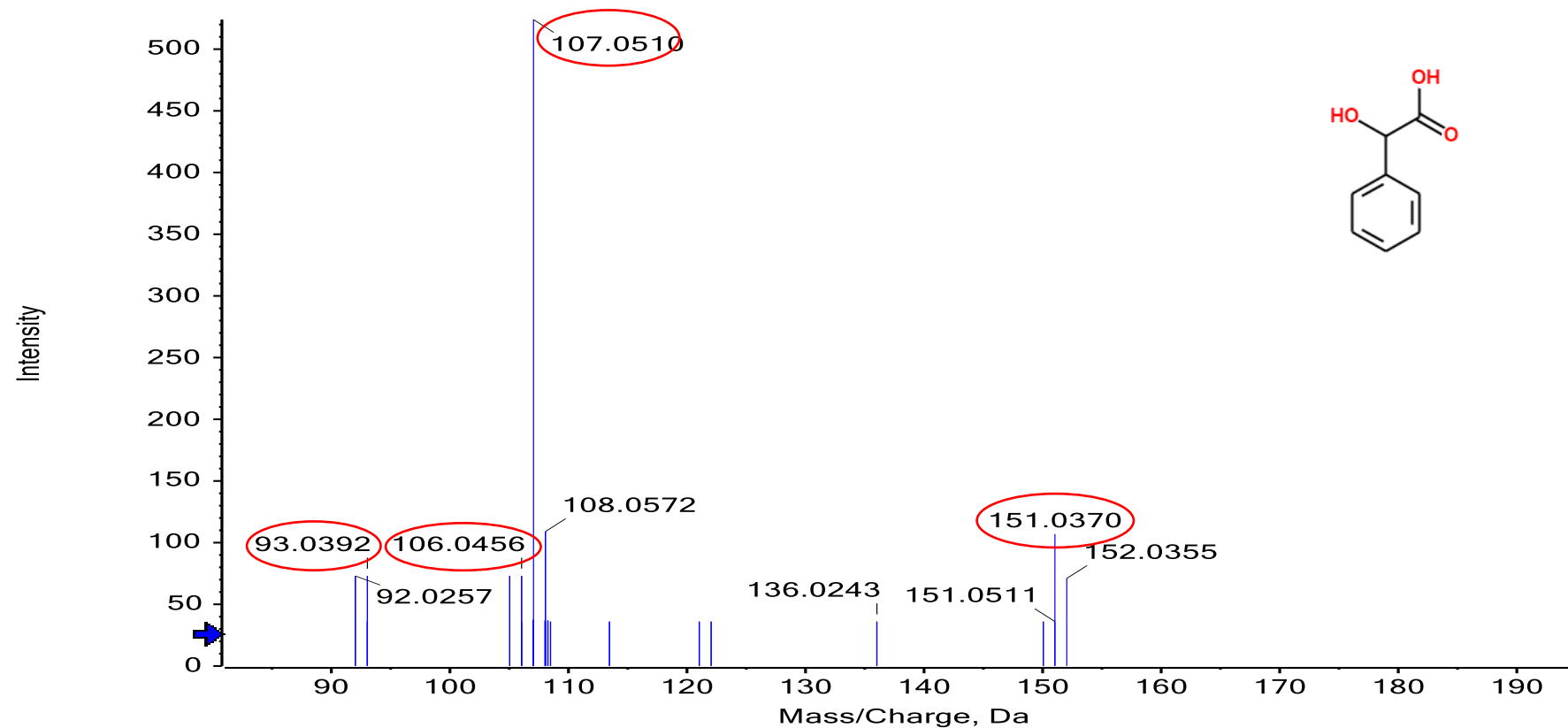


Figure (10S): LC/Ms-Ms of hydroxy phenylacetic acid of ETM in ESI negative mode

Spectrum from IDA-NEG-240116-SM0289-4.wiff (sampl...xperiment 4, -TOF MS² (50 - 1000) from 1.270 min
Precursor: 191.1 Da, Gaussian smoothed

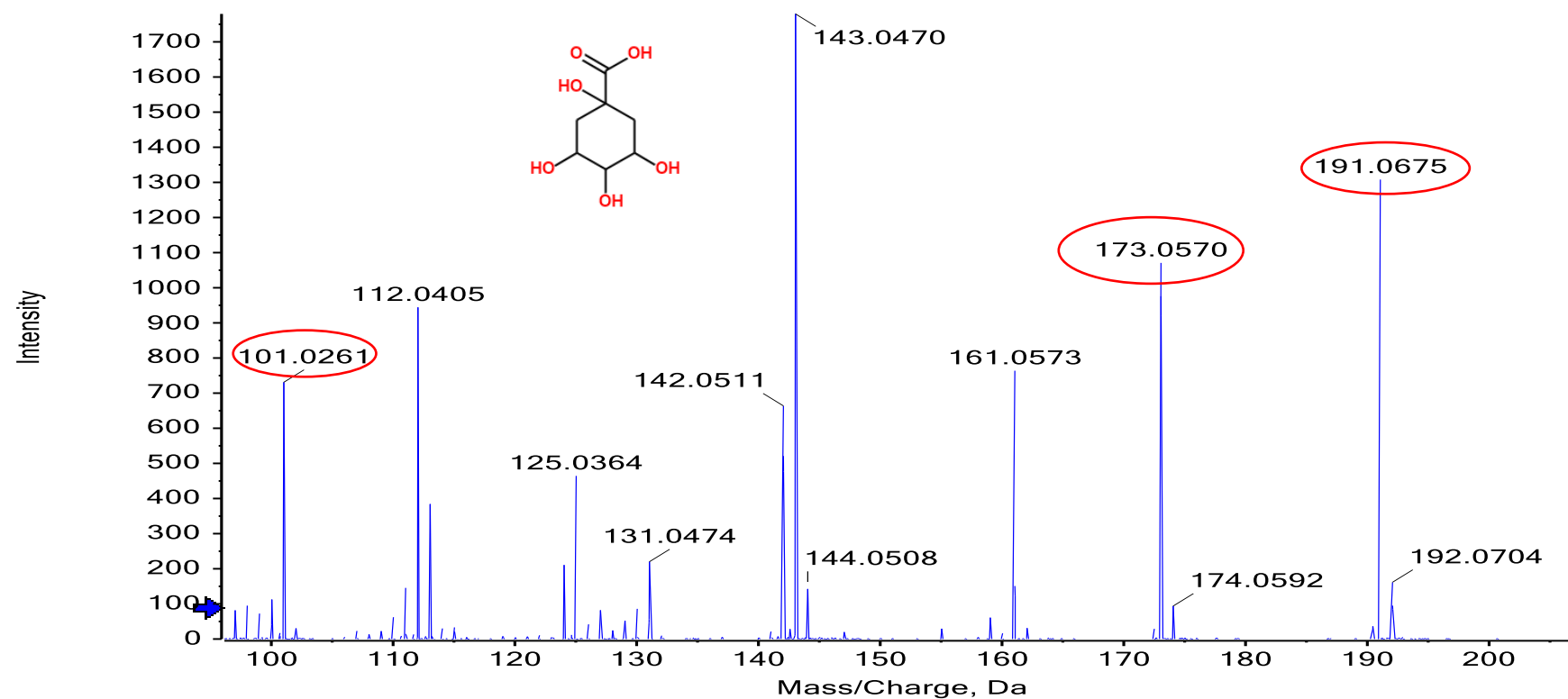


Figure (11S): LC/Ms-Ms of quinic acid of ETM in ESI negative mode

Spectrum from IDA-POS-240115-SM0289-4.wiff (sampl...xperiment 2, +TOF MS² (50 - 1000) from 1.988 min
Precursor: 123.0 Da, CE: 35.0, Gaussian smoothed

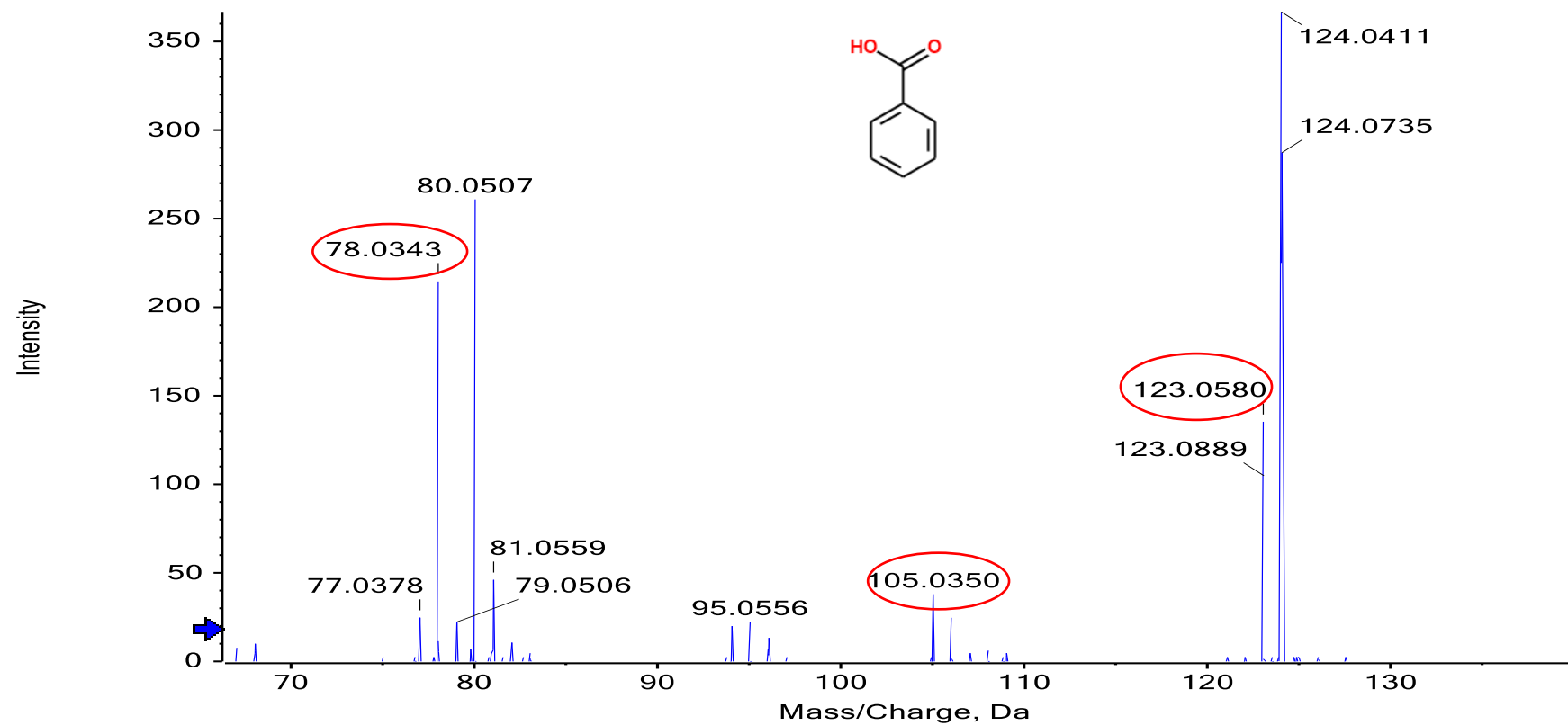


Figure (12S): LC/Ms-Ms of benzoic acid of ETM in ESI positive mode

Spectrum from IDA-POS-240115-SM0289-4.wiff (sampl...xperiment 6, +TOF MS² (50 - 1000) from 3.929 min
Precursor: 179.1 Da, CE: 35.0, Gaussian smoothed

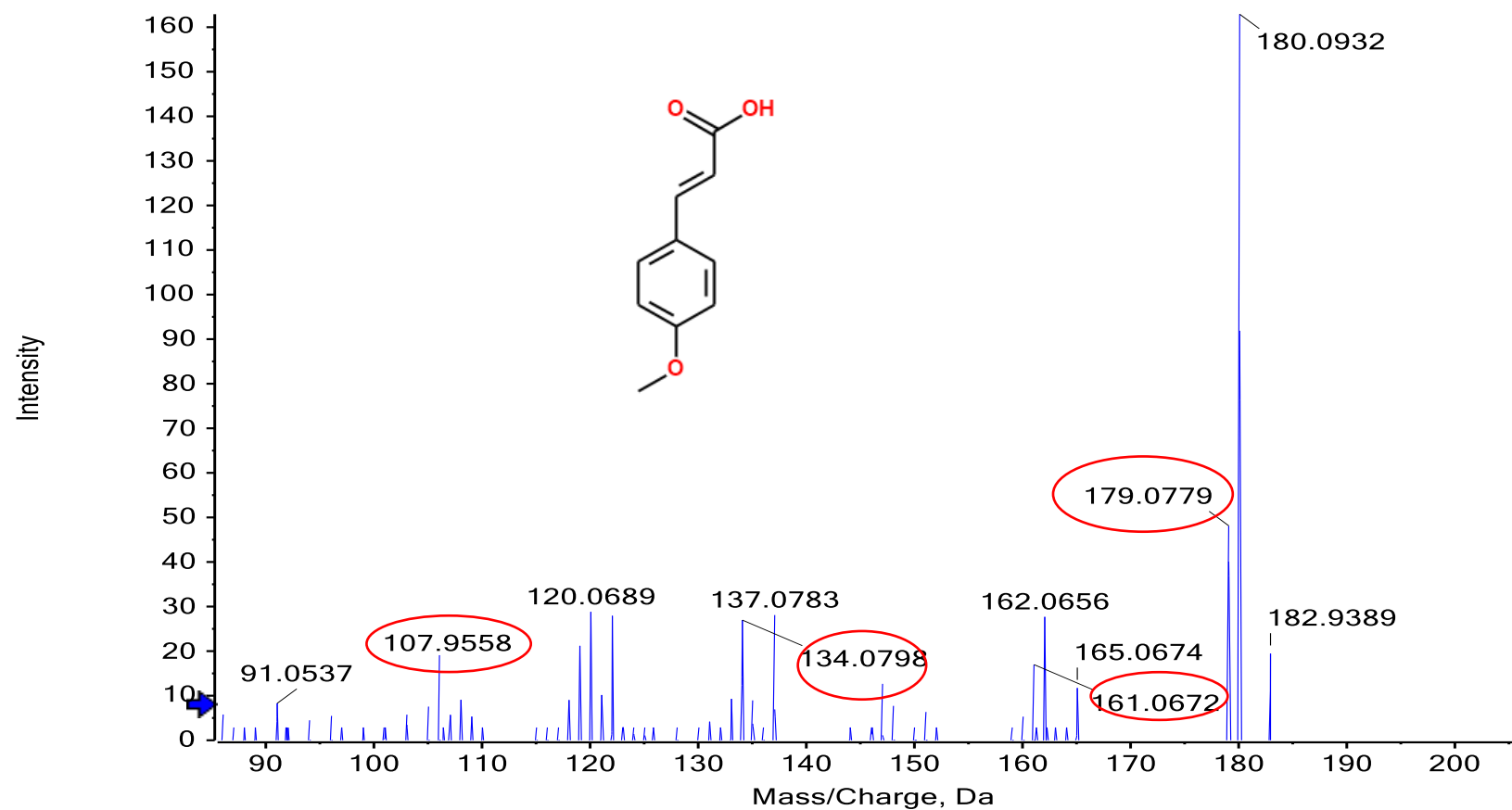


Figure (13S): LC/Ms-Ms of methoxy cinnamic acid of ETM in ESI positive mode

Spectrum from IDA-POS-240115-SM0289-4.wiff (sampl...xperiment 3, +TOF MS² (50 - 1000) from 5.814 min
Precursor: 149.1 Da, CE: 35.0, Gaussian smoothed

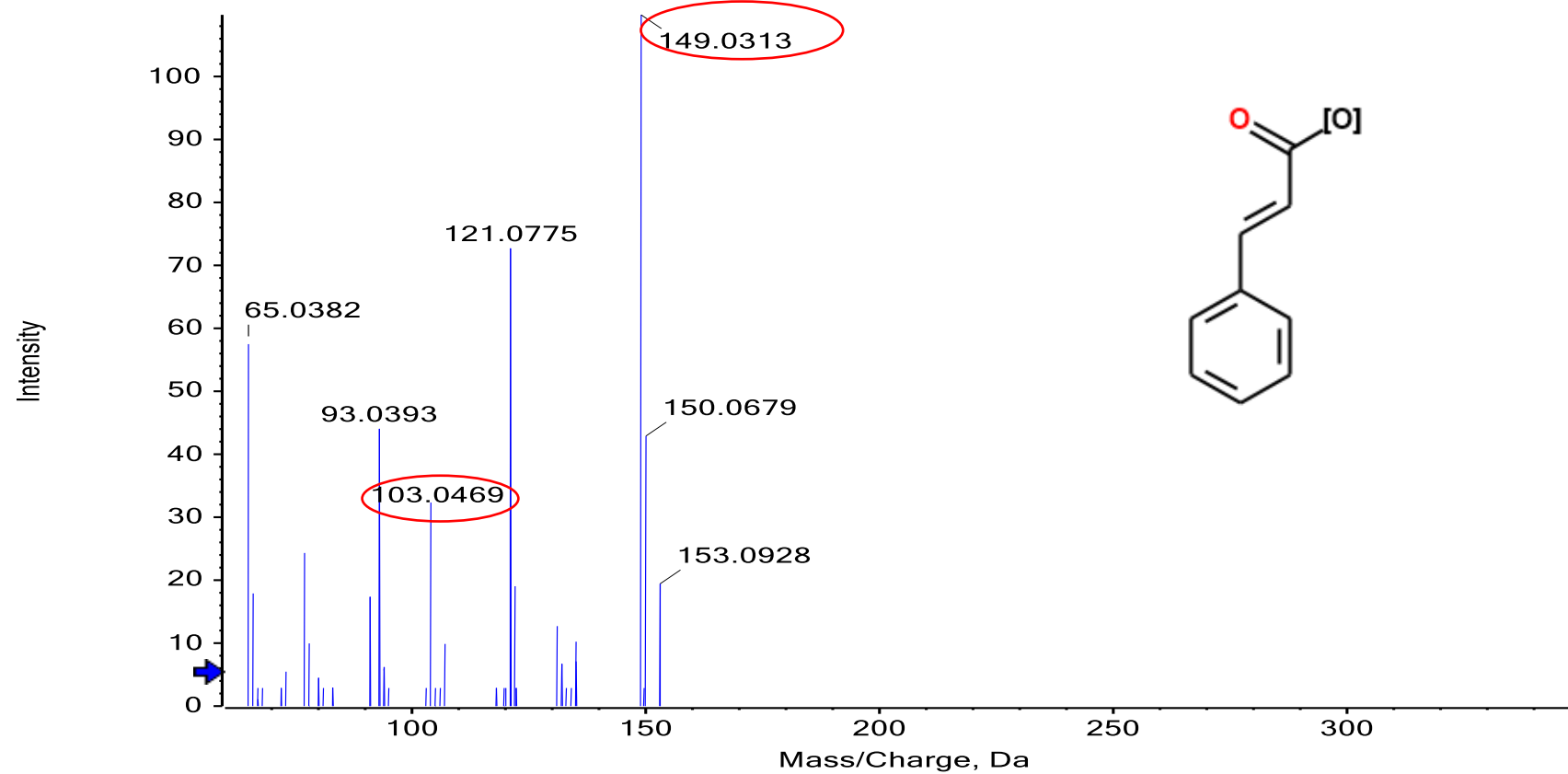


Figure (14S): LC/Ms-Ms of cinnamate of ETM in ESI positive mode