ORIGINAL RESEARCH

Diabetes Mellitus Severity and a Switch From Using Lipoprotein Lipase to Adipose-Derived Fatty Acid Results in a Cardiac Metabolic Signature That Embraces Cell Death

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***Background*—**Fatty acid (FA) provision to the heart is from cardiomyocyte and adipose depots, plus lipoprotein lipase action. We tested how a graded reduction in insulin impacts the source of FA used by cardiomyocytes and the cardiac adaptations required to process these FA.

***Methods and Results*—**Rats injected with 55 (D55) or 100 (D100) mg/kg streptozotocin were terminated after 4 days. Although D55 and D100 were equally hyperglycemic, D100 showed markedly lower pancreatic and plasma insulin and loss of lipoprotein lipase, which in D55 hearts had expanded. There was minimal change in plasma FA in D55. However, D100 exhibited a 2- to 3-fold increase in various saturated, monounsaturated, and polyunsaturated FA in the plasma. D100 demonstrated dramatic cardiac transcriptomic changes with 1574 genes differentially expressed compared with only 49 in D55. Augmented mitochondrial and peroxisomal β-oxidation in D100 was not matched by elevated tricarboxylic acid or oxidative phosphorylation. With increasing FA, although control myocytes responded by augmenting basal respiration, this was minimized in D55 and reversed in D100. Metabolomic profiling identified significant lipid accumulation in D100 hearts, which also exhibited sizeable change in genes related to apoptosis and terminal deoxynucleotidyl transferase dUTP nick-end labeling–positive cells.

***Conclusions*—**With increasing severity of diabetes mellitus, when the diabetic heart is unable to control its own FA supply using lipoprotein lipase, it undergoes dramatic reprogramming that is linked to handling of excess FA that arise from adipose tissue. This transition results in a cardiac metabolic signature that embraces mitochondrial FA overload, oxidative stress, triglyceride storage, and cell death. **(*J Am Heart Assoc*. 2019;8:e014022. DOI: 10.1161/JAHA.119.014022.)**

Key Words: diabetic cardiomyopathy • fatty acid • metabolism • metabolomics • RNA sequencing

Coronary disease is a primary basis for the increased incidence of cardiovascular disease following diabetes mellitus.[1,2] However, patients with type 1 and type 2 diabetes mellitus have also been diagnosed with reduced or low-normal diastolic function and left ventricular hypertrophy in the absence of vascular defects (labeled diabetic cardiomyopathy).[3,4] Animal models of diabetes mellitus also exhibit signs of cardiomyopathy.[5–7] Factors contributing to the development of cardiomyopathy include connective tissue and insoluble collagen accumulation, impaired sensitivity to various ligands, mitochondrial dysfunction, endoplasmic reticulum stress, renin-angiotensin-aldosterone system activation and abnormalities in Ca^{2+} sensing and regulating proteins.[5,7] Abnormalities in pathways regulating cardiac energy metabolism also contribute toward the etiology of diabetic cardiomyopathy.[8]

The earliest metabolic change occurring in the diabetic heart is reduced glucose consumption,[9] and a switch to exclusively utilize FA for energy.[10,11] This metabolic switching is likely initiated by a high-glucose–induced release of endothelial cell heparanase-1,[12] an endoglycosidase exceptional in its ability to cleave side chains of heparan sulfate proteoglycan on the cardiomyocyte cell surface, thereby instigating release of bound ligands. These include lipoprotein lipase (LPL),[13] which then traverses the interstitial space to the apical surface of the coronary lumen, where it breaks

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Accompanying Figure S1 and Tables S1 through S4 are available at https://www.ahajournals.org/doi/suppl/10.1161/JAHA.119.014022

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Clinical Perspective

What Is New?

- Using dissimilar doses of streptozotocin (55 and 100 mg/kg), a β-cell–specific toxin used to induce hypoinsulinemia, we established models of diabetes mellitus of varying intensities; despite the decline of insulin in D55, although these animals were hyperglycemic, they exhibited minimal change in average plasma fatty acid (FA) concentrations, and it was only in D100 that the predicted enlargement in FA emerged.
- With increasing severity of diabetes mellitus, when the heart is unable to control its own FA supply using lipoprotein lipase, it undergoes dramatic reprogramming like stimulation of β-oxidation in peroxisomes and mitochondria, that is linked to handling of excess FA that arise from adipose tissue.
- As high β-oxidation is not matched by elevated tricarboxylic acid cycle activity or enhanced oxidative phosphorylation, the subsequent increase of FA intermediates and their diversion to triglyceride, paired with increased reactive oxygen species formation secondary to excessive β-oxidation, provoked a gene expression program supporting cell death (lipotoxicity).

What Are the Clinical Implications?

- In guiding the clinical management of type 1 diabetes mellitus, in addition to focusing on drugs that lower plasma glucose, attention should also be placed on dyslipidemia, which could be a major link between diabetes mellitus and cardiomyopathy.

down the triglyceride core of circulating lipoproteins to release FA[14] (Figure 1E). In this way, when glucose is being underutilized and a need for FA arises, the heart can tailor LPL to meet the ATP demands of the cardiomyocyte by providing the necessary amount of FA to replace ATP otherwise derived from glucose breakdown (LPL finely tunes FA delivery to cardiomyocytes). With increasing severity and disease progression, this cardiac heparanase-1–LPL signaling axis is compromised in the diabetic heart, leading to a decline in LPL.[15] A downside to the loss of this LPL rheostat renders the diabetic heart dependent on hydrolysis of adipose tissue (AT) triglyceride to generate FA. This could be a questionable adaptation, as the site of control of FA provision to the heart changes from a measured regulated delivery by coronary LPL to the unrestrained and unregulated provision by AT.

Streptozotocin (STZ) is an agent that produces pancreatic β-cell necrosis and ensuing hypoinsulinemia. We used 2 doses (55 and 100 mg/kg IV) of STZ to differentially lower plasma insulin and produce diabetes mellitus of variable intensities. With D55, animals are moderately hypoinsulinemic, hyperglycemic, with little change in circulating FA or triglyceride and an increase in LPL. Interestingly, D100 displays striking hypoinsulinemia with augmentation of both circulating glucose and FA/ triglyceride[15–18] and a reduction in LPL. We tested how the heart adapts to this graded reduction in insulin and a switch from LPL-derived FA to those obtained from AT.

Methods

The authors declare that all supporting data are available within the article and its online supplementary files.

Experimental Animals

This investigation conformed to the *Guide for the Care and Use of Laboratory Animals* published by the National Institutes of Health, the Canadian Council on Animal Care Guidelines, and institutional guidelines at the University of British Columbia (Certificate A17-0072). Adult male Wistar rats (240–260 g; Charles River Laboratories, Wilmington, MA) were fed Laboratory Rodent Diet 5001 with a chemical composition of 5% total fat (ether extract) made up of 1.5% saturated, 1.6% monounsaturated, and 1.5% polyunsaturated FA. STZ is a β-cell-specific toxin used to induce hypoinsulinemia and diabetes mellitus. Under isoflurane anesthesia, animals were injected with a single intravenous dose of 55 (D55) or 100 (D100) mg/kg of STZ into the tail vein.[15] After 24 hours, hyperglycemia (>13 mmol/L) was confirmed in tail-tip blood samples using a glucometer and glucose test strips. Animals were euthanized after 4 days. Female rats were not used, as we have previously documented that female rodents are not as susceptible to the diabetogenic effects of D55-STZ.[19]

Metabolic Assessments

At termination, hearts were exsanguinated and blood in the thoracic cavity collected in K2-EDTA tubes and centrifuged immediately for separation of plasma that was used for determination of insulin (rat insulin ELISA; ALPCO, Salem, NH), FA (NEFA-HR; Wako Diagnostics, Mountain View, CA) and triglyceride (Stanbio Triglycerides LiquiColor Mono; Thermo Fisher Scientific, Waltham, MA). After acid-ethanol extraction, insulin content in the pancreas was assessed by ELISA.

RNA Sequencing and Analysis

Total RNA from 4 control, 6 D55, and 6 D100 rats was isolated using TRIzol (Thermo Fisher Scientific, Waltham, MA). Sequencing libraries were prepared from 400 ng total RNA using the TruSeq Stranded mRNA Sample Preparation kit (Illumina, San Diego, CA). Samples were checked for quality using a Bioanalyzer (Agilent Trchnologies, Sanra Clara, CA)

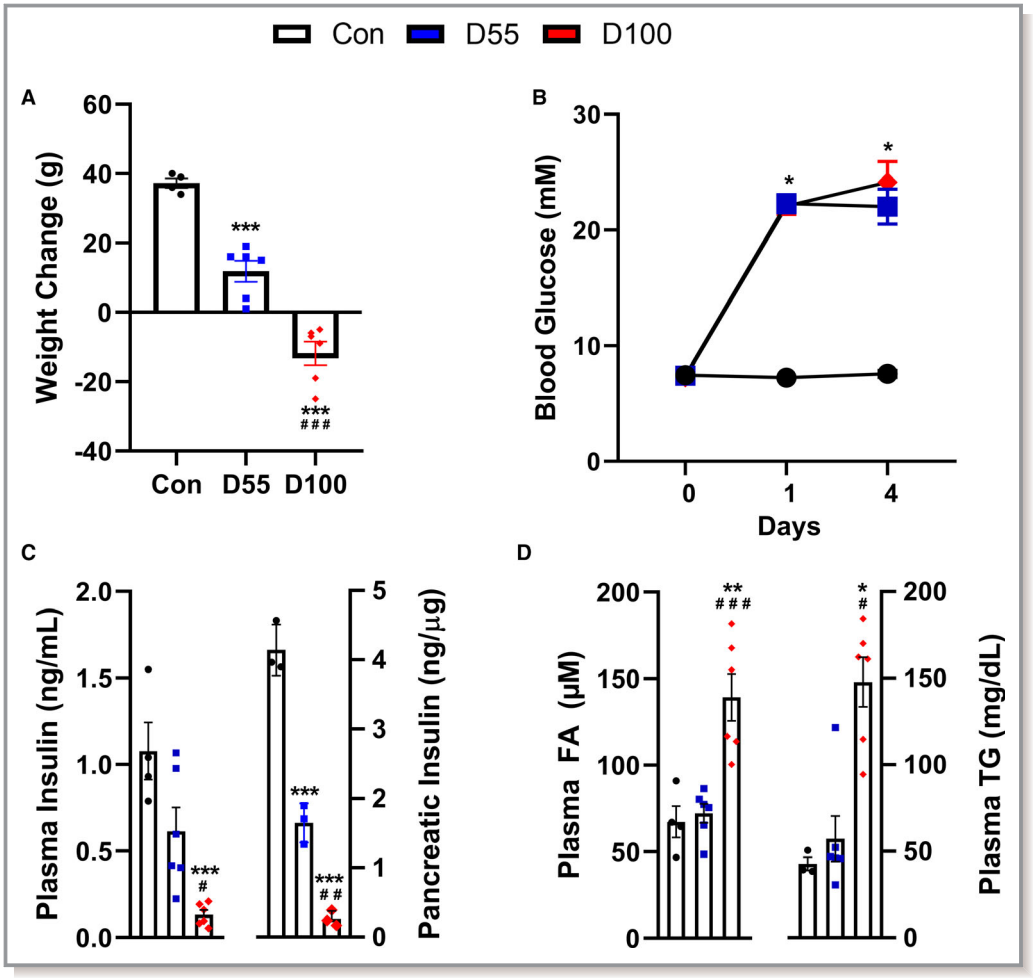

Figure 1. The severity of streptozotocin (STZ) diabetes mellitus is uncovered by measuring insulin and not glucose. Diabetes mellitus was induced by injection of 2 different doses of STZ (55 [D55] or 100 [D100] mg/kg IV) and the animals terminated 4 days later (n=4–6). At termination, weight gain (change in body weight compared with initial value) was assessed (**A**). Glucose was determined throughout the study period from tail-tip blood samples using glucose test strips and an Accu-Chek glucose monitor (**B**). Following heart extraction, blood in the thoracic cavity was collected in tubes containing K2-EDTA as anticoagulant. After centrifugation, plasma isolated from this blood was used for determination of insulin (**C**, left panel) and fatty acids (FA) and triglycerides (TG) (**D**). Pancreatic total insulin (ng) was determined following acid-ethanol extraction and measured using a rat ultrasensitive insulin ELISA normalized to total protein (μg; **D,** right panel). Lipoprotein lipase (LPL) trafficking in the heart is summarized in E with the inset (stacked bar graph that characterizes LPL activity in the 1.0 mol/L fraction redrawn from original in Wang et al[15]) representing dimeric, catalytically active LPL determined in heart homogenates loaded onto a heparin-sepharose column and eluted with increasing concentrations of NaCl. To measure LPL activity, we used in vitro hydrolysis of a [^{3}H]triolein substrate. Data are presented as mean ±SEM. Significantly different from control, $^*P<0.05$, $^{**}P<0.01$, $^{***}P<0.001$. Significantly different from the D55 group, $^{\#}P<0.05$, $^{\#\#}P<0.01$, $^{\#\#\#}P<0.001$.

and quantified using Qubit fluorometer (Thermo Fisher Scientific, Waltham, MA). Libraries were multiplexed and sequenced on the NextSeq 500 (Illumina). Following a previously published procedure,[20] multiple analysis pipelines were applied and their results combined. The output for each pipeline was a list of genes ranked by the *P* value for differential expression after correction for multiple testing. A combined list was obtained by ranking the genes according to their median rank from the various analysis pipelines. One potential outlier was detected when clustering the samples and was therefore removed for the differential expression analysis. Network analysis and function categorization were conducted using STRING (set at the highest confidence with evidence from experiments, databases, coexpression, and co-occurrence[21]). Gene ontology term enrichment and Kyoto Encyclopedia of Genes and Genomes pathway analysis (Enrichr software[22]) of differentially expressed genes were also applied to ascertain significantly enriched pathways.

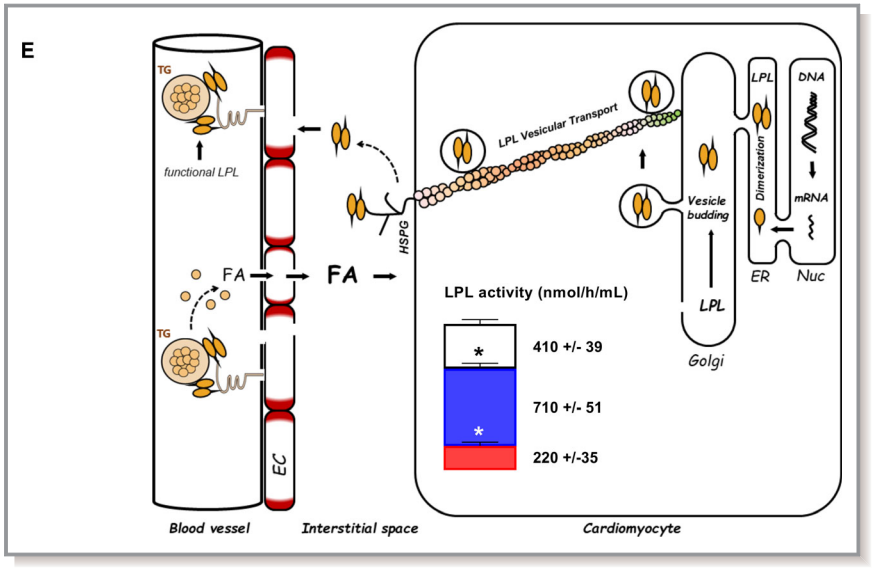

Figure 1. Continued.

Separation and Characterization of Plasma and Cardiac Lipids

Total plasma and cardiac lipids were extracted and solubilized in degassed chloroform:methanol:acetone:hexane (4:6:1:1v/v/v/v). Separation of triglyceride and FA were achieved using high-performance liquid chromatography (HPLC; Waters 2690 Alliance HPLC, Milford, MA) equipped with an auto-sampler and column heater, as previously described.[23] Lipid classes were separated on a YMC DIOL column (4.6×250 mm, YMC, Asan, Korea) and the HPLC flow was split with ≈80% flow going to a FCII fraction collector (Waters, Milford, MA) and the remaining 20% flow going to a Waters evaporative light scattering detector. Phospholipid fractions were collected, solvent evaporated under a stream of nitrogen, then derivatized with boron trifluoride (14%) in methanol. Individual FA methyl esters were then separated using an 6850 GLC (Agilent Technologies) equipped with a flame ionization detector and an SP-2330 capillary column (30 m×0.25 mm internal diameter) (Supelco, Bellefonte, PA) using hydrogen as a carrier gas. Peak areas were calculated using Chemstation software (Agilent Technologies) and FA quantified using heptadecaenoic acid (17:0) as the internal standard.

Isolation of Cardiomyocytes

Primary ventricular cardiomyocytes were prepared following previously described procedures.[17,24]

Mitochondrial Stress Test

Oxygen consumption rate (OCR) was measured using the Seahorse XFe96 extracellular flux analyzer and the Seahorse XF Cell Mito Stress Test kit (Agilent Technologies). Mitochondrial inhibitor concentrations and cell density were optimized, and protocols were based on previously published data.[25,26] Cardiomyocytes were plated at a density of 5000 cells/well and incubated overnight in 150 μL of normal culture medium (replicates of 8–12 wells per condition and cell type). The next day, cells were washed twice with warm substrate-limited assay media (XF Base Medium, 2.5 mmol/L GL, 0.1 mmol/L sodium pyruvate, 4 mmol/L L-glutamine, 0.5 mmol/L L-carnitine, 5 mmol/L HEPES, pH 7.4) and incubated with fresh assay media for 1 hour. Immediately before assay, either bovine serum albumin (BSA) 0.05 mmol/L palmitic acid (PA) or 0.1 mmol/L PA were added to the wells (PA:BSA, Agilent Technologies). The cartridge was loaded with 3 metabolic inhibitors, which were sequentially injected into the plate, and OCR measured after each addition subsequent to 3 initial baseline readings: oligomycin (2 μmol/L), carbonyl cyanide 4-(trifluoromethoxy)phenylhydrazone (FCCP; 2 μmol/L), followed by the combination of rotenone and antimycin A (2 μmol/L/10 μmol/L). At the end of the assay, OCR was normalized to protein content.

Cardiac Apoptosis

Terminal deoxynucleotidyl transferase dUTP nick-end labeling assay was carried out using a terminal deoxynucleotidyl transferase dUTP nick-end labeling kit (Promega, Madison, WI) as described previously.[23] Nuclei (n=2546, 2256, and 2382 for controls, D55, and D100, respectively) were counted from 3 different ventricular sections per animal, from 3 separate animals per group.

Metabolomic Profiling

Untargeted metabolomic analysis was performed using an Agilent 6530 quadrupole-time of flight mass spectrometer,

Agilent 1290 binary ultra performance liquid chromatography and MassHunter data acquisition software. The instrument was operated in positive ion, then negative ion for reverse phase and hydrophilic interaction (HILIC) chromatography involving a total of 4 separate runs for each sample. Negative ion tests used the same columns, but mobile phases were 5 mmol/L ammonium acetate (Fisher Optima LC/MS Grade, Thermo Fisher Scientific) in 98% water 2% acetonitrile, with pH adjusted to 9.2 using ammonium hydroxide. Reverse phase chromatography utilized a Waters BEH-C18 column, 2.1×100 mm, 1.7 μm particle size, and similar buffered mobile phases to HILIC with the exception of using methanol rather than acetonitrile. Gradient chromatography was used for both HILIC and reverse phase with starting conditions of 90% organic solvent for HILIC and 90% aqueous for reverse phase and total run times of 35 to 45 minutes. The 6530 quadrupole-time of flight mass spectrometer with Agilent Jet Spray was operated in electrospray ionization mode and used dual electrospray ionization nebulizers for simultaneous introduction of sample and reference mass solutions, data were collected at 2 scans/second with an m/z range of 65 to 1050 in all modes of operation. The quadrupole-time of flight mass spectrometer was tuned specifically for low masses following the manufacturer's instructions, operated in high-resolution mode using 4-GHz data acquisition and used Agilent's standard reference mass solution providing corrected mass accuracy of about 2 to 3 ppm. Additional runs of pooled heart samples used tandem mass spectrometry mode and specifically targeted ions of interest with collision energies of 10, 20, or 40 volts to assist in identification of analytes. Data processing used multiple Agilent Technologies software packages. Profinder version 10.0 was used for molecular feature extraction; then, all features were exported to the chemometric software Mass Profiler Professional. Data imported to Mass Profiler Professional were normalized using a 75th percentile shift algorithm, baselined to the median of all samples, then filtered to remove entities that were highly variable within any one sample group. Identification of metabolites used a number of resources including Agilent MassHunter ID Browser B.08 software and Metlin accurate tandem mass spectrometry spectral library with matching mass tolerance set at 2 mDa±5 ppm, online mass spectral libraries from the Human Metabolome Database,[27] and MassBank (https://massbank.eu/MassBank/), and our own mass spectral/retention time library created from about 200 compounds provided by British Columbia Children's Hospital Newborn Screening program.

Statistical Analysis

One-way ANOVA followed by Bonferonni post hoc comparisons test was used to determine differences between group mean values. For some analyses, Kruskal–Wallis nonparametric test followed by Dunn post hoc comparisons test was applied for nonnormal distributions. Values are presented as means±SEM with individual data points. The minimum level of statistical significance was set at $*P<0.05$.

Results

Using dissimilar doses of STZ, we established models of diabetes mellitus of varying intensities. Accordingly, weight gain over 4 days was reduced in D55 animals compared with control such that these rats had lower body weights at the time of death. Induction of a more severe diabetes mellitus in D100 rats over the same time period resulted in a loss of body weight (as compared with body weight on day 0; Figure 1A). Both D55 and D100 were equally hyperglycemic compared with control over the duration of the study, with no measurable difference between the 2 diabetic groups (Figure 1B). Intriguingly, the severity of diabetes mellitus between D55 and D100 was uncovered only following determination of insulin; D100 animals showed markedly lower plasma and pancreatic insulin compared with D55 (Figure 1C). This dramatic pancreatic β-cell destruction and hypoinsulinemia in D100 was accompanied by robust increases in plasma FA and triglyceride, effects that were essentially absent in D55 animals (Figure 1D). Our data advocate for D55 as a model of moderate type 1 diabetes mellitus with insufficient glycemic management, and an increase in cardiac LPL activity (Figure 1E, inset) to support FA provision to the heart when glucose use is curtailed. Additionally, D100 could be considered as a model of severe type 1 diabetes mellitus with poor glycemic control and dyslipidemia, resulting in a loss of LPL activity (Figure 1E, inset).

Subsequent to a reduction in circulating insulin, increased AT lipolysis attributable to lipase (adipose triglyceride lipase and hormone-sensitive lipase) hyperactivity releases FA into the circulating plasma.[28] Interestingly, despite the decline of insulin in D55, these animals exhibited minimal change in average plasma FA concentrations (Figure 2A through 2E). However, with increasing severity of diabetes mellitus and a further drop in insulin, the predicted enlargement in FA emerged. Accordingly, D100 animals exhibited close to a 2- to 3-fold increase in various types of saturated (palmitic [16:0], stearic [18:0]), monounsaturated (oleic [18:1]), and polyunsaturated (linoleic (18:2), arachidonic (20:4)] FA that made up ≈80% of the total plasma pool (Table S1 and Figure 2A through 2E). It should be noted that despite the absolute increase in plasma saturated FA, monounsaturated FA, and polyunsaturated FA in D100, the percentage composition of these FAs remained unaltered (Figure 2F). Also of interest was the observation that circulating very-long-chain FAs (VLCFAs; with ≥22 carbons; eg, docosahexaenoic acid, C22:6n3), that made up a small percentage of the total

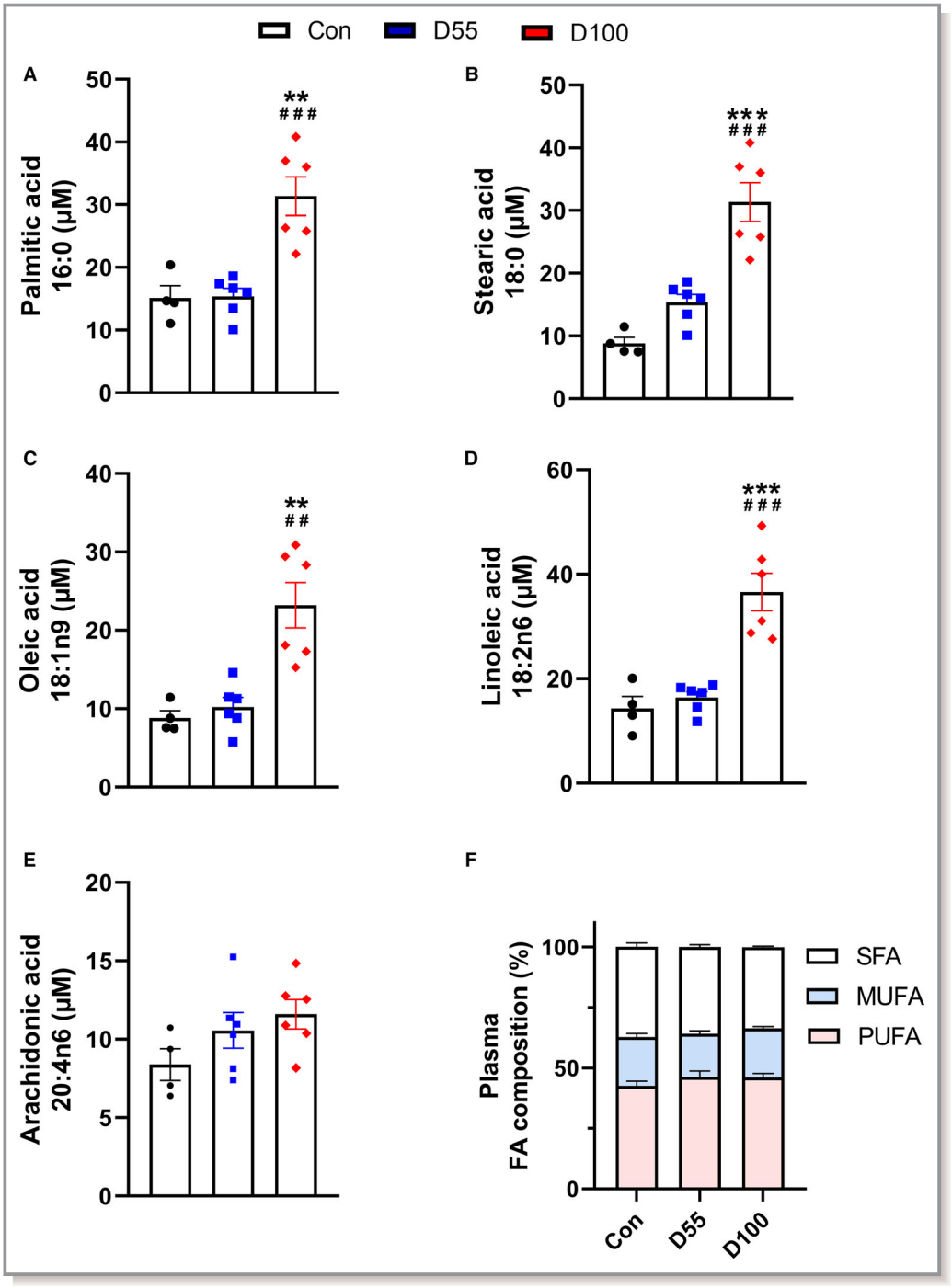

Figure 2. Plasma fatty acid (FA) composition is altered only when insulin reduction by streptozotocin (STZ) is substantial. Four days after injection of STZ, animals were terminated and plasma collected for determination of fatty acid (FA) composition (n=4–6). Plasma FAs were extracted with chloroform: methanol:acetone:hexane solvent. Separation of FAs was achieved using high-performance liquid chromatography, followed by conversion to their respective methyl esters, and quantification by gas liquid chromatography. The unadjusted baseline saturated (SFA; palmitic acid [**A**]; stearic acid [**B**]), monosaturated (MUFA; oleic acid [**C**]), and polyunsaturated (PUFA; linoleic acid [**D**]; arachidonic acid [**E**]) FA composition is shown in control (Con) rats and animals with variable degrees of hypoinsulinemia (D55 and D100). Results are also expressed as the molar percentage of each FA over the total FA measured in the plasma (**F**). Data are presented as mean±SEM. Significantly different from control, $^{**}P<0.01$, $^{***}P<0.001$. Significantly different from the D55 group, $^{\#\#}P<0.01$, $^{\#\#\#}P<0.001$.

identified FA and that must undergo initial peroxisomal β-oxidation before entering the mitochondria for ATP generation, were also increased in D100 (Table S1). Our data suggest that the D100 heart could use the substantially increased plasma concentrations of these different FAs for generation of ATP instead of FA originating from LPL action.

To determine the capacity of the heart to respond to excess LPL or AT-derived FA, we compared the ventricle transcriptome of D55 (Table S2) and D100 animals (Table S3). Figure 3A (lower panel) illustrates that in D55, there were 49 differentially regulated genes (padj <0.05 and significant in at least 5 out of the 10 analysis pipelines used), and when clustered according to function and ranked based on the false discovery rate, they were enriched largely for traditional glucose, protein, and lipid metabolic processes (Figure 3B). Strikingly, in D100, there were dramatic transcriptomic changes with 1574 genes differentially expressed (Figure 3A, upper panel). Like D55, the majority of genes were annotated as related to metabolic processes (with additional enrichment in genes related to cellular transport, mitochondrial and blood vessel organization, response to oxidative stress, and cell death [Figure 3A and 3B]). These results indicate that with the reduced glucose utilization, it is the superimposition of augmented AT-derived FA that likely determines the extent of cardiac gene expression changes following diabetes mellitus.

Glucose and FA are the major sources from which the heart derives most of its energy. However, with the development of diabetes mellitus, the ability of this organ to utilize glucose is obstructed.[5] Consistent with this finding, we observed a substantial decrease in the expression of genes controlling glucose transport (*SLC2A4*) and glycolysis (*ENO3, HK2, PFKFB2*) (Figure 4A). Furthermore, genes that modulate proteins (*PDK1* and *PDK4*) that phosphorylate and inhibit pyruvate dehydrogenase to lower glucose oxidation, increased in expression. All changes related to genes controlling cardiac glucose utilization were more pronounced in the D100 compared with D55 (Figure 4A). Because glucose use is impaired in diabetes mellitus, the heart is obliged to primarily metabolize FA and does so by enabling its mitochondrial β-oxidation followed by oxidative phosphorylation, to yield ATP. Related to this requirement, the genes controlling FA transport (*CD36, FABP4*) and mitochondrial β-oxidation (*CPT1A, HADHA, HADHB, ACADL*) exhibited increased expression and more so for D100 (Figure 4B). The expression of genes encoding peroxisomal metabolism were also found to be universally elevated in the D100 heart (Figure 4C) and corresponds to the decline in VLCFA (eg, C22:5n3; C22:6n3) in this organ (Figure 4D and inset). Intriguingly, in D100, cardiac accumulation of the major polyunsaturated FA (18:2n6) and monounsaturated FA (18:1n9) exceeded that of saturated fats like palmitic (16:0) or stearic (18:0) acids (Figure 4D). This could indicate that saturated FA entering the hearts gets preferentially used, whereas monounsaturated FA and polyunsaturated FA (which require 2 additional steps to convert unsaturated to saturated bonds) get stored as triglyceride.[29]

Mitochondrial β-oxidation of FA produces flavin adenine dinucleotide and nicotinamide adenine dinucleotide (consumed by the oxidative phosphorylation complex to produce ATP) as well as Acetyl-CoA (that enters the tricarboxylic acid [TCA] cycle to also generate nicotinamide adenine dinucleotide and flavin adenine dinucleotide). We used Enrichr analyses of the transcriptomic data from D100 hearts and determined that of the biological processes that showed the highest enrichment, a disproportionate amount (the top 10 gene ontology terms for biological processes) was those related to mitochondrial functioning (Figure 5A), implicating a significant effect of excess FA on mitochondria. Furthermore, analysis of a protein-protein interaction network in D100 identified functional networks enriched for components of mitochondrial ribosomal protein, respiratory complex 1, and ATP synthase (Figure 5B, pink squares). Closer inspection of the gene expression data revealed that core metabolic genes involved in making enzymes for the mitochondrial TCA cycle (Figure 5C) and oxidative phosphorylation (Figure 5D) were actually universally downregulated in D100 hearts. Unexpectedly, using a substrate limited medium (only low glucose; 2.5 mmol/L), measurement of basal OCR as a gauge of cardiomyocyte oxidative capacity indicated that myocytes from D100 hearts had the highest basal respiration (Figure 5E). This was possibly an outcome of metabolism of endogenous triglyceride-derived FA as addition of etomoxir (carnitine palmitoyltransferase 1 inhibitor) lowered OCR in these myocytes (Figure 5E, inset). With addition of increasing concentrations of PA, although control myocytes responded by increasing their basal respiration, this effect was minimized in D55 and reversed in D100 myocytes (Figure 5E). Similarly, using FCCP to uncouple the proton gradient and maximize oxygen consumption to calculate spare respiratory capacity, control and D55 myocytes under basal conditions had the mitochondrial capacity to respond to this augmented energy demand, an outcome that was lacking in D100 (Figure 5F). FA decreased the response of myocytes from all 3 groups to FCCP-stimulated OCR (Figure 5F).

The final products of an abnormal plasma FA profile, together with robust transcriptomic changes in the D100 heart to consume these FA, are metabolites. Using a nontargeted metabolomics approach by liquid chromatography–tandem mass spectrometry, we identified a broad set (363) of metabolites that were significantly differentially expressed in the D100 heart compared with control cardiac tissue (Table S4). We used principal component analysis (Figure 6A) and an orthogonal partial least squares discriminant analysis scores plot (Figure 6B) to identify the differences in metabolic patterns

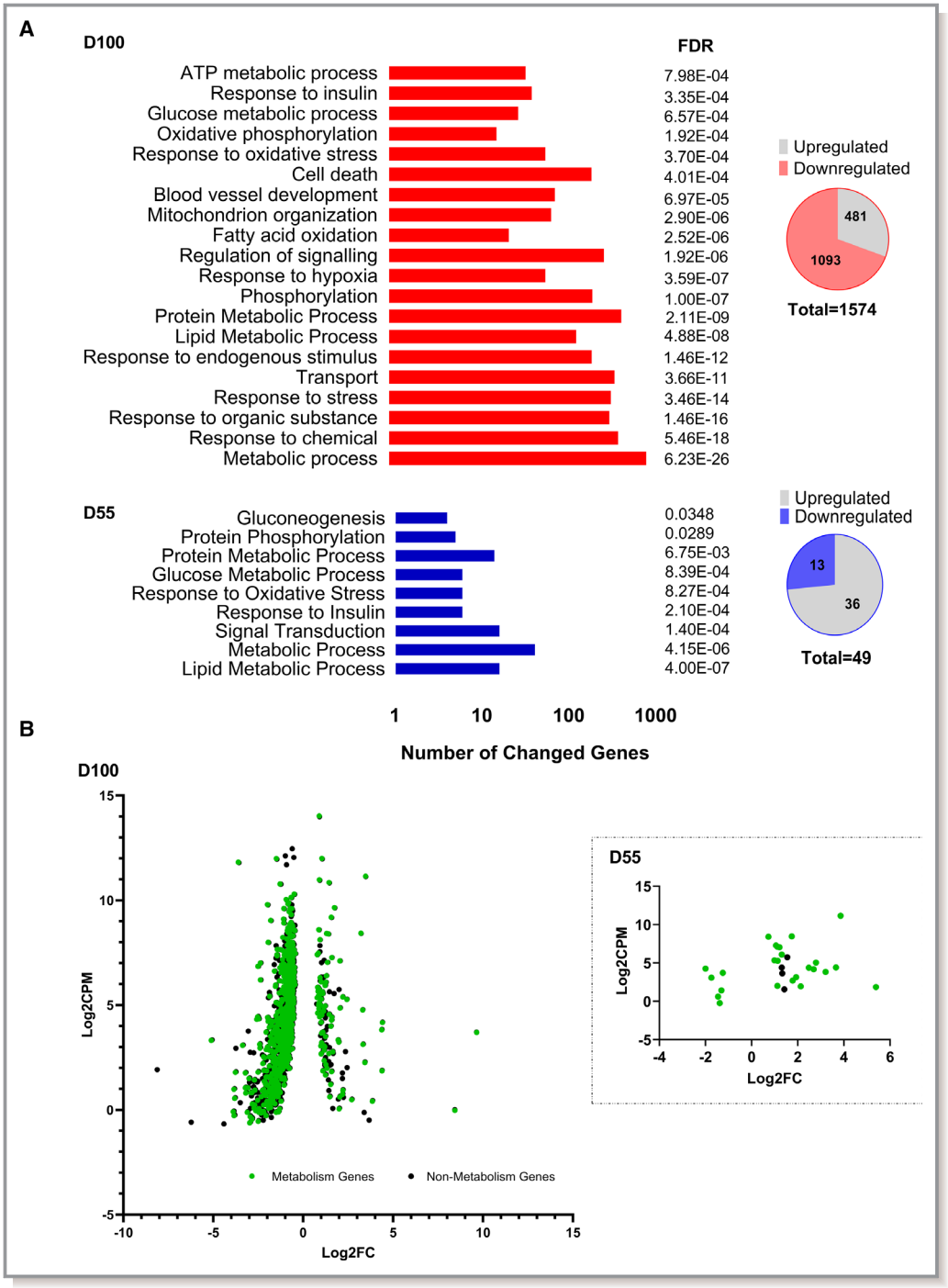

Figure 3. The largest magnitude of change in the ventricular transcriptome of rats with severe diabetes mellitus embraces metabolic pathway genes. Ventricle RNA from the different groups of rats was sequenced (n=4–6), and differentially expressed genes (padj <0.05 and significant in at least 5 of the 10 analysis pipelines used) were clustered according to function and ranked based on false discovery rate (FDR) (**A**). The insets describe the number of genes whose expression was up- or downregulated. The volcano plot (**B**) describes the profile of differentially expressed genes in D55 (inset) and D100 rats. The *x* axis represents Log_2FC expression of genes vs Log_2CPM on the *y* axis. Green circles highlight differentially expressed genes related to the metabolic process. CPM indicates counts per million.

between control and D100 hearts and found clear separation between data for the 2 groups. Moreover, the corresponding S-plot of orthogonal partial least squares discriminant analysis shows that the metabolite ions (the top 30) with the greatest influence on separation of control from D100 (ie, located furthest away from the center of the S-plot and with a large

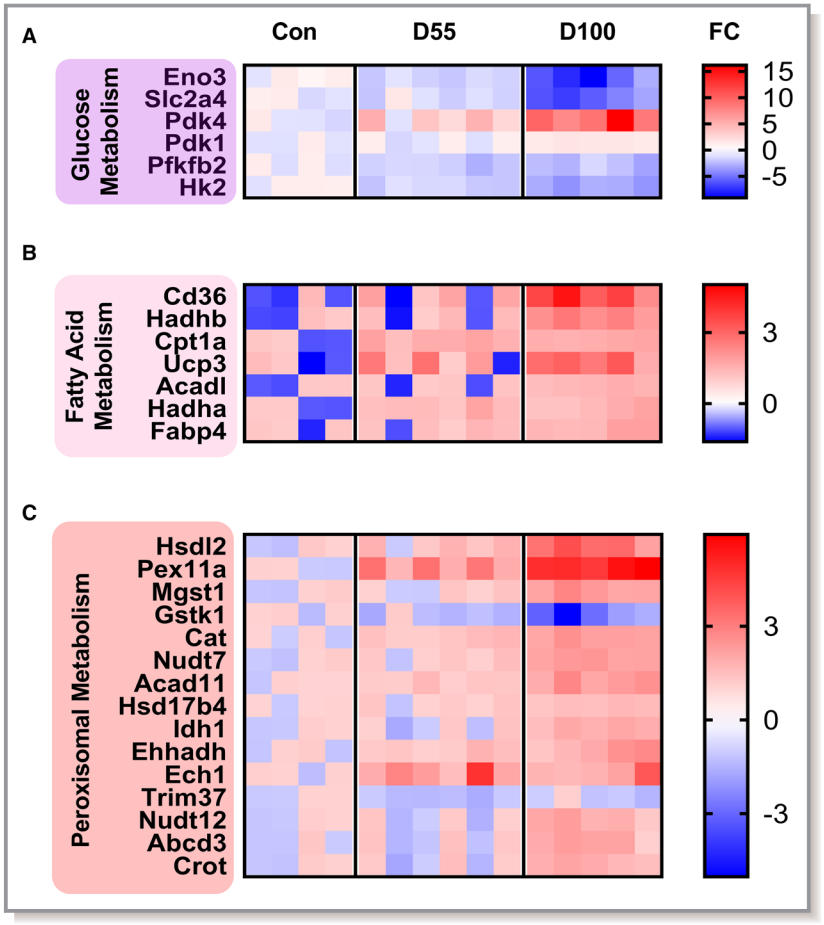

Figure 4. Metabolic gene expression reprogramming following diabetes mellitus of varying intensities emphasizes the increase in mitochondrial and peroxisomal β-oxidation. Heat map of statistically significant genes related to cardiac metabolism of carbohydrates (**A**) and fatty acid (FA; **B**). (**C**) is a heat map pattern showing relative expression values of genes encoding peroxisomal metabolism. The red (high) and blue (low) colors reflect fold change (FC). Separation of heart FAs was achieved using high-performance liquid chromatography, followed by their conversion to their respective methyl esters and quantification (μg/mg protein) by gas liquid chromatography. The FA depicted made up almost 80% of the eluted peaks and are expressed as a percentage of the total FA extracted (D). The inset in (**D**) describes the percentage composition of long-chain FA (LCFA) and very-long-chain FA (VLCFA; chain-length with 22 or more carbons) in hearts from the three groups (n=4–6). Data are presented as mean±SEM. Significantly different from control, $^{*}P<0.05$, $^{***}P<0.001$. Significantly different from the D55 group, $^{\#\#}P<0.01$, $^{\#\#\#}P<0.001$.

variable important value ≥1) included increases in many types of diglycerides (ie, 18:2/18:1, 16:1/18:0) and phospholipids (ie, phosphatidylcholine [18:2/18:2, 16:0/18:2, 18:0/20:4]; phosphatidylethanolamine [18:2/21:0, 19:0/22:6, 22:6/21:0, 18:1/19:0]; phosphatidylserine [P-20:0/18:0, P-20:0/16:0, P-20:0/18:1, P-20:0/18:2, P-20:0/22:4, O-20:0/22:4, O-16:0/20:0]), with the highest contribution identified as coming from triacid triglyceride (ie, 17:1/18:1/19:1, 14:0/20:2/20:2, 17:0/17:1/17:0, 12:0/20:0/22:5, 14:1/18:0/18:0, 16:1/18:0/18:3, 16:1/18:2/22:0, 18:2/19:1/19:1, 16:1/18:2/22:4, 12:0/12:0/12:0, 17:0/17:1/22:1) (Figure 6C and Table S4). These results, when added to the increased expression of (1) genes encoding acyl-coenzyme A thioesterase (ACOT1, 2, and 4) that contributes to the conversion of acyl-coenzyme A to FAs and coenzyme A (and thus triglyceride synthesis at the expense of FA oxidation), and (2) genes encoding glycerolipid synthesis (glycerol-3-phosphate acyltransferase, mitochondrial and glycerol-3-phosphate acyltransferase 3) (Figure 6D) implies that D100 animals with plasma lipid overload and mitochondrial dysfunction results in intracellular triglyceride accumulation (Figure 6E) and likely cell death.

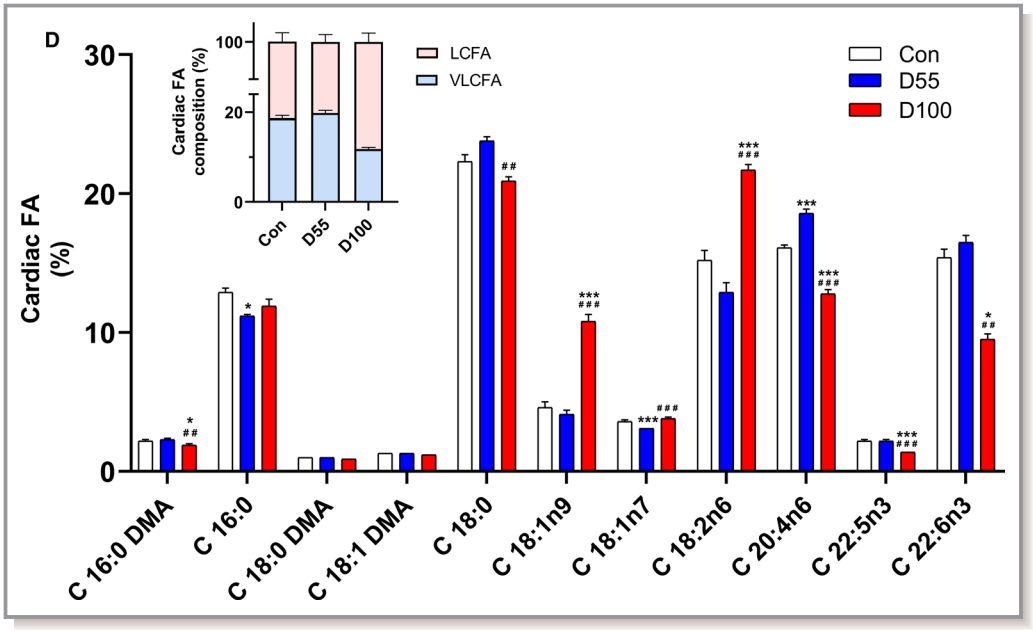

Figure 4. Continued.

Electrons from nicotinamide adenine dinucleotide and flavin adenine dinucleotide enter the electron transport chain to cause buildup of the proton motive force for oxidative phosphorylation and production of ATP. With the availability of excess FA in D100, electrons are donated to molecular oxygen, with electron leakage resulting in abnormally large amounts of reactive oxygen species generation, leading to changes in gene expression related to oxidative stress (Figure 7A) and cell death (lipotoxicity). Indeed, of the genes that were differentially expressed in D100 hearts, a large number were those related to apoptosis, with a dramatic decrease in expression of antiapoptotic and an increase in proapoptotic genes (Figure 7B) together with a significant increase in terminal deoxynucleotidyl transferase dUTP nick-end labeling–positive apoptotic cells (Figure 7C, Figure S1). Our data reveal that following severe diabetes mellitus, mitochondrial overload, incomplete FA oxidation, and oxidative stress pushes the heart toward potentially unrecoverable loss of cardiomyocytes (Figure 7D).

Discussion

Cardiovascular disease is a leading cause of death in patients with diabetes mellitus.[1] Although atherosclerosis is a primary cause for this cardiovascular disease, patients and animal models with type 1 and type 2 diabetes mellitus have also been diagnosed with heart failure in the absence of vascular defects (cardiomyopathy), with alterations in cardiac substrate metabolism contributing to this etiology.[5] We used 2 doses (55 and 100 mg/kg) of STZ to differentially lower insulin and produce models of diabetes mellitus that imitate a continuum of glycemic management in patients, from insufficient (D55) to poor (D100) control. Our data suggest that with an increasing severity of diabetes mellitus, when the diabetic heart is unable to control its own FA supply using LPL, it undergoes dramatic reprogramming that is linked to handling of excess FA that arise from AT. This transition results in a cardiac metabolic signature that embraces mitochondrial FA overload, oxidative stress, triglyceride storage, and cell death.

Using a single injection of 55 mg/kg of STZ, we produced a model of moderate diabetes mellitus that we describe as imitating insufficient glycemic management in patients with type 1 diabetes mellitus where multiple finger pricks and daily insulin injections (3–4/day) may mean variable patient compliance and repeated exposure to bouts of hyperglycemia. With this dose of STZ, the insulin reduction was insufficient to increase circulating albumin-bound FA or TG. As a result, production of energy in the diabetic heart is appropriated by LPL; there is augmented processing of this enzyme into an active dimeric form followed by its recruitment to the coronary vascular lumen.[8] Out here, it breaks down the triglyceride core of circulating lipoproteins to release FA, representing an immediate compensatory response to guarantee FA supply when glucose cannot be used.[15,16] Intriguingly, 100 mg/kg of STZ produced animals displaying striking hypoinsulinemia, hyperglycemia, and an augmented pool of circulating plasma FA and triglyceride. We label these animals as being severely diabetic, representing patients with type 1 diabetes mellitus with poor glycemic control. In these animals, the unfettered hydrolysis of AT triglyceride to generate FA

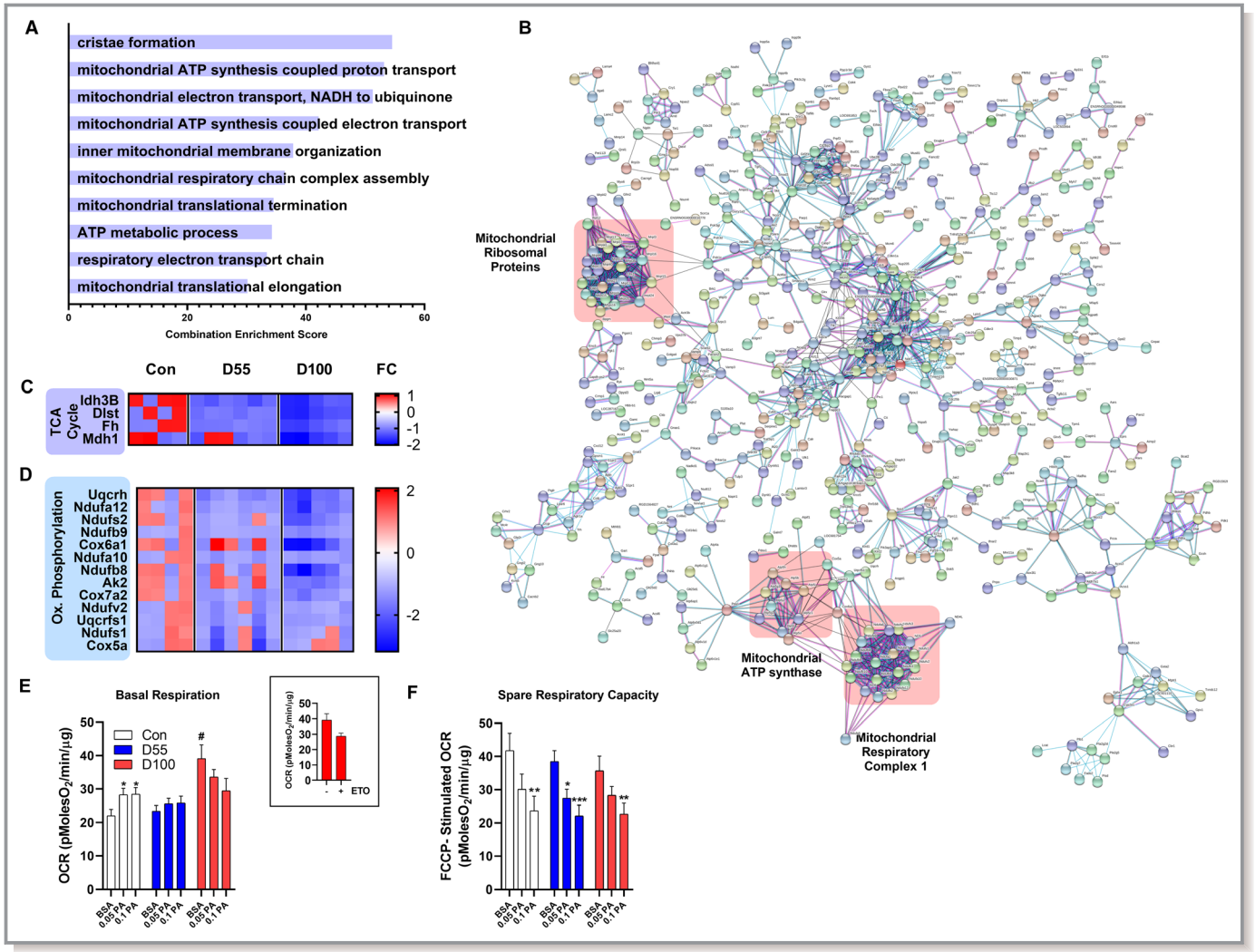

Figure 5. Mitochondrial oxidative phosphorylation is actively repressed with increasing severity of diabetes mellitus. Gene ontology enrichment analysis of biological processes using the Enrichr analysis tool (**A**). The gene signature identifying only the top 10 enriched gene ontology (GO) terms is depicted (**A**). Association network of genes that were significantly different between control (Con) and D100 hearts. The protein-protein interaction network was assembled from RNAseq data. The pink squares illustrate the differentially regulated networks that are related to mitochondrial functioning. Lines represent associations based on differential expression evidence (**B**). Heat map pattern showing relative expression values of genes encoding tricarboxylic acid (TCA) cycle activity (**C**) and mitochondrial oxidative phosphorylation (**D**). The red (high) and blue (low) colors reflect fold change (FC). Oxygen consumption rates (OCRs) in cardiomyocytes isolated from Con, D55, and D100 hearts. Immediately before assay, either bovine serum albumin (BSA), 0.05 mmol/L of palmitic acid (PA), or 0.1 mmol/L of PA was added to the wells. Cells were exposed sequentially to the 3 metabolic inhibitors oligomycin, carbonyl cyanide 4-(trifluoromethoxy)phenylhydrazone (FCCP) and rotenone plus antimycin A. OCR is expressed as pmole O_2/min per µg protein. Basal respiration (in BSA) was measured in the absence (**E**) or presence (**E**, inset) of etomoxir (ETO; 100 µmol/L), an inhibitor of carnitine palmitoyltransferase I (CPT1) (to assess the contribution of fatty acids arising from endogenous triglycerides. Spare respiratory capacity was calculated as OCR following FCCP minus baseline OCR (**F**). Three separate plates were assayed, each with cardiomyocytes isolated from 3 separate Con, D55, and D100 animals. Data are presented as mean±SEM. Significantly different compared with BSA treatment within each group, $*P<0.05$, $**P<0.01$, $***P<0.001$. Significantly different compared with BSA-Con, $^{\#}P<0.0008$.

results in the diabetic heart using this pool of FA disproportionally. Consequently, to avoid lipid oversupply, there is conversion of LPL to inactive monomers, a reduction of enzyme at the coronary lumen, and inhibition of lipoprotein triglyceride hydrolysis.[15] Our results imply that the greater the loss of glycemic control in type 1 diabetes mellitus, delivery of FA to the heart shifts from lipoprotein-triglyceride hydrolysis by coronary LPL to AT-derived FA. This is a questionable adaptation, as the site of control for FA provision to the heart changes from a measured regulated delivery by coronary LPL (which is then turned off to avoid further lipid overload) to unrestrained provision of this substrate from AT.

Therapeutic management of blood glucose and its monitoring are the foundational basis of diabetes mellitus

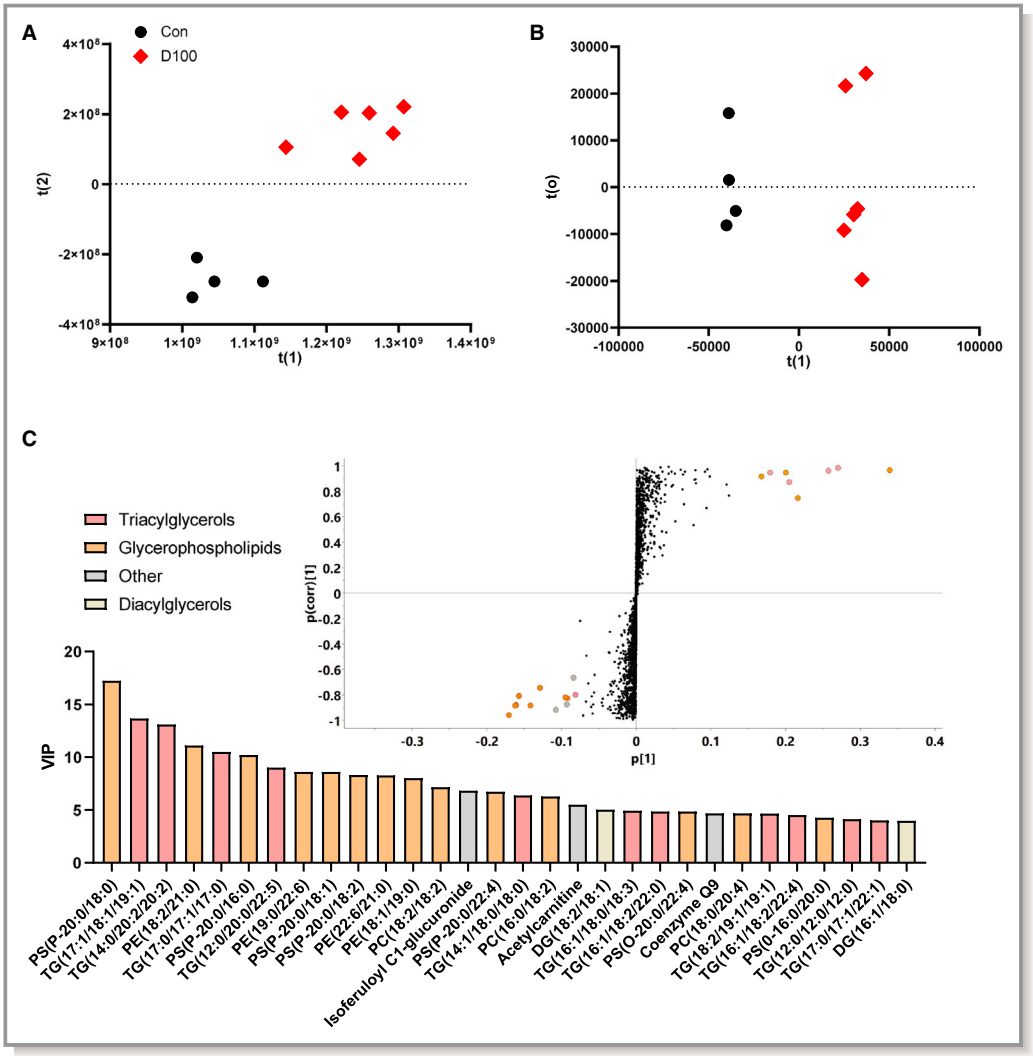

Figure 6. Substantial accumulation of lipid metabolites and triglycerides (TG) in heart tissue from D100 animals. Heart samples (5–10 mg) were powdered, transferred to a 1.7-mL microcentrifuge tube, and 4 volumes of solvent added (acetonitrile for hydrophilic interaction or methanol for reversed phase). Following brief sonication and centrifugation at 20 000*g* for 10 min, the supernatant was removed to a high-performance liquid chromatography autosampler vial. Hydrophilic interaction chromatography used a Waters BEH-Amide column 2.1×100 mm, 1.7μm particle size, and mobile phases of 5 mmol/L ammonium formate (Fisher Optima LCMS Grade)+0.1% formic acid (Sigma) in 98% water/2% acetonitrile (EMD LCMS Grade) and acetonitrile containing 2% water and 5 mmol/L ammonium formate+ 0.1% formic acid for positive ion tests, both at pH 3.5. T-tests were performed on the filtered data to determine statistical significance of $P<0.05$, and included Benjamini-Hotchberg false discovery rate for multiple hypothesis testing correction. Principal component analysis (R2X=0.992, Q2 (cum)=0.974) (**A**) and orthogonal partial least squares discriminant analysis (R2X=0.635, R2Y=0.992) (**B**) score plots acquired by liquid chromatography–tandem mass spectrometry detailing cardiac metabolomics of control and D100 hearts. The S-plot analysis (**C**, inset) and the variable important plot (**C**, top 30 metabolites) derived from the metabolite data illustrating the ions that contributed most to the separation of control from D100 hearts. Heat map of genes involved in glycerolipid synthesis in hearts from the different groups of rats (**D**). The red (high) and blue (low) colors reflect fold change. Total cardiac TG was extracted and solubilized in chloroform:methanol:acetone:hexane (4:6:1:1 v/v/v/v) and measured using high-performance liquid chromatography (n=4–6). Data are presented as mean ±SEM. Significantly different from the D55 group, $^{\#\#}P<0.01$.

treatment.[30] Regrettably, recommended glycemic goals are infrequently achieved, and this strategy often overlooks other features that are commonly part of this complex disease such as hyperlipidemia. In this respect, insulin deficiency produces activation of lipolysis in AT that results in hydrolysis of stored triglyceride and release of large amounts of FA into the

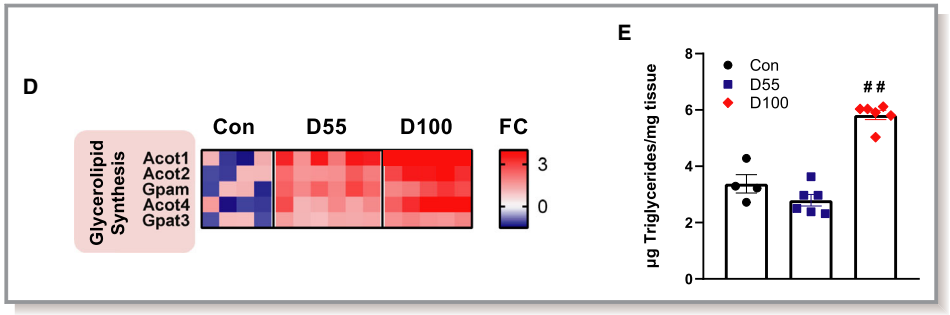

Figure 6. Continued.

plasma. This is because the primary enzymes responsible for lipolysis in adipocytes, adipose triglyceride lipase and hormone-sensitive lipase, are highly sensitive to inhibition by insulin.[31] Unexpectedly, a reduction of plasma insulin by almost 50% was insufficient to stimulate lipolysis. Contrasting with these data, it was only when insulin fell by >80% that an increase in plasma FAs was observed. It is important to note that the percentage composition of the main FAs identified in D100 plasma remained unchanged and mirrored the composition of the dietary FA ingested. Following their release, FAs enter into the portal circulation and thus the liver (where they induce biogenesis of very-low-density lipoprotein), or are delivered to the heart as a complex with albumin[10] and transferred across the plasma membrane to serve as an energy source. Given that the isolated heart exposed to equivalent concentrations of FA oxidize saturated FA, monounsaturated FA, and polyunsaturated FA at similar rates,[32] our results indicate that the augmented FA in D100 would be nonproductive, as the supply of FA might exceed the flexibility of the heart to use this excess amount of substrate.

With uninterrupted contraction being a feature of the heart, cardiac muscle has a high demand for energy. As such, this organ demonstrates substrate promiscuity, enabling it to use multiple sources of energy, including FA, carbohydrates, amino acids, and ketones.[32] Among these, carbohydrates and FA are the major participants from which the heart derives most of its energy, with FA producing almost 2.4-fold more ATP than glucose. Accordingly, in a basal setting, glucose and lactate contribute to ≈30% of ATP generation, with FA oxidation accounting for the remaining 70%.[32] Insulin plays an important role in glucose uptake and oxidation and suppression of FA oxidation in the heart.[33] It was not surprising, then, that its reduction in D55 animals was characterized by cardiac gene expression changes that emphasized defects in glucose metabolism and an enrichment in FA utilization. However, in hearts from D100 animals, it was noticeable how much more pronounced this change in the metabolism gene profile was, related not only to altered substrate utilization but also to the wide spectrum of associated downstream consequences including mitochondria organization, oxidative stress, and cell death. Whether this effect is a consequence of the high amounts of plasma FA[34] or the catastrophic loss of insulin in D100, or both, is currently unknown and can be assessed only if these results are compared with animals, where plasma FAs are increased without affecting insulin (using lipid- and heparin-induced elevation of FA).[34]

The first degradative step in the cardiac utilization of FA involves its β-oxidation in the mitochondria. However, another cytoplasmic organelle, peroxisomes, are also capable of β-oxidation of FA (especially VLCFA), with 1 key difference. Within peroxisomes, VLCFA only undergo β-oxidation for chain shortening and are incapable of being fully oxidized to CO_2 and H_2O to produce ATP[35]; the shorter chain moieties generated in the peroxisomes are in fact transferred to the mitochondria for additional β-oxidation and subsequent ATP generation. When systemic hyperglycemia was superimposed with dyslipidemia, there were more intense gene expression changes in the D100 heart that direct this organ to use FA by activating both the peroxisomal and mitochondrial β-oxidative pathways. One unappealing outcome of β-oxidation of FA in these organelles is the production of chemically reactive ROS[36,37] and, when combined with the reduction of antioxidant enzyme genes, causes oxidative stress.[38] Another drawback is that it results in the decrease of VLCFA like docosahexaenoic acid (22:6n3) and hence loss of the antioxidative and anti-inflammatory effects of this omega-3 FA.[39] Thus, in attempting to handle excess FA through stimulation of β-oxidation in peroxisomes and mitochondria, the D100 heart is exposed to oxidative damage and ultimately cellular demise.

The decrease in VLCFA may not be completely attributable to augmented oxidation but may also include a pathway to production of eicosanoids involved in an anti-inflammatory response. However, an argument against this view is that D100 hearts had an enrichment of genes annotated as related to a response to oxidative stress, and decreased coenzyme Q9. Furthermore, linoleic (LA, C18:2n-6) and oleic (OA, C18:1n-9) acid are increased in both the heart and plasma FA in D100 rats. The accumulation of LA in metabolic tissues has specifically been proposed to induce oxidative

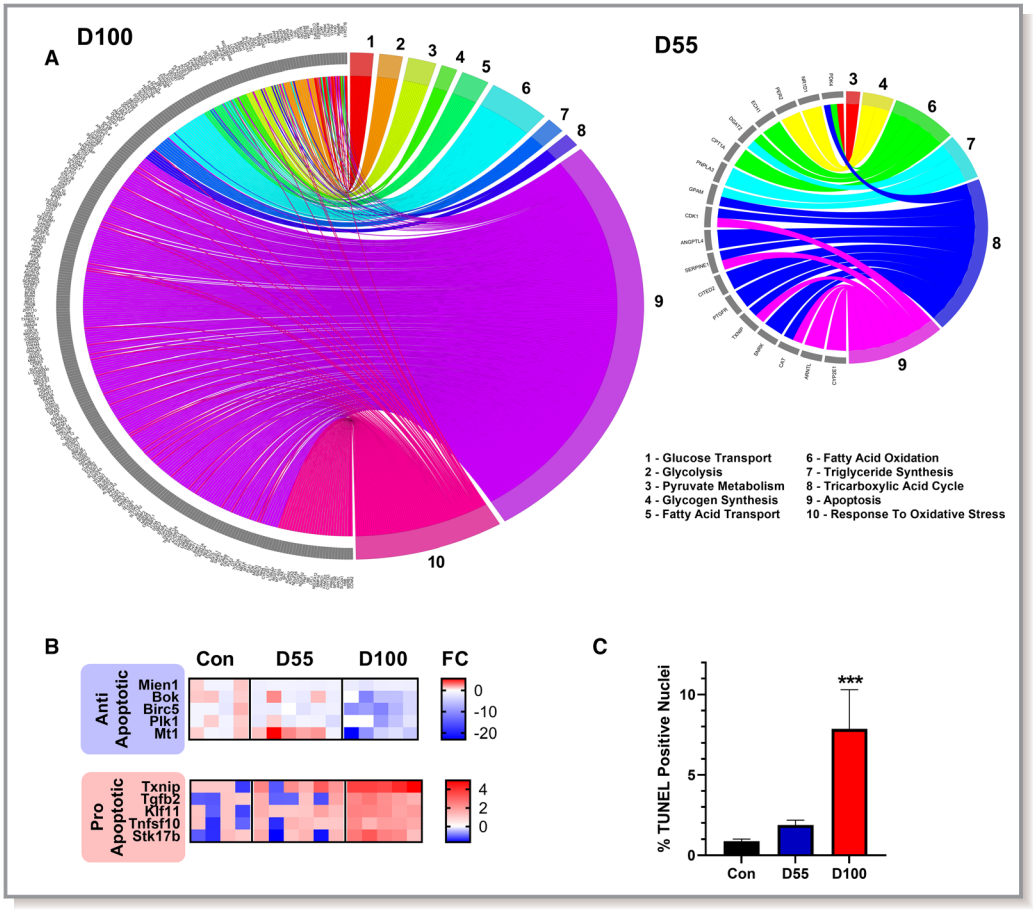

Figure 7. Significant apoptotic cell death in D100 hearts. A Circos plot was used to display the association between differentially expressed genes in D100 (**A**) and D55 (**A**, inset) hearts (n=4–6). Expression level of genes involved in the pathways is indicated as a $\log_2$ fold change (FC). The vast majority of genes are annotated as being directed towards modulation of metabolism (**A**) and cell survival mechanisms (**B**). Apoptotic cell death as identified by terminal deoxynucleotidyl transferase dUTP nick-end labeling (TUNEL) assay (**C**). Isolated rat hearts were retrogradely perfused with phosphate-buffered saline, then 10% formalin, embedded in paraffin, and 5-µm sections prepared. Nuclei were counted from 3 different ventricular sections per animal, from 3 individual animals per group. Data are presented as mean±SEM. Kruskal–Wallis nonparametric test, Dunn post hoc. Significantly different from the control, ***P<0.001. The summary diagram (**D**) illustrates that following moderate hypoinsulinemia and hyperglycemia, when plasma fatty acids (FAs) have yet to increase, lipoprotein lipase (LPL) is "switched on," and a robust expansion of coronary LPL follows. In animals with marked hypoinsulinemia and severe diabetes mellitus, there is a decline in vascular LPL. As these animals exhibit elevated plasma FA, we concluded that LPL-mediated FA delivery would be redundant in these circumstances and is "turned off." This is a questionable adaptation as the site of control of FA provision to the heart changes from a measured regulated delivery by coronary LPL to the unrestrained and unregulated provision by adipose tissue. Because of this metabolic reprogramming, FA supply exceeds the mitochondrial capacity of cardiomyocytes resulting in incomplete mitochondrial oxidation, accumulation of toxic FA metabolites, flux of excess unoxidized FA to triglycerides inducing a gene expression program supporting cell death (lipotoxicity).

stress through the generation of multiple oxidized LA compounds.[40–42] Interestingly, some of them have cardiospecific toxicities, which can range from mishandling of calcium to inflammation.[43] Such findings are also being increasingly reported in humans.[44–46] Additionally, the upregulation of OA in cardiac tissues is known to generate triglyceride,[47,48] as we see in our D100 model. While this storage of triglyceride may be adaptive, over time, such accumulation of triglyceride would cause cardiomyopathy, as has also been shown clinically.[49–51] We also emphasize that both OA and LA require additional steps by isomerases and reductases before they can be completely β-oxidized compared with PA.[52,53] Thus, PA without double bonds can undergo β-oxidation uninterrupted, is a better β-oxidation substrate than LA and OA, and gets used faster (its levels are lower in both diabetic groups). Finally, reductases use

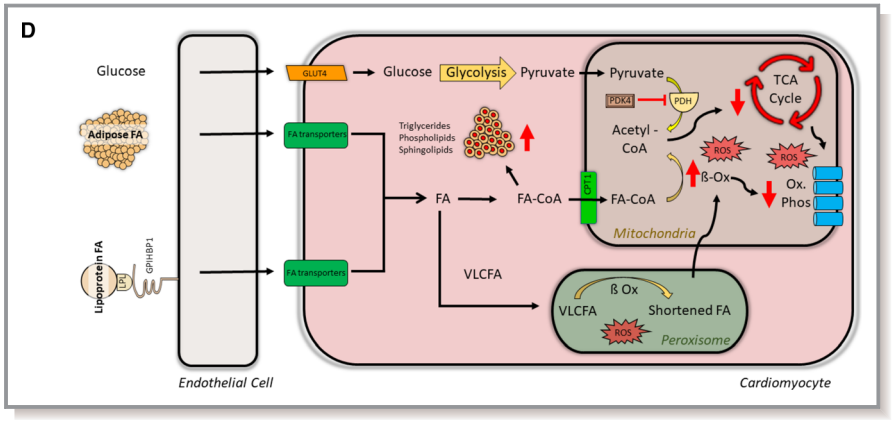

Figure 7. Continued.

nicotinamide adenine dinucleotide phosphate as the reducing equivalent donor.[54] The preference of the D100 heart to underutilize OA or LA (hence leading to their accumulation) could be an adaptive response to preserve nicotinamide adenine dinucleotide phosphate levels within myocytes to prevent further oxidative stress.

Following β-oxidation, FA catabolism resumes with sequential processing in the mitochondrial TCA cycle and oxidative phosphorylation system to yield ATP.[55] Contrary to prediction, the augmented β-oxidation was not matched by elevated TCA cycle activity or enhanced oxidative phosphorylation in D100 hearts. In fact, assessment of genes involved in mitochondrial metabolism revealed a critical decline in transcript levels of genes involved in these 2 pathways. In support of these observations, high-fat feeding is also known to increase β-oxidation but reduce TCA cycle intermediates in skeletal muscle of obese rodents.[56] As a consequence, in our study, myocytes from D100 hearts were unable to increase their respiration in response to increasing concentrations of FA under both basal conditions or when energy demand is increased. This suggests that when FA supply exceeds the mitochondrial capacity for disposal of this substrate (mitochondrial overload), incomplete oxidation of FA and ATP deficiency is an expected outcome.[56] The subsequent increase of FA intermediates and their diversion to triglyceride, paired with increased ROS formation secondary to excessive β-oxidation, can provoke a gene expression program supporting cell death (lipotoxicity). Indeed, a large number of the differentially expressed genes in D100 hearts were those involved in apoptosis. Thus, even though a recent study has suggested that hyperglycemia/hypoinsulinemia alone, without dyslipidemia, is sufficient to impair cardiac function,[57] data sets from this study indicate that with the increasing severity of diabetes mellitus, the sizeable increase in FA accounts for larger (compared with hyperglycemia alone) transcriptomic, metabolomic, and functional consequences and cardiomyocyte cell death.

In summary, our data establish the value of STZ models of diabetes mellitus with different degrees of hypoinsulinemia that imitate a continuum of glycemic management from insufficient (D55) to poor (D100) control. Globally, our data suggest that the differential reduction of insulin produced a dramatic change in cardiac gene expression largely related to substrate metabolism where glucose utilization is minimized and the heart adapts to use the robust increase in circulating FA. Unfortunately, this adaptation is nonproductive, as the supply of FA (especially monounsaturated FA and polyunsaturated FA) exceeds the flexibility of the heart to use these excess FAs resulting in triglyceride storage, oxidative stress, and cell death (lipotoxicity). These results may help guide the clinical management of type 1 diabetes mellitus, where in addition to focusing on drugs that lower plasma glucose, attention should also be placed on dyslipidemia, which could be a major link between diabetes mellitus and associated cardiomyopathy.

Limitations

The current study used a rodent model of STZ diabetes mellitus. It should be noted that most data from studies of rodent models of diabetes mellitus show minimal urinary glucose excretion when plasma glucose concentration is <22.2 mmol/L. This is a much higher capacity than what is typically observed in humans, where the renal threshold is 10 to 11 mmol/L.[58–60] Our model of diabetes mellitus in the current study is one of acute loss of insulin and its associated metabolomic, transcriptomic, and lipidomic changes. However, in a separate ongoing study, D55 animals were followed for 6 weeks. The initial hyperglycemia causes a glucose-induced pancreatic toxicity resulting in a further reduction in plasma insulin. This is accompanied by a modest increase in plasma FAs and triglycerides in D55 animals that is observed only in the long-term. In these chronically diabetic D55 animals, the sustained increase in LPL[16] together with the modest increase in adipose tissue lipolysis results in metabolomic changes that

more closely resemble what was seen in 4-day D100 hearts in the current study (Rodrigues Lab, unpublished data, 2019). It should be noted that the increase in cardiac LPL in acute D55 was unable to induce gene expression changes, oxidative stress, triglyceride accumulation, and cell death to the same magnitude as D100 hearts exposed to a robust enlargement in circulating plasma FA. This does not imply that augmentation of cardiac LPL, especially chronically, is without health risks. Cardiac-specific LPL overexpression in mice (likely to a level much higher than that seen in D55 hearts) causes severe myopathy characterized by lipid oversupply and deposition, muscle fiber degeneration, excessive dilatation, and impaired ventricular function in the absence of vascular defects, a situation comparable to diabetic cardiomyopathy.[61,62] Additionally, in chronically diabetic D55 animals, the sustained reduction in insulin, modest increase in plasma FA, and expansion of cardiac LPL led to a depressed cardiac function.[63]

Acknowledgments

Lipid analysis and ventricular metabolomics were performed at the Analytical Core for Metabolomics and Nutrition, British Columbia Children's Hospital. RNA sequencing activities were performed at the Sequencing and Bioinformatics Consortium at the University of British Columbia.

Mr. Puri was involved with data generation and collation, and writing the paper with Dr Rodrigues. Mr. Lal and Ms. Shang were responsible for diabetes mellitus induction in the rat model, helped with monitoring of the control and diabetic animals over 4 days, and contributed in part to some of the experiments performed. Dr Ghosh provided the expertise for interpretation of the lipid data. Dr Flibotte analyzed the RNAseq data. Mr Dyer generously determined plasma and cardiac lipids and conducted the ventricular metabolomics. The mitochondrial stress test was done by Ms. Hussein, who also oversaw the entire project and contributed to the editing of the manuscript. Dr Rodrigues and Puri generated the hypothesis, designed the study, and wrote the manuscript. Dr Rodrigues is the guarantor of this study.

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Disclosures

None.

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Supplemental Material

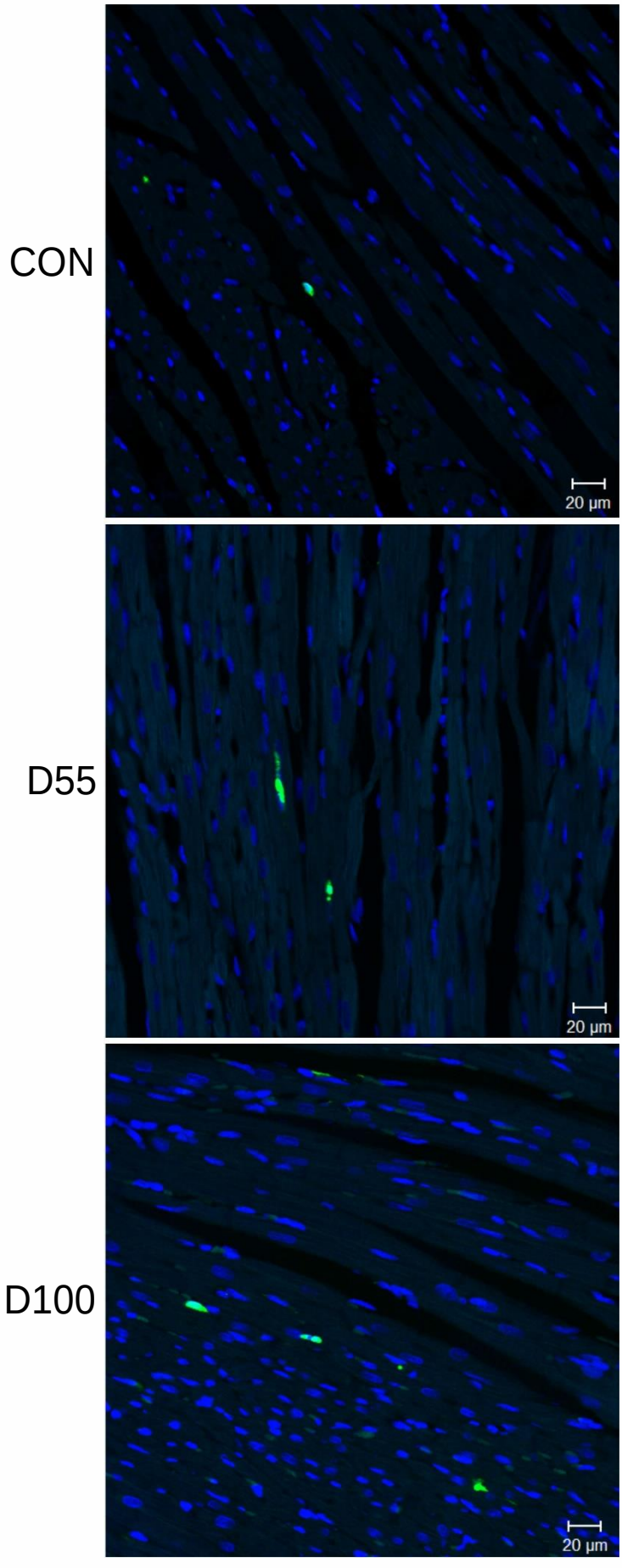

Figure S1. TUNEL assay to identify cardiomyocyte apoptosis. Apoptotic cell death was measured via TdT-mediated dUTP Nick-End Labeling (TUNEL) assay. Isolated rat hearts were retrogradely perfused with PBS, then 10% formalin, embedded in paraffin, and 5 µm sections prepared. Nuclei were counted from 3 different ventricular sections per animal, from 3 individual animals per group and were quantified in Figure 7C. Sections were visualized by fluorescence microscopy where DAPI- stained nuclei are blue, and fluorescein-12-dUTP incorporation resulted in localized green fluorescence only within the nuclei of apoptotic cells. CON, control; D55, 55 mg/kg streptozotocin- induced diabetes; D100, 100 mg/kg streptozotocin-induced diabetes.

Table S1. Micromolar FA in Plasma.

Fatty Acid	Con Mean	(+/-)	D55 Mean	(+/-)	D100 Mean	(+/-)
C 12:0	0.09	0.01	0.07	0.02	0.07	0.02
C 14:0	0.43	0.10	0.31	0.07	0.68	0.17
C 14:1	0.01	0.00	0.01	0.01	0.01	0.00
C 16:0 DMA	0.05	0.02	0.06	0.02	0.05	0.01
C 16:1 DMA	0.04	0.01	0.03	0.01	0.06	0.01
C 16:0	15.13	3.79	15.39	2.48	31.35	6.03
C 16:1n9	0.28	0.06	0.19	0.05	0.31	0.06
C 16:1n7	0.90	0.40	0.57	0.15	1.20	0.29
C 18:0 DMA	0.10	0.03	0.11	0.03	0.06	0.01
C 18:1 DMA	0.64	0.19	0.48	0.12	0.55	0.10
C 18:0	8.82	1.82	9.84	1.67	13.88	2.32
C 18:1n9	9.93	3.07	10.22	2.38	23.21	5.64
C 18:1n7	1.55	0.43	1.28	0.25	2.51	0.50
C 18:2n6	14.32	4.48	16.43	2.16	36.59	7.01
C 18:3n6	0.11	0.05	0.11	0.02	0.59	0.83
C 20:0	0.08	0.03	0.09	0.01	0.24	0.06
C 18:3n3	0.36	0.13	0.30	0.10	1.15	0.32
C 20:1n11	0.17	0.05	0.16	0.03	0.38	0.09
C 20:1n9	0.11	0.05	0.07	0.01	0.31	0.06
C 18:4n3	0.02	0.01	0.02	0.03	0.08	0.03
C 20:2n6	0.21	0.05	0.17	0.06	0.31	0.07
C 20:3n9	0.10	0.03	0.11	0.06	0.13	0.02
C 20:3n6	0.56	0.19	0.44	0.19	0.55	0.11
C 22:0	0.06	0.02	0.07	0.01	0.15	0.03
C 20:4n6	8.39	1.98	10.57	2.23	11.60	1.84
C 20:5n3	0.84	0.31	0.78	0.12	1.70	0.38
C 24:0	0.08	0.01	0.08	0.02	0.16	0.03
C 22:4n6	0.18	0.06	0.23	0.04	0.39	0.08
C 24:1	0.05	0.02	0.04	0.02	0.06	0.01
C 22:5n6	0.06	0.02	0.05	0.00	0.18	0.05
C 22:5n3	0.74	0.27	0.83	0.18	1.66	0.37
C 22:6n3	2.90	0.91	3.23	0.33	9.06	2.09

Table S2. RNA seq D55

gene_id	gene_name	log2FoldChange	log2CPM	FC
ENSRNOG00000014448	Arntl	-2	4.25	-4
ENSRNOG00000022268	Pnpla3	-1.74	3.07	-3.340351678
ENSRNOG00000009785	Cdkn3	-1.45	0.6	-2.732080514
ENSRNOG00000025302	Cdca2	-1.38	-0.24	-2.602683711
ENSRNOG00000000632	Cdk1	-1.31	1.42	-2.4794154
ENSRNOG00000028137	Mki67	-1.25	3.71	-2.37841423
ENSRNOG00000006622	Cry1	-0.8	NA	-1.741101127
ENSRNOG00000046005	Scd2	-0.68	NA	-1.602139755
ENSRNOG00000016810	Stmn1	-0.65	NA	-1.569168196
ENSRNOG00000058609	Palmd	-0.56	NA	-1.474269217
ENSRNOG00000042179	Cfap20	-0.51	NA	-1.424050196
ENSRNOG00000013293	Mccc1	-0.47	NA	-1.385109468
ENSRNOG00000042717	Ciart	5.39	1.86	41.93258892
ENSRNOG00000016983	Myh7	3.86	11.15	14.52030649
ENSRNOG00000021027	Dbp	3.66	4.41	12.64066099
ENSRNOG00000007545	Angptl4	3.21	3.82	9.253505471
ENSRNOG00000009329	Nr1d1	2.79	5.04	6.91629785
ENSRNOG00000034228	Pik3c2g	2.69	4.17	6.453134074
ENSRNOG00000018413	Per3	2.48	4.37	5.578974665
ENSRNOG00000019120	Hmgcs2	2.15	NA	4.438277888
ENSRNOG00000055221	Acot1	2.13	1.94	4.377174805
ENSRNOG00000012458	Cyp2e1	1.93	3.14	3.810551992
ENSRNOG00000048961	Bhlhe41	1.78	2.69	3.434261746
ENSRNOG00000009565	Pdk4	1.74	8.46	3.340351678
ENSRNOG00000020254	Per2	1.72	NA	3.294364069
ENSRNOG00000015850	Rbp7	1.55	5.74	2.928171392
ENSRNOG00000003228	Mid1ip1	1.43	NA	2.694467154
ENSRNOG00000015003	Pex11a	1.42	1.55	2.67585511
ENSRNOG00000001414	Serpine1	1.42	NA	2.67585511
ENSRNOG00000020308	Ech1	1.35	NA	2.549121255
ENSRNOG00000023657	Gprin3	1.33	3.64	2.514026749
ENSRNOG00000009019	Slc6a6	1.31	4.39	2.4794154
ENSRNOG00000015124	Gpam	1.31	6.09	2.4794154
ENSRNOG00000016573	Dgat2	1.22	NA	2.329467173
ENSRNOG00000046912	Nr1d2	1.21	7.04	2.313376368
ENSRNOG00000007648	Rab11b	1.14	NA	2.203810232
ENSRNOG00000056940	Cited2	1.13	5.27	2.188587403
ENSRNOG00000012363	Peli2	1.12	2	2.173469725
ENSRNOG00000046468	Ptgfr	1.12	7.11	2.173469725
ENSRNOG00000010134	Acot2	1.06	7.27	2.084931522
ENSRNOG00000021201	Txnip	1.03	NA	2.042024251
ENSRNOG00000007152	Bhlhe40	0.99	5.34	1.986184991
ENSRNOG00000014508	Mgll	0.83	NA	1.777685362
ENSRNOG00000016692	Hsdl2	0.73	8.4	1.658639092
ENSRNOG00000004050	Snrk	0.69	NA	1.613283518

ENSRNOG00000014254	Cpt1a	0.68	NA	1.602139755
ENSRNOG00000008747	Plekha5	0.68	NA	1.602139755
ENSRNOG00000008364	Cat	0.51	NA	1.424050196

Table S3. RNA seq D100.

gene_id	gene_name	log2FoldChange	log2CPM	FoldChange
ENSRNOG00000028993	RPL12	9.65	3.69	803.4141162
ENSRNOG00000017586	Snrpc	8.44	-0.03	347.2907078
ENSRNOG00000033529	Amy1a	5.24	NA	37.79176517
ENSRNOG00000010128	Slc27a2	4.67	NA	25.45716748
ENSRNOG00000034228	Pik3c2g	4.41	4.17	21.25897303
ENSRNOG00000042717	Ciart	4.38	1.86	20.82146969
ENSRNOG00000007545	Angptl4	4.37	3.82	20.67764529
ENSRNOG00000003683	Glp2r	4.1	NA	17.1483754
ENSRNOG00000018656	Ampd1	3.85	0.41	14.4200074
ENSRNOG00000017424	Chrna2	3.66	-0.53	12.64066099
ENSRNOG00000016983	Myh7	3.47	11.15	11.08087574
ENSRNOG00000055221	Acot1	3.43	2.26	10.77786861
ENSRNOG00000015581	Dnah6	3.38	-0.16	10.41073484
ENSRNOG00000012458	Cyp2e1	3.33	3.12	10.056107
ENSRNOG00000019120	Hmgcs2	3.31	4.77	9.9176616
ENSRNOG00000007810	Gdf6	3.22	NA	9.317868692
ENSRNOG00000009565	Pdk4	3.21	8.43	9.253505471
ENSRNOG00000018692	Mc4r	2.7	0.48	6.498019171
ENSRNOG00000015279	Vtcn1	2.68	NA	6.408559021
ENSRNOG00000056940	Cited2	2.43	5.27	5.388934307
ENSRNOG00000007675	Gpr63	2.43	1.99	5.388934307
ENSRNOG00000033844	LOC100912195	2.34	2.76	5.063026376
ENSRNOG00000057404	Slc47a1	2.33	NA	5.028053498
ENSRNOG00000003991	Ankar	2.22	0.56	4.658934346
ENSRNOG00000019744	Prr16	2.21	0.93	4.626752736
ENSRNOG00000019342	Sult1a1	2.2	5.39	4.59479342
ENSRNOG00000011702	Foxp3	2.19	0.74	4.563054863
ENSRNOG00000015003	Pex11a	2.17	1.47	4.500233939
ENSRNOG00000053332	Cdh26	2.17	1.73	4.500233939
ENSRNOG00000001414	Serpine1	2.05	4.86	4.141059695
ENSRNOG00000046468	Ptgfr	2.04	7.11	4.112455307
ENSRNOG00000046864	Acot4	2.03	0.61	4.084048503
ENSRNOG00000017806	RGD1564827	2	0.05	4
ENSRNOG00000015850	Rbp7	1.98	5.74	3.944930818
ENSRNOG00000043176	RGD1565355	1.98	3.23	3.944930818
ENSRNOG00000037645	Tceal7	1.94	3.33	3.837056477
ENSRNOG00000005268	Gnat3	1.94	0.48	3.837056477
ENSRNOG00000011351	Mat1a	1.83	NA	3.555370725
ENSRNOG00000021201	Txnip	1.74	9.65	3.340351678
ENSRNOG00000005906	ENSRNOG00000005906	1.7	5.54	3.249009585
ENSRNOG00000010610	Hpgd	1.69	NA	3.226567037
ENSRNOG00000021381	Ccdc68	1.69	NA	3.226567037
ENSRNOG00000016306	Adgrv1	1.65	2.67	3.138336392
ENSRNOG00000000386	Pbld1	1.64	2.77	3.116658319
ENSRNOG00000011313	Sorcs1	1.63	0.03	3.095129987

ENSRNOG00000010134	Acot2	1.59		7.27	3.010493495
ENSRNOG00000018413	Per3	1.59		4.42	3.010493495
ENSRNOG00000021209	Polr3gl	1.58		4.28	2.989698497
ENSRNOG00000054052	Ppp4r4	1.58		1.82	2.989698497
ENSRNOG00000002618	Ivns1abp	1.56		9.19	2.948538435
ENSRNOG00000030771	Dgkb	1.54		3.99	2.907945035
ENSRNOG00000004918	Kcna4	1.53		2.14	2.887858391
ENSRNOG00000010392	Nrg1	1.53		1.21	2.887858391
ENSRNOG00000020254	Per2	1.51	NA		2.848100391
ENSRNOG00000017716	Ucp3	1.49	NA		2.808889751
ENSRNOG00000052173	Ranbp3	1.48		0.62	2.789487333
ENSRNOG00000050325	Adgre4	1.48		0.64	2.789487333
ENSRNOG00000007390	Nfkbia	1.47	NA		2.770218936
ENSRNOG00000026196	Lrrd1	1.46		2.1	2.751083636
ENSRNOG00000003510	Fmo2	1.45		4.56	2.732080514
ENSRNOG00000025460	Tmem71	1.44		5.63	2.713208655
ENSRNOG00000040108	Cd36	1.44		10.85	2.713208655
ENSRNOG00000029841	Cdh19	1.44		2.96	2.713208655
ENSRNOG00000048961	Bhlhe41	1.43		2.69	2.694467154
ENSRNOG00000047077	LOC681341	1.41		0.89	2.657371628
ENSRNOG00000016692	Hsdl2	1.4		8.4	2.639015822
ENSRNOG00000037632	LOC688553	1.4		2.28	2.639015822
ENSRNOG00000031053	ND4L	1.39	NA		2.620786808
ENSRNOG00000009487	Gpr160	1.38		1.4	2.602683711
ENSRNOG00000010308	Nr2f2	1.38	NA		2.602683711
ENSRNOG00000046912	Nr1d2	1.35		7.04	2.549121255
ENSRNOG00000057221	Scn3b	1.33		2.09	2.514026749
ENSRNOG00000040201	Atp6ap1l	1.33		3.97	2.514026749
ENSRNOG00000061533	AABR07001926.3	1.33	NA		2.514026749
ENSRNOG00000046629	Zfp37	1.32		1.98	2.496661098
ENSRNOG00000008236	Decr1	1.3		8.42	2.462288827
ENSRNOG00000015036	Ctgf	1.29		6.4	2.445280555
ENSRNOG00000000633	Rhobtb1	1.29	NA		2.445280555
ENSRNOG00000003515	Ephx1	1.28	NA		2.428389769
ENSRNOG00000001843	Bcl6	1.27	NA		2.411615655
ENSRNOG00000015124	Gpam	1.26		6.09	2.394957409
ENSRNOG00000062125	Aox3l1	1.26		3.09	2.394957409
ENSRNOG00000012363	Peli2	1.26		2.16	2.394957409
ENSRNOG00000022710	Prrg4	1.26	NA		2.394957409
ENSRNOG00000004476	Wif1	1.25		1.66	2.37841423
ENSRNOG00000018911	Pfkfb3	1.25	NA		2.37841423
ENSRNOG00000009425	Fgf7	1.24		1.66	2.361985323
ENSRNOG00000032668	ENSRNOG00000032668	1.24		3.78	2.361985323
ENSRNOG00000020308	Ech1	1.24	NA		2.361985323
ENSRNOG00000047848	Cbr1	1.24		3.5	2.361985323
ENSRNOG00000004282	Arl4a	1.23		4.59	2.345669898
ENSRNOG00000034198	Tceal9	1.22		5.94	2.329467173
ENSRNOG00000005854	Angpt1	1.22		4.96	2.329467173

ENSRNOG00000004861	Itga4	1.22		2.47	2.329467173
ENSRNOG00000009019	Slc6a6	1.21		4.67	2.313376368
ENSRNOG00000039560	Omd	1.21		4.38	2.313376368
ENSRNOG00000017963	RGD1566325	1.21		4.43	2.313376368
ENSRNOG00000042679	Lcor	1.21	NA		2.313376368
ENSRNOG00000007964	Tp53inp1	1.2		3.02	2.29739671
ENSRNOG00000023657	Gprin3	1.2	NA		2.29739671
ENSRNOG00000011820	Acpp	1.2	NA		2.29739671
ENSRNOG00000002305	Slc15a2	1.19		2.31	2.281527432
ENSRNOG00000004378	Abca5	1.19		2.17	2.281527432
ENSRNOG00000025587	Plagl1	1.19	NA		2.281527432
ENSRNOG00000052467	Klrc3	1.18		2.11	2.265767771
ENSRNOG00000007250	Six4	1.17		2.84	2.250116969
ENSRNOG00000042308	LOC680200	1.17		2.35	2.250116969
ENSRNOG00000053122	Scn1a	1.17	NA		2.250116969
ENSRNOG00000060246	Klrd1	1.17		3.4	2.250116969
ENSRNOG00000003620	Fmo3	1.16		4.91	2.234574276
ENSRNOG00000015260	Lpar3	1.16		2.85	2.234574276
ENSRNOG00000006653	Slc38a4	1.16	NA		2.234574276
ENSRNOG00000013011	Dnajb4	1.15		7.14	2.219138944
ENSRNOG00000027357	Sox17	1.15		3.06	2.219138944
ENSRNOG00000031163	Nfkbiz	1.15	NA		2.219138944
ENSRNOG00000025691	Pla2g7	1.15	NA		2.219138944
ENSRNOG00000003927	Cd55	1.14		4.71	2.203810232
ENSRNOG00000003749	Xk	1.14	NA		2.203810232
ENSRNOG00000054157	Nadkd1	1.13		6.34	2.188587403
ENSRNOG00000009686	Aqp7	1.13	NA		2.188587403
ENSRNOG00000008846	Plag1	1.13	NA		2.188587403
ENSRNOG00000030418	Tmem47	1.13	NA		2.188587403
ENSRNOG00000015741	Slc2a13	1.11		2.84	2.158456473
ENSRNOG00000018648	Mppe1	1.1		3.71	2.143546925
ENSRNOG00000042630	Asb5	1.1		1.86	2.143546925
ENSRNOG00000054259	Klf11	1.1	NA		2.143546925
ENSRNOG00000006670	Rai2	1.1	NA		2.143546925
ENSRNOG00000015075	Stc1	1.1	NA		2.143546925
ENSRNOG00000012502	Stk17b	1.1	NA		2.143546925
ENSRNOG00000010775	Arrdc4	1.09		5.55	2.128740365
ENSRNOG00000045649	Arrdc3	1.09		4.68	2.128740365
ENSRNOG00000054218	Il18rap	1.09	NA		2.128740365
ENSRNOG00000018505	Cidea	1.08	NA		2.114036081
ENSRNOG00000045992	Tlr8	1.08	NA		2.114036081
ENSRNOG00000060972	Heca	1.08	NA		2.114036081
ENSRNOG00000003434	Trove2	1.08	NA		2.114036081
ENSRNOG00000011652	Sppl2a	1.07		5.63	2.099433367
ENSRNOG00000017800	Foxc1	1.07	NA		2.099433367
ENSRNOG00000006967	Xiap	1.07	NA		2.099433367
ENSRNOG00000014511	Alg10	1.07	NA		2.099433367
ENSRNOG00000018382	Inpp4b	1.06	NA		2.084931522

ENSRNOG00000049911	LOC102556347	1.06	NA		2.084931522
ENSRNOG00000000808	Hsf2	1.05	NA		2.070529848
ENSRNOG00000010940	Acad11	1.04		4.52	2.056227653
ENSRNOG00000015577	Lpar6	1.04		5.55	2.056227653
ENSRNOG00000029042	Mt-nd6	1.04		12	2.056227653
ENSRNOG00000033261	Fam107a	1.04	NA		2.056227653
ENSRNOG00000024986	Mmrn1	1.04	NA		2.056227653
ENSRNOG00000021729	Iqub	1.04	NA		2.056227653
ENSRNOG00000000073	Tmed5	1.04	NA		2.056227653
ENSRNOG00000015334	Fcho2	1.03		6.16	2.042024251
ENSRNOG00000001770	Ehhadh	1.03	NA		2.042024251
ENSRNOG00000010235	Pkig	1.03	NA		2.042024251
ENSRNOG00000007027	Hgf	1.03	NA		2.042024251
ENSRNOG00000061862	Zbtb10	1.02		3.66	2.02791896
ENSRNOG00000047439	Pot1b	1.02		3.2	2.02791896
ENSRNOG00000012278	Fgf10	1.02	NA		2.02791896
ENSRNOG00000053787	Mdfic	1.02	NA		2.02791896
ENSRNOG00000007249	Cdkn1b	1.01		5.28	2.0139111
ENSRNOG00000022066	Fam117b	1.01	NA		2.0139111
ENSRNOG00000024730	Ppm1e	1.01	NA		2.0139111
ENSRNOG00000011280	Mllt3	1.01	NA		2.0139111
ENSRNOG00000011994	Perp	1		6.11	2
ENSRNOG00000007743	Mgst1	1		4.18	2
ENSRNOG00000045733	LOC298139	1		6.34	2
ENSRNOG00000006441	Zbtb25	1		2.67	2
ENSRNOG00000001544	Cyyr1	1		7.03	2
ENSRNOG00000001827	Masp1	1	NA		2
ENSRNOG00000008524	Glcci1	1	NA		2
ENSRNOG00000002075	Cnot6l	1	NA		2
ENSRNOG00000059538	Clec2g	1	NA		2
ENSRNOG00000015906	Tgif1	0.99	NA		1.986184991
ENSRNOG00000017404	Pcmtd2	0.99	NA		1.986184991
ENSRNOG00000004616	Npm1	0.99	NA		1.986184991
ENSRNOG00000009197	Asb4	0.98		3.05	1.972465409
ENSRNOG00000016456	Il33	0.98		5.64	1.972465409
ENSRNOG00000021314	Fdft1	0.98	NA		1.972465409
ENSRNOG00000056135	Tsc22d3	0.98	NA		1.972465409
ENSRNOG00000033402	LOC501110	0.98	NA		1.972465409
ENSRNOG00000006975	Wasl	0.98	NA		1.972465409
ENSRNOG00000036913	RGD1309621	0.98	NA		1.972465409
ENSRNOG00000006206	Tmem106b	0.98	NA		1.972465409
ENSRNOG00000039110	Lsmem1	0.97		5.42	1.958840595
ENSRNOG00000004772	Cytip	0.97	NA		1.958840595
ENSRNOG00000012881	Fgl2	0.97	NA		1.958840595
ENSRNOG00000005917	Pawr	0.97	NA		1.958840595
ENSRNOG00000059460	Ttc30b	0.96	NA		1.945309895
ENSRNOG00000025372	Glce	0.96	NA		1.945309895
ENSRNOG00000005578	Zbtb44	0.96	NA		1.945309895

ENSRNOG00000010224	Rab30	0.96	NA		1.945309895
ENSRNOG00000051377	Zfp748	0.96	NA		1.945309895
ENSRNOG00000050534	Gcnt1	0.95		5.57	1.931872658
ENSRNOG00000006110	Jph1	0.95		4.12	1.931872658
ENSRNOG00000003587	Vegfd	0.95	NA		1.931872658
ENSRNOG00000028649	Tox3	0.95	NA		1.931872658
ENSRNOG00000007648	Rab11b	0.95	NA		1.931872658
ENSRNOG00000004448	Acss3	0.95		3.52	1.931872658
ENSRNOG00000020769	Crebrf	0.94		6.31	1.918528239
ENSRNOG00000010205	Mturn	0.94	NA		1.918528239
ENSRNOG00000049985	Gprasp1	0.93		5.03	1.905275996
ENSRNOG00000008364	Cat	0.93		8.12	1.905275996
ENSRNOG00000011696	Lifr	0.93		6.15	1.905275996
ENSRNOG00000008747	Plekha5	0.93	NA		1.905275996
ENSRNOG00000006418	Samhd1	0.93	NA		1.905275996
ENSRNOG00000014712	Zfp39	0.93	NA		1.905275996
ENSRNOG00000002418	Tgfb2	0.92		4.44	1.892115293
ENSRNOG00000007947	Fam13a	0.92	NA		1.892115293
ENSRNOG00000012364	Prickle2	0.92	NA		1.892115293
ENSRNOG00000049057	Znrf2	0.92	NA		1.892115293
ENSRNOG00000007345	Amot	0.92	NA		1.892115293
ENSRNOG00000034078	Mxi1	0.91		5.57	1.879045498
ENSRNOG00000024852	Tmx4	0.91		7.84	1.879045498
ENSRNOG00000025528	Efr3a	0.91		7.55	1.879045498
ENSRNOG00000013300	Atpif1	0.91	NA		1.879045498
ENSRNOG00000039582	RGD1561161	0.91	NA		1.879045498
ENSRNOG00000029342	Scn7a	0.91	NA		1.879045498
ENSRNOG00000006244	Lztfl1	0.91	NA		1.879045498
ENSRNOG00000010800	Hadhb	0.9		10.98	1.866065983
ENSRNOG00000002159	Gpat3	0.9	NA		1.866065983
ENSRNOG00000031855	Actr3b	0.9	NA		1.866065983
ENSRNOG00000006859	Insig1	0.9	NA		1.866065983
ENSRNOG00000019184	Npr3	0.9	NA		1.866065983
ENSRNOG00000020578	Ceacam1	0.9	NA		1.866065983
ENSRNOG00000000655	Ptprc	0.9	NA		1.866065983
ENSRNOG00000015095	Spryd7	0.9	NA		1.866065983
ENSRNOG00000050251	MGC105649	0.9	NA		1.866065983
ENSRNOG00000000815	Smpdl3a	0.89		5.75	1.853176124
ENSRNOG00000001607	Adamts1	0.89		5.35	1.853176124
ENSRNOG00000029971	Mt-nd5	0.89		14.03	1.853176124
ENSRNOG00000018378	Cacnb2	0.89	NA		1.853176124
ENSRNOG00000016183	Ipp	0.89	NA		1.853176124
ENSRNOG00000011929	Abcd3	0.89	NA		1.853176124
ENSRNOG00000014852	Fbxo30	0.89	NA		1.853176124
ENSRNOG00000006118	Klf10	0.88		5.1	1.840375301
ENSRNOG00000001271	Card6	0.88	NA		1.840375301
ENSRNOG00000014215	Klf9	0.88	NA		1.840375301
ENSRNOG00000016541	Enc1	0.88	NA		1.840375301

ENSRNOG00000002225	Scarb2	0.88	NA		1.840375301
ENSRNOG00000012733	Ankrd12	0.88	NA		1.840375301
ENSRNOG00000010240	Fam46a	0.88	NA		1.840375301
ENSRNOG00000061102	Taf9b	0.88		4.83	1.840375301
ENSRNOG00000004496	Rock2	0.87		8.6	1.8276629
ENSRNOG00000011921	Dusp4	0.87	NA		1.8276629
ENSRNOG00000013269	Tnfsf10	0.87	NA		1.8276629
ENSRNOG00000015020	Idh1	0.87	NA		1.8276629
ENSRNOG00000000164	Lamp2	0.87	NA		1.8276629
ENSRNOG00000052721	Kdm6a	0.87	NA		1.8276629
ENSRNOG00000015501	Ddhd2	0.86		4.99	1.815038311
ENSRNOG00000002089	Ccng2	0.86	NA		1.815038311
ENSRNOG00000001376	Mettl7a	0.85	NA		1.802500925
ENSRNOG00000010682	Clcn3	0.85	NA		1.802500925
ENSRNOG00000030021	Ccl6	0.85	NA		1.802500925
ENSRNOG00000023509	Irs2	0.85	NA		1.802500925
ENSRNOG00000002338	Dgke	0.85	NA		1.802500925
ENSRNOG00000006779	Crot	0.85	NA		1.802500925
ENSRNOG00000010017	Wee1	0.85	NA		1.802500925
ENSRNOG00000021213	Lix1l	0.84		7.48	1.790050142
ENSRNOG00000011976	Nudt7	0.84		5.43	1.790050142
ENSRNOG00000019179	Ggta1	0.84		5.75	1.790050142
ENSRNOG00000012536	Sgms1	0.84	NA		1.790050142
ENSRNOG00000004011	Nedd1	0.84	NA		1.790050142
ENSRNOG00000018719	Cir1	0.84	NA		1.790050142
ENSRNOG00000004019	Phlda1	0.84	NA		1.790050142
ENSRNOG00000003470	Fundc1	0.83		5.66	1.777685362
ENSRNOG00000022576	Nudt12	0.83	NA		1.777685362
ENSRNOG00000011946	Ptn	0.83	NA		1.777685362
ENSRNOG00000010239	Cnbp	0.83	NA		1.777685362
ENSRNOG00000012302	Gucy1a3	0.82		5.83	1.765405993
ENSRNOG00000012183	Glrx	0.82	NA		1.765405993
ENSRNOG00000012683	Abhd17c	0.82	NA		1.765405993
ENSRNOG00000005470	Atxn3	0.82	NA		1.765405993
ENSRNOG00000060107	Dnajb14	0.82	NA		1.765405993
ENSRNOG00000002125	Ccni	0.82	NA		1.765405993
ENSRNOG00000018944	Pank1	0.81	NA		1.753211443
ENSRNOG00000007034	Hipk2	0.81	NA		1.753211443
ENSRNOG00000008580	Nbn	0.8		5.85	1.741101127
ENSRNOG00000006867	Etv1	0.8		4.62	1.741101127
ENSRNOG00000016848	Fzd4	0.8	NA		1.741101127
ENSRNOG00000024849	Tor1aip2	0.8	NA		1.741101127
ENSRNOG00000006076	Steap2	0.8	NA		1.741101127
ENSRNOG00000011358	Hipk3	0.8	NA		1.741101127
ENSRNOG00000021403	Rhob	0.8	NA		1.741101127
ENSRNOG00000037658	Gprasp2	0.8	NA		1.741101127
ENSRNOG00000022946	Slc22a3	0.8	NA		1.741101127
ENSRNOG00000014084	Sp1	0.8	NA		1.741101127

ENSRNOG00000023197	Zfp608	0.79	NA		1.729074463
ENSRNOG00000013867	Fgf1	0.79	NA		1.729074463
ENSRNOG00000048043	F2r	0.79	NA		1.729074463
ENSRNOG00000008839	Pparg	0.79	NA		1.729074463
ENSRNOG00000057569	Ahnak	0.79	NA		1.729074463
ENSRNOG00000005715	Lgr4	0.78		5.35	1.717130873
ENSRNOG00000005039	Tfpi	0.78		7.41	1.717130873
ENSRNOG00000058522	Fam214a	0.78	NA		1.717130873
ENSRNOG00000003452	Asb9	0.78	NA		1.717130873
ENSRNOG00000001982	Cblb	0.78	NA		1.717130873
ENSRNOG00000000657	Nek7	0.78	NA		1.717130873
ENSRNOG00000032659	Plcl1	0.78	NA		1.717130873
ENSRNOG00000003071	Vamp4	0.78	NA		1.717130873
ENSRNOG00000034191	Fmo1	0.77	NA		1.705269784
ENSRNOG00000019892	Lrrfip1	0.77	NA		1.705269784
ENSRNOG00000046889	Dbi	0.77	NA		1.705269784
ENSRNOG00000033796	Kcnj5	0.77	NA		1.705269784
ENSRNOG00000013368	Plcl2	0.77	NA		1.705269784
ENSRNOG00000015812	Tm4sf1	0.77	NA		1.705269784
ENSRNOG00000010584	Tmem123	0.77	NA		1.705269784
ENSRNOG00000002036	Paxbp1	0.77	NA		1.705269784
ENSRNOG00000031716	Ecm2	0.77	NA		1.705269784
ENSRNOG00000001930	Ccdc50	0.77	NA		1.705269784
ENSRNOG00000000800	Man1a1	0.77	NA		1.705269784
ENSRNOG00000059968	Jak2	0.77	NA		1.705269784
ENSRNOG00000001090	Stard13	0.76	NA		1.693490625
ENSRNOG00000017243	Bnip3	0.76	NA		1.693490625
ENSRNOG00000016378	Map3k8	0.76	NA		1.693490625
ENSRNOG00000013484	Gsta2	0.76	NA		1.693490625
ENSRNOG00000005464	Lgalsl	0.76	NA		1.693490625
ENSRNOG00000022162	Pbx3	0.75	NA		1.681792831
ENSRNOG00000007047	Eps8	0.75	NA		1.681792831
ENSRNOG00000007637	Acer2	0.75	NA		1.681792831
ENSRNOG00000010748	Mtus1	0.75	NA		1.681792831
ENSRNOG00000018346	Agtr1a	0.75	NA		1.681792831
ENSRNOG00000007106	Sos1	0.75	NA		1.681792831
ENSRNOG00000002069	Slc35a5	0.75	NA		1.681792831
ENSRNOG00000014076	Mbnl1	0.75	NA		1.681792831
ENSRNOG00000011548	Ebf2	0.74	NA		1.670175839
ENSRNOG00000015117	Lrrc39	0.74	NA		1.670175839
ENSRNOG00000004749	Slc30a1	0.74	NA		1.670175839
ENSRNOG00000008151	Plscr4	0.73		5.04	1.658639092
ENSRNOG00000053869	Ppp1r3d	0.73	NA		1.658639092
ENSRNOG00000001557	Cxadr	0.73	NA		1.658639092
ENSRNOG00000054902	LOC100909709	0.73	NA		1.658639092
ENSRNOG00000002146	Pkd2	0.73	NA		1.658639092
ENSRNOG00000001657	Cldnd1	0.73	NA		1.658639092
ENSRNOG00000060460	Clec1a	0.73	NA		1.658639092

ENSRNOG00000001007	Baiap2l1	0.72	NA	1.647182035
ENSRNOG00000022196	Bmpr2	0.72	NA	1.647182035
ENSRNOG00000013683	S1pr1	0.72	NA	1.647182035
ENSRNOG00000001516	Rapgef4	0.72	NA	1.647182035
ENSRNOG00000014254	Cpt1a	0.71	NA	1.635804117
ENSRNOG00000002093	Tgfbr3	0.71	NA	1.635804117
ENSRNOG00000009552	Serinc3	0.71	NA	1.635804117
ENSRNOG00000018282	Gda	0.71	NA	1.635804117
ENSRNOG00000042848	Jam2	0.71	NA	1.635804117
ENSRNOG00000012037	Galnt7	0.71	NA	1.635804117
ENSRNOG00000020288	Slc25a20	0.7	NA	1.624504793
ENSRNOG00000021840	Cped1	0.7	NA	1.624504793
ENSRNOG00000021614	Kmt2e	0.7	NA	1.624504793
ENSRNOG00000053086	Selenop	0.69	NA	1.613283518
ENSRNOG00000061910	Igfbp3	0.69	NA	1.613283518
ENSRNOG00000048800	Nr3c1	0.69	NA	1.613283518
ENSRNOG00000014066	Jade1	0.69	NA	1.613283518
ENSRNOG00000002141	Cd200	0.68	NA	1.602139755
ENSRNOG00000005865	Ssfa2	0.68	NA	1.602139755
ENSRNOG00000004677	Zeb2	0.68	NA	1.602139755
ENSRNOG00000005642	Frs2	0.68	NA	1.602139755
ENSRNOG00000011154	Adgrf5	0.67	NA	1.591072968
ENSRNOG00000009980	Plpp1	0.67	NA	1.591072968
ENSRNOG00000024250	Wwc3	0.67	NA	1.591072968
ENSRNOG00000008927	Hbp1	0.67	NA	1.591072968
ENSRNOG00000007896	Klhl38	0.67	NA	1.591072968
ENSRNOG00000011852	Myo6	0.67	NA	1.591072968
ENSRNOG00000003151	Bfar	0.66	NA	1.580082624
ENSRNOG00000024737	Tnrc6a	0.66	NA	1.580082624
ENSRNOG00000057556	Pdzrn3	0.66	NA	1.580082624
ENSRNOG00000004050	Snrk	0.66	NA	1.580082624
ENSRNOG00000005196	Slc12a6	0.66	NA	1.580082624
ENSRNOG00000010805	Fabp4	0.66	NA	1.580082624
ENSRNOG00000003099	Ubqln2	0.66	NA	1.580082624
ENSRNOG00000012124	Trappc13	0.66	NA	1.580082624
ENSRNOG00000008709	Arhgap32	0.65	NA	1.569168196
ENSRNOG00000036918	Etfbkmt	0.65	NA	1.569168196
ENSRNOG00000023431	LOC102555635	0.65	NA	1.569168196
ENSRNOG00000004891	Arl14ep	0.65	NA	1.569168196
ENSRNOG00000013872	P2ry14	0.65	NA	1.569168196
ENSRNOG00000014450	Shprh	0.65	NA	1.569168196
ENSRNOG00000010992	Hspb3	0.65	NA	1.569168196
ENSRNOG00000010174	Enpp4	0.65	NA	1.569168196
ENSRNOG00000028557	Hibch	0.65	NA	1.569168196
ENSRNOG00000005802	Usp24	0.64	NA	1.558329159
ENSRNOG00000021719	Slfn5	0.64	NA	1.558329159
ENSRNOG00000023786	Ybx1	0.63	NA	1.547564994
ENSRNOG00000013309	Pik3ap1	0.63	NA	1.547564994

ENSRNOG00000018396	Prpf18	0.63	NA	1.547564994
ENSRNOG00000003114	B4galt4	0.63	NA	1.547564994
ENSRNOG00000016090	Mtmr10	0.63	NA	1.547564994
ENSRNOG00000020388	Inpp5f	0.63	NA	1.547564994
ENSRNOG00000005261	Fbxl5	0.63	NA	1.547564994
ENSRNOG00000008163	Atp6v1g1	0.62	NA	1.536875181
ENSRNOG00000013217	Ttc33	0.62	NA	1.536875181
ENSRNOG00000051056	Fndc4	0.62	NA	1.536875181
ENSRNOG00000000415	Asf1a	0.62	NA	1.536875181
ENSRNOG00000051960	Dnajc12	0.61	NA	1.526259209
ENSRNOG00000015121	N4bp1	0.61	NA	1.526259209
ENSRNOG00000025476	Tmem252	0.61	NA	1.526259209
ENSRNOG00000026319	Akap9	0.61	NA	1.526259209
ENSRNOG00000040110	Foxn2	0.61	NA	1.526259209
ENSRNOG00000015840	Hsd17b4	0.6	NA	1.515716567
ENSRNOG00000028822	Bex3	0.6	NA	1.515716567
ENSRNOG00000017286	Ephx2	0.6	NA	1.515716567
ENSRNOG00000024629	Hadha	0.6	NA	1.515716567
ENSRNOG00000019943	Slc7a6	0.59	NA	1.505246747
ENSRNOG00000001807	Sspn	0.59	NA	1.505246747
ENSRNOG00000016271	Itm2b	0.58	NA	1.494849249
ENSRNOG00000008049	Max	0.58	NA	1.494849249
ENSRNOG00000001247	Clip1	0.58	NA	1.494849249
ENSRNOG00000025040	Gng10	0.58	NA	1.494849249
ENSRNOG00000009824	Irf2	0.58	NA	1.494849249
ENSRNOG00000030688	Lrrc2	0.58	NA	1.494849249
ENSRNOG00000017493	Pias2	0.58	NA	1.494849249
ENSRNOG00000031328	Zfp110	0.58	NA	1.494849249
ENSRNOG00000026842	Nnt	0.57	NA	1.484523571
ENSRNOG00000050317	Uhrf1bp1l	0.57	NA	1.484523571
ENSRNOG00000056984	Baz2b	0.57	NA	1.484523571
ENSRNOG00000008666	Etl4	0.57	NA	1.484523571
ENSRNOG00000020804	Smarcc1	0.56	NA	1.474269217
ENSRNOG00000005916	Ppm1a	0.56	NA	1.474269217
ENSRNOG00000020468	Stard4	0.56	NA	1.474269217
ENSRNOG00000004464	Sel1l	0.56	NA	1.474269217
ENSRNOG00000005641	Fbxl4	0.55	NA	1.464085696
ENSRNOG00000026902	Lyve1	0.55	NA	1.464085696
ENSRNOG00000001517	Pdk1	0.55	NA	1.464085696
ENSRNOG00000022939	Gpkow	0.55	NA	1.464085696
ENSRNOG00000013340	Twsg1	0.55	NA	1.464085696
ENSRNOG00000012074	Ifngr1	0.54	NA	1.453972517
ENSRNOG00000021200	Hfe2	0.54	NA	1.453972517
ENSRNOG00000018194	Srrm1	0.54	NA	1.453972517
ENSRNOG00000009149	Jam3	0.53	NA	1.443929196
ENSRNOG00000000989	Bud31	0.53	NA	1.443929196
ENSRNOG00000007060	Plin2	0.53	NA	1.443929196
ENSRNOG00000019333	Hipk1	0.53	NA	1.443929196

ENSRNOG00000008593	Ryk	0.52	NA	1.433955248
ENSRNOG00000010765	Vcl	0.52	NA	1.433955248
ENSRNOG00000002256	Art3	0.52	NA	1.433955248
ENSRNOG00000013160	Sash1	0.52	NA	1.433955248
ENSRNOG00000008090	Txndc12	0.52	NA	1.433955248
ENSRNOG00000019341	Tmem179b	0.52	NA	1.433955248
ENSRNOG00000006338	Lrp6	0.52	NA	1.433955248
ENSRNOG00000056954	Inpp5k	0.52	NA	1.433955248
ENSRNOG00000026493	Cdnf	0.51	NA	1.424050196
ENSRNOG00000016343	Dkk3	0.51	NA	1.424050196
ENSRNOG00000012966	Acadl	0.51	NA	1.424050196
ENSRNOG00000040205	Zcchc24	0.51	NA	1.424050196
ENSRNOG00000005568	Pcnx4	0.51	NA	1.424050196
ENSRNOG00000004226	Irak3	0.51	NA	1.424050196
ENSRNOG00000061768	Slc43a3	0.5	NA	1.414213562
ENSRNOG00000003946	Tor1aip1	0.5	NA	1.414213562
ENSRNOG00000019018	Plat	0.5	NA	1.414213562
ENSRNOG00000003550	Acbd6	0.5	NA	1.414213562
ENSRNOG00000003078	Dcaf6	0.49	NA	1.404444876
ENSRNOG00000051965	Smad4	0.49	NA	1.404444876
ENSRNOG00000016526	Dsg2	0.49	NA	1.404444876
ENSRNOG00000007587	Tcp11l2	0.49	NA	1.404444876
ENSRNOG00000008587	Tek	0.48	NA	1.394743666
ENSRNOG00000022772	Prickle1	0.48	NA	1.394743666
ENSRNOG00000009639	Zrsr1	0.48	NA	1.394743666
ENSRNOG00000002342	Aldh3a2	0.47	NA	1.385109468
ENSRNOG00000045668	Ifnar2	0.47	NA	1.385109468
ENSRNOG00000005589	Dhrs7	0.46	NA	1.375541818
ENSRNOG00000029995	Herpud2	0.46	NA	1.375541818
ENSRNOG00000012035	Rnf181	0.45	NA	1.366040257
ENSRNOG00000043387	Cpe	0.45	NA	1.366040257
ENSRNOG00000002240	Dirc2	0.44	NA	1.356604327
ENSRNOG00000048205	Ube2h	0.43	NA	1.347233577
ENSRNOG00000053659	RGD1311703	0.43	NA	1.347233577
ENSRNOG00000055246	Ncor1	0.43	NA	1.347233577
ENSRNOG00000006766	Laptm4b	0.42	NA	1.337927555
ENSRNOG00000022015	Cntrl	0.42	NA	1.337927555
ENSRNOG00000016423	Tacc1	0.42	NA	1.337927555
ENSRNOG00000018251	Mrc1	0.42	NA	1.337927555
ENSRNOG00000028341	Alkbh5	0.42	NA	1.337927555
ENSRNOG00000000634	RGD1306739	0.42	NA	1.337927555
ENSRNOG00000000583	Cdk19	0.41	NA	1.328685814
ENSRNOG00000025715	Dynlrb1	0.4	NA	1.319507911
ENSRNOG00000011111	Cipc	0.4	NA	1.319507911
ENSRNOG00000010176	Map2k1	0.4	NA	1.319507911
ENSRNOG00000020737	Cdc25a	0.4	NA	1.319507911
ENSRNOG00000019169	RGD1562218	0.39	NA	1.310393404
ENSRNOG00000010964	Akap13	0.39	NA	1.310393404

ENSRNOG00000019063	Fbxo38	0.36	NA		1.283425898
ENSRNOG00000024886	Ext1	0.35	NA		1.274560627
ENSRNOG00000049975	Zfp46	0.3	NA		1.231144413
ENSRNOG00000016807	Oat	0.23	NA		1.172834949
ENSRNOG00000009956	Wnk1	-0.44		7.46	-1.356604327
ENSRNOG00000030055	Vamp3	-0.46		5.97	-1.375541818
ENSRNOG00000007895	Pdhb	-0.47		8.56	-1.385109468
ENSRNOG00000000923	Cct6a	-0.48		6.12	-1.394743666
ENSRNOG00000020646	Sdhaf2	-0.48		6.8	-1.394743666
ENSRNOG00000013505	Vdac2	-0.48		8.82	-1.394743666
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ENSRNOG00000020893	Snx27	-0.49		5.87	-1.404444876
ENSRNOG00000036742	Uqcrc2	-0.5		10.3	-1.414213562
ENSRNOG00000012106	Dnaja4	-0.51		6.77	-1.424050196
ENSRNOG00000013211	Chchd3	-0.51		7.64	-1.424050196
ENSRNOG00000019649	Cul4a	-0.52		6.34	-1.433955248
ENSRNOG00000017965	Afg3l2	-0.52		6.51	-1.433955248
ENSRNOG00000021758	Tnpo3	-0.52		5.15	-1.433955248
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ENSRNOG00000011413	Podn	-0.53		7.9	-1.443929196
ENSRNOG00000060005	Surf4	-0.53		6.02	-1.443929196
ENSRNOG00000020351	Vps4a	-0.53		5.21	-1.443929196
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ENSRNOG00000002724	Prpsap2	-0.53		4.54	-1.443929196
ENSRNOG00000013763	Erlin2	-0.53		5.07	-1.443929196
ENSRNOG00000023538	Aldh5a1	-0.54		5.35	-1.453972517
ENSRNOG00000036798	Dusp3	-0.54		6.49	-1.453972517
ENSRNOG00000002205	Ociad1	-0.54		7.05	-1.453972517
ENSRNOG00000008195	Ywhaz	-0.54		7.14	-1.453972517
ENSRNOG00000019205	Gnpat	-0.54		6.28	-1.453972517
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ENSRNOG00000029910	Golga4	-0.55		6.73	-1.464085696
ENSRNOG00000002840	Atp5b	-0.55		12.07	-1.464085696
ENSRNOG00000014058	Tomm22	-0.55		6.26	-1.464085696
ENSRNOG00000011245	Arhgap18	-0.55		5.67	-1.464085696
ENSRNOG00000011175	Hnrnpa2b1	-0.56		8.31	-1.474269217
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ENSRNOG00000049876	Prkar1a	-0.57		7.42	-1.484523571
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ENSRNOG00000003524	Lrrc59		-0.58	4.93	-1.494849249
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ENSRNOG00000046547	Rbm24		-0.58	5.87	-1.494849249
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ENSRNOG00000008279	Mrps15		-0.58	6.26	-1.494849249
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ENSRNOG00000018048	Dctn5		-0.59	5.11	-1.505246747
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ENSRNOG00000005308	Tmx2		-0.61	5.69	-1.526259209
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ENSRNOG00000008921	Dynll2		-0.62	7.42	-1.536875181
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ENSRNOG00000017730	Psmd1		-0.62	7.26	-1.536875181
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ENSRNOG00000020791	Ube2q1	-0.64	4.8	-1.558329159
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ENSRNOG00000053450	Myadm	-0.65	7.12	-1.569168196
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ENSRNOG00000007040	Timm17a	-0.65	6.24	-1.569168196
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ENSRNOG00000054352	Atp6ap1	-0.65	6.72	-1.569168196

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ENSRNOG00000017195	Ctr9	-0.65	5.16	-1.569168196
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ENSRNOG00000013492	Cap1	-0.66	5.86	-1.580082624
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ENSRNOG00000030871	Calm2	-0.66	6.81	-1.580082624
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ENSRNOG00000012085	Isca2	-0.66	5.08	-1.580082624
ENSRNOG00000016243	Casq2	-0.66	9.8	-1.580082624
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ENSRNOG00000019975	Cdc5l	-0.67	6.12	-1.591072968
ENSRNOG00000031479	Hdlbp	-0.67	7.75	-1.591072968
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ENSRNOG00000010038	Psmc5	-0.67	5.8	-1.591072968
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ENSRNOG00000011849	Ndufs1	-0.67	10.14	-1.591072968
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ENSRNOG00000015301	Elp2	-0.68	4.85	-1.602139755

ENSRNOG00000014485	Pdcd6	-0.68	5.39	-1.602139755
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ENSRNOG00000060694	Adam17	-0.68	5.86	-1.602139755
ENSRNOG00000007356	Chmp3	-0.68	5.67	-1.602139755
ENSRNOG00000010523	Naa20	-0.68	5.38	-1.602139755
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ENSRNOG00000017201	Cd2bp2	-0.68	5.12	-1.602139755
ENSRNOG00000024061	Rarb	-0.68	3.93	-1.602139755
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ENSRNOG00000010543	Srpra	-0.68	6.31	-1.602139755
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ENSRNOG00000007102	Acss1	-0.69	7.99	-1.613283518
ENSRNOG00000013837	Tp53bp1	-0.69	5.05	-1.613283518
ENSRNOG00000003506	Gosr2	-0.69	4.89	-1.613283518
ENSRNOG00000048981	Ahsa1	-0.69	5.66	-1.613283518
ENSRNOG00000001991	Atp5o	-0.69	8.61	-1.613283518
ENSRNOG00000003253	Qdpr	-0.69	4.25	-1.613283518
ENSRNOG00000028884	Atp5l	-0.69	9.24	-1.613283518
ENSRNOG00000008546	Mrpl35	-0.69	5.9	-1.613283518
ENSRNOG00000017631	Cyp20a1	-0.69	4.65	-1.613283518
ENSRNOG00000001884	Ranbp1	-0.69	4.09	-1.613283518
ENSRNOG00000005279	Ndufaf7	-0.69	4.08	-1.613283518
ENSRNOG00000001931	Fgf12	-0.69	5.18	-1.613283518
ENSRNOG00000057701	Myom1	-0.69	8.6	-1.613283518
ENSRNOG00000006094	Cd44	-0.69	4.34	-1.613283518
ENSRNOG00000027124	Tdg	-0.69	4.17	-1.613283518
ENSRNOG00000018547	Mrpl46	-0.7	3.9	-1.624504793
ENSRNOG00000002001	Itsn1	-0.7	4.06	-1.624504793
ENSRNOG00000002128	Ppat	-0.7	5.71	-1.624504793
ENSRNOG00000007234	Cyp51	-0.7	4.66	-1.624504793
ENSRNOG00000020167	Reep5	-0.7	6.97	-1.624504793
ENSRNOG00000028087	Sdhaf4	-0.7	3.89	-1.624504793
ENSRNOG00000016800	Ss18	-0.7	5.4	-1.624504793
ENSRNOG00000028783	Wdr35	-0.7	3.84	-1.624504793
ENSRNOG00000019278	Fsd2	-0.71	6.1	-1.635804117
ENSRNOG00000002050	Igfbp7	-0.71	7.14	-1.635804117
ENSRNOG00000015290	Tpi1	-0.71	8.66	-1.635804117
ENSRNOG00000016470	Ndufa10	-0.71	8.32	-1.635804117
ENSRNOG00000036664	Narf	-0.71	5.37	-1.635804117
ENSRNOG00000005053	Egln3	-0.71	7.67	-1.635804117
ENSRNOG00000060141	Epdr1	-0.71	5.57	-1.635804117
ENSRNOG00000058461	Sfpq	-0.71	6.07	-1.635804117
ENSRNOG00000007981	Klhl23	-0.71	6.16	-1.635804117
ENSRNOG00000016379	Jtb	-0.71	5.46	-1.635804117
ENSRNOG00000008676	Emp1	-0.71	7.47	-1.635804117
ENSRNOG00000004687	Thbd	-0.71	6.01	-1.635804117

ENSRNOG00000026415	Col14a1	-0.71	6.38	-1.635804117
ENSRNOG00000009888	Timm8b	-0.71	6.81	-1.635804117
ENSRNOG00000013286	Pdcl3	-0.71	4.36	-1.635804117
ENSRNOG00000030628	Eif4a1	-0.72	7.02	-1.647182035
ENSRNOG00000016923	Clptm1l	-0.72	5.18	-1.647182035
ENSRNOG00000003931	Arsg	-0.72	4.77	-1.647182035
ENSRNOG00000019811	LOC100362432	-0.72	6.72	-1.647182035
ENSRNOG00000021179	Naa40	-0.72	3.99	-1.647182035
ENSRNOG00000061928	Myo1e	-0.72	3.54	-1.647182035
ENSRNOG00000009175	Jagn1	-0.72	3.34	-1.647182035
ENSRNOG00000025285	Gfm2	-0.72	4.99	-1.647182035
ENSRNOG00000022922	Slc25a12	-0.72	6	-1.647182035
ENSRNOG00000016250	Ammecr1l	-0.72	4.88	-1.647182035
ENSRNOG00000005877	Lrpprc	-0.72	7.52	-1.647182035
ENSRNOG00000008566	Mrpl15	-0.72	6.61	-1.647182035
ENSRNOG00000014013	Map4k4	-0.72	6.15	-1.647182035
ENSRNOG00000010379	Celf1	-0.72	5.14	-1.647182035
ENSRNOG00000023467	Fam168b	-0.72	5.16	-1.647182035
ENSRNOG00000057821	AABR07015165.1	-0.72	4.17	-1.647182035
ENSRNOG00000018877	Zfp689	-0.73	4.62	-1.658639092
ENSRNOG00000016937	Mtfr1l	-0.73	7.7	-1.658639092
ENSRNOG00000042467	Ttc4	-0.73	4.09	-1.658639092
ENSRNOG00000022392	Hspb8	-0.73	7.43	-1.658639092
ENSRNOG00000014584	Odf2	-0.73	3.97	-1.658639092
ENSRNOG00000015496	Tpm4	-0.73	6.62	-1.658639092
ENSRNOG00000014109	Psmd13	-0.73	5.45	-1.658639092
ENSRNOG00000016201	Mrps9	-0.73	5.65	-1.658639092
ENSRNOG00000006369	Alg2	-0.73	3.21	-1.658639092
ENSRNOG00000033280	Pam	-0.73	9.61	-1.658639092
ENSRNOG00000015459	Heatr3	-0.73	4.09	-1.658639092
ENSRNOG00000004789	Diexf	-0.73	3.16	-1.658639092
ENSRNOG00000007316	Idh3B	-0.74	8.42	-1.670175839
ENSRNOG00000006067	Aifm1	-0.74	6.74	-1.670175839
ENSRNOG00000028448	Elovl1	-0.74	4.33	-1.670175839
ENSRNOG00000009080	Atp6v1d	-0.74	6.63	-1.670175839
ENSRNOG00000001596	Atp5g3	-0.74	9.84	-1.670175839
ENSRNOG00000012827	Mlf1	-0.74	7.25	-1.670175839
ENSRNOG00000015987	Rap1gds1	-0.74	4.46	-1.670175839
ENSRNOG00000011825	Ndufb3	-0.74	7.47	-1.670175839
ENSRNOG00000042696	Minos1	-0.74	6.26	-1.670175839
ENSRNOG00000059402	Itgb1bp1	-0.74	4.74	-1.670175839
ENSRNOG00000025629	Prpf3	-0.74	4.04	-1.670175839
ENSRNOG00000009716	Casc3	-0.74	4.98	-1.670175839
ENSRNOG00000028238	Sh3bgr	-0.75	7.35	-1.681792831
ENSRNOG00000029875	Mrpl41	-0.75	4.6	-1.681792831
ENSRNOG00000013743	Sec61a1	-0.75	4.87	-1.681792831
ENSRNOG00000013852	Med20	-0.75	3.89	-1.681792831
ENSRNOG00000005257	Prkaca	-0.75	6.76	-1.681792831

ENSRNOG00000042503	Ndufv2	-0.75	8.85	-1.681792831
ENSRNOG00000009761	Tmod1	-0.75	7.48	-1.681792831
ENSRNOG00000047118	LOC683897	-0.75	4.46	-1.681792831
ENSRNOG00000008187	Ubash3b	-0.75	2.43	-1.681792831
ENSRNOG00000008237	Unc13b	-0.75	4.68	-1.681792831
ENSRNOG00000001201	Cstb	-0.76	4.97	-1.693490625
ENSRNOG00000027230	Fhod3	-0.76	7.2	-1.693490625
ENSRNOG00000015329	Kpna2	-0.76	6.96	-1.693490625
ENSRNOG00000004206	Glrx5	-0.76	5.3	-1.693490625
ENSRNOG00000016810	Stmn1	-0.76	5.06	-1.693490625
ENSRNOG00000004401	Mrpl13	-0.76	5.96	-1.693490625
ENSRNOG00000054058	Osbpl1a	-0.76	5.33	-1.693490625
ENSRNOG00000016265	Acsl5	-0.76	4.9	-1.693490625
ENSRNOG00000026616	Ndufb2	-0.76	6.39	-1.693490625
ENSRNOG00000005009	Zfp3	-0.76	2.82	-1.693490625
ENSRNOG00000011553	Actl6a	-0.76	4.26	-1.693490625
ENSRNOG00000004807	Arf2	-0.77	4.43	-1.705269784
ENSRNOG00000046996	Pea15	-0.77	6.31	-1.705269784
ENSRNOG00000005061	Dlst	-0.77	8.5	-1.705269784
ENSRNOG00000017752	Mccc2	-0.77	6.28	-1.705269784
ENSRNOG00000005218	Sf3a1	-0.77	4.32	-1.705269784
ENSRNOG00000019211	Olfml3	-0.77	3.29	-1.705269784
ENSRNOG00000011952	Samm50	-0.77	6.66	-1.705269784
ENSRNOG00000019634	Eif4e2	-0.77	4.42	-1.705269784
ENSRNOG00000005482	Sap30bp	-0.77	3.18	-1.705269784
ENSRNOG00000001518	Itga6	-0.77	6.93	-1.705269784
ENSRNOG00000013589	Cxcl12	-0.77	7.39	-1.705269784
ENSRNOG00000017466	Kif5b	-0.77	7.92	-1.705269784
ENSRNOG00000007069	Adhfe1	-0.77	4.96	-1.705269784
ENSRNOG00000002980	Tsr1	-0.77	4.95	-1.705269784
ENSRNOG00000004577	Fez2	-0.77	5.27	-1.705269784
ENSRNOG00000021005	Mrpl16	-0.77	5.69	-1.705269784
ENSRNOG00000010950	Cep41	-0.77	1.97	-1.705269784
ENSRNOG00000020480	Fads1	-0.78	4.25	-1.717130873
ENSRNOG00000042740	Mrpl42	-0.78	5.9	-1.717130873
ENSRNOG00000018848	Eif1b	-0.78	3.89	-1.717130873
ENSRNOG00000017983	Ubac1	-0.78	5.33	-1.717130873
ENSRNOG00000002459	Fbxo40	-0.78	5.48	-1.717130873
ENSRNOG00000036835	Copz1	-0.78	5.51	-1.717130873
ENSRNOG00000010812	Osbpl6	-0.78	5.76	-1.717130873
ENSRNOG00000012415	Mpc1	-0.78	8	-1.717130873
ENSRNOG00000018281	Uqcrfs1	-0.78	9.46	-1.717130873
ENSRNOG00000006248	Trim37	-0.78	3.18	-1.717130873
ENSRNOG00000009899	Skil	-0.78	3.37	-1.717130873
ENSRNOG00000039668	Col8a1	-0.78	4.09	-1.717130873
ENSRNOG00000002403	Fam129a	-0.78	3.8	-1.717130873
ENSRNOG00000002926	Uap1	-0.78	5.21	-1.717130873
ENSRNOG00000003576	Ints2	-0.78	2.97	-1.717130873

ENSRNOG00000031232	Nrp2	-0.79	5.29	-1.729074463
ENSRNOG00000045558	Cd34	-0.79	6.73	-1.729074463
ENSRNOG00000010550	Trappc3	-0.79	4.09	-1.729074463
ENSRNOG00000033883	Stard8	-0.79	4.57	-1.729074463
ENSRNOG00000042037	Smim7	-0.79	5.47	-1.729074463
ENSRNOG00000014645	Aldh7a1	-0.79	4.92	-1.729074463
ENSRNOG00000009063	Dnajc15	-0.79	6.6	-1.729074463
ENSRNOG00000010164	Mrps2	-0.79	5.04	-1.729074463
ENSRNOG00000020317	RGD1307752	-0.79	5.23	-1.729074463
ENSRNOG00000008481	Reep1	-0.79	4.73	-1.729074463
ENSRNOG00000033824	Gpd2	-0.79	3.81	-1.729074463
ENSRNOG00000028403	Ptcd2	-0.79	3.81	-1.729074463
ENSRNOG00000003954	Il2rg	-0.79	4.61	-1.729074463
ENSRNOG00000009097	Immt	-0.8	7.86	-1.741101127
ENSRNOG00000018415	Acot13	-0.8	6.28	-1.741101127
ENSRNOG00000017619	Aldh1a1	-0.8	5.5	-1.741101127
ENSRNOG00000031802	LOC691427	-0.8	6.82	-1.741101127
ENSRNOG00000005615	Gadd45a	-0.8	4.7	-1.741101127
ENSRNOG00000052418	Cpsf3	-0.8	4.53	-1.741101127
ENSRNOG00000006148	RGD1310352	-0.8	5.88	-1.741101127
ENSRNOG00000010985	Zfp410	-0.8	4.55	-1.741101127
ENSRNOG00000002227	Kit	-0.8	3.89	-1.741101127
ENSRNOG00000014075	Clybl	-0.8	4.91	-1.741101127
ENSRNOG00000009381	Mapk6	-0.8	5.5	-1.741101127
ENSRNOG00000051450	Abracl	-0.8	3.98	-1.741101127
ENSRNOG00000001803	Dnajb11	-0.8	4.69	-1.741101127
ENSRNOG00000003977	Dusp1	-0.8	5.35	-1.741101127
ENSRNOG00000013636	Ppil3	-0.8	3.64	-1.741101127
ENSRNOG00000010799	Noct	-0.8	2.58	-1.741101127
ENSRNOG00000002615	Pmm2	-0.81	5.15	-1.753211443
ENSRNOG00000042179	Cfap20	-0.81	4.24	-1.753211443
ENSRNOG00000007600	Igsf1	-0.81	4.37	-1.753211443
ENSRNOG00000046428	Lrrc75b	-0.81	4.16	-1.753211443
ENSRNOG00000048309	Uqcc1	-0.81	6.53	-1.753211443
ENSRNOG00000020950	Syvn1	-0.81	4.81	-1.753211443
ENSRNOG00000012049	Sox7	-0.81	4.09	-1.753211443
ENSRNOG00000012482	Ndrg4	-0.81	7.66	-1.753211443
ENSRNOG00000017235	Atp6v0d1	-0.81	5.17	-1.753211443
ENSRNOG00000005602	Mthfd1	-0.81	4.05	-1.753211443
ENSRNOG00000008569	Ndufa6	-0.81	7.49	-1.753211443
ENSRNOG00000047394	Ufd1l	-0.81	5.9	-1.753211443
ENSRNOG00000018044	Phyh	-0.81	9.89	-1.753211443
ENSRNOG00000009192	Rnaseh2b	-0.81	3.34	-1.753211443
ENSRNOG00000015519	Ces1d	-0.81	5.61	-1.753211443
ENSRNOG00000018087	Vim	-0.81	7.46	-1.753211443
ENSRNOG00000030124	Ptpn11	-0.81	7.17	-1.753211443
ENSRNOG00000014310	Tmtc4	-0.82	3.28	-1.765405993
ENSRNOG00000042980	Adam19	-0.82	6.52	-1.765405993

ENSRNOG00000001062	Kmt5a	-0.82	4.55	-1.765405993
ENSRNOG00000017012	Coq7	-0.82	4.54	-1.765405993
ENSRNOG00000001331	Rnf34	-0.82	3.15	-1.765405993
ENSRNOG00000019208	P2rx5	-0.82	3.82	-1.765405993
ENSRNOG00000059750	NA	-0.82	4.83	-1.765405993
ENSRNOG00000019219	Vamp1	-0.82	4.16	-1.765405993
ENSRNOG00000018647	Mrpl20	-0.82	5.05	-1.765405993
ENSRNOG00000011732	Psmb7	-0.82	6.52	-1.765405993
ENSRNOG00000052157	Nav3	-0.82	4.05	-1.765405993
ENSRNOG00000023317	Colgalt1	-0.82	4.85	-1.765405993
ENSRNOG00000013733	Ppp4r1	-0.82	4.28	-1.765405993
ENSRNOG00000037620	Mob3c	-0.82	2.5	-1.765405993
ENSRNOG00000012062	Npc2	-0.82	5.28	-1.765405993
ENSRNOG00000058609	Palmd	-0.83	5.12	-1.777685362
ENSRNOG00000013293	Mccc1	-0.83	5.8	-1.777685362
ENSRNOG00000016367	Vasp	-0.83	4.45	-1.777685362
ENSRNOG00000015420	Stxbp1	-0.83	3.73	-1.777685362
ENSRNOG00000005577	Desi1	-0.83	3.1	-1.777685362
ENSRNOG00000004359	Wars	-0.83	4.53	-1.777685362
ENSRNOG00000020487	Coa3	-0.83	4.47	-1.777685362
ENSRNOG00000005269	Srl	-0.84	8.53	-1.790050142
ENSRNOG00000007561	Glb1l2	-0.84	3.57	-1.790050142
ENSRNOG00000007764	Frmd4b	-0.84	3.51	-1.790050142
ENSRNOG00000000064	Atp5i	-0.84	7.51	-1.790050142
ENSRNOG00000058249	Pgk1	-0.85	8.68	-1.802500925
ENSRNOG00000027919	Rdh13	-0.85	4.23	-1.802500925
ENSRNOG00000015461	Serpine2	-0.85	5.44	-1.802500925
ENSRNOG00000008103	Mdh1	-0.85	9.83	-1.802500925
ENSRNOG00000036660	Fn3krp	-0.85	3.95	-1.802500925
ENSRNOG00000001139	Suds3	-0.85	4.08	-1.802500925
ENSRNOG00000018404	Aars	-0.85	5.04	-1.802500925
ENSRNOG00000009850	St3gal4	-0.85	4.55	-1.802500925
ENSRNOG00000012140	Cep89	-0.85	2.81	-1.802500925
ENSRNOG00000042903	Cox7a2	-0.85	8.48	-1.802500925
ENSRNOG00000019760	Oxnad1	-0.85	5.4	-1.802500925
ENSRNOG00000015029	Dbt	-0.85	6.41	-1.802500925
ENSRNOG00000014785	Ykt6	-0.85	3.96	-1.802500925
ENSRNOG00000003219	Trim16	-0.85	4.7	-1.802500925
ENSRNOG00000002667	Lamc2	-0.85	4.49	-1.802500925
ENSRNOG00000005203	Sec61g	-0.85	5.68	-1.802500925
ENSRNOG00000015962	Nmnat1	-0.85	3.74	-1.802500925
ENSRNOG00000018023	Bin3	-0.85	2.64	-1.802500925
ENSRNOG00000015551	Fuca2	-0.86	4.56	-1.815038311
ENSRNOG00000010390	Hmbs	-0.86	4.48	-1.815038311
ENSRNOG00000037655	Gatb	-0.86	4.54	-1.815038311
ENSRNOG00000014798	RGD1309540	-0.86	2.59	-1.815038311
ENSRNOG00000017373	Rhobtb2	-0.86	3.81	-1.815038311
ENSRNOG00000015205	Cyb5a	-0.86	5.49	-1.815038311

ENSRNOG00000024170	Phf5a	-0.86	3.91	-1.815038311
ENSRNOG00000010852	Nup205	-0.86	3.41	-1.815038311
ENSRNOG00000057620	Slc6a8	-0.86	6.08	-1.815038311
ENSRNOG00000009756	Pacsin2	-0.87	6.65	-1.8276629
ENSRNOG00000019895	Nedd8	-0.87	5.45	-1.8276629
ENSRNOG00000000341	Nid2	-0.87	4.56	-1.8276629
ENSRNOG00000019506	Dnajb2	-0.87	5.21	-1.8276629
ENSRNOG00000047045	Sdhaf1	-0.87	4.45	-1.8276629
ENSRNOG00000026646	Ndufs5	-0.87	6.69	-1.8276629
ENSRNOG00000000809	Atat1	-0.87	2.07	-1.8276629
ENSRNOG00000007128	Nop56	-0.87	4.53	-1.8276629
ENSRNOG00000019276	RGD735029	-0.87	6.14	-1.8276629
ENSRNOG00000057042	Pcca	-0.88	6.5	-1.840375301
ENSRNOG00000000902	Hsph1	-0.88	5.63	-1.840375301
ENSRNOG00000009078	Mrpl37	-0.88	5.26	-1.840375301
ENSRNOG00000016973	Tmem242	-0.88	4.27	-1.840375301
ENSRNOG00000038372	Ndufs2	-0.88	8.56	-1.840375301
ENSRNOG00000011714	Sat2	-0.88	3.58	-1.840375301
ENSRNOG00000015505	Mfap5	-0.88	4.2	-1.840375301
ENSRNOG00000000122	Ak2	-0.88	4.36	-1.840375301
ENSRNOG00000009071	Gripap1	-0.88	4.2	-1.840375301
ENSRNOG00000055471	Ywhah	-0.88	7.87	-1.840375301
ENSRNOG00000007821	Dyrk2	-0.88	4.86	-1.840375301
ENSRNOG00000024605	Fam220a	-0.88	3.65	-1.840375301
ENSRNOG00000030120	Ormdl2	-0.88	3.52	-1.840375301
ENSRNOG00000019085	Xpo5	-0.88	3.88	-1.840375301
ENSRNOG00000006947	Pdhx	-0.89	6.19	-1.853176124
ENSRNOG00000036689	P4hb	-0.89	7.56	-1.853176124
ENSRNOG00000058007	Nde1	-0.89	4.72	-1.853176124
ENSRNOG00000024972	Cox10	-0.89	5.4	-1.853176124
ENSRNOG00000026745	Acsl6	-0.89	4.46	-1.853176124
ENSRNOG00000009550	Sqle	-0.89	2.63	-1.853176124
ENSRNOG00000016543	Trim63	-0.9	5.63	-1.866065983
ENSRNOG00000046333	Ablim1	-0.9	6.41	-1.866065983
ENSRNOG00000018225	Tp53inp2	-0.9	8.15	-1.866065983
ENSRNOG00000019648	Col6a3	-0.9	6.93	-1.866065983
ENSRNOG00000018574	Qsox2	-0.9	2.25	-1.866065983
ENSRNOG00000019403	Afap1l1	-0.91	5.09	-1.879045498
ENSRNOG00000022657	Tmem97	-0.91	1.93	-1.879045498
ENSRNOG00000003703	Mcm6	-0.91	2.26	-1.879045498
ENSRNOG00000029490	Znf768	-0.91	3.97	-1.879045498
ENSRNOG00000016234	Ciapin1	-0.91	4.62	-1.879045498
ENSRNOG00000010628	Sec13	-0.91	4.07	-1.879045498
ENSRNOG00000033608	Cd276	-0.91	3.95	-1.879045498
ENSRNOG00000010184	Brk1	-0.91	5.1	-1.879045498
ENSRNOG00000008673	Arpc3	-0.91	4.32	-1.879045498
ENSRNOG00000010646	Tmem229b	-0.91	2.79	-1.879045498
ENSRNOG00000047213	Gnpda1	-0.92	3.85	-1.892115293

ENSRNOG00000021678	Alkbh3		-0.92	5.41	-1.892115293
ENSRNOG00000015437	Tmem14c		-0.92	5.92	-1.892115293
ENSRNOG00000003287	Fbxw10		-0.92	2.75	-1.892115293
ENSRNOG00000039593	Ecscr		-0.92	3.39	-1.892115293
ENSRNOG00000047276	NA		-0.92	6.1	-1.892115293
ENSRNOG00000056216	Casp7		-0.92	4.43	-1.892115293
ENSRNOG00000046639	Itgae		-0.92	2.71	-1.892115293
ENSRNOG00000027175	Cnpy4		-0.92	3.21	-1.892115293
ENSRNOG00000019817	Ddx28		-0.92	2.39	-1.892115293
ENSRNOG00000020692	Tmem216		-0.92	2.74	-1.892115293
ENSRNOG00000001205	Agpat3		-0.92	5.18	-1.892115293
ENSRNOG00000039980	Slc25a5		-0.93	6.83	-1.905275996
ENSRNOG00000050585	Pgam1		-0.93	6.72	-1.905275996
ENSRNOG00000000250	Jmjd6		-0.93	2.77	-1.905275996
ENSRNOG00000043192	Hacd1		-0.93	5.57	-1.905275996
ENSRNOG00000024689	Hopx		-0.93	4.38	-1.905275996
ENSRNOG00000000825	Fam26e		-0.93	3.52	-1.905275996
ENSRNOG00000014665	Dhdds		-0.94	6.05	-1.918528239
ENSRNOG00000013603	Dffa		-0.94	4.9	-1.918528239
ENSRNOG00000003626	Atp5h		-0.94	8.41	-1.918528239
ENSRNOG00000021399	RGD1306954		-0.94	3.78	-1.918528239
ENSRNOG00000025143	Icam2		-0.94	4.44	-1.918528239
ENSRNOG00000048194	LOC100912380		-0.94	4.7	-1.918528239
ENSRNOG00000045747	Capns1		-0.94	4.7	-1.918528239
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ENSRNOG00000015191	Phc1		-0.94	3.2	-1.918528239
ENSRNOG00000000924	Slc7a1		-0.94	2.91	-1.918528239
ENSRNOG00000010944	Hyou1		-0.94	5.62	-1.918528239
ENSRNOG00000012559	Man1b1		-0.94	4.44	-1.918528239
ENSRNOG00000017571	Ndufa2		-0.94	6.29	-1.918528239
ENSRNOG00000020822	Atp8b2		-0.94	4.36	-1.918528239
ENSRNOG00000055281	Dcbld2		-0.94	5.62	-1.918528239
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ENSRNOG00000001720	Hes1		-0.94	3.51	-1.918528239
ENSRNOG00000004263	Ints7		-0.94	2.81	-1.918528239
ENSRNOG00000010028	Polr3d		-0.95	3.62	-1.931872658
ENSRNOG00000018184	Tpm1		-0.95	11.72	-1.931872658
ENSRNOG00000003084	Parp1		-0.95	5.98	-1.931872658
ENSRNOG00000000493	Snrpc		-0.95	3.8	-1.931872658
ENSRNOG00000002653	Kcnk2		-0.95	3.75	-1.931872658
ENSRNOG00000017847	Rps19bp1		-0.95	3.19	-1.931872658
ENSRNOG00000000697	Coro1c		-0.95	4.57	-1.931872658
ENSRNOG00000015212	Hspa14		-0.95	3.57	-1.931872658
ENSRNOG00000003357	Col3a1		-0.95	10.04	-1.931872658
ENSRNOG00000037162	Slbp		-0.95	4.17	-1.931872658
ENSRNOG00000004857	L2hgdh		-0.95	4.29	-1.931872658
ENSRNOG00000017405	Raly		-0.95	6.03	-1.931872658
ENSRNOG00000007367		43347	-0.95	4.38	-1.931872658

ENSRNOG00000016135	Fars2	-0.95	3.4	-1.931872658
ENSRNOG00000046493	Pnpo	-0.96	5.47	-1.945309895
ENSRNOG00000009227	Aplnr	-0.96	6.05	-1.945309895
ENSRNOG00000014201	Manf	-0.96	4.7	-1.945309895
ENSRNOG00000017913	Atg16l1	-0.96	4.1	-1.945309895
ENSRNOG00000002450	Rrp15	-0.96	2.98	-1.945309895
ENSRNOG00000012828	Emg1	-0.96	3.51	-1.945309895
ENSRNOG00000011535	Gcsh	-0.96	5.31	-1.945309895
ENSRNOG00000007302	Fbn1	-0.96	7.35	-1.945309895
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ENSRNOG00000018992	Dpysl3	-0.97	3.6	-1.958840595
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ENSRNOG00000010889	Fbxw7	-0.97	4.75	-1.958840595
ENSRNOG00000010116	Leo1	-0.98	3.48	-1.972465409
ENSRNOG00000029571	Coq10a	-0.98	5.62	-1.972465409
ENSRNOG00000001194	Rrp1b	-0.98	3.59	-1.972465409
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ENSRNOG00000004941	Gpn1	-0.98	3.41	-1.972465409
ENSRNOG00000052070	Aldh1a3	-0.98	2.98	-1.972465409
ENSRNOG00000058752	Popdc2	-0.98	6.69	-1.972465409
ENSRNOG00000051624	Hspe1	-0.99	5.87	-1.986184991
ENSRNOG00000024625	Proser3	-0.99	2.9	-1.986184991
ENSRNOG00000005539	Thg1l	-0.99	2.07	-1.986184991
ENSRNOG00000010691	Cmtm3	-0.99	2.95	-1.986184991
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ENSRNOG00000012343	Pdp2	-0.99	3.56	-1.986184991
ENSRNOG00000015691	Fam212b	-1	5.39	-2
ENSRNOG00000018825	Dcaf11	-1	6.86	-2
ENSRNOG00000018207	Dynlt1	-1	2.71	-2
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ENSRNOG00000052389	AABR07031489.1	-1	3.68	-2
ENSRNOG00000010558	Ppif	-1	5.67	-2
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ENSRNOG00000018293	Strip1	-1	3.95	-2
ENSRNOG00000050051	Pin4	-1	4	-2
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ENSRNOG00000025890	Opa3	-1.02	4.34	-2.02791896
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ENSRNOG00000009421	Ivd	-1.02	6.76	-2.02791896
ENSRNOG00000021099	Lysmd1	-1.02	2.69	-2.02791896
ENSRNOG00000006622	Cry1	-1.03	2.25	-2.042024251
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ENSRNOG00000011509	Agk	-1.03	3.32	-2.042024251
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ENSRNOG00000050741	Rbm4	-1.04	2.65	-2.056227653
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ENSRNOG00000037199	Spink8	-1.05	7.39	-2.070529848
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ENSRNOG00000045860	U2af1	-1.05	4.18	-2.070529848
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ENSRNOG00000020373	Dap3	-1.05	4.72	-2.070529848
ENSRNOG00000004821	Sntb1	-1.05	4.66	-2.070529848
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ENSRNOG00000014675	Pi4k2a	-1.05	3.69	-2.070529848
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ENSRNOG00000000166	Apex2	-1.06	1.18	-2.084931522
ENSRNOG00000016635	LOC361646	-1.06	2.63	-2.084931522
ENSRNOG00000026049	Qrsl1	-1.07	3.94	-2.099433367
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ENSRNOG00000053753	Rn50_8_0646.1	-1.07	5.41	-2.099433367
ENSRNOG00000001171	Coq5	-1.07	4.53	-2.099433367
ENSRNOG00000016826	Pla2g2d	-1.07	3.07	-2.099433367
ENSRNOG00000021670	Frem2	-1.07	2.2	-2.099433367
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ENSRNOG00000012817	Lrrc17	-1.08	2.48	-2.114036081
ENSRNOG00000055450	Ckmt2	-1.08	9.61	-2.114036081
ENSRNOG00000022099	Trim72	-1.08	6.5	-2.114036081
ENSRNOG00000015599	Mall	-1.08	2.18	-2.114036081
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ENSRNOG00000008101	Tmem251	-1.08	1.66	-2.114036081
ENSRNOG00000016559	Tm2d2	-1.09	5.22	-2.128740365
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ENSRNOG00000008642	Snx11	-1.09	2.84	-2.128740365
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ENSRNOG00000003917	Uck2	-1.1	2.46	-2.143546925
ENSRNOG00000053172	Ssr4	-1.1	3.95	-2.143546925
ENSRNOG00000010947	Mmp14	-1.1	4.34	-2.143546925
ENSRNOG00000010381	Mknk1	-1.11	3.67	-2.158456473
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ENSRNOG00000020467	Nrep	-1.13	4.34	-2.188587403
ENSRNOG00000022144	LOC100361993	-1.13	3.32	-2.188587403
ENSRNOG00000008405	Taco1	-1.14	2.59	-2.203810232
ENSRNOG00000050347	Ptges3l	-1.14	3.94	-2.203810232
ENSRNOG00000016166	Pdlim1	-1.14	5.26	-2.203810232
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ENSRNOG00000016723	Phpt1	-1.14	4.51	-2.203810232
ENSRNOG00000016913	Stk36	-1.14	1.93	-2.203810232
ENSRNOG00000018898	Mpi	-1.15	4.25	-2.219138944
ENSRNOG00000056596	Alas1	-1.15	7.17	-2.219138944
ENSRNOG00000019079	Polr1c	-1.15	3.13	-2.219138944
ENSRNOG00000006086	Lynx1	-1.15	4.96	-2.219138944
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ENSRNOG00000059344	Tpcn1	-1.15	4.48	-2.219138944
ENSRNOG00000012503	Dnajc16	-1.15	2.74	-2.219138944
ENSRNOG00000023312	Lonrf2	-1.15	3.18	-2.219138944
ENSRNOG00000037446	Pxmp2	-1.15	4.7	-2.219138944
ENSRNOG00000007755	Pm20d2	-1.16	1.91	-2.234574276
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ENSRNOG00000021155	Ctsk	-1.16	3.5	-2.234574276
ENSRNOG00000058975	Iqsec2	-1.16	4.88	-2.234574276
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ENSRNOG00000000858	Sapcd1	-1.16	1.94	-2.234574276
ENSRNOG00000010133	Bpgm	-1.16	4.61	-2.234574276
ENSRNOG00000017260	Cdr2	-1.16	2.93	-2.234574276
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ENSRNOG00000037505	Ulk1	-1.16	5.24	-2.234574276

ENSRNOG00000059956	Bcl6b	-1.17	5.6	-2.250116969
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ENSRNOG00000020975	Mrpl49	-1.17	3.19	-2.250116969
ENSRNOG00000010386	H2afx	-1.17	3.53	-2.250116969
ENSRNOG00000011831	Nudt18	-1.17	3.76	-2.250116969
ENSRNOG00000023162	Car14	-1.18	5.54	-2.265767771
ENSRNOG00000021866	Bola3	-1.18	4.71	-2.265767771
ENSRNOG00000003596	Itgb1bp2	-1.18	6.56	-2.265767771
ENSRNOG00000020918	Ccnd1	-1.18	5.27	-2.265767771
ENSRNOG00000032788	Dysf	-1.18	5.71	-2.265767771
ENSRNOG00000019482	Gnao1	-1.18	2.73	-2.265767771
ENSRNOG00000020244	Perm1	-1.19	6.93	-2.281527432
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ENSRNOG00000032780	Mrpl58	-1.19	4.47	-2.281527432
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ENSRNOG00000050780	Fpgs	-1.19	2.31	-2.281527432
ENSRNOG00000005042	Ranbp17	-1.19	0.78	-2.281527432
ENSRNOG00000045568	Rbm14	-1.19	2.45	-2.281527432
ENSRNOG00000046005	Scd2	-1.2	5.12	-2.29739671
ENSRNOG00000043426	Kyat3	-1.2	4.13	-2.29739671
ENSRNOG00000012720	Irx4	-1.2	3.03	-2.29739671
ENSRNOG00000017282	Tesk2	-1.2	1.47	-2.29739671
ENSRNOG00000019550	Slc11a2	-1.21	4.13	-2.313376368
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ENSRNOG00000004377	Lpin1	-1.21	4.83	-2.313376368
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ENSRNOG00000019202	PVR	-1.22	2.02	-2.329467173
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ENSRNOG00000050169	Pet100	-1.23	3.55	-2.345669898
ENSRNOG00000011863	Gins3	-1.23	0.41	-2.345669898
ENSRNOG00000016831	Serpinh1	-1.23	6.56	-2.345669898
ENSRNOG00000001044	Aimp2	-1.23	3.31	-2.345669898
ENSRNOG00000001300	P2rx4	-1.23	2.45	-2.345669898
ENSRNOG00000006444	Fkbp4	-1.24	6.74	-2.361985323
ENSRNOG00000002072	Eva1c	-1.24	1.53	-2.361985323
ENSRNOG00000007720	Rnf26	-1.24	2.28	-2.361985323
ENSRNOG00000047796	Pcbd2	-1.24	2.56	-2.361985323
ENSRNOG00000007726	Mcam	-1.25	5.44	-2.37841423
ENSRNOG00000028207	Colgalt2	-1.25	1.8	-2.37841423
ENSRNOG00000008942	RGD1304963	-1.25	3.69	-2.37841423
ENSRNOG00000016412	Fxyd6	-1.25	3.8	-2.37841423
ENSRNOG00000029535	Nrbp2	-1.25	4.06	-2.37841423
ENSRNOG00000030269	Atp2b2	-1.25	2.54	-2.37841423
ENSRNOG00000016313	Ctnnbip1	-1.25	2.58	-2.37841423
ENSRNOG00000008786	Ap1b1	-1.26	4.44	-2.394957409
ENSRNOG00000020688	Ccdc51	-1.26	2.68	-2.394957409

ENSRNOG00000030848	Myl2	-1.26	10.79	-2.394957409
ENSRNOG00000033389	Susd2	-1.26	3.37	-2.394957409
ENSRNOG00000012149	Gpsm2	-1.26	0.48	-2.394957409
ENSRNOG00000005413	Creb3l1	-1.26	1.81	-2.394957409
ENSRNOG00000027784	Tsku	-1.27	1.61	-2.411615655
ENSRNOG00000049063	NA	-1.27	0.83	-2.411615655
ENSRNOG00000021051	Cyth2	-1.27	3.64	-2.411615655
ENSRNOG00000019265	Pcdh12	-1.28	5.01	-2.428389769
ENSRNOG00000006898	Mrps16	-1.28	4.72	-2.428389769
ENSRNOG00000033700	Wbscr22	-1.28	1.62	-2.428389769
ENSRNOG00000001766	Tfrc	-1.28	7.65	-2.428389769
ENSRNOG00000023587	Dhtkd1	-1.28	1.93	-2.428389769
ENSRNOG00000043094	Oxct1	-1.29	10.78	-2.445280555
ENSRNOG00000000812	RGD1302996	-1.29	4.51	-2.445280555
ENSRNOG00000000473	Pfdn6	-1.29	3.69	-2.445280555
ENSRNOG00000010208	Timp1	-1.29	2.18	-2.445280555
ENSRNOG00000012067	Fam111a	-1.29	1.98	-2.445280555
ENSRNOG00000013027	Rgl3	-1.29	1.7	-2.445280555
ENSRNOG00000016754	Bcs1l	-1.3	3.31	-2.462288827
ENSRNOG00000008064	Naga	-1.3	3.21	-2.462288827
ENSRNOG00000021025	Ppp2r5b	-1.3	3.48	-2.462288827
ENSRNOG00000054890	Flna	-1.3	6.78	-2.462288827
ENSRNOG00000020776	Dhcr7	-1.3	0.83	-2.462288827
ENSRNOG00000021463	Ppara	-1.31	3.38	-2.4794154
ENSRNOG00000025310	Pop7	-1.31	1.79	-2.4794154
ENSRNOG00000006789	Ddit3	-1.31	3.62	-2.4794154
ENSRNOG00000061085	Fancd2	-1.31	0.89	-2.4794154
ENSRNOG00000004968	Ncapg2	-1.31	4.35	-2.4794154
ENSRNOG00000059362	Has3	-1.31	0.04	-2.4794154
ENSRNOG00000005424	Odc1	-1.32	6.15	-2.496661098
ENSRNOG00000043033	Lace1	-1.32	3.16	-2.496661098
ENSRNOG00000003171	Mpz	-1.32	0.63	-2.496661098
ENSRNOG00000016109	Neurl4	-1.32	3.9	-2.496661098
ENSRNOG00000014166	Smoc2	-1.33	2.86	-2.514026749
ENSRNOG00000001170	Cox6a1	-1.33	5.58	-2.514026749
ENSRNOG00000008761	Ncs1	-1.33	3.61	-2.514026749
ENSRNOG00000002186	Nudt9	-1.33	3.02	-2.514026749
ENSRNOG00000045989	Hba-a3	-1.33	4.24	-2.514026749
ENSRNOG00000020440	Fads2	-1.34	2.94	-2.531513188
ENSRNOG00000019305	Sh3tc2	-1.34	1.6	-2.531513188
ENSRNOG00000018371	Tubb6	-1.34	2.32	-2.531513188
ENSRNOG00000011979	Mrps24	-1.34	3.32	-2.531513188
ENSRNOG00000060381	Col15a1	-1.35	7.14	-2.549121255
ENSRNOG00000005935	A3galt2	-1.35	1.86	-2.549121255
ENSRNOG00000045821	Slc41a3	-1.35	4.92	-2.549121255
ENSRNOG00000010105	S100a11	-1.36	3.78	-2.566851795
ENSRNOG00000030238	Fndc5	-1.36	5.72	-2.566851795
ENSRNOG00000018677	Akt2	-1.36	5.05	-2.566851795

ENSRNOG00000048050	Tmem120b	-1.36	1.28	-2.566851795
ENSRNOG00000051620	Tspan9	-1.36	5.57	-2.566851795
ENSRNOG00000050090	Slc6a17	-1.37	4.83	-2.584705661
ENSRNOG00000051699	Zdhhc4	-1.37	3.21	-2.584705661
ENSRNOG00000005758	Btbd11	-1.37	1.59	-2.584705661
ENSRNOG00000028517	Rhno1	-1.37	1.08	-2.584705661
ENSRNOG00000054957	Sfrp4	-1.37	-0.1	-2.584705661
ENSRNOG00000004640	Mtfp1	-1.38	4.09	-2.602683711
ENSRNOG00000005767	Tulp3	-1.38	2.27	-2.602683711
ENSRNOG00000007327	Pars2	-1.38	1.22	-2.602683711
ENSRNOG00000059073	Slamf1	-1.38	1.09	-2.602683711
ENSRNOG00000054140	Myl6	-1.38	6.5	-2.602683711
ENSRNOG00000021268	LOC681292	-1.38	0.38	-2.602683711
ENSRNOG00000021153	Fkbp2	-1.39	2.94	-2.620786808
ENSRNOG00000026037	Plb1	-1.39	0.63	-2.620786808
ENSRNOG00000020357	Msto1	-1.39	1.91	-2.620786808
ENSRNOG00000013408	Npas2	-1.39	3.27	-2.620786808
ENSRNOG00000050624	Lysmd4	-1.4	2.19	-2.639015822
ENSRNOG00000053334	Stmn4	-1.4	0.86	-2.639015822
ENSRNOG00000018706	Il15ra	-1.4	1.76	-2.639015822
ENSRNOG00000014218	Tmem25	-1.4	1.42	-2.639015822
ENSRNOG00000020642	Flad1	-1.4	4.05	-2.639015822
ENSRNOG00000020721	Nme6	-1.4	2.25	-2.639015822
ENSRNOG00000016777	R3hcc1	-1.41	3.07	-2.657371628
ENSRNOG00000013445	Aaas	-1.41	1.52	-2.657371628
ENSRNOG00000020653	S1pr2	-1.42	3.65	-2.67585511
ENSRNOG00000011316	Fam167a	-1.42	2.07	-2.67585511
ENSRNOG00000018232	Srf	-1.42	4.67	-2.67585511
ENSRNOG00000014743	Hagh	-1.42	3.34	-2.67585511
ENSRNOG00000012051	Ncaph	-1.42	0.64	-2.67585511
ENSRNOG00000058883	NEWGENE_1589866	-1.42	0.61	-2.67585511
ENSRNOG00000018552	Slc25a38	-1.42	2.01	-2.67585511
ENSRNOG00000016468	Tpmt	-1.43	3.83	-2.694467154
ENSRNOG00000007687	Sema7a	-1.43	3.78	-2.694467154
ENSRNOG00000012543	Mcm3	-1.43	1.08	-2.694467154
ENSRNOG00000017206	Igfbp5	-1.44	7.66	-2.713208655
ENSRNOG00000020246	Myl9	-1.44	5.07	-2.713208655
ENSRNOG00000005492	Hpcal1	-1.44	3.02	-2.713208655
ENSRNOG00000027891	Dhrs11	-1.45	4.22	-2.732080514
ENSRNOG00000003172	Serpinf1	-1.45	5.1	-2.732080514
ENSRNOG00000009373	RGD1562690	-1.45	4.67	-2.732080514
ENSRNOG00000034254	Actb	-1.45	7.35	-2.732080514
ENSRNOG00000018351	Thap4	-1.45	2.76	-2.732080514
ENSRNOG00000004162	Pfkfb2	-1.46	4	-2.751083636
ENSRNOG00000037449	Pole	-1.46	1.03	-2.751083636
ENSRNOG00000048812	Gpx1	-1.46	7.4	-2.751083636
ENSRNOG00000020617	Mus81	-1.46	1.81	-2.751083636
ENSRNOG00000015063	Dhodh	-1.47	1.35	-2.770218936

ENSRNOG00000024705	Rarres2	-1.47	3.72	-2.770218936
ENSRNOG00000010077	Smarcd3	-1.47	3.7	-2.770218936
ENSRNOG00000038600	Dnaaf3	-1.47	4.14	-2.770218936
ENSRNOG00000014170	Dbn1	-1.47	2.99	-2.770218936
ENSRNOG00000003546	Tnfrsf12a	-1.47	1.65	-2.770218936
ENSRNOG00000016827	Slc38a3	-1.47	3.78	-2.770218936
ENSRNOG00000019675	Pycard	-1.48	2.18	-2.789487333
ENSRNOG00000050015	LOC687508	-1.48	3.32	-2.789487333
ENSRNOG00000005555	LOC100911101	-1.48	6.33	-2.789487333
ENSRNOG00000030467	Ube2l6	-1.48	2.45	-2.789487333
ENSRNOG00000023809	Opcml	-1.48	1.22	-2.789487333
ENSRNOG00000009892	Adamts15	-1.49	3.44	-2.808889751
ENSRNOG00000000130	Dnajb5	-1.49	4.28	-2.808889751
ENSRNOG00000008536	Actc1	-1.49	11.99	-2.808889751
ENSRNOG00000008074	Cyp11a1	-1.5	3.39	-2.828427125
ENSRNOG00000016484	Gstk1	-1.5	3.97	-2.828427125
ENSRNOG00000058288	Tcf19	-1.5	0.96	-2.828427125
ENSRNOG00000003915	Tmem206	-1.5	1.76	-2.828427125
ENSRNOG00000004666	Prr5l	-1.5	-0.12	-2.828427125
ENSRNOG00000003724	Mrpl27	-1.5	4	-2.828427125
ENSRNOG00000006108	Gngt2	-1.51	3.75	-2.848100391
ENSRNOG00000016838	Pla2g5	-1.51	5.12	-2.848100391
ENSRNOG00000018143	Hpdl	-1.51	1.51	-2.848100391
ENSRNOG00000015318	Heyl	-1.51	4.49	-2.848100391
ENSRNOG00000042897	Nmrk2	-1.51	2.29	-2.848100391
ENSRNOG00000017259	Tacc3	-1.52	1.64	-2.867910496
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ENSRNOG00000011668	Nfil3	-1.52	2.25	-2.867910496
ENSRNOG00000019573	Lcat	-1.52	0.79	-2.867910496
ENSRNOG00000001404	Agfg2	-1.53	2.92	-2.887858391
ENSRNOG00000018666	Gpsm1	-1.53	5.96	-2.887858391
ENSRNOG00000011483	S100a9	-1.53	1.84	-2.887858391
ENSRNOG00000029195	Uba7	-1.53	2.78	-2.887858391
ENSRNOG00000007235	Atp5g1	-1.53	7.84	-2.887858391
ENSRNOG00000010797	Esm1	-1.53	2.47	-2.887858391
ENSRNOG00000019428	Higd1a	-1.54	5.89	-2.907945035
ENSRNOG00000007883	Timm10	-1.54	4.36	-2.907945035
ENSRNOG00000005695	Mgp	-1.54	7.24	-2.907945035
ENSRNOG00000015077	Acsf3	-1.54	3.62	-2.907945035
ENSRNOG00000008373	Colec11	-1.54	1.98	-2.907945035
ENSRNOG00000008738	Tp53i11	-1.54	3.63	-2.907945035
ENSRNOG00000033110	Svep1	-1.54	1.69	-2.907945035
ENSRNOG00000060356	Kif15	-1.54	1.56	-2.907945035
ENSRNOG00000008595	Ttc12	-1.54	0.23	-2.907945035
ENSRNOG00000013774	Lmnb1	-1.55	1.89	-2.928171392
ENSRNOG00000019082	Sbk1	-1.56	3.64	-2.948538435
ENSRNOG00000000245	Slc16a6	-1.56	2.06	-2.948538435
ENSRNOG00000016689	Fanci	-1.56	1.15	-2.948538435

ENSRNOG00000017063	Fcna	-1.57	1.82	-2.969047141
ENSRNOG00000053498	Dnajc22	-1.57	0.19	-2.969047141
ENSRNOG00000036859	Gdpd5	-1.57	2.08	-2.969047141
ENSRNOG00000020803	Meox1	-1.57	0.29	-2.969047141
ENSRNOG00000022555	LOC497899	-1.58	0.69	-2.989698497
ENSRNOG00000027035	Sgo2	-1.58	1.44	-2.989698497
ENSRNOG00000021220	Cpxm1	-1.58	2.22	-2.989698497
ENSRNOG00000000662	Srrd	-1.58	0.62	-2.989698497
ENSRNOG00000032929	Incenp	-1.59	0.74	-3.010493495
ENSRNOG00000055300	Ncapd2	-1.59	1.69	-3.010493495
ENSRNOG00000006841	Ano4	-1.6	1.15	-3.031433133
ENSRNOG00000015085	Dmpk	-1.6	6.62	-3.031433133
ENSRNOG00000012481	Ppm1j	-1.6	1.92	-3.031433133
ENSRNOG00000018929	Kif20b	-1.6	1	-3.031433133
ENSRNOG00000049598	LOC100912571	-1.6	3.81	-3.031433133
ENSRNOG00000016254	Sema4c	-1.6	2.74	-3.031433133
ENSRNOG00000028047	Mecr	-1.61	3.08	-3.052518418
ENSRNOG00000013727	Ndc80	-1.61	1.46	-3.052518418
ENSRNOG00000000704	Cmklr1	-1.62	2.51	-3.073750363
ENSRNOG00000026604	Cercam	-1.62	1.94	-3.073750363
ENSRNOG00000043044	Cnn2	-1.62	2.03	-3.073750363
ENSRNOG00000018910	Abhd11	-1.62	2.26	-3.073750363
ENSRNOG00000047000	Fuom	-1.62	2.55	-3.073750363
ENSRNOG00000002693	Nme1	-1.63	2.42	-3.095129987
ENSRNOG00000023023	Trpt1	-1.63	1.32	-3.095129987
ENSRNOG00000006604	Thy1	-1.63	0.6	-3.095129987
ENSRNOG00000033057	Gapdh-ps2	-1.63	4.95	-3.095129987
ENSRNOG00000052725	RGD1566029	-1.64	2.02	-3.116658319
ENSRNOG00000047098	LOC103694855	-1.64	6.93	-3.116658319
ENSRNOG00000011654	Plk4	-1.64	1.18	-3.116658319
ENSRNOG00000018319	Pisd	-1.64	2.41	-3.116658319
ENSRNOG00000057357	AABR07001054.2	-1.65	0.51	-3.138336392
ENSRNOG00000024885	Asb10	-1.65	2.43	-3.138336392
ENSRNOG00000018069	Ngdn	-1.66	3.38	-3.160165247
ENSRNOG00000013196	Dok5	-1.67	0.85	-3.182145935
ENSRNOG00000050181	Chid1	-1.68	2.75	-3.20427951
ENSRNOG00000056069	Kif11	-1.68	2.17	-3.20427951
ENSRNOG00000012962	Nudt16	-1.68	0.83	-3.20427951
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ENSRNOG00000007837	Acot11	-1.68	2.29	-3.20427951
ENSRNOG00000059997	Brip1	-1.69	0.46	-3.226567037
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ENSRNOG00000003984	Apln	-1.71	4.21	-3.271608234
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ENSRNOG00000006916	Sardh	-1.71	3.7	-3.271608234
ENSRNOG00000024468	Traf3ip1	-1.72	0.76	-3.294364069
ENSRNOG00000009339	Cenpe	-1.73	1.73	-3.317278183

ENSRNOG00000000525	Pi16	-1.73	3.93	-3.317278183
ENSRNOG00000018785	Slc16a13	-1.73	0.32	-3.317278183
ENSRNOG00000020165	Ahsp	-1.73	1.2	-3.317278183
ENSRNOG00000003870	C1qtnf2	-1.74	2.52	-3.340351678
ENSRNOG00000003784	Rilp	-1.75	2.78	-3.363585661
ENSRNOG00000019472	Ackr2	-1.75	0.4	-3.363585661
ENSRNOG00000022921	Dact2	-1.75	-0.07	-3.363585661
ENSRNOG00000021056	Kcnj14	-1.76	0.93	-3.386981249
ENSRNOG00000036684	Pcyt2	-1.76	4.03	-3.386981249
ENSRNOG00000006033	Spon2	-1.76	0.93	-3.386981249
ENSRNOG00000048088	Mest	-1.77	1.33	-3.410539567
ENSRNOG00000046607	Cited4	-1.77	1.3	-3.410539567
ENSRNOG00000019965	Tgfb1i1	-1.77	2.83	-3.410539567
ENSRNOG00000060410	Pcdh1	-1.77	2.46	-3.410539567
ENSRNOG00000009785	Cdkn3	-1.78	0.51	-3.434261746
ENSRNOG00000012318	Aspm	-1.78	1.9	-3.434261746
ENSRNOG00000024650	Ckap2	-1.78	1.47	-3.434261746
ENSRNOG00000015921	Esco2	-1.78	1.04	-3.434261746
ENSRNOG00000001715	Ece2	-1.78	0.66	-3.434261746
ENSRNOG00000016156	Nptxr	-1.78	0.28	-3.434261746
ENSRNOG00000001245	Pcbp3	-1.79	3.28	-3.458148925
ENSRNOG00000043167	Itga9	-1.79	3.26	-3.458148925
ENSRNOG00000017981	Mcm10	-1.8	1.61	-3.482202253
ENSRNOG00000009334	Knstrn	-1.8	-0.4	-3.482202253
ENSRNOG00000047134	Gtf2f1	-1.8	3.15	-3.482202253
ENSRNOG00000019100	Kif2c	-1.81	-0.12	-3.506422885
ENSRNOG00000029886	Hba-a2	-1.81	9.04	-3.506422885
ENSRNOG00000037302	Rad51	-1.81	0.11	-3.506422885
ENSRNOG00000014448	Arntl	-1.81	4.26	-3.506422885
ENSRNOG00000058539	Ccnb1	-1.82	0.61	-3.530811985
ENSRNOG00000000521	Cdkn1a	-1.82	3.51	-3.530811985
ENSRNOG00000021256	Adra1d	-1.82	1.4	-3.530811985
ENSRNOG00000013552	Scd	-1.82	0.48	-3.530811985
ENSRNOG00000015222	Fam46c	-1.83	1.09	-3.555370725
ENSRNOG00000020185	Wdr6	-1.83	3.24	-3.555370725
ENSRNOG00000058916	Ccdc65	-1.84	1.55	-3.580100284
ENSRNOG00000004479	Aurka	-1.85	0.26	-3.60500185
ENSRNOG00000020951	Slc4a1	-1.87	3.47	-3.655325801
ENSRNOG00000006116	Hk2	-1.87	5.42	-3.655325801
ENSRNOG00000018681	Nes	-1.87	3.98	-3.655325801
ENSRNOG00000016403	Olah	-1.87	0.98	-3.655325801
ENSRNOG00000007206	LOC361016	-1.87	0.01	-3.655325801
ENSRNOG00000000167	Alas2	-1.88	3.94	-3.680750602
ENSRNOG00000036701	LOC100361457	-1.88	5.47	-3.680750602
ENSRNOG00000061215	Crym	-1.88	2.84	-3.680750602
ENSRNOG00000046379	LOC100912604	-1.88	2.09	-3.680750602
ENSRNOG00000037871	Sfxn5	-1.89	1.59	-3.706352248
ENSRNOG00000016337	Slc22a1	-1.89	0.43	-3.706352248

ENSRNOG00000021032	Sphk2	-1.89	2.53	-3.706352248
ENSRNOG00000015449	Tmem171	-1.9	1.62	-3.732131966
ENSRNOG00000008831	Hcn2	-1.9	3.6	-3.732131966
ENSRNOG00000059903	Thbs3	-1.91	1.7	-3.758090997
ENSRNOG00000054582	LOC100134871	-1.91	5.6	-3.758090997
ENSRNOG00000018267	B3gnt7	-1.91	0.25	-3.758090997
ENSRNOG00000006984	Mapk11	-1.92	0.08	-3.784230587
ENSRNOG00000049642	Smim5	-1.93	1.76	-3.810551992
ENSRNOG00000061876	Tas1r2	-1.95	4.22	-3.863745316
ENSRNOG00000047321	Hba-a2	-1.95	7.99	-3.863745316
ENSRNOG00000024365	Ect2	-1.95	0.85	-3.863745316
ENSRNOG00000001469	Eln	-1.96	5.34	-3.89061979
ENSRNOG00000057760	Stil	-1.97	0.21	-3.91768119
ENSRNOG00000009436	Hemgn	-1.97	0.78	-3.91768119
ENSRNOG00000008170	Jph2	-1.97	4.32	-3.91768119
ENSRNOG00000001859	Sdf2l1	-1.98	1.17	-3.944930818
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ENSRNOG00000058105	Hbb	-1.99	9.8	-3.972369982
ENSRNOG00000055314	Msrb1	-1.99	3	-3.972369982
ENSRNOG00000036692	Gcgr	-1.99	1.57	-3.972369982
ENSRNOG00000007541	Fhl3	-2.01	3.34	-4.0278222
ENSRNOG00000005936	Foxm1	-2.02	0.4	-4.055837919
ENSRNOG00000027098	Sez6l2	-2.03	1.01	-4.084048503
ENSRNOG00000020383	Dapk3	-2.03	1.86	-4.084048503
ENSRNOG00000007799	Fam151a	-2.04	1.7	-4.112455307
ENSRNOG00000000281	Prodh1	-2.05	2.88	-4.141059695
ENSRNOG00000028137	Mki67	-2.06	3.71	-4.169863043
ENSRNOG00000025302	Cdca2	-2.06	-0.28	-4.169863043
ENSRNOG00000008450	LOC100359539	-2.06	1.57	-4.169863043
ENSRNOG00000000231	Kctd17	-2.08	0.68	-4.228072162
ENSRNOG00000022178	Dcdc5	-2.09	2.36	-4.25748073
ENSRNOG00000014080	Kif23	-2.09	1.55	-4.25748073
ENSRNOG00000015423	Ccna2	-2.09	1.22	-4.25748073
ENSRNOG00000015308	Pbk	-2.09	0.69	-4.25748073
ENSRNOG00000006731	Spc25	-2.09	0.3	-4.25748073
ENSRNOG00000021812	Scx	-2.11	1.33	-4.316912946
ENSRNOG00000021847	Ska3	-2.12	0.22	-4.34693945
ENSRNOG00000021611	Clip2	-2.13	1.58	-4.377174805
ENSRNOG00000012557	Lgals5	-2.14	1.64	-4.407620464
ENSRNOG00000011189	Acy1	-2.15	2.48	-4.438277888
ENSRNOG00000003262	Cacng4	-2.15	-0.14	-4.438277888
ENSRNOG00000023303	Dpep2	-2.17	1.36	-4.500233939
ENSRNOG00000005659	Aurkb	-2.17	0.87	-4.500233939
ENSRNOG00000020030	Crlf1	-2.17	0.75	-4.500233939
ENSRNOG00000008165	Tpx2	-2.19	1.88	-4.563054863
ENSRNOG00000011332	Clspn	-2.19	-0.11	-4.563054863
ENSRNOG00000020239	Capn15	-2.19	0.97	-4.563054863
ENSRNOG00000003807	Wnt9b	-2.2	0.23	-4.59479342

ENSRNOG00000001082	Abcb9	-2.2	0.68	-4.59479342
ENSRNOG00000017684	Fbxl22	-2.21	2.54	-4.626752736
ENSRNOG00000018484	Plk3	-2.21	-0.07	-4.626752736
ENSRNOG00000038572	Ncapg	-2.22	0.58	-4.658934346
ENSRNOG00000002711	Nuf2	-2.23	0.8	-4.691339797
ENSRNOG00000003388	Cenpf	-2.24	2.21	-4.723970646
ENSRNOG00000005115	Asf1b	-2.25	-0.53	-4.75682846
ENSRNOG00000006617	Cntnap2	-2.25	0.38	-4.75682846
ENSRNOG00000051372	Mycn	-2.27	0.92	-4.823231311
ENSRNOG00000008056	Ankrd9	-2.29	1.46	-4.890561111
ENSRNOG00000020197	LOC100911932	-2.3	2.6	-4.924577653
ENSRNOG00000016377	Cep55	-2.33	0.46	-5.028053498
ENSRNOG00000008986	Diaph3	-2.33	0.6	-5.028053498
ENSRNOG00000011145	Crhr2	-2.33	0.63	-5.028053498
ENSRNOG00000015529	Cdca3	-2.34	-0.15	-5.063026376
ENSRNOG00000004781	Crmp1	-2.34	-0.29	-5.063026376
ENSRNOG00000026143	Ckap2l	-2.37	0.09	-5.169411323
ENSRNOG00000001143	Cit	-2.37	-0.05	-5.169411323
ENSRNOG00000016561	Ns5atp9	-2.37	-0.23	-5.169411323
ENSRNOG00000017226	Slc2a4	-2.38	6.2	-5.205367422
ENSRNOG00000017786	Acta1	-2.38	7.01	-5.205367422
ENSRNOG00000019627	Mybpc2	-2.39	0.45	-5.241573615
ENSRNOG00000053047	Top2a	-2.4	2.95	-5.278031643
ENSRNOG00000001005	Fcer2	-2.42	3.13	-5.351710219
ENSRNOG00000016962	Neu2	-2.42	-0.09	-5.351710219
ENSRNOG00000022911	Hjurp	-2.43	0.23	-5.388934307
ENSRNOG00000027787	Cdc6	-2.45	0.06	-5.464161027
ENSRNOG00000054286	Rrm2	-2.46	-0.12	-5.502167273
ENSRNOG00000015904	Wfdc1	-2.48	4.34	-5.578974665
ENSRNOG00000004682	Parpbp	-2.5	-0.55	-5.656854249
ENSRNOG00000046192	Nsun4	-2.51	1.8	-5.696200782
ENSRNOG00000004078	Eno3	-2.52	6.85	-5.735820992
ENSRNOG00000018113	Anlnl1	-2.52	0.26	-5.735820992
ENSRNOG00000007906	Bub1b	-2.53	0.46	-5.775716782
ENSRNOG00000010872	Ckb	-2.53	4.44	-5.775716782
ENSRNOG00000038035	Kif4a	-2.56	0.8	-5.897076869
ENSRNOG00000024428	Kif20a	-2.56	1.34	-5.897076869
ENSRNOG00000014343	Anln	-2.57	0.53	-5.938094283
ENSRNOG00000001736	Bdh1	-2.58	4.32	-5.979396995
ENSRNOG00000023008	Fam131c	-2.59	1.3	-6.02098699
ENSRNOG00000015131	Ube2c	-2.63	-0.05	-6.190259974
ENSRNOG00000018953	Cblc	-2.69	0.94	-6.453134074
ENSRNOG00000027894	Iqgap3	-2.7	0.24	-6.498019171
ENSRNOG00000000632	Cdk1	-2.71	1.42	-6.543216468
ENSRNOG00000033658	Kntc1	-2.71	0.32	-6.543216468
ENSRNOG00000013598	Melk	-2.73	0.08	-6.634556367
ENSRNOG00000016483	Myo16	-2.76	0.79	-6.773962499
ENSRNOG00000013057	Prc1	-2.79	2.7	-6.91629785

ENSRNOG00000004351	Slc25a29	-2.79	1.07	-6.91629785
ENSRNOG00000032994	Myom3	-2.79	2.72	-6.91629785
ENSRNOG00000038047	Mt1	-2.79	1.33	-6.91629785
ENSRNOG00000055111	AABR07000658.1	-2.8	0.21	-6.964404506
ENSRNOG00000028415	Cdc20	-2.83	0.28	-7.110741449
ENSRNOG00000029055	Ttk	-2.84	0.83	-7.160200567
ENSRNOG00000037080	Adamts17	-2.85	-0.42	-7.210003701
ENSRNOG00000011777	Spag5	-2.86	0.3	-7.260153243
ENSRNOG00000004438	Cntn1	-2.86	-0.47	-7.260153243
ENSRNOG00000018815	Plk1	-2.88	NA	-7.361501205
ENSRNOG00000018214	Bok	-2.91	0.82	-7.516181994
ENSRNOG00000047653	Crybb1	-2.91	0.63	-7.516181994
ENSRNOG00000020407	Atcay	-2.95	-0.33	-7.727490631
ENSRNOG00000011824	Trh	-2.97	-0.62	-7.835362381
ENSRNOG00000017130	Rhd	-2.97	0.04	-7.835362381
ENSRNOG00000007227	Mien1	-2.98	2.72	-7.889861636
ENSRNOG00000020985	Atp4a	-3	NA	-8
ENSRNOG00000050315	Dcxr	-3.01	1.5	-8.0556444
ENSRNOG00000049033	Racgap1	-3.02	1.29	-8.111675838
ENSRNOG00000020281	Kif22	-3.07	1.05	-8.397733469
ENSRNOG00000020277	Cntnap1	-3.09	3.74	-8.51496146
ENSRNOG00000018122	Tspan17	-3.11	-0.12	-8.633825892
ENSRNOG00000011427	Hr	-3.19	0.8	-9.126109727
ENSRNOG00000016148	Gtse1	-3.21	NA	-9.253505471
ENSRNOG00000014336	Mcm5	-3.22	1.05	-9.317868692
ENSRNOG00000027742	Adamtsl2	-3.22	1.76	-9.317868692
ENSRNOG00000022268	Pnpla3	-3.37	3.08	-10.33882265
ENSRNOG00000050819	Birc5	-3.51	NA	-11.39240156
ENSRNOG00000049766	Sctr	-3.54	0.31	-11.63178014
ENSRNOG00000025757	Myh6	-3.61	11.82	-12.21007367
ENSRNOG00000012835	Espl1	-3.63	NA	-12.38051995
ENSRNOG00000020097	Inha	-3.77	1.79	-13.64215827
ENSRNOG00000022932	Serhl2	-3.78	2.92	-13.73704698
ENSRNOG00000049604	Mvk	-3.81	0.55	-14.02569154
ENSRNOG00000007142	B3gat1	-3.84	-0.28	-14.32040113
ENSRNOG00000000885	Auts2	-3.85	0.98	-14.4200074
ENSRNOG00000015682	Kel	-3.89	-0.09	-14.82540899
ENSRNOG00000021713	Kif18b	-4.45	-0.71	-21.85664411
ENSRNOG00000030174	NA	-5.11	3.32	-34.53530357
ENSRNOG00000008040	Fam64a	-6.27	-0.63	-77.17170097
ENSRNOG00000011096	Hmgb3	-8.17	1.89	-288.0149721

Table S4. Metabolites D100

Compound	Mass	Retention mode	CON 1	CON 2	CON 3	CON 4	D100 1	D100 2	D100 3	D100 4	D100 5	D100 6
1-Palmitoyllysophosphatidylcholine	495.3336	5.656 HILICpos	19215830	19365632	18956040	17963440	14947183	17430056		11259519	10686738	10490630
(-)-?-Himachalene	204.1876	12.597 Rpneg	8830	8056	7311	9184	4314	3201	4888	5225	4284	3583
(-)-?-Himachalene Esi-12.383001	204.1873	12.383 Rpneg	4835	4574	2228	4457	2153	959	2291	3866	2012	1843
(-)-11-hydroxy-9,10-dihydrojasmonic acid 11-beta-D-glucos	390.188	6.734 Rpneg	6032	7864	4593	8433	8806	5023	4940	6069	8709	6374
(-)-11-nor-9-carboxy-?9-THC-d3	694.4392	0.994 HILICneg	1383469	1968034	1410345	1709892	553957	1	588958	732357	233913	248693
Acetylcarnitine	203.1157	1.075 Rppos	8.52E+07	9.26E+07	1.04E+08	1.01E+08	6.97E+07	6.39E+07	7.06E+07	7.27E+07	6.59E+07	5.92E+07
(-)-Chimonanthine	346.2157	10.592 Rpneg	8254	3169	2984	3555	3686	1	9587	8116	2140	11314
(-)-Jamine	675.588	27.391 Rppos	310120	307186	340621	345136	251506	490088	305382	333000	318941	417565
(-)-Neolinderatin	590.3625	11.927 Rpneg	5671	1091	7724	6177	8112	3702	4508	5098	5763	5151
(-)-Tortuosamine	326.1958	1.617 HILICpos	638565	891948	386728	894230	996698	1003880		952056	902069	721762
(-)-trans-C75	236.1411	7.464999 Rppos	405932	379536	334817	456305	423635	329007	457494	476854	490176	496983
(-)-trans-C75	254.1527	9.395001 Rpneg	3093	5992	2558	5250	6103	2701	3041	5567	7102	4773
(+)-20-Methyl-docosanoic acid	354.3495	13.653 Rpneg	257109	104002	54754	95499	80818	59525	82203	72456	90234	57559
(+)-20-Methyl-docosanoic acid	354.3496	0.977 HILICneg	166054	115027	85912	146145	134526	68799	139322	162497	335984	152036
(+)-24-Methyl-hexacosanoic acid	410.4104	14.311 Rpneg	19500	8943	3073	5816	8133	6073	5972	5649	4997	1402
(+)-beta-thujone	152.1191	0.994 HILICneg	34390	50460	68048	48113	58932	27746	36963	45285	124751	81188
(+)-CP 47,497	317.2718	7.673999 Rppos	290128	329173	397965	447453	301706	376465	404332	466649	490879	510382
(+)-CP 47,497 Esi+7.1920004	317.2708	7.192 Rppos	80889	100595	128972	141313	100500	123030	131048	130448	139560	130110
(+)-CP 47,497 Esi+7.325	317.2709	7.325 Rppos	98018	121863	148736	172603	115989	157106	147289	161110	80956	176808
(+)-CP 47,497 Esi+7.492999	317.2709	7.492999 Rppos	226907	254840	300156	314929	256452	296400	329260	340461	351089	370604
(+)-Prosopinine	359.2661	12.477 Rpneg	4289	3180	2442	3246	3590	3071	2703	2670	3238	1803
(+)-trans-alpha-Irone	206.1673	12.739 Rpneg	15855	21115	59183	19020	95981	36074	41644	16553	19615	30503
(+)-trans-alpha-Irone	206.1674	0.926 HILICneg	818351	327567	110281	264934	1105545	179102	110006	246506	224740	337621
(+)-trans-alpha-Irone Esi-13.277	206.1675	13.277 Rpneg	11339	9638	11912	11516	7307	7454	10879	8021	10810	10383
(+)-Villanovane-13alpha,19-diol	322.2491	12.653 Rpneg	6820	7219	8553	10028	3981	1	4096	4121	1	3232
(+/-)-2,16,16-trimethyl-5,8,11,14-all-cis-tricosatetraenoyl-2	415.3575	20.978 Rppos	808804	731480	1236308	954896	790964	946808	947459	947832	589991	534017
(+/-)-6-Hydroxy-3-oxo-alpha-ionol	224.1412	11.219 Rpneg	2156	3115	3287	3400	2768	3381	2709	3902	4435	4524
Carnitine	161.1052	7.645999 HILICpos	49671540	51932548	58096220	56164116	63099888	55919800		58202452	48590492	55589712
(±)-1,4-Nonanediol diacetate	243.1815	15.667 Rppos	276965	157507	349848	156387	101680	99270	195884	136894	130528	55350
Choline	103.1002	5.191 HILICpos	32395980	29873590	27230764	29043788	47010608	36982584		40752208	38743212	34448672
(±)-1,4-Nonanediol diacetate	244.1678	7.714999 Rpneg	9442	13772	8099	15544	24910	8858	7815	14421	21377	11625
(±)12-HETE	320.2338	12.851 Rpneg	1	4248	3326	5311	5239	1	3251	6416	4227	3907
(±)12-HETE	320.2359	1.185 HILICneg	774425	797791	487380	516627	579057	651716	426994	335132	488737	462320
(±)12-HETE Esi-11.798001	320.2354	11.798 Rpneg	10385	15993	14783	15198	14877	15683	16686	23363	26957	10910
(±)16-HETE	320.234	11.799 Rpneg	19746	14541	6480	7924	11994	13728	15769	22914	23176	11310
(±)16-HETE Esi-11.674	320.2341	11.674 Rpneg	7473	15335	5759	14500	7923	13573	6481	1	9862	9523
(±)16-HETE Esi-12.352999	320.2336	12.353 Rpneg	4047	5873	6143	9360	3420	1	5719	1	5956	7068
(±)-2-Octanol	130.136	9.947 Rpneg	16057	19515	16573	16723	18402	15021	13116	16520	20100	15875
(±)-Conen	625.1722	19.718 Rppos	1165023	1396272	1292391	1325874	1219336	1354270	1337744	1381624	1413028	1477208
(±)-Myristoylcarnitine	371.304	2.118 HILICpos	3100718	1201217	1308297	1015386	1036951	960487		673997	1036960	1167067
(±)-Sulfobutanedioic acid	197.9839	0.715 Rpneg	15833	26497	2635	17255	18768	2453	14224	5879	28529	39081
(±)-Taxifolin	304.0587	6.362999 HILICneg	316827	385078	399394	399615	413469	329237	345291	395192	350763	348595
(1(10)E,4a,5E)-1(10),5-Germacradiene-12-acetoxy-4,11-diol	313.2286	2.559 HILICpos	358128	154350	144168	110100	148379	99078		107381	92417	202032
(10S)-Juvenile hormone III diol	330.2042	9.060999 Rpneg	21541	19427	15739	18915	20189	15522	15663	19408	23073	17001
(10S)-Juvenile hormone III diol Esi-8.498	330.2038	8.498 Rpneg	5976	4910	4458	6166	14367	3740	3584	5019	5028	3956
(10S)-Juvenile hormone III diol Esi-8.814001	330.2041	8.814001 Rpneg	12099	9463	7334	9814	10962	8105	7246	9085	11526	8047
(10S)-Juvenile hormone III diol Esi-9.079001	284.1978	9.079001 Rpneg	24138	17319	17296	28068	55476	17710	16824	21692	23173	16978
(10S)-Juvenile hormone III diol Esi-9.678	330.2018	9.678 Rpneg	1	6250	3715	1	12450	2137	3069	5195	7622	1
(14alpha,17beta,20S,22R)-14,20-Epoxy-17-hydroxy-1-oxow	470.2649	4.132 HILICneg	224387	223561	193481	195655	49742	1	53777	1	1	38855
DG(16:1/18:0)	594.5241	27.274 Rppos	1.39E+07	1.59E+07	1.80E+07	1.65E+07	2.53E+07	4.11E+07	3.05E+07	3.30E+07	2.95E+07	3.11E+07
(17Z)-1?,25-dihydroxy-26,27-dimethyl-17,20,22,22,23,23-	448.3363	16.038 Rppos	218237	250387	627431	443953	488683	140784	233865	225535	227010	211016
(1R,2R)-3-oxo-2-pentyl-cyclopentanehexanoic acid	250.1914	9.152 Rppos	209561	245471	313995	317923	247105	298812	314939	369538	335123	335251
DG(18:2/18:1)	618.5225	25.623 Rppos	1.65E+07	1.90E+07	2.37E+07	1.79E+07	3.48E+07	5.36E+07	4.03E+07	4.49E+07	4.55E+07	4.14E+07
(1R,2R,3S,1'R)-Nepetalinic acid	200.1046	5.164001 Rppos	553693	1049330	1083217	960625	1010068	707770	671474	691634	1113142	1319783
(1R,4R,5S)-5-Hydroxyfenchone glucoside	376.1733	6.055 Rpneg	12150	13384	7557	15518	16827	7535	6692	10784	16189	9778
(1S,2S)-3-oxo-2-pentyl-cyclopentanehexanoic acid	268.2038	11.752 Rpneg	53382	23616	19569	23354	25584	15079	38001	40727	26937	32418
(1S,2S)-3-oxo-2-pentyl-cyclopentanehexanoic acid Esi-11.86	268.2023	11.863 Rpneg	10587	9028	25226	6792	11881	4007	6159	11408	1	1
(1S,2S)-3-oxo-2-pentyl-cyclopentanehexanoic acid Esi-12.32	268.202	12.326 Rpneg	5849	5526	3730	3827	6510	3864	5028	5348	4216	4396
Eicosanoyl-EA	337.3344	18.392 Rppos	9851915	12952001	17164784	10109084	28450392	12694044	39074816	17692536	13462789	6295982
(1S,2S,4R,8R)-p-Menthane-1,2,8,9-tetrol	425.2982	7.535001 Rppos	61789	435380	84237	371638	523272	86420	94238	319799	700085	304865
(1S,3R,4R)-p-Menthane-1,3-diol	172.1455	0.837 HILICneg	22660	19578	17828	11669	19419	1	6354	13354	24649	10054
Isoferuloyl C1-glucuronide	370.0935	0.7 HILICpos	2.38E+08	1.06E+08	2.4E+08	96731832	71707544	2.46E+08		75836984	2.15E+08	1.23E+08
(20S,22E)-3beta-Hydroxychola-5,16,22-trien-24-oic Acid	370.249	12.853 Rpneg	2275	3529	1	1	753	1574	3764	2055	4506	2056
(22E)-(24S)-1?,24,25-trihydroxy-22,23-didehydrovitamin D	430.3051	11.616 Rpneg	6889	4933	4074	3091	947	1	909	1366	1943	1451
(22E)-3?-Hydroxychola-5,16,22-trien-24-oic Acid	370.2483	13.383 Rpneg	21346	10906	4104	7448	21629	1	19181	9139	11510	11036
(22E,24E)-1?,25-dihydroxy-22,23,24,24a-tetradehydro-24a	422.3222	17.247 Rppos	153426	197963	169951	206970	82412	170663	265415	237319	198687	152021
(22R)-3?,7?,22-Trihydroxy-5?-cholan-24-oic Acid Esi+15.14	407.3017	15.141 Rppos	231661	109001	162084	124618	66665	39207	131123	57122	94768	40275
(22S)-3?,7?,22-Trihydroxy-5?-cholan-24-oic Acid	425.312	8.793 Rppos	105803	73917	10610	36052	59018	261989	43860	54898	118368	139645
(25R)-11alpha,20,26-trihydroxyecdysone	572.3183	9.667 Rpneg	3202	1194	1865	1410	1	1	1	1108	2161	1
(25R)-12alpha-hydroxy-24R,26R-dimethyl-26,27-cyclo-chol	456.3229	11.407 Rpneg	737	1	1	3797	1992	5058	1	1807	3465	2603
(25R)-spirost-5en-3beta-ol 3-O-alpha-L-rhamnopyranosyl-(1	900.5076	24.714 Rppos	1669095	1693656	1364652	1194028	1817997	1413213	1278102	1309251	1378216	1308289
Kaempferol 3-[6'''-p-coumarylglucosyl-(1->2)-rhamnoside]	740.1897	0.705 HILICpos	1.84E+08	63747872	92435888	87308568	65390880	2.28E+08		68587784	1.84E+08	1.1E+08
(25S)-26,26,26-trifluoro-1?,25-dihydroxyvitamin D3 / (25S)	487.3283	1.4 HILICpos	642262	478379	72904	85492	298894	214440		117624	169957	82243
(2S,2'S)-Oscillol 2,2'-di(?-L-fucoside)	892.5384	13.276 Rpneg	6467	3173	3683	4018	2203	1980	3220	2345	3661	3191
(2xi,6xi)-7-Methyl-3-methylene-1,2,6,7-octanetetrol	226.1211	5.694 HILICpos	343723	253885	192594	630448	215428	175262		480937	265293	326206
(3b,6b,8a,12a)-8,12-Epoxy-7(11)-eremophilene-6,8,12-trim	326.2116	12.609 Rpneg	105705	59794	46298	66037	48245	34118	53507	62760	72435	48011
(3beta,5alpha,9alpha,22E,24R)-5,9-Epidioxy-3-hydroxyergo	488.3125	8.214999 Rpneg	27190	23685	25476	27479	20883	23148	22408	26604	25610	28215
PC(16:0/18:2)	757.5638	1.542 HILICpos	1.03E+08	1.35E+08	1.14E+08	99402560	1.44E+08	1.67E+08		1.69E+08	1.65E+08	1.37E+08
PC(16:0/20:4(5Z,8Z,10E,14Z)(12OH[S]))	779.5495	22.004 Rpneg	9468855	1.01E+07	1.02E+07	9329975	4927756	4418650	6393217	6500134	3827598	1759775
(3-Methylcrotonyl)glycine methyl ester	217.0956	5.832 HILICneg	235580	314036	303940	344213	107932	90169	163043	174459	92598	149602
(3-Methylcrotonyl)glycine methyl ester Esi-7.033	217.0958	7.033 HILICneg	49560	120501	138064	113388	60002	41279	48720	26093	62566	33494
(3R,4S)-(6S,7R)-Diepoxy-9Z-heneicosene	322.2861	13.107 Rpneg	12937	10242	4153	7656	5660	4115	6097	6133	5834	4519
PC(16:0/22:5)	789.5678	23.347 Rppos	19211756	12654232	24303476	26880332	14702829	11793965	11076525	9109469	11067940	12979723
(3R,7R)-1,3,7-Octanetriol	162.1254	6.572999 Rppos	631654	1923512	1297076	960409	1067701	1649659	628003	690536	1231593	741286
(3S,5R,6R,7E)-3,5,6-Trihydroxy-7-megastigmen-9-one	242.1524	8.806 Rpneg	1	1	1	11522	13139	1	7647	9268	18175	9227
(4S,5S)-(+)-Germacrone 4,5-epoxide	234.1624	0.901 HILICneg	417378	287513	88024	158702	616890	35869	98835	271174	204821	272111
(5b,7a,12a)-(1,3-dihydro-5-nitro-1,3-dioxo-2H-isoindol-2-yl	595.3271	11.748 Rppos	400060	354688	523303	554941	467929	484899	373165	339891	362360	316083
(5R,6S)-5,6-Epoxy-7-megastigmen-9-one	208.1459	9.788001 Rpneg	2647	1725	1715	1812	1777	1817	1777	1906	1881	2081
(5R,6S)-5,6-Epoxy-7-megastigmen-9-one	243.1831	0.975 HILICpos	1342924	1840410	1471219	1028005	1999648	675189		455541	552487	1115866

(5Z,10Z)-19-fluoro-1?-hydroxyvitamin-D3/(5Z,10Z)-19-fluo	464.3302	13.574	Rpneg	47268	154149	61507	1	26377	21975	62825	40903	107717	147227	
(6R)-vitamin D3 6,19-sulfur dioxide adduct / (6R)-cholecalci	896.6041	4.845	HILICneg	954576	917257	915717	1091257	690929	634534	705377	699329	632598	567722	
(6S)-vitamin D2 6,19-sulfur dioxide adduct / (6S)-ergocalcife	460.2979	13.202	Rpneg	5221	4525	2924	4653	3541	3019	3905	4057	5048	5359	
(6S)-vitamin D3 6,19-(4-phenyl-1,2,4-triazoline-3,5-dione) a	563.3514	5.96	Rppos	365602	533194	358972	511188	655789	369018	330667	507667	636001	435489	
(8R,8'R)-Secoisolariciresinol 9-glucoside	584.2481	7.441001	Rpneg	1569	1754	2742	1422	2471	2256	2395	1904	1152	912	
(9R,10S,12Z)-9,10-Dihydroxy-8-oxo-12-octadecenoic acid	328.2236	10.987	Rpneg	16776	10273	7789	10853	11466	12020	8471	10275	8391	7610	
(9R,10S,12Z)-9,10-Dihydroxy-8-oxo-12-octadecenoic acid E	328.2238	10.77	Rpneg	12100	6378	3420	5509	3556	8617	6449	6776	3737	3713	
(9R,10S,12Z)-9,10-Dihydroxy-8-oxo-12-octadecenoic acid E	328.2228	9.056	Rpneg	2079	5270	2165	1	8135	1	1793	3775	5223	3626	
(9R,10S,12Z)-9,10-Dihydroxy-8-oxo-12-octadecenoic acid E	328.2222	9.057	Rpneg	2104	4057	2118	6102	8255	2385	1592	3775	4439	3685	
(E)-2-Methyl-2-buten-1-ol O-beta-D-Glucopyranoside	247.1425	1.603	Rppos	3922565	1182844	1104448	994047	8869034	1.98E+07	1.75E+07	1.89E+07	2.47E+07	1.77E+07	
(E)-2-Methyl-2-buten-1-ol O-beta-D-Glucopyranoside	248.1259	5.335	Rpneg	13687	19545	6928	21135	22499	4576	11037	16550	22360	5425	
(E)-3,7-Dimethyl-2,6-octadienyl decanoate	308.271	12.973	Rpneg	1340599	1076939	708668	1093036	816022	583587	841325	1054339	886776	828679	
(E)-3,7-Dimethyl-2,6-octadienyl decanoate	308.2722	1.042	HILICneg	1051952	1224721	997038	1058416	1164971	403320	875444	965943	1056672	912748	
(E)-Urocanic acid	138.0428	1.222	Rpneg	351965	1521324	102194	1794458	2938340	151985	236420	2147112	2990566	1469727	
PC(18:0/20:4)	807.5765	23.147	Rppos	1.08E+08	92669936	1.24E+08	1.18E+08	79794832	88041432	93131696	87273392	85785624	90507168	
(R)(-)-Allantoin	158.0438	5.662	HILICneg	129312	211263	193508	158051	214732	200389	171286	175707	199496	194061	
(R)-(+)-2-Pyrrolidone-5-carboxylic acid	129.0423	7.566001	HILICneg	1501496	337154	241968	324834	385582	283952	280587	276851	363756	318515	
PC(18:2/18:2)	781.5636	1.533	HILICpos	2.62E+08	2.68E+08	2.83E+08	2.79E+08	2.09E+08	2.22E+08		2.37E+08	2.44E+08	1.99E+08	
(R)-(+)-2-Pyrrolidone-5-carboxylic acid	129.0427	0.806	Rpneg	86426	91480	166665	103196	258947	111078	137349	101904	80160	83515	
(R)-(+)-2-Pyrrolidone-5-carboxylic acid Esi-7.683999	147.0527	7.683999	HILICneg	128175	43354	33752	34462	27614	32673	31289	30079	35365	34225	
PC(20:5/15:1)	763.5172	22.69	Rppos	3.65E+07	3.57E+07	3.38E+07	3.77E+07	2.61E+07	2.69E+07	3.17E+07	2.69E+07	2.26E+07	2.59E+07	
(R)-2-Hydroxy-7,8-dimethoxy-2H-1,4-benzoxazin-3(4H)-one	447.1381	12.596	Rpneg	4364	3325	2039	2340	2364	1019	1097	1686	1053	766	
(R)-2-Hydroxysterculic acid	310.2481	12.784	Rpneg	9203	7241	6002	5467	6373	7672	5650	5370	7534	5904	
(R)-3-((R)-3-Hydroxybutanoyloxy)butanoate	172.0735	5.038001	Rppos	274185	433339	32153	375013	447492	79623	230055	278586	565956	456673	
(R)-3,4-Dihydro-2-methyl-2-(4,8,12-trimethyl-3,7,11-tridec	382.2871	13.006	Rpneg	3224	5027	3113	4149	5067	2271	4542	6149	2881	3128	
(R)-Dihydromaleimide	99.0317	7.037	HILICneg	25160	71689	18801	28435	24045	21886	37294	43379	26378	51000	
(R)-Rhazinilam	294.1712	12.082	Rpneg	5861	9433	6389	10106	4226	5010	8167	11339	5563	7737	
(R)-Stearoylcarnitine	427.3653	1.875	HILICpos	7823598	2400118	2349707	2667253	3099139	3144086		3283410	3657033	3407536	
(S)-3-Hydroxytetradecanoyl-CoA	997.2803	18.813	Rppos	610661	727579	718004	782364	395124	450423	445763	492617	847655	529019	
(S)-3-Octanol glucoside	292.1882	6.942	Rppos	443947	964286	615344	960837	1027181	865434	635405	840008	1164193	833625	
PE(18:1(9Z)/19:0)	759.5771	1.55	HILICpos	1.77E+08	2.12E+08	1.91E+08	1.34E+08	1.04E+08	1.12E+08		1.41E+08	1.05E+08	88386104	
(S)-3-Octanol glucoside	292.1906	1.033	HILICpos	446354	574920	319157	551281	1076394	274692		313240	482973	534899	
(x)-2-Heptanol glucoside	278.1753	1.05	HILICpos	201660	634484	410041	579637	1061927	454487		410180	443089	566827	
(Z)-2-Tetracos-15-enamidoethanesulfonic acid	473.3533	13.489	Rpneg	10340	7019	5501	8381	6290	3644	6541	5091	6166	5520	
(Z)-Methyl 3-(methylsulfinyl)-1-propenyl disulfide	181.9884	0.748	Rpneg	4474	16887	2720	15698	14521	1	1	7146	19382	14524	
(Z)-Tamarindienal	126.0314	0.699	Rpneg	1281	8019	2711	5625	7899	1	2297	6196	7898	2992	
?-15,16-DiHODE	358.2351	10.04	Rpneg	10140	7684	7418	8011	8572	7064	6723	7105	7710	6834	
?-15,16-DiHODE Esi-9.513	358.2343	9.513	Rpneg	5203	3406	3448	3886	5060	3697	3399	4168	4133	3558	
?-9,10-DiHODE	311.2453	9.819	Rppos	357533	480146	630477	795489	481260	555358	693909	853559	946827	1036663	
?-9,10-DiHODE	312.2277	10.866	Rpneg	1	4462	3202	5950	1	2053	3296	5752	4299	3863	
?-Caprolactam	113.084	1.417	HILICpos	158879	149131	186004	385480	241793	184799		301658	194136	235518	
?-Glutamyl-?-cyanoalanine	243.0833	0.907	Rpneg	36000	36481	54676	39583	24903	30324	28436	31298	26990	29651	
?-Hydroxyisobutyrate Esi-1.051	104.0471	1.051	Rpneg	1	12482	6710	1	22740	27764	22015	15181	32282	22272	
?-Rhodomycinone	428.1134	10.173	Rpneg	2709	2077	2361	1589	2622	2308	1752	1394	1221	1066	
[3-[1-Formyl-2-(2-furanyl)ethenyl]]-2-(2-furanyl)-5-(2-furanyl	419.1002	5.179	HILICneg	18979	60511	45618	55045	28238	26457	24052	22843	14064	22682	
[6]-Gingerdiol 3,5-diacetate	380.2233	10.733	Rpneg	7550	9162	5781	9058	14432	4945	5966	7942	11305	7244	
[6]-Gingerdiol 3,5-diacetate Esi-11.614999	380.222	11.615	Rpneg	4200	1	1854	3349	3751	2184	3147	3573	4727	3230	
[6]-Gingerdiol 3,5-diacetate Esi-12.072999	380.222	12.073	Rpneg	2317	2501	2049	2533	1	1639	1	2001	2350	2042	
PE(18:2/21:0)	785.5949	1.542	HILICpos	2.49E+08	3.05E+08	4.01E+08	2.59E+08	3.86E+08	4.43E+08		6.07E+08	4.63E+08	3.9E+08	
PE(18:3/20:3)	763.5168	4.887001	HILICneg	2.44E+07	2.69E+07	2.64E+07	2.93E+07	1.76E+07	1.42E+07	2.02E+07	2.02E+07	1.56E+07	1.97E+07	
PE(22:6/21:0)	833.6094	1.525	HILICpos	1.97E+08	1.57E+08	2.29E+08	2.26E+08	1.38E+08	1.42E+08		1.31E+08	1.15E+08	1.18E+08	
PG(15:0/19:1)	748.5263	1.149	HILICneg	14545125	10518913	12475207	15255894	4677737	2970466	5882595	5183681	5084275	5891000	
PS(O-16:0/22:0)	787.6091	27.018	Rppos	97294048	1.09E+08	1.37E+08	1.05E+08	1.19E+08	1.74E+08	1.54E+08	1.16E+08	1.48E+08	1.24E+08	
PS(O-20:0/22:4)	835.6078	25.165	Rppos	70439424	56790184	86193592	87685672	47385240	58235452	52923008	46520324	43820352	54719844	
PS(P-20:0/16:0)	757.5624	23.28	Rppos	1.74E+08	2.21E+08	1.92E+08	1.73E+08	2.67E+08	3.07E+08	2.71E+08	2.92E+08	2.95E+08	2.83E+08	
1-(10-methyl-hexadecanoyl-2-(8-[3]-ladderane-octanyl)-sn-g	616.5453	13.124	Rpneg	60316	49513	53383	46024	47763	46354	46579	41165	45069	43228	
PS(P-20:0/17:0)	771.5773	24.253	Rppos	3623432	5084830	4162713	3478955	8125165	1.15E+07	6797163	9552314	1.41E+07	1.08E+07	
1-(14-methyl-pentadecanoyl)-2-(8-[3]-ladderane-octanyl)-sn	602.526	12.973	Rpneg	22178	18862	13274	13988	13820	11119	15032	17363	26650	13164	
1-(5-Hydroxy-2-pyrimidinyl)piperazine	180.0993	1.043	Rpneg	2755	3346	4173	1837	1	1098	1	3818	5955	3976	
1-(5-Phosphoribosyl)-4-(N-succinocarboxamide)-5-aminoim	835.2308	19.809	Rppos	1.00E+07	1.13E+07	1.01E+07	1.06E+07	8262332	8550881	8094190	8610024	1.06E+07	8981136	
1-(6-[3]-ladderane-hexanoyl)-2-(8-[3]-ladderane-octanyl)-sn-	745.503	0.854	HILICneg	777967	343557	380056	378433	343075	520757	336482	362736	514526	364350	
1-(6-[3]-ladderane-hexanoyl)-2-(8-[3]-ladderane-octanyl)-sn-	805.5271	13.972	Rpneg	10968	1	1	1	6328	5693	1839	4772	1	2943	
1-(6-[3]-ladderane-hexanoyl)-2-(8-[3]-ladderane-octanyl)-sn-	745.5044	4.774001	HILICneg	77113	84956	85745	80487	67406	65908	71612	69287	67140	70501	
1-(6-[5]-ladderane-hexanyl)-2-(8-[3]-ladderane-octanyl)-sn-gl	606.4982	13.122	Rpneg	4219	2548	3110	2888	2486	2210	2476	2475	2870	2278	1-
(8-[3]-ladderane-octanoyl)-2-(8-[3]-ladderane-octanyl)-sn-	773.5371	4.696	HILICneg	1.17E+07	1.05E+07	1.08E+07	1.16E+07	1.11E+07	9945274	1.13E+07	1.08E+07	1.09E+07	1.14E+07	
1-(8-[3]-ladderane-octanoyl-2-(8-[3]-ladderane-octanyl)-sn-g	650.5271	1.45	HILICpos	865935	765314	972949	1209201	1237898	782119		938510	991935	875853	
1-(8-[5]-ladderane-octanoyl)-2-(8-[3]-ladderane-octanyl)-sn-	771.521	4.722	HILICneg	1284757	1432544	1679646	1537209	1415121	974664	1149558	1383381	1012590	1474461	
1-(9Z,12Z,15Z-Octadecatrienoyl)-2-(11Z-eicosenoyl)-sn-glyc	644.5388	27.396	Rppos	10553515	10074403	10426073	10706218	9111415	13134757	10154537	9633535	9224739	9774251	
1-(Methylthio)ethyl 2-propenyl disulfide	226.0177	13.016	Rpneg	1	1011	1	1	1199	5121	1	2618	5803	7651	
1-(O-alpha-D-glucopyranosyl)-3-keto-(1,25R)-hexacosanedio	574.4438	1.124	HILICneg	433441	340940	308445	314379	459870	323155	381419	402861	425330	375235	
1-(O-alpha-D-mannopyranosyl)-25-keto-(1,3R,27R)-octacosa	636.496	1.02	HILICneg	407617	1	1	1	315287	210108	344895	376423	446479	359652	
1-(O-alpha-D-mannopyranosyl)-3-keto-(1,27R)-octacosanedi	602.4797	1.094	HILICneg	1038804	697819	699416	633855	1550279	142404	1195584	1320805	1553206	1406297	
1,1'-(1,4-Dihydro-4-nonyl-3,5-pyridinediyl)bis[1-decanone]	575.4892	0.977	HILICneg	266247	220509	247594	329686	329365	1	276461	364753	363454	354352	
1,1'-[1,12-Dodecanediylbis(oxy)]bisbenzene	354.2549	12.912	Rpneg	2977	2176	2048	2397	1455	1054	1849	1682	1	1618	
1,1-Cyclopropanedicarboxylic acid	130.0271	1.26	HILICneg	168080	133230	71876	103889	189612	39568	104745	106621	93324	172829	
1,1-Cyclopropanedicarboxylic acid	148.038	1.043	Rpneg	15274	16968	23364	11374	8772	8378	11452	9814	27643	12417	
1,1-Diphenyl-2-(4-methoxyphenyl)propene	346.1563	11.59	Rpneg	1	2876	3740	6317	10812	2431	4401	7024	7638	5233	
1,1'-Thiobisethanethiol	153.994	0.749	Rpneg	4407	34891	5159	33583	33306	3944	6254	18349	42477	27799	
1,2,3-Tris(1-ethoxyethoxy)propane	308.2187	6.849	Rppos	824836	2100298	886767	1943185	2359198	1132901	1004512	1614071	2757791	1547069	
1,2-dihydrostilbene	364.2187	1.07	HILICneg	929261	834824	572724	832041	846074	1	352491	563968	356935	410467	
1,2-Epoxy-1,2,7,7',8,8',11,12-octahydro-psi,psi-carotene	604.4794	1.085	HILICneg	388850	266495	174043	173659	769617	174479	577599	646377	674338	782371	
1,2-Glyceryl dinitrate	182.0173	1.018	Rpneg	10256	1	11056	13137	11066	13281	8843	12482	12481	11658	
1,2-Propanediol, 3-[[2-(2-methoxyphenoxy)ethyl]amino]	240.1486	1.16	Rppos	204664	332363	335991	151528	391952	343744	271739	337089	335334	203517	
1,3,5-Trihydroxy-10-methylacridone	303.0733	5.113999	Rpneg	63037	39033	55777	59694	24763	40081	35342	51900	30958	40870	
1,3,5-Trihydroxy-10-methylacridone	303.0747	5.475999	HILICneg	65467	152845	227521	109191	147905	190057	419081	670101	605263	355752	
1,3-Dipropyl-8-cyclopentylxanthine [DPCPX]	303.2029	6.272999	Rppos	283912	160899	77441	76992	180455	144719	174443	161947	189322	207468	
PS(P-20:0/18:0)	785.5926	25.299	Rppos	2.26E+08	3.10E+08	2.90E+08	2.31E+08	4.85E+08	5.65E+08	5.02E+08	5.38E+08	5.78E+08	5.40E+08	
1,3-Dipropyl-8-cyclopentylxanthine [DPCPX] Esi+6.4159994	303.2011	6.415999	Rppos	185959	121107	55123	67683	92473	98254	157786	106160	152368	154295	
1,4-beta-D-Glucan	536.1614	2.647	Rppos	4309128	2991420	3530596	4030254	3267860	5076532	1976766	5140994	4638694	4077215	
1,5-Dihydroxy-3-methoxy-2-prenylxanthone	326.1163	6.17	HILICneg	55766	117138	101392	98411	59047	59850	53546	51821	27118	44382	
1,8-Diazacyclotetradecane-2,9-dione	226.1679	5.317	Rpneg	13095	4738	3958	6039	5714	2921	3895	4635	1	7119	
1?,25-dihydroxy-11-(4-hydroxymethylphenyl)-9,11-didehyd	537.3817	16.451	Rppos	208741	208797	228346	179649	193080	290384	214526	241819	299756	240544	

1?,25-dihydroxy-11?-phenylvitamin D3 / 1?,25-dihydroxy-1	492.3591	14.9	Rpneg	62963	45386	1	46151	70462	62656	1406	33578	42563	23658
1?,25-dihydroxy-21-nor-20-oxavitamin D3 / 1?,25-dihydrox	386.2831	8.199999	Rppos	313203	253241	290783	239391	361076	319724	345751	380677	281235	365107
1?,25-dihydroxy-22-oxavitamin D3 / 1?,25-dihydroxy-22-ox	418.3096	19.001	Rppos	992440	790706	13148272	1206170	645091	1899747	674055	689914	1020176	596227
1?,25-dihydroxy-22-oxavitamin D3 / 1?,25-dihydroxy-22-ox	418.309	17.668	Rppos	2686018	2415329	5262332	5513677	5384006	4943503	5402870	5116951	5205992	1879560
1?,25-dihydroxy-25,25-diphenyl-26,27-dinorvitamin D3 / 1	540.3593	13.807	Rpneg	5925	24628	34040	35882	46994	47432	32933	52328	45406	61016
1?,25-dihydroxy-25,25-diphenyl-26,27-dinorvitamin D3 / 1	540.3601	1.2	HILICneg	75266	172597	126595	146850	136302	94509	129886	89657	89550	136297
1?,25-dihydroxy-25,25-diphenyl-26,27-dinorvitamin D3 / 1	600.3811	12.304	Rpneg	28996	8400	7569	13236	4797	1	5367	6935	6483	1
1?,25-dihydroxy-25,25-diphenyl-26,27-dinorvitamin D3 / 1	600.381	12.304	Rpneg	27158	8400	7569	13236	4753	1	5367	6820	6603	1
1?,25-dihydroxy-25,25-diphenyl-26,27-dinorvitamin D3 / 1	600.3829	12.304	Rpneg	20421	7822	7084	10580	6393	1	5245	6066	6430	1
1?,25-dihydroxy-25,25-diphenyl-26,27-dinorvitamin D3 / 1	586.369	5.734001	HILICneg	150675	157200	157253	160338	138905	98382	149179	131177	124926	113087
1?,25-dihydroxy-3-deoxyvitamin D3 / 1?,25-dihydroxy-3-de	400.3337	13.308	Rpneg	25060	16969	6760	16751	12890	9291	12355	12570	13706	6864
1?-hydroxy-18-[m-(1-hydroxy-1-ethylpropyl)-benzyloxy]-23,	522.3723	0.883	HILICpos	254336	357797	272023	415017	288619	172023		166398	358604	224039
1?-hydroxy-23-[3-(1-hydroxy-1-methylethyl)phenyl]-22,22,	474.3115	13.354	Rpneg	1139	14797	10060	1665	2807	1143	6263	2108	1927	4994
10,11-Dihydro-10,11-dihydroxyprotriptyline	611.3749	20.755	Rppos	668284	681615	628448	683462	650172	629295	696341	675159	625678	646764
10,11-Epoxy-3,7,11-trimethyl-2E,6E-tridecadienoic acid	248.1783	8.552001	Rppos	191292	204322	226431	273298	124941	233995	234043	280406	261575	276570
10,20-Dihydroxyeicosanoic acid	408.3095	13.736	Rpneg	48936	22110	36239	33390	33231	27873	39823	46738	20882	31670
10,20-Dihydroxyeicosanoic acid Esi-13.813002	390.2969	13.813	Rpneg	19747	6872	17344	9417	8820	10190	12177	15793	31142	12829
10-Deoxymethynolide	295.2154	8.497001	Rppos	268352	303563	672078	245132	340496	245882	321261	332479	340838	390728
10E,12Z-Tetradecadienyl acetate	252.2092	1.132	HILICneg	287637	242526	231637	252896	228068	144992	270430	282547	322757	299586
10E,12Z-Tetradecadienyl acetate	252.2094	12.165	Rpneg	107504	74737	34264	68990	93386	65589	66362	137528	160859	134926
10-hydroxy-11-dodecenoic acid	214.1569	10.509	Rpneg	22838	14272	8267	10052	10594	8417	12647	11387	13793	14125
10-Hydroxy-8-nor-2-fenchanone glucoside	362.1561	5.474999	Rpneg	38226	41175	4374	5668	5249	2646	5251	7509	13751	7987
10-hydroxy-hexadecan-1,16-dioic acid	284.1984	7.827001	Rppos	829722	594096	927721	906809	592167	857313	1493217	616811	593362	592065
10-keto stearic acid	280.2381	9.387	Rppos	38262	76370	107458	123955	72565	150752	121252	102828	99880	102983
10-keto stearic acid	298.2503	11.707	Rpneg	41630	31951	29415	28568	31098	24022	31355	36909	38973	38445
10-keto stearic acid	298.2504	1.171	HILICneg	589618	553873	252149	376471	756135	1	384898	450979	448670	427659
10-keto stearic acid Esi-1.344	298.2521	1.344	HILICneg	291041	1	304676	236233	349901	451304	321935	382193	364050	397088
10-keto stearic acid Esi-11.968001	298.2505	11.968	Rpneg	17270	14035	1	42131	14240	32321	11424	14437	15744	10814
10-keto stearic acid Esi-11.968001 :1	298.2504	11.968	Rpneg	18546	13834	1	33036	34936	48468	38925	15042	15118	11160
10-keto stearic acid Esi-12.0165	298.2502	12.0165	Rpneg	54155	15040	44126	40230	41829	45952	12254	32559	15782	48379
10-methyl-hexadecanoic acid	270.2557	12.971	Rpneg	1310559	1123068	808546	1032527	955401	890393	914853	1637761	1629709	1002568
10-methyl-hexadecanoic acid Esi-12.905999	270.2559	12.906	Rpneg	1003569	739820	380204	716958	603877	462315	560534	454322	1	1
10-methyl-hexadecanoic acid Esi-12.906	270.2558	12.906	Rpneg	1003393	739997	379435	716943	601511	463007	559964	454127	1630376	317557
PS(P-20:0/18:1)	783.5767	23.424	Rppos	6.05E+07	8.17E+07	7.34E+07	6.00E+07	1.24E+08	1.26E+08	1.30E+08	1.36E+08	1.75E+08	1.41E+08
11,12,15-trihydroxy palmitic acid	286.2152	9.611	Rppos	560045	592499	631647	684220	584924	609753	719567	627292	671694	658763
11?-Misoprostol	399.2993	9.912001	Rppos	153825	154913	219735	181299	437598	160293	130703	146389	197809	153794
11?-Prostaglandin F1?	356.2556	11.657	Rpneg	14156	6508	3410	6757	11328	8684	4867	7543	9822	7963
11-Docosenyl acetate	366.3509	0.975	HILICneg	1138573	967363	612624	751287	558049	187082	595605	506775	793917	526239
11E,13Z-Hexadecadienyl acetate	280.2408	5.465	HILICneg	39103	131668	94456	115825	142470	104646	141598	138031	155372	121703
11-Hydroxyeicosatetraenoate glyceryl ester	440.2803	12.948	Rpneg	12691	5110	3437	5711	4456	1788	6941	5757	7422	2987
11S-hydroxy-hexadecanoic acid	272.2349	12.262	Rpneg	1	7639	5049	1	8074	5800	7558	7841	5753	5948
11S-hydroxy-hexadecanoic acid Esi-13.11	272.2362	13.11	Rpneg	7735	4483	3607	6298	3395	1	3928	3006	3322	3533
11Z,14Z,17Z-Eicosatrienyl isobutyrate	362.3177	13.315	Rpneg	9469	7543	5151	7898	5928	4502	5566	6751	6059	5795
11Z-octadecen-9-ynoic acid	278.2255	1.116	HILICneg	1090084	1370087	1356866	1223840	1131834	343519	1217379	1497697	891890	918369
11Z-tetradecenoyl-CoA	979.27	24.722	Rppos	14992883	16895324	13476324	14557647	13207200	11486773	10197294	12033509	16396095	12700902
12,13-epoxy-9-octadecenoic acid	296.2345	11.559	Rpneg	16625	47579	56592	36891	53569	51867	60527	78460	76666	74699
12,13-epoxy-9-octadecenoic acid	296.2365	1.314	HILICneg	556427	703412	736433	529103	851584	339936	794511	913075	708294	798715
12,13-epoxy-9-octadecenoic acid Esi-11.775001	296.2353	11.775	Rpneg	1	16233	12700	8393	28193	1	7858	17912	9804	8753
12,14-Triacontanedione	450.4424	14.598	Rpneg	67059	33264	10963	35909	29761	14740	17173	20542	9484	6280
12,15-epoxy-13,14-dimethyleicosa-12,14-dienoic acid	350.2823	12.982	Rpneg	14685	15660	22185	23698	8195	5991	15590	12208	11673	9928
12,15-epoxy-13,14-dimethyleicosa-12,14-dienoic acid Esi-1	350.2783	12.576	Rpneg	7561	6480	5677	7604	7563	5659	6278	5391	5867	1
12:0 Cholesteryl ester	614.5309	12.86	Rpneg	40847	32478	28294	28174	37688	40301	38726	46822	44781	42057
12:0 Cholesteryl ester Esi-12.858999	628.544	12.859	Rpneg	8339	6007	5204	5576	6080	8351	7865	8774	7430	7067
12alpha-12-Hydroxy-7,13-abietadien-18-oic acid	300.2093	9.835	Rppos	170202	178329	191521	206402	177211	182357	197069	181552	188216	207762
PS(P-20:0/18:2)	781.561	22.976	Rppos	3.84E+08	3.80E+08	3.93E+08	4.16E+08	3.10E+08	3.43E+08	3.57E+08	3.30E+08	2.97E+08	3.17E+08
12alpha-Fluoro-11beta,17beta-dihydroxyandrosta-1,4-dien	366.1852	12.451	Rpneg	3569	2728	7965	2310	2630	2860	2189	1744	1	2384
12-Heptadecynoic acid	266.2239	12.408	Rpneg	22711	16540	6551	15320	11956	7477	15250	15906	17762	10533
12-HETE-Gly	377.2603	12.859	Rpneg	13440	3635	1923	4396	7861	7390	13569	14196	13476	11091
12-hydroxy-10-dodecenoic acid	214.1576	7.547	Rppos	875771	988487	615328	2247466	818421	710493	602580	1142728	639831	1271719
PS(P-20:0/20:2)	809.5933	20.29	Rppos	1.44E+08	97218808	92766800	1.03E+08	1.08E+08	70795992	1.15E+08	80272232	89693568	75933672
12-hydroxy-3Z-dodecenoic acid	213.1718	7.211	Rppos	369555	366960	821982	444604	343364	420618	738863	530280	491853	416071
12-hydroxy-8E,10E-heptadecadienoic acid	264.2087	8.617999	Rppos	343017	420052	458649	501323	415232	469835	509158	527365	519671	532061
12-oxo-9Z-octadecenoic acid	278.2232	9.767999	Rppos	173051	102117	146050	91605	147050	214079	184624	303032	197795	287948
12S-HpOME(13E)	314.2458	10.586	Rpneg	13322	8913	11430	13468	17915	9944	7138	9415	8437	11557
12S-HpOME(13E) Esi-10.5859995	314.2453	10.586	Rpneg	13047	8611	11430	13579	13806	9984	7043	9145	8422	8321
12S-HpOME(13E) Esi-10.907999	314.2436	10.908	Rpneg	13002	4510	8332	1	7329	4784	5242	10701	6783	5805
12S-HpOME(13E) Esi-11.054	314.2438	11.054	Rpneg	3632	2410	8903	3196	2251	3175	2258	7556	1	5854
12S-HpOME(13E) Esi-12.880999	314.2464	12.881	Rpneg	10101	6456	5063	6978	5852	4088	4372	5609	7343	8412
13(14)-EpDPE	344.2372	11.799	Rpneg	34081	21042	21582	18483	15737	16393	21015	33725	33899	20047
13(14)-EpDPE Esi-11.798999	344.2376	11.799	Rpneg	34332	21353	22011	18545	15669	17737	21186	34992	33595	19673
13(14)-EpDPE Esi-11.798999 :1	344.2375	11.799	Rpneg	34362	21871	22223	18329	15570	17580	21265	34651	33550	19984
13,14-dihydroxy-docosanoic acid	418.3288	14.319	Rpneg	92877	28861	97174	62955	29866	98733	29211	113673	82799	82830
13,16-Docosadienoic acid	336.3	0.987	HILICneg	118844	124144	109109	121909	177385	26951	93278	108352	131087	102648
13,16-Docosadienoic acid	336.3031	13.24	Rpneg	97477	69136	37468	66180	55481	39313	56305	65474	58762	56462
13-Cyclohexyltridecanoic acid	314.2817	13.203	Rpneg	5137	8017	4177	238012	1	1	5149	4189	4940	1
13E-Docosenamide	337.3346	14.853	Rpneg	215537	196122	231032	314861	719994	200054	575711	228532	122994	57374
13E-Docosenamide	337.3348	0.975	HILICpos	5664983	1660324	1966033	2543004	5137878	942867		2958401	1353694	5306471
13E-Docosenamide Esi-14.739	337.3345	14.739	Rpneg	200517	169436	222222	347368	638511	189970	753245	271535	125865	46491
13-Hydroxy-9-methoxy-10-oxo-11-octadecenoic acid	342.2385	11.665	Rpneg	4298	10481	5315	7523	6393	3712	1	8962	1	4356
13-Hydroxy-9-methoxy-10-oxo-11-octadecenoic acid	359.2662	7.858001	Rppos	302936	181939	133740	138944	252182	249119	293854	323175	251658	337721
13-methoxy-heneicosanoic acid	356.3292	13.421	Rpneg	20371	8784	5199	10261	7320	5753	6772	7739	7189	5817
13-methyl-hexadecanoic acid	270.2555	1.106	HILICneg	1037098	836728	662854	782937	1304890	248199	597856	740445	1305669	876044
14,15-EE-8(Z)-E	324.264	12.692	Rpneg	12437	6777	1835	6942	2852	2382	2864	2894	6422	4813
14,19-Dihydroaspidospermatine	340.2132	12.856	Rpneg	2117	1509	1096	1088	2376	1711	2232	2595	2747	2324
14,19-Dihydroaspidospermatine	340.2173	1.037	HILICneg	210044	341062	275289	267760	212836	1	143282	140933	156677	175303
14:0 Cholesteryl ester	642.5604	13.17	Rpneg	13722	8508	6558	7088	7995	7249	8981	8206	9449	9601
14'-apo-beta-carotenal	328.2404	13.452	Rpneg	75096	98814	101093	116047	42592	12485	24429	17619	9377	25024
14'-apo-beta-carotenal Esi-13.451002	328.2402	13.451	Rpneg	77523	65094	66945	94845	1	19121	22485	14910	12734	8103
14-fluoro-myristic acid	292.2054	0.717	HILICneg	22077	11806	20527	21278	23843	35985	19723	53607	49729	12618
14-fluoro-myristic acid	292.2065	12.375	Rpneg	12409	13574	7974	9592	13109	10279	7685	15757	9841	11825
14-fluoro-myristic acid Esi-0.70800006	306.2215	0.708	HILICneg	22171	11556	22073	20570	18493	27742	19354	36201	34826	11826
14-hydroxy-12-tetradecenoic acid	242.1885	11.534	Rpneg	43818	24447	15322	18816	21321	14906	25922	27226	26834	29024

1-Naphthylacetylspermine	387.2983	8.625	Rppos	449473	306475	374818	295973	389853	310878	346930	433061	282796	347643
1-Naphthylacetylspermine	430.2966	12.536	Rpneg	18276	5286	5710	10452	7799	2845	4623	7034	7274	5171
1-Naphthylacetylspermine Esi+11.002999	369.2891	11.003	Rppos	464990	442111	503570	558471	470904	474866	521897	483584	505136	469817
1-Naphthylacetylspermine Esi+8.78	387.2983	8.78	Rppos	380330	203371	272437	187319	252262	278617	314529	327738	263694	340627
1-NM-PP1	331.1803	11.61	Rpneg	2406	2193	1502	1922	1	1	1051	1	1	1
1-Octadecanol	269.3079	11.079	Rppos	447156	222115	212273	196450	303524	167449	186135	243951	199218	166737
1-Oleoyl-2-acetyl-sn-glycerol	397.319	10.162	Rppos	251676	811126	807838	852068	1713805	1441447	596926	1028464	1231675	1501798
1-Oleoyl-2-acetyl-sn-glycerol	415.3331	2.859	HILICpos	3681590	1300607	1206704	970602	589407	922558		952493	1455742	1629645
1-Oleoyl-2-acetyl-sn-glycerol	458.3256	12.919	Rpneg	30316	11351	12817	18525	12976	6943	6960	9293	10552	4404
1-Oleoyl-2-acetyl-sn-glycerol Esi+10.041	415.3296	10.041	Rppos	672806	851931	1239067	1091117	1168067	761968	814890	1003854	659706	815110
1-Oleoyl-2-acetyl-sn-glycerol Esi+10.282999	415.3297	10.283	Rppos	520972	450008	742574	547161	597650	541835	656351	664708	514734	561475
1-Oleoyl-2-acetyl-sn-glycerol Esi+10.995001	397.3165	10.995	Rppos	171083	264603	464342	189119	425839	322155	346308	201962	264593	129212

1-Oleoyl-2-acetyl-sn-glycerol Esi+27.100002	813.6355	27.1 Rppos	987595	940831	1117030	940353	1033112	1553912	1264521	1247827	1509781	1426117
1-Oleoyl-2-acetyl-sn-glycerol Esi-12.651	458.321	12.651 Rpneg	10226	4000	4249	5629	4423	1	3236	1	1	1
1-Oleoyl-2-acetyl-sn-glycerol Esi-12.917	458.3238	12.917 Rpneg	30316	11351	12817	1	12970	6943	2419	9293	10552	2018
1-Palmitoyllysophosphatidylcholine	495.3321	12.928 Rppos	1.96E+07	1.78E+07	1.95E+07	1.85E+07	1.18E+07	1.67E+07	1.41E+07	1.22E+07	1.16E+07	1.08E+07
1-Palmitoyllysophosphatidylcholine Esi+12.372001	495.3329	12.372 Rppos	1882274	1769337	1846415	1768101	1394067	1916893	1571663	1568019	1468377	1311391
1-Phenyl-1,3-eicosanedione	386.3156	13.241 Rpneg	9662	7769	5772	6792	5706	5146	5959	5456	6098	4672
1-Phenyl-1-propanol	136.089	6.623 Rppos	320267	418436	500460	434790	436995	536916	456023	430218	462335	475801
1-Phenyl-5-mercaptotetrazole	224.0358	13.05 Rpneg	3253	6707	6439	5437	6512	15486	4063	9321	13853	9229
1-Phenyl-5-mercaptotetrazole	224.0374	0.892 HILICneg	198492	153746	422706	188489	125226	1568042	278139	510493	284035	213984
1-Phenylethylamine	121.0894	3.085 HILICpos	561359	562132	598848	633717	637723	601871		547111	550593	679344
2-(?-D-Mannosyl)-3-phosphoglycerate	348.0465	0.795 Rpneg	47063	194259	203324	116767	116930	34409	210121	29569	46372	55818
2-(2-Methylbutanoyl)-9-(3-methyl-2E-pentenoyl)-2b,9a-dihy	430.27	11.058 Rpneg	14409	11979	1655	6746	8637	19916	6900	7769	14130	16184
2(3H)-Furanone	84.0208	0.904 Rpneg	9505	11206	21495	12812	12515	17186	17542	8752	14687	11860
2(3H)-Furanone Esi-0.904	84.0206	0.904 Rpneg	9589	11834	19824	13142	12490	15510	17639	8175	13220	10936
2-(4-Chloro-3,5-dimethylphenoxy)-N-(2-phenyl-2H-benzotri	466.1416	10.703 Rpneg	4395	5288	4537	2898	2753	3016	5005	4194	4083	4041
2-(4-Chloro-3,5-dimethylphenoxy)-N-(2-phenyl-2H-benzotri	466.1429	10.993 Rpneg	3339	4766	3214	2473	2303	2244	3572	3735	3251	3198
2-(8-[3]-ladderane-octanyl)-sn-glycero-3-phosphoethanolam	533.3069	5.795 HILICneg	50293	59081	51890	52954	35979	30610	36043	30991	29560	29420
2-(8-[3]-ladderane-octanyl)-sn-glycero-3-phosphoethanolam	565.3354	13.229 Rpneg	116414	12406	9582	12871	2754	1	10660	12471	4311	6548
2-(Fluoromethoxy)-1,1,3,3,3-pentafluoro-1-propene (Comp	226.0067	0.889 Rpneg	23934	17542	17303	14827	11962	13067	7462	12299	9812	8412
2-(Fluoromethoxy)-1,1,3,3,3-pentafluoro-1-propene (Comp	226.0077	1.035 Rpneg	12509	12345	12396	11161	15185	15791	15720	6197	9620	8329
2-(Methylthio)ethanol	92.03	12.007 Rpneg	4119	5774	5241	3505	5719	10488	3497	6942	11294	10765
2-(Methylthio)ethanol Esi-13.377	92.0294	13.377 Rpneg	1	1	5208	5056	3673	10155	3996	6122	11877	9442
2-(Methylthio)ethanol Esi-13.639	92.0295	13.639 Rpneg	11416	10884	11205	6138	6067	8241	4954	8791	13600	10262
2-(Octylthio)ethanol	250.1593	11.243 Rpneg	1	35063	10415	24709	31063	1	7662	19475	39323	16821
2,2,4,4-Tetramethyl-6-(1-oxobutyl)-1,3,5-cyclohexanetrion	234.1255	7.692 Rppos	419657	484362	478861	497941	443804	475350	500468	516460	537444	522330
2,2,9,9-tetramethyl-undecan-1,10-diol	229.2404	8.266999 Rppos	1023203	1097952	1194977	1124215	1063165	1163080	1089398	1162408	1100073	1054366
2,2-Dimethyloxirane	72.0575	1.125 Rpneg	8919	1	1	1	12413	14452	9015	13653	17588	14115
2,3,4-Trimethyl-3-pentanol	129.1516	5.184 Rppos	985264	1422100	1014795	1180433	1497009	1070685	1021883	1115759	1346818	1151233
2,3,4-Trimethyl-3-pentanol Esi+6.866	129.1514	6.866 Rppos	299031	305059	323413	281196	251603	351139	310352	275374	263557	304835
2,3,5-Trimethyl-6-[4-(methylthio)butyl]pyrazine	270.1379	0.943 HILICneg	324175	239631	135523	275233	278753	82220	64694	342780	135409	108223
2,3-Butanediol	89.0836	0.838 Rppos	177717	949653	847864	1040383	626469	935781	313051	385910	709869	486828
PS(P-20:0/22:4)	833.5921	24.462 Rppos	2.93E+08	2.5E+08	3.16E+08	3.24E+08	2.42E+08	2.75E+08	2.63E+08	2.38E+08	2.17E+08	2.41E+08
2,3-dihydro-1,4-benzodioxin-2-ylmethyl dimethylcarbamat	237.0994	6.31 Rpneg	3170	11240	1057	9707	16001	1195	1445	11609	21002	7681
2,3-Dihydroxy-2,4-cyclopentadien-1-one	112.0139	0.923 Rpneg	144748	111035	154256	136476	88008	110140	74754	121290	100861	98340
2,3-Dihydroxy-2,4-cyclopentadien-1-one Esi-0.6999999	112.0162	0.7 Rpneg	20899	24112	15711	23553	33104	16852	18071	10175	28590	18768
2,3-Dihydroxy-2,4-cyclopentadien-1-one Esi-0.9250001	112.0141	0.925 Rpneg	121039	169790	143698	120130	117565	127998	103567	108622	131966	89741
2,3-Dimethylsuccinic acid	146.058	6.341 HILICneg	601975	549962	181506	407730	391078	84504	42567	36444	15898	31959
2,3-dinor Fluprostenol	430.1615	5.055 Rpneg	5576	3437	3359	3947	2975	3202	2603	3949	3213	5126
2,3-dinor Thromboxane B1	344.2198	9.363 Rpneg	75881	46912	40914	49454	51037	49399	40103	48493	55402	38337
2,3-dinor Thromboxane B1 Esi-10.32	344.2202	10.32 Rpneg	1	5726	4584	5840	10081	3088	4188	6947	4061	1896
2,3-dinor Thromboxane B1 Esi-10.741999	344.2193	10.742 Rpneg	1	3164	2935	3246	4356	1908	2860	3864	2465	1514
2,3-dinor Thromboxane B1 Esi-9.079001	344.2195	9.079001 Rpneg	23516	19384	17049	25555	59907	18617	16714	20179	23862	16789
2,3-dinor Thromboxane B1 Esi-9.581	344.2192	9.581 Rpneg	5464	7504	3864	5420	5904	4535	4139	5341	4346	1
2,3-dinor Thromboxane B1 Esi-9.852999	344.221	9.852999 Rpneg	2738	4846	4332	5178	5599	3461	4665	6198	5912	6314
2,4,6-Triethyl-1,3,5-trioxane	191.1517	5.152 HILICpos	281962	260218	191124	190753	442930	271422		130894	137937	256400
2,4,6-Trimethyl-1,3,5-trithiane	226.0153	12.913 Rpneg	1	1956	1586	1	1541	7480	1169	3828	8912	11800
2,4-Dichlorobenzoate	235.9648	5.312 HILICneg	1595803	1281278	1267237	1248726	1085245	572478	714554	783284	618350	722501
2,4-Dihydroxy-7,8-dimethoxy-2H-1,4-benzoxazin-3(4H)-one	287.0661	1.106 HILICneg	98126	160920	120431	162358	190456	43343	89317	106061	74015	179660
2,4-Dihydroxybenzoic acid	154.0268	5.705 Rpneg	90254	45194	32919	37863	57102	56009	56076	75928	53067	38641
2,4-dimethyl-2-eicosenoic acid	338.3208	0.985 HILICneg	909621	639246	487830	578420	691791	196130	541682	582491	697061	536141
2,4-dimethyl-2E-tetradecenoic acid	254.2255	5.497001 HILICneg	71598	78425	31200	46921	63137	36641	41959	104234	56977	33928
2,4-dimethyl-2E-tetradecenoic acid	272.2356	12.661 Rpneg	37756	28274	15798	24894	22271	22133	22685	27882	27963	23947
2,4-dimethyl-2E-tetradecenoic acid Esi-12.9522	254.2247	12.9522 Rpneg	12925	6144	8084	20795	19445	6620	13524	17923	23630	31395
2,4-Dimethyl-2-pentacosenoic acid	408.3952	13.907 Rpneg	24792	5434	4650	4897	5814	4249	3791	1435	3916	1
2,4-Dimethylbenzaldehyde	138.0423	1.493 Rppos	475689	1486263	168346	1828546	4578334	310719	320514	3482287	4805008	2214790
2,6,10-trimethyl-undecanoic acid	227.2248	11.126 Rpneg	194220	211536	261503	265955	221136	250460	260100	247550	264438	288478
2,6,10-trimethyl-undecanoic acid	228.2089	12.316 Rpneg	2687713	2349927	1780195	2291650	2118282	1751519	2058151	2223351	2400755	1890198
2,6,10-trimethyl-undecanoic acid Esi-12.107001	228.2092	12.107 Rpneg	25289	18955	9055	16379	16734	11134	12093	16174	12038	9598
2,6,10-trimethyl-undecanoic acid Esi-12.316001	228.2089	12.316 Rpneg	2690920	2337845	1781731	2294547	2117990	1753748	2066898	2224860	2406618	1894652
2,6,10-trimethyl-undecanoic acid Esi-12.667	228.2092	12.667 Rpneg	4260	5452	3999	4599	5039	6862	5989	7160	7045	6651
2,6,10-trimethyl-undecanoic acid Esi-12.9609995	228.209	12.961 Rpneg	4735	5694	10501	1	8119	9709	9178	8764	9404	9824
2,6,10-trimethyl-undecanoic acid Esi-13.380999	228.2094	13.381 Rpneg	5832	3286	4659	4321	1	6399	3385	9000	8324	21153
2,6-Dichlorobenzamide	188.977	1.071 HILICneg	73947	111549	70491	75908	108884	65403	95578	91878	83951	79575
2,6-Dimethyl-1,8-octanedioic acid	202.1208	7.093 Rppos	540197	506288	575740	432445	592305	437892	379222	727374	1116433	540508
2,6-Dimethyl-1,8-octanedioic acid	202.1209	1.504 HILICneg	34545	31908	1	29804	50783	31021	11576	22773	27596	1
2,6-Dimethyl-7-octene-1,6-diol 8-O-glucoside	316.1877	7.752999 Rppos	826767	876785	839818	906255	900196	876328	761784	800562	1060479	905910
2?-(3-Hydroxypropyl)-1?,25-dihydroxy-19-norvitamin D3	444.361	20.29 Rppos	720176	787152	1188564	589002	1197756	1459920	1007013	1130355	1090598	1019964
2?-(3-Hydroxypropyl)-1?,25-dihydroxy-19-norvitamin D3 Es	444.3618	18.919 Rppos	268159	272156	1	309623	129574	222838	341899	262789	327965	280183
2?-(3-Hydroxypropyl)-1?,25-dihydroxy-19-norvitamin D3 Es	484.3532	19.172 Rppos	277689	291117	225244	349499	134648	366856	359871	291374	440232	314495
2?-(3-Hydroxypropyl)-1?,25-dihydroxy-19-norvitamin D3 Es	444.3616	19.173 Rppos	623557	755279	672344	768082	209919	689522	791222	531921	972263	682138
2?-(3-Hydroxypropyl)-1?,25-dihydroxy-19-norvitamin D3 Es	444.3615	19.525 Rppos	360621	715615	654365	442771	278172	599777	453702	341578	493842	421146
2?-(3-Hydroxypropyl)-1?,25-dihydroxy-19-norvitamin D3 Es	444.3604	20.077 Rppos	368167	315437	617960	448696	548940	464887	500965	471282	503649	488347
2?-(3-Hydroxypropyl)-1?,25-dihydroxy-19-norvitamin D3 Es	444.3611	21.587 Rppos	380647	326709	496445	438390	528054	515494	556765	374622	557338	431752
2?-Fluoro-19-nor-22-oxa-1?,25-dihydroxyvitamin D3	424.3023	7.443999 Rppos	216943	1219353	292456	1070851	1573386	254637	295584	890536	1913198	858830
2-[4-(3-Hydroxypropyl)-2-methoxyphenoxy]-1,3-propanedio	238.1204	7.303001 Rppos	538358	1151414	1151630	1296235	1092028	1144276	955818	1014771	1381434	1084581
2-[4-(3-Hydroxypropyl)-2-methoxyphenoxy]-1,3-propanedio	273.1585	5.922 Rppos	403151	591435	638967	483276	374212	402674	529545	376144	447832	428777
20:2(5Z,9Z)(11Me,15Me,19Me)	350.3186	13.347 Rpneg	7424	4412	3061	5309	4286	3517	4579	4376	4478	5144
20:2-Glc-Campesterol	852.6857	24.322 Rppos	1415977	747713	1138568	1086749	1262229	1306284	1413334	1280494	998442	1092089
20-Tetracosene-1,18-diol	385.3899	17.733 Rppos	416222	276965	230129	213731	280416	246153	265748	233852	208721	245292
22:0-Glc-Cholesterol	869.7442	22.422 Rppos	141297	224083	314933	246479	457960	407419	655890	555512	213303	690694
22:2(5Z,9Z)(13Me,17Me,21Me)	424.3536	13.241 Rpneg	7156	3867	1	3921	3397	2012	3228	2298	2289	1
22:2(5Z,9Z)(13Me,17Me,21Me) Esi-13.240999	424.354	13.241 Rpneg	7156	3867	1	3921	3397	2012	3228	2298	2289	1
22:3(5Z,9Z,19Z)(13Me,17Me,21Me)	376.3317	0.937 HILICneg	1	74702	95105	88250	96757	15282	98784	91344	1	71367
22:4(7Z,13Z,16Z,19Z)	332.2712	12.913 Rpneg	1166081	1163342	902066	1305071	743520	547710	675075	819176	793655	807637
22-iso-teinemine	461.3546	13.56 Rpneg	12803	8615	8304	10143	9224	8838	9467	9875	13172	11392
22-Tricosenoic acid	352.3331	13.489 Rpneg	166339	52075	64397	46187	56300	54695	60881	48793	59333	43132
24-Nor-5?-chol-22-ene-3?,12?-diol	346.29	14.497 Rpneg	877629	454340	316384	628697	809248	658167	829371	894031	470315	408988
24-Nor-5?-chol-22-ene-3?,12?-diol Esi-12.701999	346.2901	12.702 Rpneg	43424	43042	52302	41453	84985	111514	92389	85088	76176	90541
24-Nor-5?-chol-22-ene-3?,12?-diol Esi-12.706	346.2901	12.706 Rpneg	56735	52149	63437	47753	108025	121259	96650	94110	84157	99454
24-Nor-5?-chol-22-ene-3?,12?-diol Esi-13.039	346.2901	13.039 Rpneg	39014	243874	292691	217410	304140	375258	38908	433661	441497	276729
24-Nor-5?-chol-22-ene-3?,12?-diol Esi-13.050001	346.2902	13.05 Rpneg	224976	371494	438625	325632	378159	438383	283434	246298	348186	372975
24-Nor-5?-chol-22-ene-3?,12?-diol Esi-14.550001	346.2899	14.55 Rpneg	877629	757090	1	1	759891	799451	623449	659542	167627	231054

24R-methylcholest-22E-en-3beta,4beta,5alpha,6alpha,8bet	574.338	12.448	Rpneg	2294	1004	1089	1445	2242	834	1189	1834	3583	1
25:0(18Me)	413.4215	19.436	Rppos	470871	392651	338145	387104	373601	366454	303376	344376	292250	307378
25:0(23Me)	396.3938	0.962	HILICneg	103768	102118	49052	96469	84326	54560	91300	106165	182186	73182
26-(2-Glucosyl-6-acetylglucosyl]-1,3,11,22-tetrahydroxyerg	842.4293	11.932	Rpneg	11854	2039	15684	12324	14759	7267	8599	9514	12455	11063
26,26,26,27,27,27-hexafluoro-1?,25-dihydroxyvitamin D3	584.2879	11.882	Rpneg	3964	1886	1163	1279	1157	1117	2801	1234	2336	1440
26,26,26,27,27,27-hexafluoro-1?,25-dihydroxyvitamin D3	524.2743	12.562	Rpneg	1	1	1	1	5065	4717	5808	11019	9258	10163
26,26,26-trifluoro-25-hydroxyvitamin D3 / 26,26,26-trifluo	454.3045	12.129	Rpneg	1	1	1	1	2403	2304	3837	4681	5595	4536
26,27-dinor-3alpha,6alpha,12alpha-trihydroxy-5beta-chole	452.312	10.893	Rpneg	6378	4085	4243	3998	4033	4205	3671	3863	3783	4025
27:3(5Z,9Z,20Z)	404.366	0.933	HILICneg	282959	174823	240549	234531	233424	108394	263549	248081	244326	187398
28:2(5Z,9Z)(6Br)	498.3073	12.567	Rpneg	2462	4871	2021	3675	2174	1213	2475	2079	3420	3362
2-Acetyl-1,5,6,7-tetrahydro-6-hydroxy-7-(hydroxymethyl)-4	199.0822	0.985	Rpneg	34036	30326	22346	28843	52235	42890	40453	81314	72017	63080
2-Acetylthiazole	127.0116	0.848	Rpneg	40072	33675	42554	35974	35898	45019	47762	41383	33047	39659
2-amino-14,16-dimethyloctadecan-3-ol	335.3174	16.929	Rppos	99412	162913	221403	127831	456586	142580	569164	221838	164574	52408
2-Amino-3-methyl-1-butanol	103.0998	0.834	Rppos	7243067	4745297	4120581	5898217	9088376	6417088	6637399	10300815	6878420	7892504
2-amino-tetradecanoic acid	243.2191	9.192	Rppos	205334	202073	242308	248296	219368	235160	226155	238290	263750	253719
2-Angeloyl-9-(3-methyl-2E-pentenoyl)-2b,9a-dihydroxy-4Z,1	873.5358	23.455	Rppos	394381	509682	179352	355596	806588	573169	589921	663929	732439	509228
2-Benzoxazolol	135.0325	2.176	HILICpos	1427652	1479614	1091249	962421	903312	746155		1215033	141795	937349
2-BROMOETHANOL	169.959	1.032	Rpneg	5540	5719	5416	4834	21849	23963	28157	2501	6225	3840
2-Butoxyethanol	117.1155	1.602	Rppos	190679	357622	344380	451868	503854	707681	507079	467746	506894	440185
2-Carboxy-4-dodecanolide	288.1576	6.570001	Rpneg	13176	17231	8024	18533	22598	8810	8067	14626	21563	12959
2-carboxy-Pyrimidine	294.0599	5.312	HILICneg	210022	221127	178916	195919	157441	87755	128501	117096	107441	109099
2-chloro-3-Deazaadenosine	646.1283	0.991	HILICneg	35483	70963	56184	55098	75443	1	67570	80713	87333	59195
2-Chloro-3-oxoadipate	240.0016	0.99	Rpneg	46282	49728	47688	46384	45170	38653	51599	40409	36153	42023
2-C-Methyl-D-erythritol 2,4-cyclodiphosphate	277.9982	0.993	Rpneg	15560	12757	11908	13394	17175	19228	14277	12216	12673	12609
2-Deoxy-5-keto-D-gluconic acid	178.0461	0.805	Rpneg	2839	10414	10430	9696	10813	1	3707	10259	8712	7743
2-Diethylaminoethanol	117.1153	5.014	HILICpos	3132887	3506403	3420004	6108076	6771893	2098504		3133122	4625176	5856619
2-Diethylaminoethanol	117.1169	0.941	Rppos	1407496	3641997	1532229	2370981	3674013	2041798	713908	2021086	5054882	2160626
2-Diethylaminoethanol Esi+3.5429997	117.1156	3.543	HILICpos	3699822	3234021	3291525	4160864	8238466	3054683		3796848	4640614	5581709
2-Dimethylamino-5,6-dimethylpyrimidin-4-ol	167.1059	7.41	HILICpos	77531	69166	61175	104303	298127	138190		177522	288485	284240
2-Dodecylbenzenesulfonic acid	326.1923	12.451	Rpneg	257628	185129	484141	177847	166033	133316	153955	153647	153225	114697
2-Dodecylbenzenesulfonic acid Esi-12.215	326.1918	12.215	Rpneg	114671	80685	1	73474	71515	72681	73501	73432	64985	68643
2-Dodecylbenzenesulfonic acid Esi-12.216001	326.1917	12.216	Rpneg	100150	67208	73159	60976	59328	60811	61578	61170	57619	57007
2-Dodecylbenzenesulfonic acid Esi-12.451001	326.1924	12.451	Rpneg	257507	185022	545120	177847	166137	133316	153955	154077	125022	114697
2-Dodecylbenzenesulfonic acid Esi-12.451001:1	326.1922	12.451	Rpneg	257521	185129	544332	177847	167235	133316	154041	155057	153225	23833
2E,6E-Octadienyl acetate	150.1043	6.606999	Rppos	1828291	1956063	1539076	1651056	1753726	1776357	1704255	1619888	1688418	1674091
2-Ethoxythiazole	175.0316	5.013	HILICneg	127615	361568	285853	382534	171295	179330	157337	149860	100069	217431
2-Ethyl-1-hexanol sulfate	210.0931	10.042	Rpneg	4673	16151	5444	10288	12754	5916	5257	9557	16009	8961
2-Heptyl butyrate	200.1776	11.644	Rpneg	1630955	1549065	1417020	1450277	1517259	1415078	1434119	1474609	1491395	1405733
2-Heptyl butyrate Esi-11.641999	200.1777	11.642	Rpneg	13607	1548874	1405722	6679	1517259	1425699	1426531	1475068	1490062	5777
2-Heptyl butyrate Esi-12.472	200.1779	12.472	Rpneg	2719	2618	3737	3450	3341	3494	3379	4142	7443	7543
2-heptyl-nonanoic acid	256.2404	12.93	Rpneg	298446	320052	276131	306417	306119	288939	113089	340983	319423	296746
2-heptyl-nonanoic acid Esi-13.192999	256.2407	13.193	Rpneg	106957	127568	116929	124288	303688	13034	107270	106666	51521	47497
2-heptyl-nonanoic acid Esi-13.194	256.2409	13.194	Rpneg	131901	52646	119763	55806	41346	52431	50471	52733	14027	48005
2-heptyl-nonanoic acid Esi-13.773001	256.2409	13.773	Rpneg	58109	1	43443	24307	1	6021	13290	77464	45102	1683
2-heptyl-nonanoic acid Esi-13.809999	256.2403	13.81	Rpneg	105169	1	43443	24307	48861	6021	8642	36677	13920	2539
2-heptyl-nonanoic acid Esi-14.801	256.2396	14.801	Rpneg	51535	165081	93674	139816	95380	129139	124568	164034	143937	146990
2-hydroxy palmitic acid	272.2351	12.547	Rpneg	319285	200169	180245	257672	176466	173853	172098	230416	282951	205121
2-hydroxy palmitic acid Esi-12.073999	272.2349	12.074	Rpneg	1	7759	7784	7758	9452	6254	8409	7796	1	11428
2-Hydroxy-22-methyltetracosanoic acid	398.3738	13.679	Rpneg	19182	7263	3546	6854	5146	4395	5645	5669	6115	3152
2-Hydroxy-24-keto-octacosanolide	452.3834	13.411	Rpneg	10510	4431	1265	5298	3002	1632	3232	1952	2018	1836
2-Hydroxy-dAMP	347.063	1.297	Rppos	134096	256528	384254	213618	168472	81173	649930	108288	109131	144966
2-Hydroxyfelbamate	300.096	8.463999	HILICneg	62507	48213	51637	56706	56820	102634	66520	72687	58224	53862
2-Hydroxyhepta-2,4-dienedioate	218.0432	4.123001	HILICneg	214809	1	105493	169036	179860	1	60040	1	1	14543
2-Hydroxyhexadecanoic acid	272.2355	12.45	Rpneg	59015	41837	30957	44038	36052	26373	42639	35854	42432	39157
2-Hydroxyhexadecanoic acid	272.2356	1.404	HILICneg	143200	103235	94629	177859	162706	201786	91948	147329	111297	91125
2-Hydroxyhexadecanoic acid Esi-11.349	272.2348	11.349	Rpneg	12150	15534	13078	14008	18267	11401	13799	13063	11361	8858
2-Hydroxyhexadecanoic acid Esi-11.349:1	272.2338	11.349	Rpneg	14123	13294	12966	13632	17774	9844	12023	12432	11091	12813
2-Hydroxyhexadecanoic acid Esi-5.833	272.2358	5.833	HILICneg	19439	51605	32385	54246	36687	30013	28984	26501	36507	26775
2-Hydroxynicotinic acid	139.0271	2.277	Rpneg	10083	124535	12483	72342	172629	11879	13313	61816	148709	44367
2-Hydroxypropylphosphonate	280.0471	5.186	HILICneg	1923040	5428911	5630641	5510207	4371151	3112299	3546545	3441179	3241530	3143996
2-hydroxy-tricosanoic acid	370.3426	13.508	Rpneg	19020	8222	5237	8899	8564	5345	7969	7328	6623	5668
2-Iodophenol	265.9423	1.028	Rpneg	10262	9336	8723	8858	39069	43387	52258	4734	10291	7466
2-Isopropyl-1,4-hexadiene	124.1248	12.596	Rpneg	5493	5184	4018	3930	6291	1	5661	6313	5094	6010
2-Keto valeric acid	116.0466	11.63	Rpneg	5742	6842	3780	6589	3132	3699	7698	6791	10060	5943
2-Keto valeric acid	116.0473	5.108	HILICneg	160730	51937	65296	75696	104001	119355	121237	141531	125664	131868
2-Linoleoyl Glycerol	400.2816	10.961	Rpneg	18719	10590	11365	12227	11080	12301	9268	12025	12493	10363
2-Linoleoyl Glycerol Esi-10.751	400.2806	10.751	Rpneg	5662	4386	2043	1	1	5154	2204	3385	5256	4559
2-methoxy-hexadecanoic acid	285.2658	7.417	Rppos	144998	168068	172394	183330	161140	170216	177783	182429	205081	208008
2-Methyl-?-pyrrolidinobutiophenone	231.163	12.25	Rpneg	4635	4735	3931	4400	4975	4646	4269	5012	4968	4264
2-Methyl-1,4-naphthalenediol bis(dihydrogen phosphate)	333.9998	1.446	Rppos	525141	442457	486115	520223	387128	511718	381825	492720	441141	496779
2-Methyl-2-hexacosenoic acid	454.4004	13.541	Rpneg	23890	7502	10472	13294	6010	7811	6258	4622	7080	2588
2-Methyl-3-hydroxybutyric acid	118.0628	5.64	HILICneg	35236	32488	36350	21652	57570	128706	175454	112870	97436	83973
2-Methyl-3-hydroxybutyric acid Esi-4.996	118.0612	4.996	HILICneg	1	156978	29650	1	151705	168359	140869	164842	153945	118016
2-methylbacteriohopane-32,33,34,35-tetrol	560.4835	12.318	Rpneg	4772	2777	1774	2465	2708	1718	2011	2388	2909	1942
2-Methylbutylamine	87.1048	3.728	HILICpos	905162	918963	573240	2827406	854924	629815		2774804	1250718	849138
2-Methylbutyroylcarnitine	245.1638	3.893	HILICpos	2286307	1139668	965669	1683315	790460	643297		755755	562960	669400
2-Methylbutyroylcarnitine	228.1361	6.223	Rppos	452719	595445	242950	564470	535055	269290	552313	557144	602994	267042
2-Naphthalenesulfonic acid	208.0195	0.759	HILICneg	21769	32819	1	16372	139933	122307	34073	37045	44919	8440
2'-Norberbamunine	582.2736	11.566	Rpneg	5609	3019	2102	1884	4294	1656	5084	2604	1904	2993
2-O-(beta-D-galactopyranosyl-(1-6)-beta-D-galactopyranosyl	574.2605	23.713	Rppos	356571	420943	354677	538245	575828	589897	516854	512314	536603	478879
2-O-(beta-D-galactopyranosyl-(1-6)-beta-D-galactopyranosyl	554.2914	11.925	Rpneg	101542	20600	139441	105343	148540	60510	74999	84787	104184	94503
2-Octaprenylphenol	655.5508	0.885	HILICpos	610305	401216	204166	235303	174872	107739		90452	1	49044
2-Oxo-3-hydroxy-4-phosphobutanoate	213.9867	5.91	Rpneg	394726	198493	118060	163709	710762	739200	708660	93945	228679	141233
2-Oxosuberate	188.0683	1.543	Rpneg	1589	108871	1	65052	85775	5117	4151	46297	104091	46406
2-Phenylethanol glucuronide	298.1051	6.859	Rpneg	4997	3654	3811	4317	3963	6206	4267	6299	3890	6083
2-Piperidinecarboxamide(PPX)	464.3175	0.963	HILICneg	186379	219935	121982	132072	128362	1	70038	70896	92364	62432
2R-aminoheptanoic acid	145.1101	5.911	HILICpos	4332314	4646578	4117864	4168756	5117241	5031601		3877456	4646534	3977346
2R-aminoheptanoic acid Esi+3.0839999	145.1102	3.084	HILICpos	1703449	1921112	1351503	1133129	1337831	1667572		1208324	960531	773583
2R-hydroxylauric acid	198.1618	9.611	Rppos	338373	385839	364186	413129	360562	380538	466789	398428	413384	432919
2S-aminohexadecanoic acid	271.2507	7.391	Rppos	192045	205055	211556	230265	198011	211574	223545	212681	229151	236934
2-Stearyl citrate	444.3068	12.297	Rpneg	7618	2395	2569	3943	3618	1	1	1974	1	1
2-Stearyl citrate Esi-12.667	444.3087	12.667	Rpneg	10219	5752	6159	9311	1	3040	5321	5159	5163	2841

2-Stearyl citrate Esi-12.891999	444.3073	12.892	Rpneg	8852	3319	3755	4102	2890	1238	1	2158	1	1
2-Tetracosanamidoethanesulfonic acid	475.369	13.653	Rpneg	26487	16676	16678	23548	15676	11129	15494	11482	14763	12162
2-Undecyl-4(1H)-quinolinone N-oxide	331.2331	4.219	HILICpos	1532325	722036	295547	296411	268838	526676		416361	628976	610608
2-Undecyl-4(1H)-quinolinone N-oxide	331.2357	7.244	Rppos	185640	107628	89910	72624	465835	127940	201506	198400	162691	228146
2Z,6Z,8Z,12E-hexadecatetraenoic acid	248.1775	11.565	Rpneg	2250	2690	1540	1509	1526	821	1616	3078	976	1300
2Z-Dodecenedioic acid	210.1249	6.668	Rppos	241309	491483	467677	555538	596032	604585	447052	550945	373337	315144
3-(2-(Methylamino)ethyl)-1H-indol-5-ol	194.0822	5.405	Rppos	79264	147107	1	159252	217449	80119	85536	150669	227592	130697
3'-(2'',3'',4'',6''-Tetrakisgalloylglucosyl)-phloroacetophenone	998.1669	13.774	Rpneg	6907	5566	5936	9151	9584	3598	7408	1	6239	5949
3-(2-Furanyl)-2-propenal	122.0372	12.852	Rpneg	7814	5243	6225	5894	15908	6335	14118	13906	11357	14114
3-(2-Furanyl)-2-propenal Esi-12.597	122.037	12.597	Rpneg	9104	4826	18752	4739	6218	3825	2596	32198	7830	3830
3-(2-Heptenyloxy)-2-hydroxypropyl undecanoate	356.2917	14.728	Rppos	366619	237987	491885	373296	625028	953123	951024	1046764	831825	699801
3-(2-Heptenyloxy)-2-hydroxypropyl undecanoate	356.2927	13.069	Rpneg	43410	19896	19261	15911	14896	15985	14090	14527	15196	6695
3-(2-Heptenyloxy)-2-hydroxypropyl undecanoate Esi+14.29	356.2924	14.299	Rppos	237077	312142	301438	379122	515689	847316	699723	769316	564975	846407
3-(2-Heptenyloxy)-2-hydroxypropyl undecanoate Esi-11.532	356.2911	11.533	Rpneg	13926	9079	8846	9594	10579	6013	7106	9162	9033	7959
3-(2-Heptenyloxy)-2-hydroxypropyl undecanoate Esi-13.069	356.2904	13.069	Rpneg	43837	20144	19261	15911	14672	15985	14099	14494	15792	6702
3-(2-Heptenyloxy)-2-hydroxypropyl undecanoate Esi-13.072	356.2927	13.072	Rpneg	43960	5993	20359	3897	16728	15985	14099	15513	17775	10302
3-(2-Hydroxyphenyl)propionic acid	148.0524	6.668	Rppos	687304	947632	868039	958127	1019260	933560	861350	922038	1007955	903244
3-(2-Hydroxyphenyl)propionic acid Esi+7.9159994	148.052	7.915999	Rppos	97738	289276	230625	303506	395116	192768	237716	327736	355421	250248
3-(3,5-Dihydroxyphenyl)-2-propenoic acid	180.0426	5.76	Rpneg	1	26546	1004	18100	30813	1243	1018	13458	31522	11076
3-(3'-Methylthio)propylmalic acid	222.0568	8.326001	Rppos	91777	131651	118221	145931	97165	118865	129829	119672	143053	148943
3-(6'-Methylthio)hexylmalic acid	264.1066	7.507	HILICpos	115457	192641	109094	130051	419122	104493		499658	1769036	15769407
3-(Carboxymethylamino)propanoic acid	129.0417	1.445	Rppos	65030	323368	42123	311639	593815	73357	56773	383955	612601	311742
3-(Imidazol-4-yl)-2-oxopropyl phosphate	280.0462	1.304	Rpneg	50931	43999	49749	58599	16237	50123	36849	33609	33804	30251
3,11-dihydroxy myristoic acid	242.1883	8.735	Rppos	225022	233635	193223	349653	219946	217921	296356	187272	264084	234843
3,12-dihydroxy palmitic acid	287.2451	8.516	Rppos	326695	351022	390005	365562	357091	352980	360988	365337	380151	366333
3,3'-Thiobispropanoic acid	224.0361	11.008	Rpneg	3108	4525	4713	3183	4267	11652	2157	5980	11116	13406
3,3'-Thiobispropanoic acid Esi-13.377001	224.0356	13.377	Rpneg	3993	11859	11315	8874	3241	9798	11819	8767	11013	19095
3,4,5,2',4',6'-Hexahydroxychalcone 2'-glucoside	466.1138	1.074	HILICneg	2415857	3039076	974083	2110646	5627599	268949	696021	1501168	829701	1586745
3,4-Dihydro-4-[(5-methyl-2-furanyl)methylene]-2H-pyrrole	183.0662	1.534	HILICpos	2569521	2016672	2520137	2467282	1919776	2116238		2473756	2505315	2267526
3,4-Dihydroxybutyric acid	120.0423	0.896	Rpneg	19131	18179	17782	24284	16253	38069	38792	27247	35921	36261
3,4-Methylenedioxybenzoic acid	166.027	12.854	Rpneg	8597	54366	7971	6613	13103	12724	12795	35133	16722	26424
3,4-Methylenedioxybenzoic acid Esi-12.593001	166.0269	12.593	Rpneg	10429	40181	5094	7161	9960	20123	6456	46228	78104	1
3',5'-Cyclic dGMP	329.0555	9.261001	HILICneg	71624	72288	59500	64108	56589	52402	58670	62540	61036	56052
3,5-Dimethylhexanal	128.1204	9.947	Rpneg	6657	8078	6613	6713	7289	5680	5343	6653	8431	6272
3,8-Dihydroxy-6-methoxy-7(11)-eremophilen-12,8-olide	296.1612	10.599	Rpneg	3246	3904	3375	1	4272	6462	1765	6963	4944	4191
3?,12?-Dihydroxy-5?-chol-6-en-24-oic Acid	372.2659	8.793	Rppos	253364	164907	26043	51154	156334	499512	86826	85448	179364	200831
3?,12?-Dihydroxy-5?-chol-7-en-24-oic Acid	390.2787	1.425	HILICpos	1830677	741450	533162	690714	467786	1750954		1918276	532550	1576587
SM(d17:1/17:0)	702.567	22.758	Rppos	3.00E+07	2.81E+07	2.86E+07	3.23E+07	3.74E+07	4.16E+07	3.77E+07	3.97E+07	4.14E+07	3.85E+07
3?,12?-Dihydroxy-5?-chol-7-en-24-oic Acid Esi+0.915	390.2799	0.915	HILICpos	329932	259083	209130	311439	488077	1		1	429257	321889
3?,12?-Dihydroxy-7-oxo-5?-cholestan-26-oic acid	447.3351	10.637	Rppos	362489	893701	1230775	1272559	1235616	1183237	948380	1045043	1230707	1351540
3?,15?,18-Trihydroxy-5?-cholan-24-oic Acid	430.2696	8.793	Rppos	363404	291187	48562	114552	218681	854664	155132	155560	350160	371066
3?,15?-Dihydroxy-5?-cholan-24-oic Acid	392.2923	11.561	Rpneg	33417	18376	4411	3159	10462	13945	17362	2944	24007	10214
3?,15?-Dihydroxy-5?-cholan-24-oic Acid Esi-10.758001	392.292	10.758	Rpneg	5211	3560	1164	2121	2288	3477	1377	1285	2408	2228
3?,15?-Dihydroxy-5?-cholan-24-oic Acid Esi-10.758001 :1	392.29	10.758	Rpneg	5974	3633	1164	2111	2288	3112	1232	1	2408	2228
3?,7?,12?-Trihydroxy-24-nor-5?-cholan-23-al	773.5774	25.406	Rpos	258931	158130	232489	264163	78406	172995	173940	76727	76432	147072
3?,9?,11?-Trihydroxy-5?-cholan-24-oic Acid	408.2869	11.057	Rpneg	82009	50270	5798	21323	32716	127177	23968	25770	68090	88581
3?,9?,11?-Trihydroxy-5?-cholan-24-oic Acid	408.2887	6.224999	HILICneg	119912	118167	15378	47876	92573	367323	71239	67741	159328	184800
3?,9?,11?-Trihydroxy-5?-cholan-24-oic Acid Esi-10.061	408.2871	10.061	Rpneg	27732	14774	2816	5451	3605	14221	1196	1	8500	6182
3?,9?,11?-Trihydroxy-5?-cholan-24-oic Acid Esi-5.5040007	408.2864	5.504001	HILICneg	47220	44090	7093	11802	6118	37804	3007	1	7248	5066
3?-Hydroxy-5?-chol-8-en-24-oic Acid	374.2776	12.283	Rpneg	3792	1	1	2247	1122	1200	2129	2707	2111	1124
38:4(23Z,26Z,29Z,32Z)	591.5595	0.975	HILICpos	2916378	2948745	2113293	2228540	3431280	3342427		3236358	3432500	3552870
3alpha,7alpha,12alpha-Trihydroxy-24-methyl-5beta-Choles	446.3415	19.315	Rppos	4430603	2851604	3306836	2759197	2687572	2788019	1910162	2544249	3064578	2812341
3alpha,7alpha,12alpha-Trihydroxy-24-methyl-5beta-Choles	463.3653	16.038	Rppos	158809	201803	562505	401061	417569	146184	213585	181866	184236	158088
3alpha,7alpha,12alpha-Trihydroxy-24-methyl-5beta-Choles	446.3418	19.561	Rppos	1279156	693731	1383515	1071071	929013	903901	982120	1221592	1169011	1373094
3-Amino-4-hydroxybenzoic acid	153.0427	4.775001	Rpneg	2667	14851	2602	9303	21722	1957	2628	8466	16505	5898
3beta-(3-methyl-butanoyloxy)-villanovane-13alpha,17-diol	438.2969	11.294	Rpneg	8045	6553	5727	5872	5672	6008	5817	5548	5170	4955
3-Carboxy-7-chloro-1,2,4-benzothiadiazine-1,1-dioxide	319.9875	10.413	Rpneg	43314	45360	40895	41827	47897	39690	39289	43047	45628	41570
3-Deoxy-3-azido-25-hydroxyvitamin D3	896.6759	0.885	HILICneg	1	169474	269216	164867	1	1	139069	1	1	132251
3-Deoxyguanosine	267.0967	5.118	Rpneg	98180	76009	112199	122827	50994	83137	85205	104131	65358	86182
3-Deoxyguanosine	267.0973	5.487999	HILICneg	47935	170805	217091	143709	172833	267635	456434	696284	685350	513925
3-Deoxyguanosine	267.0976	5.035	HILICpos	52970656	29894416	38264624	43805380	43281868	36713380		36084456	17047064	19323144
3E,13Z-Octadecadienyl acetate	308.2709	12.973	Rpneg	1337760	1075717	707777	1091582	814843	582349	839309	1052479	884590	827212
3-Guanidinopropanoate	131.0691	0.912	Rppos	1.07E+08	1.06E+08	1.12E+08	1.06E+08	1.01E+08	1.06E+08	1.1E+08	1.08E+08	56402868	1.04E+08
3-Guanidinopropanoate	131.0696	0.915	Rpneg	160994	163393	195750	168447	151442	144031	189927	145347	129122	154776
3-Guanidinopropanoate	131.0696	8.188	HILICpos	7810517	6819819	8069129	8196328	5142732	7865417		10609291	10426200	9919607
3-hexanoyl-NBD Cholesterol	662.446	21.979	Rppos	1.07E+08	1.10E+08	1.12E+08	1.18E+08	9.73E+07	9.76E+07	9.93E+07	9.65E+07	1.03E+08	1.05E+08
3-Hydroxy-10'-apo-b,y-carotenal	392.2725	0.985	HILICneg	640240	541168	426254	342208	445340	68237	228924	280492	573731	302490
3-Hydroxy-1-phenyl-1-hexadecanone	332.2721	0.994	HILICneg	1967883	2570113	1879203	2360108	1771422	318989	1216907	1242705	1098193	1148952
3-Hydroxy-1-phenyl-1-hexadecanone	332.2745	13.20422	Rpneg	30756	351754	110515	37912	1	23785	67257	59782	64563	73415
3-Hydroxy-1-phenyl-1-hexadecanone Esi-12.912001	332.2722	12.912	Rpneg	1025683	1060416	756701	1234817	92966	643033	670958	687071	728273	738093
3-Hydroxy-3-methyl-2-oxo-Butyric acid	132.0408	0.772	Rpneg	7158	19753	10872	15703	20543	5344	5663	13401	22432	11137
3-Hydroxy-3-methyl-2-oxo-pentanoic acid	146.0585	12.173	Rpneg	28529	4323	4104	3642	3673	10032	4006	5180	3960	4335
3-Hydroxy-3-methyl-glutaric acid	162.0528	0.906	Rpneg	4114	21117	12638	30102	25431	16399	19941	19432	18234	20815
3-Hydroxyisovalerylcarnitine	261.1588	6.572999	HILICpos	1118212	1086055	1067514	1124234	508555	345632		826663	398880	292841
3-Hydroxynitrazepam	343.0803	1.512	HILICneg	20880	40040	45966	48615	47643	6807	50927	31487	22919	32291
3-Hydroxynonyl acetate	202.1569	10.717	Rpneg	5362	5811	4887	5647	6305	4774	4679	5927	6320	5389
3-Hydroxytetradecanedioic acid	256.1664	9.069	Rpos	161029	169647	178032	176989	162929	155588	182085	191881	183225	187905
3-Ketolactose	386.1048	11.905	Rpneg	6729	2325	9348	6315	8272	3209	4177	4828	5665	5329
3-methoxy Limaprost	411.2981	8.442	Rppos	152747	182791	215672	141207	400388	188357	240910	361755	169685	300253
3-methoxy Limaprost Esi+8.558	411.2986	8.558	Rppos	262471	204407	230635	166139	339278	277855	351339	439695	225893	363818
3-Methoxy-19-nor-17alpha-pregna-1,3,5(10),20-tetraen-17	312.2085	12.923	Rpneg	7662	6782	6044	6795	6465	6522	6615	5738	5691	4954
3-Methoxy-4,5-methylenedioxybenzoic acid	196.0377	5.693	Rpneg	1	89358	5271	58817	80761	4769	4116	39752	100749	32369
3-Methoxy-4-Hydroxyphenylglycol Sulfate	310.0346	5.314	HILICneg	382430	396182	313612	358370	325515	152644	227846	222198	185819	218201
3-Methyl-2-thiohydantoin	190.0418	4.139	HILICneg	8171	1	36020	45782	24488	23000	19465	1	9866	22865
3-Methyl-2-thiohydantoin Esi-7.102	320.0622	7.102	HILICneg	15245	22865	20229	22736	14349	11707	16092	15069	8312	13878
3-Methyl-3-butenyl apiosyl-(1-6)-glucoside	380.167	12.601	Rpneg	4727	2393	1	1	2880	2045	2595	2694	1946	1
3-Methylbutyl 3-oxobutanoate	172.1086	1.802	HILICneg	100171	108240	131888	137108	192764	252885	83562	162159	107915	61510
3-Methylbutyl 3-oxobutanoate	172.1096	12.493	Rpneg	32004	3763	3892	4662	3320	5581	3587	4540	2785	2244
3-Methylbutyl 3-oxobutanoate Esi-7.6920004	172.1098	7.692	Rpneg	4202	5463	2403	7217	9212	2280	1	3447	7187	3762
3-Methylbutyl propanoate	190.1206	6.715	Rpneg	8251	1	5448	6615	3679	3198	2494	5466	7368	4177
3-methyl-tetradecanoic acid	242.2227	1.139	HILICneg	765754	698240	455294	704450	731632	1	510737	606308	1336001	623938
3-Nitrophenylhydrazine	153.0513	0.923	Rpneg	169102	136492	152152	148869	114566	120318	116203	129093	110330	121324

3-O-acetylecdysone 2-phosphate	646.3113	12.556 Rpneg	13077	10255	17678	20260	8356	4292	14211	10937	8014	9530
3-O-acetylecdysone 2-phosphate Esi-12.556	646.3132	12.556 Rpneg	13077	10255	17678	20260	8356	4292	14211	10937	8014	9530
3-Oxochola-1,4,6-trien-24-oic Acid	368.2363	1.417 HILICpos	1105431	1045478	423042	413543	762590	515017		339172	468017	348736
3-oxoglutaric acid	146.0216	0.698 Rpneg	86119	65595	67297	70565	80077	88792	85970	77769	72474	63452
3-oxo-nonadecanoic acid	312.2635	0.891 HILICpos	352791	460319	400783	441636	313548	207643		189388	312262	271725
3-oxo-nonadecanoic acid	312.264	12.223 Rpneg	21329	15628	17452	19026	20360	15949	13722	10332	8607	1
3-oxo-pentadecanoic acid	255.22	8.059999 Rppos	344975	293931	373036	298188	332572	284974	350583	327649	313814	284901
3-oxo-tetracosanoic acid	382.3413	13.009 Rpneg	14957	12114	1	9883	8651	6048	1	8544	7694	8440
3-oxo-tetracosanoic acid	382.342	19.744 Rppos	227131	223028	236716	277306	216438	211756	189575	213424	307196	190343
3S,7S-dimethyl-hexadecan-2-ol	270.2909	13.21 Rpneg	13973	22624	10135	16768	10555	10158	13016	11250	15350	12001
3-Sulfinoalanine	153.0097	4.126 HILICneg	776079	1	775842	663454	821191	1	787603	1	1	698602
3-Sulfinoalanine Esi-5.339	153.0101	5.339 HILICneg	211300	281338	270762	246434	268704	241091	292106	307676	254400	258088
3'-UMP	324.0353	0.782 Rpneg	7326	18345	22319	12187	6688	4042	15074	4819	5425	5958
3Z,6Z,9Z,11Z-Nonadecatetraene	260.2503	1.032 HILICneg	328457	521952	404924	449643	329087	1	300099	280723	219633	257403
3Z,6Z,9Z,11Z-Nonadecatetraene	260.2504	12.752 Rpneg	264836	271403	331740	172096	286675	230980	295461	355786	267501	298551
3Z,6Z,9Z,11Z-Nonadecatetraene Esi-12.615999	260.2508	12.616 Rpneg	24670	23991	21851	27676	18801	17844	21262	23926	22229	25788
3Z,6Z,9Z,12Z,15Z-Tricosapentaene	331.3238	1.532 HILICpos	188956	274696	171955	218633	216065	240162		229215	424602	251278
3Z,6Z,9Z-Pentacosatriene	368.3443	5.249 HILICpos	738489	888390	694637	1024660	689672	602300		902116	811785	831644
3Z,6Z,9Z-Pentacosatriene Esi+0.961	368.3418	0.961 HILICpos	1008575	965233	876110	867888	972589	653343		492695	746031	934152
4-(4-Hydroxyphenyl)-2-butanol	212.1059	1.865 HILICneg	10904	38799	37050	27066	52030	81605	18421	35362	68177	56029
4-(Trimethylammonio)but-2-enoate	143.0945	7.163001 HILICpos	5776595	5214140	4255357	7417593	4608848	6540299		5293060	5612483	4415815
4,4'-Biphenyldithiol	218.0231	0.885 Rpneg	6468	7406	10508	7027	1	2159	1	3682	1	1
4,4'-Sulfonyldiphenol	500.0603	7.637 HILICneg	159621	143863	161122	134583	173775	159710	167840	158336	162814	159144
4,5-Dihydrovomifoliol	226.1575	8.257001 Rpneg	88601	84490	86783	81930	84915	83697	83979	84150	81773	80727
4,5-Dihydroxyphthalate	244.0226	0.719 HILICneg	126289	65073	77932	44184	74497	37446	56911	54105	85493	69032
4,5-Dimethyloxazole	79.0423	1.672 Rppos	345997	380338	413091	381242	353079	399149	407657	421414	402932	390509
4,5-seco-Dopa	229.0595	1.11 HILICneg	1659603	4868325	2840080	4435833	4492204	1561752	1748571	1919429	1245519	5048627
4,6-Dihydroxysulfadiazine	282.0452	5.191001 HILICneg	623214	1866767	1740732	1702082	1381627	1118200	1117435	1083758	1036477	999647
4-[2-(5-Carboxy-2-hydroxy-3-methoxyphenyl)-2-oxoethylide	375.0451	7.637 HILICneg	144234	131894	143018	121298	151853	139836	145682	143269	133569	140371
4alpha-methyl-24-methylene-cholestan-3beta,8beta,11bet	468.3588	19.91 Rppos	2193817	2227793	2297268	2548278	1179510	3043399	2781755	2299459	2990469	2561470
4'-Apo-beta,psi-caroten-4'-al	542.3761	1.188 HILICneg	108299	244156	134213	195161	299991	137363	176541	151469	158842	181032
4-Benzyloxy-2'-hydroxy-3',4',5',6'-tetramethoxychalcone	450.1663	1.193 HILICneg	136192	145773	80398	166564	220838	4953183	102279	226320	201022	129867
4-Carboxy-4'-sulfoazobenzene	306.0303	0.982 Rpneg	282902	187541	180274	231525	160047	202362	104230	229756	205938	186033
4-Carboxy-4'-sulfoazobenzene	306.0332	9.563001 HILICneg	35243	22685	28126	21287	31581	43164	31200	54579	46553	22879
4E,10Z-Tetradecadienyl acetate	252.209	12.345 Rpneg	20435	1	6178	11465	10684	6410	11197	14744	15880	11971
4-Fluoromethamphetamine	380.2307	1.032 HILICneg	423643	110927	320113	447924	437897	1	438492	448086	368875	411218
4-Formylsalicylic acid	166.0262	16.038 Rppos	869187	1127523	3094416	2146858	2070116	715345	883806	951470	966591	935422
4-Formylsalicylic acid Esi+7.37	148.0156	7.37 Rppos	126671	785452	601366	329510	310729	690728	166215	177320	471528	239530
4-Formylsalicylic acid Esi+8.836999	166.0264	8.836999 Rppos	316529	456920	481465	508343	401998	453836	472336	476164	577738	494057
4-Formylsalicylic acid Esi+8.974	148.0161	8.974 Rppos	663957	811273	888433	937873	791181	872320	919341	1017246	1023895	1039281
4-hydroxy caproaldehyde	116.0832	1.668 HILICneg	149398	56564	67014	45826	60874	70290	78004	122105	69269	88156
4-hydroxy caproaldehyde Esi-0.973	116.0835	0.973 HILICneg	62300	32871	28610	58351	32329	1	31967	84531	130723	50993
4-Hydroxy-6-docosanone	339.3492	19.886 Rppos	135368	106433	225324	112067	202770	126396	262394	153649	123150	82287
4-Hydroxy-6-docosanone	340.3341	13.573 Rpneg	358535	176058	103133	183321	159835	92862	149540	131916	157291	127319
4-Methyl-3-heptyl palmitate	368.3656	0.969 HILICneg	366891	342411	188677	275928	289092	558101	249404	279162	551409	228386
4-Methyl-5-thiazoleethanol	189.0463	5.18 Rpneg	47738	17982	11990	16557	33737	21552	26629	13819	11715	15292
4-methyl-decanoic acid	186.1614	1.233 HILICneg	118311	96573	50761	111345	116599	58782	127240	178435	152951	65900
4-O-alpha-D-Galactopyranosylcalystegine B2	674.2779	0.912 HILICneg	590070	496402	465873	412547	741645	279609	1140159	383647	1077038	768800
4-Oxatetradecanoic acid	230.1885	11.649 Rpneg	3652	4680	4737	4662	5068	3897	4672	4598	5128	4706
4-oxo-docosanoic acid	354.3088	12.826 Rpneg	16970	4516	11454	6401	9472	8982	7703	1	1	1
4-Quinolinemethanol, 2,8-bis(trifluoromethyl)-	294.061	1.437 Rpos	676069	461851	531163	601525	393068	536162	318848	541853	433094	407530
4-Quinolone-3-Carboxamide CB2 Ligand	468.263	12.232 Rpneg	1222	3524	866	1818	1309	1	1249	1402	1779	1241
4R-hydroxylauric acid	216.1719	1.357 HILICneg	119840	139385	43404	113197	101047	35301	103775	92883	108070	108569
4R-hydroxylauric acid	216.1727	11.012 Rpneg	25654	14724	10284	12149	11471	9395	12890	11214	15581	14215
4R-hydroxylauric acid Esi-11.226999	216.1729	11.227 Rpneg	11590	13124	12101	12928	13697	11547	12512	12958	13866	12464
4-Sulfocatechol	189.9937	2.679 Rpneg	105436	78320	54364	70094	70210	90097	61244	85644	43801	46513
4Z-Tridecenyl acetate	240.2073	1.112 HILICneg	202153	120896	86452	127449	262740	1	146812	118216	187876	158211
5-(10,13-Nonadecadienyl)-1,3-benzenediol	790.6139	5.515999 HILICneg	139082	88010	113565	126296	110769	47385	109848	109019	138061	125932
5(S),6(R)-Lipoxin A4-d5	731.5403	8.785001 Rppos	51306	412059	69960	370332	626580	48986	68772	341614	717399	342373
5(S)-HEPE	318.2177	11.496 Rpneg	5792	5470	3304	3642	1	1	2305	9550	7615	1
5(S)-HETE lactone	302.224	12.383 Rpneg	1304365	1323283	702120	1232131	622323	289551	685501	1052898	524748	505692
5(S)-HETE lactone	302.2252	1.064 HILICneg	1854097	3491689	2280063	2372532	1649429	374877	1684752	1826525	1164797	1092667
5,14,15-trihydroxy-6,8,10,12-Eicosatetraenoic acid	352.2287	12.839 Rpneg	47903	19386	9836	17333	20230	9740	21796	37282	51223	18661
5,6-dihydroxy-8,11,14-eicosatrienoic acid	338.2435	12.774 Rpneg	13046	9223	6737	7262	9027	7205	8413	7256	8782	6832
5,6-Indolequinone-2-carboxylic acid	237.0286	0.883 Rpneg	43512	30156	33703	31956	16908	16089	14157	21123	15761	18068
5,7,3',5'-Tetrahydroxy-3,6,8,4'-tetramethoxyflavone 3'-gluc	614.1488	0.815 Rpneg	9353	4449	5102	6633	3337	5292	4429	4759	3174	3298
5,8,11,14-all-cis-docosatetraenoylethanolamine	421.3182	0.789 HILICneg	106392	121612	192234	188597	68749	32545	77558	81227	43034	71053
5,9-Tetracosadienoic acid	364.3313	0.98 HILICneg	112193	103424	75245	95615	72322	53530	95160	92947	85417	50385
5,9-Tetracosadienoic acid	364.3347	13.447 Rpneg	66767	35757	22225	38027	30841	21237	30926	29528	29365	25824
5?-Chol-8(14)-en-24-oic Acid	358.2874	13.014 Rpneg	66157	65560	45573	67735	86617	63035	68827	101912	97488	60096
5?-Chol-8(14)-en-24-oic Acid	358.2856	0.985 HILICneg	440446	417212	315526	372249	422447	163698	257052	307909	289405	225653
5?-Chol-8(14)-en-24-oic Acid Esi-13.419999	358.2871	13.42 Rpneg	9706	4623	1	6366	1270	2558	3067	1	3391	2812
5?-Chola-3,11-dien-24-oic Acid	356.2722	12.877 Rpneg	52896	59043	46495	57640	37661	25170	32797	47286	38897	27312
5?-Chola-3,11-dien-24-oic Acid	356.2707	0.978 HILICneg	698379	553284	562630	406550	387473	97885	410261	280805	462833	222452
5?-Cholan-24-oic Acid	360.3031	13.165 Rpneg	22169	20530	16668	22995	22835	22002	19683	24291	27583	24688
5?-Cholest-25-ene-3?,7?,12?-triol	400.3357	17.753 Rpos	639241	458982	435356	587512	247478	546181	505912	595727	693566	868703
5?-Cholestane-3?,6?,7?,25,26-pentol	469.3692	2.57 HILICpos	785803	47681	43618	52852	1	40108		96412	85193	37228
5?-Cholestane-3?,7?,25,26-tetrol	453.3786	1.814 HILICpos	1817874	144594	111299	118611	126613	125764		79226	133275	137044
5alpha-Androstane-2alpha-fluoro-17beta-ol-3-one acetate	350.2294	7.275001 Rppos	193312	576654	238542	532115	641548	449968	252997	601997	978058	467930
5-Aminoimidazole ribonucleotide	295.0582	5.956 HILICneg	185942	455269	625454	645889	352831	384394	486737	499761	403866	396102
5-Androstene-3b,16a,17a-triol	306.2188	12.278 Rpneg	8086	9083	6079	9807	7538	5484	6866	7726	9201	7970
5-Androstene-3b,16a,17a-triol Esi-11.291	306.2179	11.291 Rpneg	4837	2132	1	3052	1363	1294	2301	3504	3069	910
5beta-cholestan-3-one	368.3437	22.388 Rppos	338404	495532	840795	570466	352945	817000	438498	480359	646220	657709
5beta-Pregnane-3alpha,17alpha,20alpha-triol	336.2669	25.578 Rppos	263881	290154	445346	300505	476699	681733	549026	649812	537405	542296
5beta-scymnol sulfate	594.3097	12.692 Rpneg	1	75603	53554	77952	56659	40752	35903	35453	35821	66938
5beta-scymnol sulfate Esi-12.689001	594.3097	12.689 Rpneg	1	75603	53554	77947	56659	40752	7963	11760	8684	66938
5beta-scymnol sulfate Esi-12.849999	594.3109	12.85 Rpneg	1	1	10292	1	10200	5946	12568	14195	9655	12019
5-bromo-3-pheny Salicylic Acid	337.9789	0.986 Rpneg	23378	27824	25938	22775	26370	17988	32427	19291	17132	21809
5-Carboxyamino-1-(5-phospho-D-ribosyl)imidazole	385.0521	11.925 Rpneg	2677	1	3066	1435	4038	950	973	910	1271	1
5-Chloro-1,2,4-trihydroxybenzene	159.9929	8.951999 HILICneg	185050	206718	201587	197274	203045	205784	158227	212469	164323	146469
5-Cholestene-3?,7?,12?,24,25-pentol	432.3262	18.559 Rppos	5494527	3292235	815695	4124854	4115463	4115878	3059641	4250627	4534387	4136708
5-Cholestene-3?,7?,12?,25,26-pentol	450.3304	11.857 Rpneg	3485	2256	1131	1571	1	1136	1570	1337	1710	1725

5-Diazoimidazole-4-carboxamide	183.0396	7.262 HILICneg	462509	461330	356261	450705	338181	324938	337531	334350	289428	361653
5E-eicosenoic acid	310.2867	13.166 Rpneg	1353605	1227369	810712	1108606	1206683	1078031	1291562	1518648	1451999	1503998
5E-eicosenoic acid	310.2882	1.019 HILICneg	1177475	1453621	1298596	1167823	1953476	341156	1631391	1845042	1547561	1876353
5-epi-5-F2c-IsoP	354.2401	11.615 Rpneg	1	7141	1	7096	15757	3363	4508	5068	18081	8951
5-epi-5-F2c-IsoP Esi-11.614999	372.2491	11.615 Rpneg	1	6986	1	9755	14186	6344	6934	18791	13035	12394
5-Ethyl-4-methyl-2-pentyloxazole	408.2994	4.784 HILICneg	12241	15502	18052	15957	33247	39575	33638	49863	74402	52359
5-Ethyl-7-methyl-3E,5E,7E-undecatriene	192.1879	12.594 Rpneg	24042	23143	19579	25334	12633	9404	11663	14860	11070	9767
5-Ethyl-7-methyl-3E,5E,7E-undecatriene	192.188	0.994 HILICneg	72824	109460	82248	113830	42093	1	34967	34303	37127	27036
5-Fluorouridine monophosphate	388.033	0.982 Rpneg	103383	59853	56639	80470	48839	70144	27336	80487	72285	60615
5-Heptyltetrahydro-2-oxo-3-furancarboxylic acid	274.1414	5.599 Rpneg	5595	6682	1405	7095	8117	1746	1	5156	8820	4576
5-Hydroxy-3,4-dihydrocarbostyryl	145.0533	6.208 Rppos	635478	619315	568332	570866	604533	564223	599374	577992	525795	552151
5-Hydroxy-6-desmethylprimaquine	522.2924	1.245 HILICneg	73421	100685	53146	72806	26470	1	47911	48693	1	86244
5-Hydroxy-7-tetracosanone	368.3651	13.786 Rpneg	608344	228430	125319	213425	172818	121391	182225	158163	172872	102560
5-Hydroxyconiferyl alcohol	196.0737	0.883 HILICpos	658251	815003	829589	842922	502100	443848		450485	618177	559959
5-methyl-octadecanoic acid	298.2871	13.252 Rpneg	309281	199713	115037	187502	193124	160626	192736	224877	247476	220480
5-methyl-octadecanoic acid Esi-13.252001	298.2872	13.252 Rpneg	293148	199798	114953	186357	192948	160538	192736	211608	247476	220480
5-Methylthio-D-ribose	240.0675	11.008 Rpneg	2352	3787	3383	2231	3509	10304	1705	5541	10399	12255
5-Nitrosalicylate	183.0172	6.748 Rpneg	9627	39503	6184	23535	33351	17109	10605	16600	37459	14409
5-Nitrosalicylate Esi-6.0950003	183.0167	6.095 Rpneg	2878	27783	4117	12783	22208	1	2501	12983	25521	8338
5-O-(1-Carboxyvinyl)-3-phosphoshikimate	327.9978	7.645 Rppos	488277	585176	623418	687559	617468	660711	702428	752312	757831	807640
5-O-(1-Carboxyvinyl)-3-phosphoshikimate	648.0504	6.487001 HILICneg	91149	93840	87916	97716	94794	89604	96305	101677	98859	101223
5S-HETE di-endoperoxide	402.2258	9.762 Rppos	1088695	1369108	1614256	1461287	1444838	1277886	1376823	1496172	1335377	1405538
5'-S-Methyl-5'-thioinosine	344.0792	4.393001 Rpneg	8153	8652	8407	9481	8393	18466	18896	7924	8113	8507
5-tert-Butyl-4-hydroxymethylfuran-2-carboxylic acid	198.0898	5.224 Rppos	93564	211463	243829	145599	222683	252103	55541	136944	153382	130101
5-trans U-44069	350.2491	12.907 Rpneg	26773	13227	8587	11894	12216	5974	12551	16084	21325	8951
5-trans U-44069	367.2715	2.215 HILICpos	716292	292788	278857	221024	253576	309555		210456	264521	320131
5Z-octadecenoic acid	282.2568	13.79 Rpneg	17470	10174	13050	10465	11779	13776	12461	16238	30199	12361
5Z-octadecenoic acid	282.2574	1.07 HILICneg	2.01E+07	3.20E+07	3.09E+07	2.36E+07	4.60E+07	5499580	3.49E+07	4.39E+07	3.26E+07	4.10E+07
6-(2-Chloroallylthio)purine	272.0116	0.866 Rpneg	26747	18448	20299	20652	16403	17652	13670	19386	16307	17408
6-(2-Chloroallylthio)purine	272.012	7.724 HILICneg	75151	65997	65098	74486	73536	72177	75646	77139	74631	76573
6-(Isopropylthio)purine	240.0677	13.049 Rpneg	2308	4235	4873	3791	4489	11801	2256	7662	11427	7921
6-(Isopropylthio)purine	240.0688	0.882 HILICneg	318550	113296	369559	118451	162263	203659	423549	968350	199819	308568
6-(Isopropylthio)purine Esi-0.882	258.0775	0.882 HILICneg	254302	1	214766	102178	1	138425	376078	650966	1	285811
6-(Isopropylthio)purine Esi-13.378	240.0673	13.378 Rpneg	4254	7593	5017	3730	4456	7547	3771	9245	11932	10351
6,8a-Seco-6,8a-deoxy-5-oxoavermectin "2a" aglycone	603.3828	0.933 HILICpos	965829	1498045	1306083	1231615	6722779	1597820		1044909	1282374	1178634
6,8-dihydroxy-octanoic acid	176.1045	5.66 Rpneg	4657	13000	4480	11773	13372	2800	1	7833	15276	7396
6,8-Dihydroxypurine	152.0336	6.213 HILICneg	168831	247450	194921	196814	121863	83539	111842	81593	69121	112687
6,8-Dihydroxypurine	152.0333	5.244 HILICpos	802603	589171	524917	811081	427472	401765		716392	517980	545373
6alpha,9-Difluoro-11beta-hydroxypregn-4-ene-3,20-dione	366.2002	9.363 Rpneg	1956	1590	1439	1685	1794	1736	1541	1933	2510	1440
6alpha-Fluoro-11beta,17-dihydroxypregn-4-ene-3,20-dione	386.1878	1.1 HILICpos	978589	1131531	469788	1858959	2581071	1304374		632737	914053	1543629
6alpha-Methylprogesterone	328.2395	12.596 Rpneg	3457185	3327611	2833867	3568504	2161303	1609297	2022465	2504599	2021695	1785661
6alpha-Methylprogesterone	328.2426	0.999 HILICneg	4.14E+07	5.57E+07	3.55E+07	4.78E+07	2.61E+07	1898789	1.52E+07	1.85E+07	9733451	9914838
6beta,17-Dimethyl-5alpha-androstane-3beta,17beta-diol	320.2704	12.948 Rpneg	11258	11058	5171	9569	6162	4614	6199	7067	7840	5706
6-Bromo-5E,9Z,13Z,24Z-heptacosatetraenoic acid	954.4719	23.672 Rppos	500569	374450	357635	417448	501338	258702	278134	382290	166631	318305
6-bromo-eicosa-5E,9Z-dienoic acid	386.1854	11.89 Rpneg	280461	211218	162086	138685	111277	110918	177312	151832	126609	144394
6-Deoxoteasterone	480.3807	14.425 Rpneg	11478	6416	4817	8849	10347	8561	10097	5105	4599	5084
6-Deoxotyphasterol	438.3478	19.369 Rppos	453832	430150	131089	311202	1	545090	479568	429001	395061	242163
6E,9E-octadecadienoic acid	280.2396	12.8368 Rpneg	41819	20239	5240	25519	29598	58538	32779	31121	30448	66965
6E,9E-octadecadienoic acid	280.2422	1.099 HILICneg	3.12E+07	4.80E+07	3.83E+07	3.81E+07	4.97E+07	3391398	4.41E+07	4.58E+07	2.76E+07	3.72E+07
6E-Dodecen-1-ol	184.1842	12.007 Rpneg	20728	21131	19995	22747	20211	21273	20206	1	27384	21308
6-Ethyl-4-methyl-3E,5E,7E-decatriene	178.1722	12.596 Rpneg	5608	5220	4500	5547	2785	2055	2529	3040	2827	2494
6-hydroxy-4-tridecanolide	228.1735	11.058 Rpneg	15710	4162	2379	4152	2744	1509	1837	2915	4730	2293
6-Hydroxymelatonin	248.1141	9.049 Rpneg	1690	4301	1925	2257	1949	2373	2345	1	4266	3601
6-Hydroxymethyletoricoxib	374.0515	12.433 Rpneg	2029	4045	2601	1428	3536	12231	1500	8023	17390	21802
6-Hydroxymethyletoricoxib Esi-12.627	374.0535	12.627 Rpneg	1	1480	1	1	1215	6250	1	3315	6438	7489
6-Hydroxyshogaol	292.168	11.262 Rpneg	5795	7400	6568	8031	10082	5568	5888	13531	11574	7798
6-Hydroxyshogaol Esi-11.377	292.1674	11.377 Rpneg	3961	4449	5497	4799	5619	3871	4344	1	6398	4724
6-Hydroxyshogaol Esi-11.489999	310.1788	11.49 Rpneg	2631	2888	7021	4966	6730	2116	2767	1	4693	4256
6'-Hydroxysiphonaxanthin ester/ 6'-Hydroxysiphonaxanthin	811.6099	21.729 Rppos	1219866	836286	875643	981156	671916	964418	1014606	794842	1092902	1020968
6-hydroxy-tetradecanoic acid	244.2043	11.857 Rpneg	33677	18926	14189	17260	12806	12548	20631	17473	18822	19307
6-hydroxy-tetradecanoic acid Esi-11.591001	244.2042	11.591 Rpneg	5159	4771	4292	4492	5058	4414	5119	4870	5175	4901
6-hydroxy-tetradecanoic acid Esi-12.004999	244.2042	12.005 Rpneg	18687	17495	16623	18992	17488	16102	17521	19734	21027	17590
6-Methyl lauric acid	214.1935	11.893 Rpneg	106249	91578	48644	71851	71487	51166	56976	67519	65212	44215
6-Methyl lauric acid Esi-11.892999	214.1935	11.893 Rpneg	120583	91609	48644	71807	71393	50941	56965	67519	65190	44175
6-Methyl lauric acid Esi-12.015	214.1936	12.015 Rpneg	75730	74728	47102	65880	74799	50295	52235	62760	60360	47926
6-Methylnonan-3-ol	157.183	6.761001 Rppos	297929	297895	293618	293861	291515	305326	290465	296071	288793	290597
6-Methyltetrahydropterin	181.0964	4.296 HILICpos	3707205	3356967	4084826	4014886	4116817	3914747		4279391	4402223	2998921
6''-O-Acetylglycitin	488.1318	11.003 Rpneg	2049	1587	2506	1486	1601	1382	2041	2008	1814	1433
6''-O-alpha-D-Galactopyranosylciceritol	680.2395	15.315 Rpneg	604530	561414	647908	576759	488857	645534	586704	537108	554849	483420
6-oxo capric acid	168.1149	6.606 Rppos	885461	496718	917614	873222	980494	886582	874670	904206	838533	885489
6-oxo capric acid Esi+5.7109995	168.114	5.711 Rppos	100405	158502	114997	162623	159009	138138	120774	124649	149423	154081
6-oxo capric acid Esi+6.4229994	186.1258	6.422999 Rppos	129019	308756	368861	502123	623979	695642	152199	242758	638689	148697
6-oxo-Nonan-1-ol	157.1465	7.475999 Rppos	770652	916187	886901	904207	847433	900989	879577	871637	1011842	956207
6-oxo-Nonan-1-ol Esi+7.6780005	157.1464	7.678001 Rppos	81588	181409	146568	151066	120071	158987	116607	111929	194080	119756
6-Tridecynoic acid	227.1881	1.083 HILICpos	943645	820934	814552	773557	1350062	634123		486871	595438	895620
6-Tridecynoic acid Esi+0.97999996	210.1621	0.98 HILICpos	757564	955688	740185	590008	955078	286915		267675	342415	649771
6-Tridecynoic acid Esi+0.97999996 :1	227.1889	0.98 HILICpos	730395	929915	707298	550671	870877	338337		261973	321129	643073
6Z-Nonen-2S-ol	188.1413	10.07 Rpneg	6187	12809	8003	7444	8540	6127	4950	7221	9262	7197
7(14)-Bisabolene-2,3,10,11-tetrol	272.1986	9.18 Rpneg	9606	8647	7153	8580	11527	7302	6599	8636	10537	7698
7,10-Heptadecadiynoic acid	266.1665	8.867999 Rppos	184619	280559	289297	321078	268355	306574	365656	354670	273978	377901
7',8'-Dihydro-8'-hydroxycitraniaxanthin	488.3276	13.635 Rpneg	9735	6026	5205	6603	5762	5272	4975	5403	6862	5858
7?,12?,26-Trihydroxy-5?-cholestan-3-one	434.3374	13.071 Rpneg	74425	13750	11708	13366	11381	5355	8456	7206	15369	3265
7?,12?,26-Trihydroxy-5?-cholestan-3-one Esi-12.837999	434.3355	12.838 Rpneg	8736	2337	2232	2608	1917	752	1	1332	3632	1
7?,12?-Dihydroxy-5?-cholan-24-oic Acid	392.2921	11.674 Rpneg	7373	5246	1779	16369	12113	4405	4998	2533	22339	3502
7?,25,27-trihydroxycholesterol	451.3668	1.875 HILICpos	1277908	65058	163073	47289	42841	55576		44073	45753	120251
7a-Hydroxy-O-carbamoyl-deacetylcephalosporin C	432.0976	0.847 Rpneg	7029	5874	13899	7460	9664	16492	20509	11052	7897	11456
7-Dehydrocholesterol	366.3299	19.371 Rppos	797314	698932	574685	596731	722810	693313	793273	729942	617749	403357
7-Dehydrocholesterol Esi+21.392	366.3283	21.392 Rppos	347561	405713	533351	533957	408723	453340	595630	672012	423035	789306
7E-Dodecenyl acetate	226.1936	11.956 Rpneg	258945	139822	47159	118088	99132	54775	77015	99223	101109	59871
7E-Dodecenyl acetate Esi-11.955001	226.1927	11.955 Rpneg	258793	139695	47303	117977	101284	54820	76976	99280	101210	1
7E-Dodecenyl acetate Esi-11.956	226.1935	11.956 Rpneg	258961	140073	47280	117963	99966	54766	77015	99251	101141	59871
7-Hexadecen-1-ol	240.2457	14.065 Rpneg	6585	3892	4004	4855	8900	10959	10817	8207	8119	9280

7-Hydroxyrisperidone	486.2261	12.035 Rpneg	1	8516	5388	4107	13073	1	1421	7484	9156	11639
7-hydroxytetradecanoic acid	244.2032	1.348 HILICneg	162709	97101	70009	103137	241562	44453	158742	52489	146135	62546
7-hydroxytetradecanoic acid Esi-1.3579999	244.2036	1.358 HILICneg	1	97044	69986	91696	1	45861	1	52489	64671	63624
7-Ketodeoxycholic acid	406.2701	10.079 Rpneg	15796	22499	1	2052	1616	16398	1098	1	10068	6274
7-methoxy-dodec-4-enoic acid	210.1618	7.487001 Rppos	3079778	2516273	4249323	2811129	2747724	2520735	4268458	3336332	2642138	2597892
7-methoxy-dodec-4-enoic acid Esi+15.141001	227.1869	15.141 Rppos	362856	194795	301565	226194	128891	71683	212413	93927	173251	45430
7-methyl-4-oxo-octanoic acid	172.111	6.46 Rppos	399819	206186	318682	389774	378216	178445	246440	264011	348744	372178
7-methyl-4-oxo-octanoic acid Esi+6.0089993	171.1259	6.008999 Rppos	336339	329899	312217	224465	176516	113542	250696	191549	194069	187521
7-methyl-nonanoic acid	172.1462	9.985 Rpneg	3188	3601	2838	9471	5051	3005	3916	3900	10819	4458
7-methyl-nonanoic acid	172.1462	1.275 HILICneg	468767	473329	236681	370252	573833	139051	202906	579896	345523	380518
7-O-Acetylaustroinulin	364.2589	12.857 Rpneg	8622	7707	5941	6768	8387	8129	8302	9182	9962	8804
7Z,10Z,13Z-docosatrienoic acid	334.2867	1 HILICpos	1078958	611138	436300	588030	1664184	343493		598371	525904	2026212
7Z,10Z-octadecadienoic acid	280.2401	12.601 Rpneg	3904961	3748865	3304883	3472279	5039881	4606311	5082914	6104413	5327793	5617851
7Z,10Z-octadecadienoic acid Esi-12.928999	280.2408	12.929 Rpneg	22403	49722	10408	36780	69981	62538	82108	17137	90808	15234
7Z,10Z-octadecadienoic acid Esi-12.932	280.2403	12.932 Rpneg	1	1	1	1	70785	32157	85746	69015	91790	56650
7Z,10Z-octadecadienoic acid Esi-12.936998	280.2407	12.937 Rpneg	33773	44500	43508	1	70534	63192	84951	117480	92389	99029
7Z,10Z-octadecadienoic acid Esi-13.248	280.2407	13.248 Rpneg	1	28406	4464	1	39544	7849	36113	53353	49770	1
7Z,10Z-octadecadienoic acid Esi-13.249	280.2405	13.249 Rpneg	1	30067	4464	6512	39113	7849	37143	1	46967	58442
7Z,10Z-octadecadienoic acid Esi-13.520002	280.2402	13.52 Rpneg	37649	36094	53661	32817	39902	32962	62085	30223	42325	34434
7Z,10Z-octadecadienoic acid Esi-13.520998	280.2403	13.521 Rpneg	35492	23834	36453	30966	39902	33360	62639	11750	34070	27784
7Z,9E-Dodecadienyl acetate	224.178	11.599 Rpneg	51745	23693	14661	24797	19285	8328	13206	20045	17258	16195
8,24-Tritricontadiene	967.0071	6.637 HILICneg	1217221	1496476	1009372	1477282	1545740	640458	904912	874029	586869	1069008
8,24-Tritricontadiene Esi-1.9139998	967.0073	1.914 HILICneg	606160	622858	650603	649115	687375	476148	569738	521237	621158	328815
8,9-EE-14(Z)-E	342.2711	12.665 Rpneg	1	1	15489	1	27653	8218	18657	27811	8970	9241
8-Acetoxy-4-acoren-3-one	277.2047	11.815 Rppos	412280	439020	415062	445689	396733	412472	481148	507823	504327	478050
8E-Heptadecenedioic acid	298.214	11.343 Rpneg	5183	4540	4443	5207	5512	4114	4187	4782	5487	4671
8E-Hexadecenyl acetate	282.2557	12.857 Rpneg	6014104	5661975	4674824	5387965	6207893	6142193	6375428	7397338	7134728	7011584
8E-Hexadecenyl acetate	282.2569	5.438 HILICneg	82259	167638	122407	129518	199131	135004	155370	127977	180515	143498
8E-Hexadecenyl acetate Esi-13.189001	282.2561	13.189 Rpneg	72312	23935	34761	111839	46598	106613	147322	123888	80687	135920
8E-Tetradecenyl acetate	254.2245	12.498 Rpneg	4236175	3363740	1164150	2969247	2659562	1981934	2336239	3054219	3222140	2474402
8E-Tetradecenyl acetate	254.2257	1.124 HILICneg	1635133	2054791	1391745	1704928	1727399	193490	1402263	1475009	2739766	1355676
8E-Tetradecenyl acetate Esi-12.498	254.2246	12.498 Rpneg	4240371	3368755	1167963	2974419	2672554	1982820	2341606	3060717	3235203	2485636
8E-Tetradecenyl acetate Esi-12.662001	254.2256	12.662 Rpneg	33347	25578	1	13506	20527	20713	19095	20831	25419	12659
8E-Tetradecenyl acetate Esi-12.889626	254.2254	12.88963 Rpneg	24712	22298	1	24554	21139	2841	17090	15858	13390	1
8-hydroxy-2'-deoxy Guanosine	283.092	2.845 Rppos	1054555	653193	641483	1002937	843892	1520424	518772	1747442	1490403	1771916
8-iso Prostaglandin F1?	355.2721	9.886001 Rppos	342103	289551	358668	335707	477965	334722	313601	355737	404113	400409
8-methyl-hexadecanedioic acid	300.2286	10.186 Rpneg	7469	7417	5233	7431	8811	5365	5392	7514	10410	5459
8-methyl-hexadecanedioic acid Esi-11.813	300.2313	11.813 Rpneg	5483	11227	6055	7749	5837	7466	1	13633	1	5697
8R-HOME(9Z)	298.2522	5.772 HILICneg	26660	85281	31552	58647	69701	58004	72052	48008	77382	75375
8R-HOME(9Z)	298.2542	12.655 Rpneg	60190	45826	53486	56597	30096	43993	35992	47650	51910	49163
8R-HOME(9Z) Esi-11.816001	298.2504	11.816 Rpneg	44395	50529	93696	114342	127733	80664	114618	39274	36344	35764
8R-HOME(9Z) Esi-11.819	298.2511	11.819 Rpneg	1	42662	88143	56757	142135	101704	35917	63034	45354	12154
8Z,10Z-Pentadecadienyl acetate	266.2244	12.54 Rpneg	8317	8086	4522	6919	6717	10625	3855	9314	4304	1
8Z-Tridecenyl acetate	240.2094	12.257 Rpneg	273380	164282	32852	141763	105361	55439	82206	108835	101141	46823
8Z-Tridecenyl acetate Esi-12.260001	240.2093	12.26 Rpneg	273380	164282	4327	141763	105361	55439	82206	108835	101141	7408
8Z-Tridecenyl acetate Esi-12.261001	258.2199	12.261 Rpneg	301882	189803	58725	169820	131049	76984	106302	141827	136466	79526
8Z-Tridecenyl acetate Esi-12.261001 :1	258.2199	12.261 Rpneg	302188	190091	58726	169805	131144	76944	105921	141991	136466	79695
9-(Methylthio)nonanenitrile	245.1454	11.243 Rpneg	9461	4588	12848	6437	2912	2373	4326	1864	1091	3402
9(Z),11(E),13(E)-Octadecatrienoic Acid ethyl ester	306.2557	12.751 Rpneg	264006	270295	330877	314876	285374	230374	294651	354181	266031	297306
9(Z),11(E),13(E)-Octadecatrienoic Acid ethyl ester Esi-12.755	306.256	12.756 Rpneg	201651	195711	330808	171925	285411	230376	294651	354181	266031	297306
9(Z),11(E),13(E)-Octadecatrienoic Acid ethyl ester Esi-12.757	324.2665	12.757 Rpneg	207071	198455	94526	174602	290301	234804	302027	358550	270710	301973
9,10-Epoxy-18-hydroxystearate	314.2457	12.093 Rpneg	4951	3713	1	3903	3971	4380	4985	6672	11446	3622
9,10-Epoxy-18-hydroxystearate	331.2727	1.022 HILICpos	85365	163682	94929	358511	418893	96926		143061	256078	344337
9,10-Epoxyoctadecane	268.2758	14.656 Rpneg	8166	1392	1192	1898	11434	10140	4511	8457	3519	3112
9-bromo-nonanoic acid	236.0437	0.889 Rpneg	4016	2171	2281	2005	1571	2269	1	1317	2495	1840
9-Docosene	325.3668	1.525 HILICpos	103756	102745	67211	92340	136767	100204		87210	179030	120492
9E-Pentadecenyl acetate	268.2402	12.681 Rpneg	1073562	784341	243175	657346	598465	394405	543050	687942	599634	443449
9E-Pentadecenyl acetate	268.2408	1.099 HILICneg	1	163855	123236	172247	357747	100694	125330	151387	650699	141827
9E-Pentadecenyl acetate Esi-12.682	268.2403	12.682 Rpneg	1073802	784738	4838	675832	615214	397807	539668	689635	613793	443865
9E-Undecenyl acetate	212.1773	11.612 Rpneg	6050	6422	2570	4403	3277	1685	2189	2336	2635	2003
9-Heneicosene	311.3556	1.542 HILICpos	338654	446964	303310	428788	388197	346850		531091	891105	379080
9-Hexacosenoic acid	394.3776	0.97 HILICneg	256618	352096	183943	286802	196252	85178	247926	182282	150830	162817
9-Hexacosenoic acid	412.3897	13.802 Rpneg	100314	53822	26078	49055	33517	20030	39431	36161	23680	17471
9-Hexacosenoic acid Esi-13.807001	394.3798	13.807 Rpneg	49216	18946	12799	19689	13629	11135	15382	10981	10740	5117
9-hydroxy-13-oxo-10-octadecenoic acid	312.2257	1.494 HILICneg	62324	56842	70404	1	86317	188401	73582	1	275299	80934
9-hydroxy-13-oxo-10-octadecenoic acid	312.2297	10.195 Rpneg	10729	8686	7025	8281	14309	8152	7313	7353	10173	13730
9-hydroxy-13-oxo-10-octadecenoic acid Esi-10.197	330.2383	10.197 Rpneg	10984	8412	6280	10703	9404	1	6719	10839	20256	10107
9-hydroxy-13-oxo-10-octadecenoic acid Esi-10.558999	312.23	10.559 Rpneg	4694	4001	4529	3868	8892	7923	5081	6819	5020	6246
9-hydroxy-13-oxo-10-octadecenoic acid Esi-11.632	330.2401	11.632 Rpneg	1	1492	1	4385	3549	1670	4680	3254	3579	5460
9-Hydroxyrisperidone	486.228	12.043 Rpneg	1	8516	1	8443	13073	1	3215	7484	9156	11639
9-Nonadecene	549.6207	24.631 Rppos	10082072	17380256	8666238	9338041	16944556	15746820	15596976	16660188	15688359	14771007
9-Pentacosene	367.4169	17.533 Rppos	847437	471042	467650	440907	448373	308816	349675	383898	487034	594417
9R,10S-dihydroxy-stearic acid	338.2436	9.387 Rppos	41432	103036	133581	188033	88462	192324	172661	142381	155431	133799
9S,10R-Epoxy-1,3Z,6Z-heneicosatriene	303.2924	8.479999 Rppos	758555	1233682	1358505	1434484	1933596	1004322	1159908	1536381	1539696	1286542
9S,12S,13S-trihydroxy-10E-octadecenoic acid	330.2379	9.591 Rpneg	24014	3842	1	4259	22995	19111	1	29729	6292	4543
9-Thiastearic Acid	284.2193	11.093 Rppos	328336	300819	348772	358076	311904	336018	361264	338776	373038	364484
9Z,11E,13-Tetradecatrienyl acetate	250.1923	1.171 HILICneg	227787	250680	198527	427244	235957	260538	226638	250655	230057	253654
A 922500	488.1972	0.789 HILICneg	12176	1	10380	6541	57199	1	72734	74269	46605	49816
Acetaldehyde diisoamyl acetal	201.2092	7.567 Rppos	509628	520841	552300	559403	509055	520435	565411	568353	581534	609814
Acetic acid	60.0215	8.951999 HILICneg	1545526	1157238	1132076	1640784	1139210	1112185	1629498	1775900	1650359	1584956
Acetic acid Esi-0.974	60.0215	0.974 HILICneg	568841	576491	483090	770098	600712	353823	771032	1162135	920362	847713
Acetic anhydride	102.032	8.553 HILICneg	36709	35570	37547	37894	36940	29415	46111	39462	45947	57651
Acetic anhydride Esi-0.89399993	102.0317	0.894 Rpneg	17659	26213	30661	22907	28818	37792	62382	48132	36274	63075
acetoacetate	102.0311	1.036 Rpneg	10239	32736	16659	27497	12842	1	1	34795	36971	31748
acetoacetate	102.0315	0.902 Rpneg	17319	28541	31604	52927	33698	38635	57986	45287	33269	52624
Acetylcarnitine	203.1159	5.673 HILICpos	1.22E+08	1.19E+08	1.17E+08	1.19E+08	36616984	52197032		58433148	90493536	43148508
Acetylenic acids; 10-Heptadecen-8-ynoic acid, 7-hydroxy-	282.2171	12.316 Rpneg	3477	2320	1507	2187	2718	1969	2173	1983	2366	1781
Acetylsalvipisone	354.1824	12.398 Rpneg	4798	2354	1	2694	1596	2096	2042	2267	2045	2254
Acoric acid	268.1658	7.636001 Rppos	316370	293256	257086	253743	286012	405903	440874	310417	295970	248849
Acrimarine H	535.1582	19.668 Rppos	1599478	1564127	1515569	1612538	1541596	1608791	1676643	1600726	1667769	1698484
Acrimarine H	535.1588	0.701 HILICpos	16348040	10281764	9164691	13307791	12240085	26047304		21038992	18765348	23265342
Acrimarine H Esi+0.671	535.1584	0.671 HILICpos	15196605	4174529	21426610	7281998	8910485	20953416		17217986	18961616	20033592

Acutilol A	304.2395	12.616 Rpneg	2659080	2684677	2432332	2994534	2206578	2106140	2416473	2657393	2554655	2740812
Acutilol A Esi-12.936998	304.2412	12.937 Rpneg	23887	26763	35976	15132	2228	1	1	1	25615	19035
Acutilol A Esi-13.483001	304.2406	13.483 Rpneg	17901	20423	27210	35415	9491	26093	13637	12609	1	7448
Acutilol A Esi-13.483001 :1	304.2404	13.483 Rpneg	28432	11976	22377	31716	9621	24287	14338	12805	1	7427
Adenine	135.0546	5.118 Rpneg	217837	166424	229093	256283	116511	171325	175135	219776	144834	182938
Adenine Esi-2.36	135.0541	2.36 Rpneg	47546	7956	13647	8300	2529	1	11215	6589	3614	1
adenosine	267.0969	3.212 Rppos	6155380	6600607	6518576	9327095	6203561	5697156	5266098	7994899	6620384	5693562
Aerophobin 1	473.9526	0.991 Rpneg	2983	3504	3287	3020	4650	4037	5103	2172	2405	2779
AFN911	557.2753	12.592 Rpneg	44579	1	7390	14347	5536	2699	6766	8969	6898	5756
Agecorynin B	418.1251	7.232 Rpneg	10100	10992	5395	8414	5613	11755	5483	8309	5615	6255
Agrocybenine	458.2897	1.255 HILICneg	264295	167520	73353	131046	313889	475551	109457	132461	120343	163229
Akeboside Ste	895.5284	21.934 Rppos	505831	517088	569616	469576	793696	893765	947283	984714	880325	894869
AL 8810 ethyl amide	918.5574	1.029 HILICneg	1	1	1	1	145913	30840	262376	61008	222796	215427
AL 8810 ethyl amide	875.5654	20.879 Rppos	580744	463886	614441	495217	144202	144126	164041	87446	496468	623859
Ala Ala Arg	316.1833	9.701 Rpneg	2159	2374	8008	4687	1965	3109	3984	1301	1	2223
Ala Ala His	616.2708	23.457 Rppos	233274	254893	244762	205403	401801	397170	369227	393400	457645	418216
Ala Ala His Esi+23.130001	616.2705	23.13 Rppos	215508	214332	235211	196555	243240	231785	252298	230233	250633	235124
Ala Thr His	654.3106	0.71 HILICneg	232088	271729	191089	295897	355993	362011	354128	322865	525936	324214
Ala-Asp-OH	358.0641	5.312 HILICneg	58212	145694	155493	133948	145493	116257	105302	120285	92468	86162
Alanyl-Glycine	146.069	0.859 Rpneg	191442	190529	160010	139518	151070	248715	177574	186644	307526	244123
Alcoifosfamide	324.0427	9.162001 Rpneg	10228	3614	5706	4495	10587	4931	4362	2116	3084	2315
Aldoifosfamide	336.0408	0.942 Rpneg	11254	8882	9591	10234	5982	8002	4247	9156	8203	7598
Alkaloid A6	699.1912	20.665 Rppos	600655	671968	667126	700434	672375	710950	693729	646127	676728	715165
Allochenodeoxycholic acid	392.2929	4.605 HILICneg	114698	57758	10958	14045	66384	68571	15027	12120	91977	46302
Allopurinol	136.0387	1.117 Rpneg	193433	138086	138400	149929	116638	85488	111373	101000	87947	109158
Allopurinol	136.0388	4.299 HILICpos	28995380	25890172	26466816	26137176	26861700	25372772		27540912	29075634	22959372
Allopurinol	136.0396	1.445 Rppos	17816490	13079195	13878490	15089065	12031830	14148667	10096048	14215693	12071450	12564274
Allopurinol Esi-0.93200004	136.0388	0.932 Rpneg	38449	25381	20233	28415	21919	19236	16740	28827	23775	17634
Allopurinol Esi-0.93200004 :1	136.0383	0.932 Rpneg	39165	24305	26134	27009	20986	18891	16740	28827	24674	22091
Allopurinol Esi-1.7349999	136.0387	1.735 Rpneg	23983	31490	33403	54459	43397	27750	33471	27592	43694	59507
Allopurinol Esi-6.3629994	136.0385	6.362999 HILICneg	199524	350906	344770	346485	293128	373450	219468	247305	299848	284967
alpha-Carboxy-delta-nonalactone	182.0943	5.164001 Rppos	205569	317595	309940	383871	763537	244518	377659	534371	709329	473994
alpha-Crocetin glucosyl ester	490.2232	1.121 HILICneg	1	53826	163749	54248	1	1	224061	153550	436019	310551
alpha-Cypermethrin	876.1508	0.872 HILICneg	57783	28437	66625	44205	45032	352361	86855	201761	70533	69041
alpha-Cyperone	234.1627	11.698 Rpneg	5130	5343	6421	4709	6500	5628	5798	5380	5157	6025
alpha-D-Mannose 1-phosphate	260.0293	0.772 Rpneg	6278	162968	445623	258680	256415	438742	748935	464309	438946	468501
alpha-Furyl methyl diketone	138.0332	4.435 Rpneg	9361	15764	44799	9948	22383	10282	7851	15394	23073	9103
alpha-L-Rhamnosyl-(1-3)-alpha-D-galactosyl-diphosphounde	1234.741	13.703 Rpneg	4982	1486	4023	10968	2649	2117	1376	4517	1698	3997
alpha-Santalyl phenylacetate	338.2253	1.3 HILICpos	415997	515222	90996	110525	461780	302948		113443	171503	183120
alpha-Tocopherolquinone	428.3651	19.914 Rppos	6266691	6090578	5909379	7831282	3385772	8689706	8342860	6789242	9032506	7259845
alpha-Tocopherolquinone Esi+22.117002	428.3654	22.117 Rppos	5240309	5092897	6582964	7006699	5581145	6326247	6313115	5248075	5269871	5139337
Alvimopan	424.2353	12.344 Rpneg	4846	7308	5517	8725	6966	3034	4739	6372	6405	4557
Ambroxol	375.9755	0.991 Rpneg	9718	10119	9371	9635	11576	11261	12645	7940	8525	8266
AMC Arachidonoyl Amide	461.2904	13.343 Rpneg	3619	4088	3023	4375	6101	4218	5292	5395	6554	5001
Aminocaproic acid	131.0947	1.727 Rpneg	256519	204821	140969	177673	355846	268524	280397	442481	395180	374146
Amitrole	84.043	0.94 Rpneg	14398	9566	14425	18675	17895	10921	1	14364	25856	19212
Ammodendrine	416.3146	0.974 HILICneg	288642	537973	413360	383202	547013	139828	333868	345951	308971	410090
Amorilin	974.4948	20.88 Rppos	808623	597403	708276	534508	224188	249565	220010	119550	469988	565067
Amorilin Esi+25.464998	974.4943	25.465 Rppos	1025720	739692	414609	783817	767095	537015	491948	568040	501103	500712
Amritoside	643.1395	20.544 Rppos	681289	590476	605188	706341	692463	612881	620153	743826	725103	724757
Anandamide (20:2, n-6)	351.3135	0.97 HILICneg	438019	264413	269205	241326	172913	64237	284867	173521	432802	164937
Anandamide (20:2, n-6)	351.3145	0.992 HILICpos	2028300	1328826	1163126	1371822	2568202	1		1	1078055	2178497
Anandamide (20:2, n-6)	351.3151	13.365 Rpneg	27516	26145	47778	91472	15073	19338	34933	13034	13225	14654
Anandamide (20:l, n-9)	353.3316	13.36 Rpneg	26266	19076	33411	51786	14764	15101	24459	11373	12244	11240
Anandamide (22:6, n-3)	371.281	13.415 Rpneg	6239	5179	6322	7844	4206	3379	3751	3834	4651	4214
Anandamide 0-phosphate	871.5301	22.935 Rppos	1200267	790845	724585	781955	2067741	1821718	962741	1817065	1703173	1736830
Androstane-3,17-diol dipropionate	421.3224	2.025 HILICpos	433485	193744	200792	107617	129949	143426		214525	306269	262199
Anhwiedelphinine	698.3094	13.075 Rpneg	1	3248	5352	4704	1697	1666	4582	2254	4828	3742
Annoglaxin	670.4601	12.573 Rpneg	41401	16950	25288	19963	16684	5843	11693	10893	11505	1
anteiso (4E,14-methyl-d16:1) sphingosine	284.2827	8.266 Rpos	424025	494791	534816	575374	466125	511068	559403	595851	614781	630624
Anthralin	208.0529	7.36 Rpos	577623	637855	708149	769235	615151	679586	746983	780928	825058	859336
Antibiotic X 14889C	614.4035	12.343 Rpneg	20556	4435	4660	8951	3585	1745	3075	3391	3505	1835
Antibiotic X 14889C	614.4047	1.149 HILICneg	374688	1	1	114107	417883	224673	90686	143708	1	222877
Antibiotic X 14889C Esi-12.274001	614.4009	12.274 Rpneg	26955	2596	2533	8960	1607	1745	2120	1830	1801	919
Antillatoxin B (red color)	565.3501	14.319 Rpneg	6288	6999	7891	8602	6899	5709	9856	8970	11520	3503
Antillatoxin B (red color)	565.3527	0.901 HILICneg	4401406	2123708	860973	1404299	6059880	603757	1589521	1447051	2181009	2537578
Antillatoxin B (red color) Esi-13.036001	565.3488	13.036 Rpneg	2817	2080	3040	2680	1427	1	1724	2270	3160	921
Apigenin 7-sulfate	350.01	6.719 Rpneg	7306	3773	2115	2571	1	1	1	1	1	1
Apo-12'-violaxanthal	382.2481	1.107 HILICneg	978181	718570	525249	946167	1450850	137802	981942	1136650	621910	1253066
Apo-12'-violaxanthal	382.2547	12.846 Rpneg	3121	2747	21963	6178	1	1	7390	2697	2827	3429
Apo-12'-violaxanthal	399.2777	1.344 HILICpos	334493	419023	170817	1	330440	200999		133485	102201	103972
Aprindine	368.2422	12.601 Rpneg	1	9350	13860	7857	3577	5041	5977	6267	4571	5343
Aprobarbital	210.1024	9.086999 Rpneg	16868	67934	17912	62886	67592	16638	18069	40163	112018	54533
Arabinosylhypoxanthine	268.0805	1.734 Rpneg	2055569	1659923	1630611	1913948	1658398	1801767	1283430	1868129	1883238	1884662
Arabinosylhypoxanthine	268.0808	2.649 Rppos	20993392	17532260	19070380	20380068	17526584	23464630	15337668	22427218	21354740	20304016
Arabinosylhypoxanthine Esi-1.0430001	268.0807	1.043 Rpneg	27713	5257	24661	10900	1	46706	1	60385	35495	37931
Arabinosylhypoxanthine Esi-12.007	314.0855	12.007 Rpneg	1108	1611	1280	964	1187	3233	1	1600	3279	3070
Arachidonic Acid Leelamide	571.4732	0.976 HILICneg	350190	301196	266776	354443	309478	136968	273665	308613	333764	309732
Arachidonyl carnitine	445.3915	0.926 HILICneg	271818	372731	436943	447989	406026	200008	399760	349006	466724	367348
Arachidyl carnitine	455.3954	1.768 HILICpos	734744	245734	62967	184282	236390	186726		897851	643452	425935
Araliacerebroside	731.5604	0.884 HILICpos	245119	281143	209428	396064	1	1		57601	1	1
Araliacerebroside	753.5346	23.922 Rppos	623157	742741	771386	566086	456916	680280	545317	707457	626853	678423
Arg Arg Arg	486.3125	13.353 Rpneg	8933	7538	6412	7588	9997	8937	11830	10516	11669	12804
Arg Asp Pro	386.1894	1.071 HILICneg	1221625	706532	476033	667310	1768607	546593	539442	769467	803607	740241
Arg Ile His	865.5342	25.419 Rppos	691980	1201497	581228	1268100	921892	904625	1208668	1132911	1289327	1053070
Arg Ile His Esi+25.182001	865.5342	25.182 Rppos	141081	166962	644553	1351645	364376	529948	617542	645561	585640	679541
Arg Lys Gln	490.2869	12.842 Rpneg	3115	3138	2264	5315	2981	1348	4242	4899	4867	1592
Arg Lys Gln Esi-12.955999	490.2867	12.956 Rpneg	1964	1913	1121	2353	941	846	1820	2092	2037	845
Arg Lys Tyr	525.2901	13.037 Rpneg	144320	110564	121313	149979	96618	90224	123697	123534	105994	112930
Arg Lys Tyr Esi-13.037001	525.2893	13.037 Rpneg	144604	110623	121313	151957	96619	90224	123707	123657	106100	112930
Arg Phe Pro	418.2313	12.859 Rpneg	3920	2951	2978	3266	3303	3918	3922	3049	3494	3306
Arg Ser Glu	390.1881	6.557 Rpneg	3631	5202	3645	7263	6407	3945	3921	5474	7467	5705

Aristolodione	614.1741	20.76 Rppos	485221	515558	519568	495889	489576	495851	503974	473813	487414	480918
Armillarivin	384.1974	13.124 Rpneg	1877	1106	890	880	1035	708	1	1	1	1
Arnamiol	450.181	11.627 Rpneg	7289	9578	4703	6147	3831	6062	13630	7385	15300	9110
Artemoin D	550.4975	0.936 HILICpos	1047508	1264789	1025173	1207786	1493813	1735542		1770819	1587102	1744977
Artoindonesianin A	570.266	11.924 Rpneg	22429	4690	30787	22657	33913	12473	15572	18096	22787	20032
AS-252424	305.0177	8.972 Rpneg	1	4944	1	2884	5602	1	955	3251	6245	2558
Ascorbate 2-sulfate	209.9835	0.764 Rpneg	10827	9987	7597	8753	15522	11166	10684	9967	16230	14577
Ascorbyl Palmitate	460.2684	9.145999 Rpneg	4352	4440	3606	4563	5645	3852	4324	4451	4898	4369
Asn Arg Asp	449.1837	1.071 HILICneg	1531905	955136	587209	960481	2962057	1	490762	1283524	880699	1300499
Asn Glu Gly	364.1224	11.928 Rpneg	7271	1630	9466	7364	10399	4724	5166	6180	7859	7083
Asn Leu Gln	355.1849	5.764 Rppos	264692	240456	249726	227899	259532	247174	238127	234863	234027	230427
Asn-Gly-OH	296.0762	9.377 Rppos	95587	98707	124804	120223	95271	122174	136384	132762	141322	160085
Asn-Gly-OH Esi+8.326999	296.0759	8.326999 Rppos	83116	130728	136034	105589	108347	139582	149972	134903	169053	154605
Asp Ala Cys	307.0837	1.29 Rppos	6568332	4454565	6693709	5532174	5595277	5770149	8007162	5738011	3992619	4388429
Asp Gln Glu	390.1378	1.276 Rpneg	5869	5348	7284	1	5469	11061	12241	6046	10535	8340
Asp Gln Glu Esi-1.2699999	390.1382	1.27 Rpneg	5869	5348	7284	6911	1	11061	12241	1	10535	1
Asp Ser Cys	369.0835	1.287 Rpneg	16202	15266	20592	18661	12509	24194	29376	14637	13033	15567
Asp-Ser-OH	374.0658	0.926 HILICneg	1	69720	76899	59078	66533	1	1	108005	108139	71315
Astaxanthin diglucoside/ Astaxanthin ?-D-diglucoside	937.5158	21.937 Rppos	273130	312303	288244	238681	303577	356744	361811	365032	230910	279911
Astaxanthin glucoside	656.4025	0.921 HILICneg	570121	283563	1	247836	778053	293755	170205	225656	266366	328514
Asterosterol	370.3203	13.006 Rpneg	1	1	16330	1	14637	11328	12777	11318	15820	1
Austalide B	474.2248	11.628 Rpneg	33268	34704	18693	25979	22913	20450	40679	26304	45625	29804
Avenanthramide L	325.0981	8.515 Rpneg	30929	23283	28377	18403	24731	30486	23477	19655	14753	15580
Avenanthramide L Esi-8.794999	325.0981	8.794999 Rpneg	22974	16607	21028	13087	18670	22409	18749	14820	10311	10908
Avermectin A2a	964.5423	0.96 HILICneg	107866	109796	72257	91866	108845	54289	135579	50397	91381	66356
Avermectin B2a	889.5166	23.214 Rppos	808647	747498	856459	725064	710961	615835	672434	1098665	518880	686536
Avocadene 4-acetate	328.259	10.941 Rpneg	10133	6479	6934	7550	6119	6766	6554	7402	7108	6213
Axillarenic acid	398.3395	13.421 Rpneg	159757	51411	45829	57188	44741	44134	35752	27289	37723	19479
Axillarenic acid	398.3413	1.118 HILICneg	104129	45402	8565	1	87465	297247	90674	1	101948	59573
Axillarenic acid Esi-12.207	398.3369	12.207 Rpneg	6111	7716	4439	14252	7314	2549	5342	5038	5718	4302
Axillarenic acid Esi-13.196	398.3405	13.196 Rpneg	24909	12031	10458	15043	8105	8925	1	6619	1	1
Axillarenic acid Esi-13.1970005	398.3409	13.197 Rpneg	25382	14237	10581	15418	9044	10958	53386	7421	10845	4857
Axillarenic acid Esi-13.421	398.3397	13.421 Rpneg	159425	51411	45829	57082	44741	44134	41914	27289	37723	19479
Axillarenic acid Esi-13.421 :1	398.3389	13.421 Rpneg	159757	51411	45829	57315	44741	44134	41955	27289	44233	19479
Azaspiracid	845.4743	24.524 Rppos	897386	936095	575409	638884	913823	897001	806568	767842	777671	747016
azido-FTY720	370.2344	7.826001 Rppos	243742	216581	233852	220863	220799	224236	256442	196669	186853	202738
Azithromycin	794.5126	13.899 Rpneg	138611	85855	97456	147637	21244	21034	37940	27663	10566	15091
Azithromycin Esi-12.579001	808.5288	12.579 Rpneg	1	12249	1617	13821	16135	1	2608	9393	21544	11553
azosemide	370.0106	7.927001 HILICneg	827328	845301	771917	785348	877336	755109	914959	869446	897601	896937
Bacterio-pheophytins	948.6001	13.293 Rpneg	9045	3837	3719	6430	1922	851	4045	3648	5027	3500
Bacteriorubixanthinal	596.4233	12.457 Rpneg	12023	5054	5207	6235	5107	2393	3679	2899	4132	3171
Bacteriorubixanthinal	596.425	1.111 HILICneg	832105	319517	239185	361386	968373	245009	273675	463576	575647	531994
Bacteriorubixanthinal Esi-12.263	642.431	12.263 Rpneg	7415	2498	1903	2702	1831	1	1	954	1111	1
Behenoyl-EA	382.3872	18.392 Rppos	82551	139912	123178	74981	221235	95536	285126	128262	120511	43120
Behenyl alcohol	325.3706	10.27 Rppos	237304	246602	576939	290626	280729	217756	244305	242666	291381	247499
Benzaldehyde glyceryl acetal	162.0684	8.647001 Rppos	226644	508237	489527	452315	543110	379898	436789	481652	454850	414483
Benzanthrone	230.0748	0.898 Rpneg	961	1	1	1	2347	9027	4971	5185	15182	4619
Benzthiazuron	207.0473	1.024 Rpneg	3217	2556	4296	2491	10113	9486	8322	6127	7489	7197
Benzyl cinnamate	238.0987	4.701 Rpneg	22669	15069	23581	19389	16880	22052	20530	18910	16372	23441
Benzyl cinnamate	238.0996	4.973 HILICneg	147011	243206	219726	232381	342913	167085	210967	185118	212916	192734
Benzyl cinnamate Esi-4.5299997	238.0987	4.53 Rpneg	16991	10523	17833	16210	14246	16750	15546	14580	13113	18222
Betaine	117.0789	0.87 Rppos	9325204	9316271	8936324	10043412	7848831	12390143	6912416	7102286	11224164	9608168
Betaine	117.0795	7.168 HILICpos	33641832	32908236	32601732	35226992	29523340	38850968		26415608	34057340	31607716
beta-Micropteroxanthin	792.6036	27.729 Rppos	1	49081	51063	15312	294087	523592	312226	322977	511221	349055
Betavulgaroside IV	794.4062	0.916 HILICneg	850110	485887	312088	381876	1317362	256485	285975	285368	537316	462259
Betavulgaroside VII	810.4062	0.917 HILICneg	1978261	840901	321228	619642	3257974	103573	299460	454052	732526	700312
b-Glucose	180.0629	0.894 Rpneg	23102	48899	43267	56306	64988	74665	67380	58814	69586	70834
BHT	220.1829	13.07 Rpneg	4394	4936	5807	4273	4671	5336	5092	3463	4301	4164
Bis (2-hydroxypropyl) amine	133.1094	5.109001 HILICpos	171448	364339	280317	537890	1288416	217418		269152	793781	856444
Bis(2-hydroxyethyl)dithiocarbamic acid	181.0239	1.024 HILICneg	1067421	996180	862186	956341	824355	356726	597582	654058	432508	529353
Bis(2-hydroxyethyl)dithiocarbamic acid Esi-1.4560001	181.0243	1.456 HILICneg	139618	214364	180520	139048	118272	15093	103025	74348	69116	53958
Bis(4-nitrophenyl)phosphate	340.0115	0.694 HILICpos	1915131	1057343	1658227	1979007	1830496	1999404		1746543	1512537	1841023
Bisacurone epoxide	268.1674	10.086 Rpneg	8310	21229	11641	24409	18381	4950	10399	12195	24526	20074
Bisacurone epoxide Esi-10.25	268.1675	10.25 Rpneg	3833	11824	1	1	11146	3822	3867	8224	16225	1
Bluensidine	282.1157	9.669 HILICneg	162481	322860	280295	286601	463135	189931	201815	168741	139365	138431
Blumenol C glucoside	418.2199	7.709001 Rpneg	24305	29238	26311	31632	37712	26631	26799	29499	34243	28529
Blumenol C glucoside Esi-7.6169996	418.2194	7.617 Rpneg	8781	9406	7910	9879	12634	7298	7368	8987	10583	8390
Boesenbergin B	386.1862	8.197999 Rppos	2853887	2166147	2502622	2143380	1920484	2149464	2471031	2303975	2147149	2291493
Bornyl isovalerate	238.1927	12.094 Rpneg	7055	6185	5059	8432	1	1	1	1	1	1
Botrydial	310.1786	7.751 Rppos	3599288	3609338	3936230	3977403	3663730	3821406	3864435	4119389	3974780	3936458
Bouillonamide A	877.5245	5.127999 HILICneg	292044	311814	339374	286128	330323	291324	324007	270097	251953	252033
Bremazocine	361.229	12.38 Rpneg	7933	5130	2659	4822	5972	4826	9070	6850	5845	5890
Butalbital	224.1182	9.163001 Rpneg	29630	16723	28222	25453	36557	22174	26834	13618	23777	22823
Butoctamide hydrogen succinate	690.427	1.071 HILICneg	2875381	3729975	1121550	2209486	6300542	164644	664726	1288138	672109	1108267
Butyl 1-(methylthio)propyl disulfide	210.0561	5.083 Rpneg	3297	2759	2879	4154	3896	2296	1832	2486	4156	2866
Butyl butyryllactate	216.1361	5.192 Rpneg	7789	28230	4195	24054	41485	5176	3601	17813	38425	15045
Butyl dodecanoate	256.2418	1.124 HILICneg	2.83E+07	2.97E+07	2.98E+07	2.80E+07	3.00E+07	3.45E+07	2.31E+07	2.58E+07	2.31E+07	2.33E+07
Butyl dodecanoate Esi-0.9440001	256.2407	0.944 HILICneg	34146	42359	49307	42881	59303	1	59984	99472	71992	20081
Butyl ethyl malonate	188.1051	7.957 HILICneg	98808	75978	60514	86124	72834	185656	79649	77417	76351	81964
butyrylcarnitine	231.1472	4.404 Rppos	167788	147257	223305	187486	282196	338491	257715	249594	313580	282297
butyrylcarnitine	231.148	4.449 HILICpos	3498725	832557	1008153	1081214	776882	990923		800050	741060	776177
Byakangelicin	380.1093	5.303001 HILICneg	221337	642333	538434	634409	408491	297504	338594	326325	253429	263165
Sphingosine-1-phosphate	831.2325	19.811 Rppos	82416504	92886016	85264888	89178904	68119464	70802760	68050776	72709136	89492024	76683720
Cadiamine	282.1958	12.856 Rpneg	5842	5084	4433	4364	5596	5501	5176	6640	6641	6571
Caffeoyl aspartic acid	295.0724	9.676001 Rpneg	9772	60659	16185	36381	54039	14878	12122	31714	68623	28081
Caffeoyl aspartic acid Esi-8.791	295.0723	8.791 Rpneg	3357	17010	3343	10920	15538	4013	3252	9752	19485	8094
Caffeoyl aspartic acid Esi-9.766	295.0725	9.766 Rpneg	13055	21491	16185	14587	19053	14878	4519	11469	24162	10350
Calusterone	316.2412	12.555 Rpneg	52319	46377	27295	41357	24077	13866	24739	30331	20133	16686
Candletoxin A	668.3235	13.278 Rpneg	322075	280146	370293	344912	208020	217746	315595	244052	331439	299054
Candletoxin A Esi-12.475999	654.3085	12.476 Rpneg	65533	47292	49465	19900	12063	11028	15771	16142	18124	17092
Candletoxin A Esi-12.663001	654.3083	12.663 Rpneg	151735	90441	108343	29333	18164	14951	22605	24315	26039	22937
Candletoxin A Esi-12.663001 :1	654.3059	12.663 Rpneg	151849	90441	108343	29333	18164	14951	22605	24315	26039	22937

Candletoxin A Esi-12.726	668.3221	12.726 Rpneg	3273	2961	2272	4743	1001	1	1	1	1	1
Candletoxin A Esi-13.277	654.3079	13.277 Rpneg	35132	32240	43214	39935	24440	26065	36304	30989	38918	36547
Candoxatril	515.2907	9.996 Rpneg	5156	1685	1027	3859	1	1	1	1	1	1
Capsiate	306.1845	11.53 Rpneg	13395	12297	11424	12352	13158	8943	11511	12187	7569	11084
Capsiate Esi-11.614999	306.185	11.615 Rpneg	1	7778	5257	1	9074	1	7853	5340	9390	7211
Carbamazepine N-Glucuronide	400.1246	5.928001 HILICpos	267556	212472	195265	228426	291418	278137		288452	299364	226564
Carbamazepine N-Glucuronide	446.1348	5.056 Rpneg	6498	5323	4960	4947	4279	4464	4156	5362	5132	7206
Carbaprostacyclin-biotin	706.4397	13.649 Rpneg	7153	6166	2793	5760	5062	2668	1	4756	3022	4331
Carbocysteine sulfoxide	195.0207	1.091 HILICneg	1028837	3220097	4230456	4078932	2960288	1	2190890	2789232	1329026	4037451
Carboxyifosfamide	292.013	0.983 Rpneg	10345	8352	7811	9111	7203	7158	5101	7829	7768	7250
Carnitine	161.1049	0.86 Rppos	3.67E+07	4.23E+07	4.33E+07	3.85E+07	4.56E+07	4.93E+07	5.63E+07	5.01E+07	5.25E+07	4.70E+07
Carnitine Esi+0.9239999	143.0945	0.924 Rppos	1316818	1376079	1280330	1300601	1393967	1675797	741129	958944	1688310	1017598
Carnosifloside VI	926.5253	20.887 Rppos	1365427	1077189	1489894	987689	427303	448468	418871	302696	762666	1245962
Carpaine	524.3854	1.008 HILICneg	147752	79718	112248	1	124210	1	127860	50804	247278	79246
Caulerpin	444.1346	5.018 Rpneg	1	1	1	1	2014	2457	2685	1768	5517	4053
Cavipetin D	418.2701	13.573 Rpneg	5681	5609	5031	5390	2302	1664	2493	1980	1	1
CAY10401	382.255	13.123 Rpneg	2776	2066	1712	1	1193	1304	1613	1656	1643	1835
CAY10412	460.2658	9.048999 Rpneg	3943	3002	3251	3637	4721	2773	2952	3593	3698	3252
CAY10412 Esi-8.697999	446.2491	8.697999 Rpneg	2342	2613	3048	4087	5942	2934	2373	2599	3010	2130
CAY10429-d3	634.4899	1.01 HILICneg	543014	765885	1	735747	753331	1	474966	540172	512589	1
CAY10465	362.0078	5.275001 HILICneg	40970	92716	80062	89608	61600	56272	64591	60293	56062	52423
CAY10580	341.2567	2.326 HILICpos	391743	218151	208228	90338	151842	141903		115360	150734	171005
CAY10621	435.3347	16.037 Rppos	352407	472198	1353527	936237	844064	343220	416465	438047	458619	412125
CCG-1423	250.0289	0.841 Rpneg	3767	3455	6413	3784	8133	9460	11964	6184	5124	6941
CE(14:1(9Z))	640.5466	12.973 Rpneg	14250	5389	3791	5134	3685	2740	4056	3910	3937	3663
Cefadroxil	363.0872	0.983 Rpneg	4026	2911	1945	3159	4988	4693	3075	8405	7436	5720
Cefamandole nafate	490.0712	0.744 Rpneg	1	6022	14105	8395	4984	14924	16172	11666	8435	10206
Cefazolin	500.0313	4.635001 Rpneg	16104	16673	14838	17695	10733	3819	8422	4278	4346	5674
Cepagenin	446.302	11.245 Rpneg	5027	3503	3357	3503	3171	3178	3440	3683	3236	3339
Cephamycin C	909.2496	22.15 Rppos	8441003	9219110	8442970	8927860	6100698	5846338	6034445	2619121	7635164	6429188
Cepharadione A	305.0697	5.113999 Rpneg	20360	13962	17483	19548	9569	13070	11858	18421	11177	13665
Cepharadione A	305.0712	5.474 HILICneg	17659	49407	60374	41821	59128	64418	135860	208010	155903	153010
Cer(d15:1/22:0)	625.5616	13.451 Rpneg	5783	37717	40048	29344	1	1	1	24771	48641	32960
Cer(d16:1/18:0)	519.501	22.901 Rppos	76192	100359	63885	224494	230596	293610	216663	339779	477068	200251
Cer(d16:1/18:0)	537.5087	0.966 HILICneg	335338	229768	315698	411091	523324	383807	432732	598689	758267	611231
Cer(d16:1/20:0)	547.5316	25.065 Rppos	161911	246578	166066	101290	219046	337882	201363	163898	319505	165703
Cer(d16:1/20:0)	565.5423	14.031 Rpneg	1	9735	1	19019	63936	62815	40840	10384	1	13952
Cer(d16:1/20:0) Esi-13.060999	565.5427	13.061 Rpneg	19336	21928	17607	18516	23066	23104	15890	25814	25087	29248
Cer(d16:1/20:0) Esi-13.064001	565.5433	13.064 Rpneg	7562	13640	15513	1	19593	7718	14924	22660	23659	15055
Cer(d16:1/20:0) Esi-14.298002	565.542	14.298 Rpneg	9963	11831	17597	13875	10579	15996	16531	17275	9903	7388
Cer(d16:2(4E,6E)/18:0)	535.494	0.955 HILICneg	508846	264335	82179	221773	764254	288488	137634	150244	200840	184118
Cer(d16:2(4E,6E)/20:0(2OH))	578.536	26.405 Rppos	817423	946561	904920	897288	522987	561695	689853	692167	962318	731548
Cer(d16:2(4E,6E)/20:0)	563.5249	0.959 HILICneg	267881	230244	208403	230074	613259	271974	359215	556285	436721	671812
Cer(d16:2(4E,6E)/22:0)	591.5587	0.951 HILICneg	394899	542982	481978	517626	896049	326895	1076005	1037916	936351	1496591
Cer(d16:2(4E,6E)/22:0)	591.5597	14.375 Rpneg	39009	80945	62605	69392	73746	79286	57555	106055	89902	79276
Cer(d16:2(4E,6E)/22:0) Esi-13.685999	669.5902	13.686 Rpneg	26691	28478	22819	21161	17864	1	31779	1	31249	29990
Cer(d16:2(4E,6E)/24:0)	619.5897	0.943 HILICneg	444784	681665	764907	707413	861673	269943	918451	1018645	923185	1296477
Cer(d18:1/24:1(15Z))	647.6166	13.594 Rpneg	1	1	1	17848	1	5719	14303	9466	25686	25317
Cer(d18:1/24:1(15Z))	647.6191	0.946 HILICneg	859796	1278637	1195397	1525520	1230545	1	1380721	1618247	1512174	1766270
Cer(d18:2/23:0)	633.6051	28.923 Rppos	1081801	1075405	970287	590503	1113684	2025418	1426269	1479285	1676385	1754165
Cer(t20:0/18:0(2OH))	627.5855	27.607 Rppos	470986	377711	403357	337945	441590	639235	535982	542261	507121	572014
Cerberin	622.3404	13.031 Rpneg	127578	554192	543804	715663	543722	423930	333146	494124	454547	728404
Cerberin Esi-13.031	622.3398	13.031 Rpneg	152841	550229	474487	711398	543696	423870	332974	494124	454160	724562
Cerebroside C	775.5603	1.531 HILICpos	803080	802476	1434753	2380996	730690	1274751		1970089	1817903	1840198
CerP(d18:1/20:0)	695.5207	1.042 HILICpos	435894	479948	201162	261098	179102	163276		380386	467354	141807
CerP(d18:1/22:0)	683.5615	23.931 Rppos	916466	1069035	848413	867594	1	1	662838	284010	1	1
Cetyl myristoleate	450.4421	14.598 Rpneg	61680	33163	10963	35623	29331	14740	17173	20542	9484	6280
Chalcomoracin	652.208	12.929 Rppos	288096	255887	285331	259985	182817	241763	210993	170954	173521	163772
Chimyl alcohol	315.3139	9.45 Rppos	665013	551048	963752	1	1	1	1	1	1	1
Chimyl alcohol Esi+9.938	315.3132	9.938 Rppos	516075	406476	740426	1	1	1	1	1	1	1
Chivosazole B	851.4866	0.906 HILICneg	969896	418973	286474	368688	1031613	85833	257995	341021	586214	473394
Chivosazole D	859.45	22.79 Rppos	438722	407282	351707	357050	709685	601400	493422	593415	673975	581192
Chivosazole E	823.4488	4.789001 HILICneg	220023	174363	154992	128845	171252	155054	174330	220987	244651	185809
Chloroform	235.8273	4.417 HILICneg	90314	85020	81462	48670	57193	15552	51210	27166	32603	45102
Chlorophyll a	929.5461	5.042 HILICpos	1554042	930189	1149121	1142154	1380279	945078		901482	483268	549838
Chloroprene	222.0227	0.846 HILICneg	45611	134278	84165	64856	31614	38708	48652	41485	65353	48776
Chlorthiophos	419.9809	0.984 Rpneg	32960	34329	30481	30445	29795	23708	31404	24583	23652	27669
Cholest-5-ene	387.3847	1.517 HILICpos	166592	190562	194563	181544	182272	145732		171806	177754	229406
cholesterol sulfate	466.3132	0.883 HILICpos	237645	289960	277377	329947	210352	176863		174101	194540	192546
cholesterol sulfate	466.3113	13.505 Rpneg	171893	123289	98919	116882	149309	74782	135963	166790	135856	99947
cholesterol sulfate	483.3398	7.769 Rppos	16225	334504	39019	260095	398094	31972	52998	246960	539927	215407
Cholic Acid Methyl Ester	439.3298	9.498 Rppos	197879	788495	1075124	828580	1799963	1101254	1391790	2049699	914995	1515249
Cholic Acid Methyl Ester	439.3316	2.801 HILICpos	1782067	792295	521953	394015	447910	587417		890008	1230188	1119286
Cholic Acid Methyl Ester Esi+10.179	421.3187	10.179 Rppos	28385	171811	335350	248822	599924	308178	445809	564550	264382	374903
Cholic Acid Methyl Ester Esi+16.033003	421.3197	16.033 Rppos	575288	767907	1824551	1393443	1349635	413589	627662	503423	650855	647733
Cholic Acid Methyl Ester Esi+9.676001	439.3297	9.676001 Rppos	206910	411795	742421	459684	984918	781235	1089142	1453453	678012	914429
Chromanol 293B	324.1141	11.888 Rpneg	9584	4661	11657	13170	10438	7563	8643	8897	13467	7071
Cibulins	92.0297	0.889 HILICneg	60324	41604	198258	54986	80219	29264	93806	214630	84191	73287
Cichorine	193.0739	5.068 Rpneg	10242	11188	11795	11174	5140	5917	8235	5251	7351	7316
Cidofovir	279.0635	6.799 HILICneg	26100	27017	18945	24695	21427	13991	12891	13701	10156	14310
Cilazprilat	389.1951	11.641 Rpneg	4186	4196	3957	4624	3772	4029	4647	4163	4945	4675
Cinitapride	402.2262	1.256 HILICneg	423283	208560	82937	174379	609710	112320	101655	129782	115314	321661
Cinnarizine	368.2262	12.521 Rpneg	9143	6992	6986	6017	8426	1	7278	6190	7142	5658
cis-(7S,8R)-Epoxy-2-methyleicosane	310.3236	12.163 Rpneg	2803	2578	2073	3225	1767	2683	3217	3641	3737	1
cis,cis-2,4-Dihydroxy-5-methyl-6-oxo-2,4-hexadienoate	172.0348	0.926 Rpneg	132377	117209	149265	135811	132156	145563	114548	120875	143951	152505
cis,cis-2,4-Dihydroxy-5-methyl-6-oxo-2,4-hexadienoate Esi-	172.035	0.926 Rpneg	131801	181581	149299	134926	128772	146661	113817	119432	145365	105584
cis,cis-2,4-Dihydroxy-5-methyl-6-oxo-2,4-hexadienoate Esi-	172.0346	0.974 Rpneg	49437	167560	47762	57643	116202	126261	100958	37893	130776	45444
cis-2-Carboxycyclohexyl-acetic acid	168.0788	4.956 Rppos	73908	323025	268874	336912	522055	78153	253283	306236	269584	710775
cis-3-(3-Carboxyethenyl)-3,5-cyclohexadiene-1,2-diol	200.0697	1.405 Rpneg	6899	1	22371	1	20901	33509	1	13329	26304	14326
cis-p-Coumaroylcorosolic acid	622.3622	24.287 Rppos	523305	551181	569621	524338	521283	593763	506764	585705	682832	617524
cis-p-Menthane-1,7,8-triol	188.1405	1.633 HILICneg	188276	152500	95492	96830	101203	56918	107858	94011	86174	98245
cis-p-Menthane-1,7,8-triol	188.1409	9.72 Rpneg	13545	7503	3618	4594	4540	3708	4787	4337	6085	5020

cis-Zeatin	219.1115	7.100999 HILICneg	984477	1527288	1663322	1577306	529174	556323	758233	781695	362921	611478
Citalopram	324.16	9.043 Rpneg	6546	12823	5373	7817	9678	5467	5677	7587	14075	8667
Citiolone	219.0554	1.499 HILICneg	1	47601	65692	87594	48982	4252	39708	29872	24469	82517
citric acid	192.0271	0.7 Rpneg	90737	64661	73891	68607	64304	76490	80716	68381	50696	54543
Citrusin A	584.2078	4.55 HILICneg	95947	110070	68688	73441	16949	10771	16965	8875	8211	14166
CL(1'-[18:2(9Z,12Z)/0:0],3'-[18:2(9Z,12Z)/0:0])	924.5148	13.281 Rpneg	36571	10941	28032	32437	6095	4210	8535	5826	9887	7387
CL(1'-[18:2(9Z,12Z)/0:0],3'-[18:2(9Z,12Z)/0:0]) Esi-13.07499	924.5163	13.075 Rpneg	14654	9004	12696	12891	12529	7639	13588	17978	22290	17262
CL(1'-[18:2(9Z,12Z)/18:2(9Z,12Z)],3'-[18:2(9Z,12Z)/0:0])	1186.741	13.74 Rpneg	47011	32385	39435	53785	32326	18734	31156	41661	38365	38147
CL(1'-[18:2(9Z,12Z)/18:2(9Z,12Z)],3'-[18:2(9Z,12Z)/18:2(9Z,	1448.983	4.588 HILICneg	647033	257637	181076	130339	255476	75550	99939	35993	126689	128200
CL(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/20:3(8Z,11Z,14Z)/18:2(9Z,	1617.023	13.88 Rpneg	25658	26089	19444	28835	21083	17849	21022	26044	21434	19977
Cochineal Red A	583.9872	0.983 Rpneg	21902	15784	13600	17557	14244	14606	9804	15539	14538	14025
Coenzyme Q9	794.6258	0.883 HILICpos	53670224	70774328	63768976	68249792	42823264	33762432		33008630	49189144	43482968
Coenzyme Q9	794.6195	24.589 Rppos	12151531	6547865	11465696	10379357	14420189	10621067	15542341	14294612	11021205	12125437
Cofaryloside	574.2971	8.100999 Rpneg	5449	5745	5586	6440	8168	5891	5952	5895	6722	5938
Cofaryloside Esi-7.732	560.2832	7.732 Rpneg	2294	2631	2181	2667	4109	2027	1691	2290	3219	2912
Cohibin D	576.5151	0.916 HILICpos	5166810	3613094	2853001	3024817	5590805	6301828		6415742	5836706	6462032
Cohibin D Esi+1.4589999	598.4947	1.459 HILICpos	639853	500129	677187	804828	528651	462894		447649	407281	408333
Colupox b	849.544	24.723 Rppos	845611	1100951	770349	816863	1094858	816963	810468	917548	838752	778923
Concanamycin A	865.5171	22.937 Rppos	1787748	1463978	1613235	726593	1454523	1495495	1648004	1159137	1511450	1097544
Concanamycin A Esi+22.186998	865.5182	22.187 Rppos	100465	94571	50627	52063	426250	603284	498728	389356	691175	621341
Coriose	210.0745	0.888 Rpneg	11762	31343	37923	40438	42132	58010	57554	42544	35713	53600
Corossoline	562.4615	19.692 Rppos	2428015	2854637	2526992	2760108	1854704	1942637	1994259	2112250	2570188	2112256
Corrinoid	352.1911	9.999 Rpneg	11398	16151	10837	14305	19849	9147	9748	13503	19480	13578
CP 339818	364.2206	12.595 Rpneg	25024	19966	12707	24222	1	1	1	20419	1	1
creatine	131.0699	8.462999 HILICneg	64312	49825	56311	55957	46393	84373	65860	45420	60362	59678
creatinine	113.0593	5.694 HILICpos	6827232	5918335	5305216	9865479	5796528	5157353		8871885	6403142	7488703
Crustecdysone	480.3071	10.498 Rpneg	5229	3603	3587	3598	3611	3258	3519	3425	3474	2910
Cucujolide IX	240.139	10.021 Rpneg	4477	4326	3782	4098	5340	5658	2993	4739	6301	4315
Cyclohexane-1,2-dione	112.0512	1.108 Rpneg	1	39970	4690	25630	26264	2206	1	22587	32288	17870
Cyclohexylammonium	99.1046	4.894001 HILICpos	1736435	1809325	2482513	2645115	2998634	2247026		2763321	1853742	2382913
Cyclopassifloic acid B	520.3744	19.925 Rppos	806770	591577	536146	606013	582453	494568	504431	483109	474865	550820
Cyclopassifloic acid B	520.3794	13.707 Rpneg	14249	4208	2149	4944	3771	3116	3147	3192	3467	1667
Cyclopassifloic acid B Esi-13.520998	580.3972	13.521 Rpneg	6720	3730	3961	3871	2726	1501	3625	3356	2517	3396
Cyclothialidine	641.2035	17.325 Rppos	476629	552574	584748	604718	483116	557404	704443	688578	624660	752631
Cyclovariegatin	354.0365	7.943 HILICneg	904600	811174	828911	910775	971307	886171	999238	970646	478287	968834
Cysteinyl-Cysteine	224.0274	0.982 Rpneg	249167	188921	183854	216762	166462	188874	125972	208405	194133	184287
Cytosine	111.0435	6.478 HILICpos	1637724	1429813	1395374	1114964	916912	961622		972445	638753	816768
Cytosine	111.0434	1.268 Rppos	1667002	1378381	1342468	1173758	957481	1014434	1155551	1117376	805016	924635
D-1-[(3-Carboxypropyl)amino]-1-deoxyfructose	247.106	0.984 Rpos	428991	425102	595862	463487	778132	933088	782241	689329	1601529	1064889
D-4-Hydroxy-2-oxoglutarate	162.0173	0.79 Rpneg	20399	46977	49213	44546	32064	31646	48416	36203	37440	37994
D-4'-Phosphopantothenate	299.0761	0.722 Rpneg	14646	15126	19268	14613	12895	19797	15906	19513	15931	16850
d-6-Methyloctanoic acid	158.1301	1.333 HILICneg	513435	385443	195738	269629	611643	104369	204304	400402	465768	378929
d-6-Methyloctanoic acid	158.1309	10.004 Rpneg	45854	39570	35332	39964	39512	29463	23380	35296	48660	30569
d-6-Methyloctanoic acid Esi-14.003999	158.1307	14.004 Rpneg	34431	1894	16403	13422	1	13051	1097	4400	1	1
Davidigenin	240.0786	7.36 Rpos	903423	956926	1077939	1133683	954884	995228	1120614	1169214	1219854	1253740
Deazaflavin	259.0583	0.91 Rpneg	5414	6433	9878	5627	4732	3685	6944	4641	3532	4953
Deazaflavin Esi-11.198999	259.0602	11.199 Rpneg	6152	5363	5484	4884	5896	5513	6005	5581	5806	5811
Decanoic acid, 9-amino-, (1)-	374.3084	0.951 HILICneg	111675	44685	38680	49088	54569	1	41288	44193	1	1
decyl octanoate	284.2717	5.427001 HILICneg	27307	54848	37109	57651	43906	85440	92353	37372	72792	34542
Dehydroxymethylflazine	278.0678	2.776 HILICneg	134272	162446	150363	192579	142365	111117	140690	150735	129323	124639
Deoxycytidine	227.0916	6.478 HILICpos	3592246	2569666	2408286	1740184	1298058	1342654		1414742	690872	1054645
Deoxycytidine	227.0911	6.172 HILICneg	111791	119363	105268	93423	69664	56889	72810	72095	48523	60064
Deoxycytidine	273.0957	0.831 Rpneg	7190	5896	9434	7152	5352	8798	8332	7092	5585	6854
Depdecin	210.0891	6.668 Rpos	1484117	1957667	1692257	2001805	2101395	1894380	1761354	1892293	2086137	1804047
Dermatan	477.0794	0.806 Rpneg	5171	3660	6700	5200	1346	6781	5611	4908	2801	4222
D-erythro-3-Hydroxyaspartate	344.0698	5.382 HILICneg	57772	48984	60962	63341	74616	37847	58000	72948	70138	70499
D-Erythroascorbic acid 1'-a-D-xylopyranoside	278.0665	0.907 Rpneg	7215	5684	8204	6201	5474	6264	5969	6447	1	5703
D-erythro-Sphingosine C-15	239.2233	8.277 Rpos	150163	195204	234466	231328	161134	206639	218122	235103	237727	243552
D-erythro-Sphingosine C-20	309.3017	16.276 Rpos	542284	629571	386245	612852	1367999	624756	1694705	871694	651179	298955
D-erythro-Sphingosine C-20	327.3131	14.137 Rpneg	4678	1	1	1478	4919	1784	4476	1497	1176	1530
Desacetylvindoline	431.2459	1.1 HILICpos	332405	441396	172375	722057	855520	430265		237667	234591	338939
Desmethylondansetron	278.1541	16.035 Rpos	367296	718366	1500728	1041234	1026011	305381	502543	453634	412439	335107
Dexpanthenol	205.1308	5.119 Rpneg	21352	58445	8078	53923	91495	8894	9470	57730	91737	45350
Dexpanthenol	205.1316	4.551 Rpos	126372	574262	61647	560182	833972	161830	165421	616035	903222	496704
Dexpanthenol Esi+6.0100007	187.1209	6.010001 Rpos	583097	525181	472956	392931	419505	292811	350610	349766	468728	353806
DG(13:0/17:0/0:0)[iso2]	522.4678	19.687 Rpos	1964674	2023599	1845003	1957178	1365575	1413273	1466842	1438458	1916699	1596576
DG(14:0/17:0/0:0)[iso2]	536.484	20.574 Rpos	901162	1124076	973963	977477	772257	1035978	751139	925192	1058032	801727
DG(14:1(9Z)/22:5(7Z,10Z,13Z,16Z,19Z)/0:0)	612.4784	24.055 Rpos	199977	261654	423225	424529	327584	513718	436954	477561	384962	413197
DG(15:0/0:0/15:0) (d5)	562.5309	0.995 HILICpos	799052	1297132	1298932	1061956	3099599	3618100		2031039	2327598	2313617
DG(15:0/17:0/0:0)[iso2]	585.5389	27.21 Rpos	427554	470369	542131	590897	527494	1080587	717639	836908	683307	909796
DG(15:1(9Z)/18:2(9Z,12Z)/0:0)[iso2]	576.4816	20.579 Rpos	1428924	1338872	1401976	1181659	1074267	1162480	676344	1288994	1145683	924121
DG(16:0/16:0/0:0)	550.4973	22.846 Rpos	732348	1055960	725138	675122	857652	752750	674481	649567	1139763	747645
DG(16:0/16:0/0:0) Esi+27.214	550.5026	27.214 Rpos	462566	460925	534280	580155	570093	1137093	801064	803371	648174	862066
DG(16:0/17:0/0:0)[iso2]	628.5215	1.107 HILICneg	404504	257458	1	189063	682709	140800	1	258441	332633	346238
DG(16:1(9Z)/18:0/0:0)[iso2] Esi+23.554998	611.5512	23.555 Rpos	1447199	1233681	1644635	1504705	257560	454160	814808	481396	1017766	1319018
DG(17:0/0:0/17:0) (d5)	623.5564	25.494 Rpos	360561	346857	418525	335081	413051	451325	378536	470716	317328	417288
DG(18:0/0:0/18:0) (d5)	651.5885	27.463 Rpos	296766	333188	379437	308049	594338	1406244	802298	982051	1079051	1009825
DG(18:0/0:0/18:0) (d5) Esi+27.936	651.5899	27.936 Rpos	153778	173448	236453	176110	307355	494794	364706	459580	372331	430266
DG(18:0/18:1(11Z)/0:0)	639.5775	27.365 Rpos	465893	508572	556976	499848	943387	1841051	1153318	1282948	1414827	1316678
DG(18:1(11Z)/16:1(9Z)/0:0)	574.5019	25.478 Rpos	317054	496475	633847	505982	697095	873198	709682	1022381	673153	737487
DG(18:1(11Z)/18:3(6Z,9Z,12Z)/0:0)	616.5072	24.019 Rpos	7462109	8599140	1.07E+07	7585696	1.57E+07	2.04E+07	1.87E+07	2.09E+07	1.78E+07	1.84E+07
DG(18:1(11Z)/18:3(6Z,9Z,12Z)/0:0) Esi+18.787	633.5351	18.787 Rpos	578745	457494	197074	557857	193368	146861	287302	166711	554459	593348
DG(18:1(11Z)/20:4(8Z,11Z,14Z,17Z)/0:0)	659.5499	25.144 Rpos	1260621	1270220	999040	1356784	131158	198775	135900	126772	58593	79984
DG(18:1(11Z)/20:4(8Z,11Z,14Z,17Z)/0:0) Esi+23.638	642.5342	23.638 Rpos	615074	997856	1336770	1216345	211260	612120	791008	171971	909207	1211196
DG(18:1(11Z)/22:4(7Z,10Z,13Z,16Z)/0:0)	686.5916	16.111 Rpos	73032	72150	72199	62520	103548	196949	140110	222289	187084	194119
DG(18:1(11Z)/22:5(7Z,10Z,13Z,16Z,19Z)/0:0)	685.5663	26.829 Rpos	1920996	2012607	2164744	2291067	1280178	1348469	1389731	1327940	799534	859675
DG(18:1(11Z)/22:5(7Z,10Z,13Z,16Z,19Z)/0:0)	668.5359	0.888 HILICpos	1057624	1288476	1335209	1417657	919932	543501		306615	475667	443703
DG(18:1(11Z)/22:5(7Z,10Z,13Z,16Z,19Z)/0:0) Esi+28.00200	668.5451	28.002 Rpos	428867	472902	824973	639534	982146	1080040	1125321	1139907	1230200	1126937
DG(18:1(9Z)/18:4(6Z,9Z,12Z,15Z)/0:0)	614.4951	21.113 Rpos	1373008	1085230	1376423	1311117	719615	640687	875487	619241	1300264	849354
DG(18:1(9Z)/18:4(6Z,9Z,12Z,15Z)/0:0) Esi+22.83	631.5216	22.83 Rpos	99159	120430	127136	105411	135319	142125	155150	194322	182825	156571
DG(18:1(9Z)/18:4(6Z,9Z,12Z,15Z)/0:0) Esi+25.123	614.4941	25.123 Rpos	193774	291826	196790	107997	151828	334749	210720	180460	211714	270920
DG(18:2(9Z,12Z)/18:1(11Z)/0:0)	618.5271	0.896 HILICpos	4030875	4332951	2861056	2541509	6441902	4918803		5344819	6073304	7361303

DG(18:2(9Z,12Z)/18:1(11Z)/0:0) Esi+21.323	635.5521	21.323	Rppos	1529281	1232202	1783196	1380840	518130	521852	734788	488133	1422709	1614858
DG(18:2(9Z,12Z)/20:4(8Z,11Z,14Z,17Z)/0:0)	622.4989	22.689	Rppos	305081	298901	259016	383848	209805	237703	247692	231744	202007	206557
DG(18:3(6Z,9Z,12Z)/16:1(9Z)/0:0)	634.4921	1.007	HILICneg	1102916	751385	581109	712529	573414	352430	545666	598370	470972	592284
DG(18:3(6Z,9Z,12Z)/20:3(5Z,8Z,11Z)/0:0)	657.5326	24.564	Rppos	2349851	3215653	2032305	2069164	1293517	838360	1055098	1011614	699286	570586
DG(18:3(6Z,9Z,12Z)/20:3(5Z,8Z,11Z)/0:0)	635.5542	0.891	HILICpos	1522154	2810380	2411413	2622181	1195385	676232		651874	789905	582704
DG(18:3(6Z,9Z,12Z)/20:3(5Z,8Z,11Z)/0:0)	640.5059	0.938	HILICneg	988614	1865004	1309730	1685258	951777	352899	703111	856792	688547	1182220
DG(18:3(6Z,9Z,12Z)/20:3(5Z,8Z,11Z)/0:0) Esi+23.619001	657.5359	23.619	Rppos	1203751	1122729	672991	845287	435224	391394	453652	682472	481549	511809
DG(18:3(6Z,9Z,12Z)/22:3(10Z,13Z,16Z)/0:0)[iso2]	650.5302	24.514	Rppos	479072	497704	516801	533430	477575	511083	672101	486526	541541	516312
DG(18:3(9Z,12Z,15Z)/20:3(5Z,8Z,11Z)/0:0)	640.5101	21.316	Rppos	2270094	1733638	2511256	1953328	840673	790146	1082629	669776	1996956	2180441
DG(18:4(6Z,9Z,12Z,15Z)/20:3(8Z,11Z,14Z)/0:0)	638.4875	18.782	Rppos	1162320	975965	1109315	1158483	427914	395481	703816	396670	1267484	894363
DG(19:1(9Z)/16:0/0:0)[iso2]	625.5642	27.435	Rppos	1778877	1763557	1994806	1660687	3235963	6170799	3933764	4388386	4726330	4529859
DG(19:1(9Z)/18:2(9Z,12Z)/0:0)[iso2]	649.5672	25.623	Rppos	558572	1109554	948745	753016	1348454	1826950	1525202	1599877	1708847	1934067
DG(19:1(9Z)/18:2(9Z,12Z)/0:0)[iso2]	696.5528	14.41	Rpneg	157458	90018	109732	75795	58116	74244	87355	70923	89030	99390
DG(19:1(9Z)/20:5(5Z,8Z,11Z,14Z,17Z)/0:0)[iso2]	700.5235	0.894	HILICneg	1069069	1793780	1563597	1932721	982590	132928	716064	755498	602408	335995
DG(19:1(9Z)/22:4(7Z,10Z,13Z,16Z)/0:0)[iso2]	684.5681	14.511	Rppos	56534	71066	45031	50844	97423	137256	168441	215083	130922	145557
DG(19:1(9Z)/22:5(7Z,10Z,13Z,16Z,19Z)/0:0)[iso2]	728.5599	0.931	HILICneg	1290428	1934552	1704061	1936174	404243	240044	1020424	1121382	888236	953863
DG(19:1(9Z)/22:6(4Z,7Z,10Z,13Z,16Z,19Z)/0:0)[iso2]	726.5459	0.882	HILICneg	443190	1481718	1449746	878614	717423	189472	887246	841438	675906	762593
DG(20:3(5Z,8Z,11Z)/16:1(9Z)/0:0)	616.508	23.566	Rppos	984507	489512	1198238	1086594	365562	164587	462351	472984	436051	823811
DG(20:3(5Z,8Z,11Z)/20:4(5Z,8Z,11Z,14Z)/0:0)	683.5496	24.723	Rppos	775553	1103744	665269	738378	487945	423366	519327	475041	343943	193478
DG(20:3(5Z,8Z,11Z)/20:5(5Z,8Z,11Z,14Z,17Z)/0:0)	681.5366	23.247	Rppos	1165483	1173861	973682	1086807	385113	291152	441094	481659	268865	179316
DG(20:3(5Z,8Z,11Z)/22:5(7Z,10Z,13Z,16Z,19Z)/0:0)	738.544	5.544	HILICneg	85533	53737	73148	84138	69617	41563	74279	85475	106355	92438
DG(20:4(5Z,8Z,11Z,14Z)/22:6(4Z,7Z,10Z,13Z,16Z,19Z)/0:0)[	688.5076	24.72	Rppos	292749	374939	275066	301726	220388	169622	232301	188279	143968	122507
DG(20:4(8Z,11Z,14Z,17Z)/22:5(4Z,7Z,10Z,13Z,16Z)/0:0)	690.522	26.824	Rppos	2352331	2598960	2827592	2981997	1665051	1659354	1706383	1626156	981712	1074767
DG(22:5(7Z,10Z,13Z,16Z,19Z)/22:5(7Z,10Z,13Z,16Z,19Z)/0:	733.5651	24.219	Rppos	817516	499718	539767	946646	327901	460395	606413	803133	442590	786122
DG(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/20:4(8Z,11Z,14Z,17Z)/0:0	688.5081	14.398	Rpneg	4859	3360	2118	3265	1	1	1	7961	1	1
DG(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/20:5(5Z,8Z,11Z,14Z,17Z)/	686.4895	23.201	Rppos	629593	373446	473887	604808	85481	48069	182514	87620	40826	31344
DG(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/22:6(4Z,7Z,10Z,13Z,16Z,1	729.5376	22.547	Rppos	1048256	1170432	559350	969034	1	1	1	1	1	1
D-Glycerate 2-phosphate	185.9932	0.718	Rpneg	55477	38624	95541	53344	31919	92241	29802	31935	9554	17584
D-glycero-D-manno-Heptose 1,7-bisphosphate	416.012	0.722	Rpneg	9397	5370	13334	6958	1261	10488	3683	2420	1	1267
Diacetyl	86.0371	0.706	Rpneg	12712	37527	13033	35453	37021	13628	12454	27025	47635	27703
Diacetyl Esi-11.627999	86.0373	11.628	Rpneg	8536	9178	4188	8269	6418	4305	10163	5750	11265	8729
Diacetyl Esi-12.670999	86.0353	12.671	Rpneg	3756	1	2086	1	1705	2395	1	1843	1426	1884
Dianhydroaurasperone C	578.1171	0.686	HILICpos	2248828	1425416	2400479	1385720	1495168	2403974		1	795495	2015482
Dibromoacetic acid	215.8397	0.808	HILICneg	21046	95738	126898	137039	110661	83540	125486	99818	81688	104277
Dichlorvos	265.9513	5.841	Rpneg	3558	2788	4104	2908	2829	3220	4699	2831	1729	2256
Dichlorvos	265.9532	4.251999	HILICneg	356868	1	678039	628096	454221	253002	455500	1	405459	470790
Dichlorvos Esi-7.6419992	265.9527	7.641999	HILICneg	72239	59295	63290	55534	65800	60094	66479	60443	59370	61017
Diethyl decanedioate	258.1831	8.53	Rpneg	9815	11223	7770	9902	15516	8757	7101	9663	14648	7821
Diethyl phthalate	204.0788	8.974	Rppos	455775	522961	568569	598112	522450	570095	625222	638814	641782	665822
Diethyl succinate	174.0888	12.445	Rpneg	7235	984	986	994	894	1491	981	846	1	1248
Digallate	326.0008	7.645	Rppos	471331	586558	639050	723785	611701	680731	723019	716756	738639	770602
Dihydro Isorescinnamine	636.3013	0.906	HILICpos	5969253	20368344	1174814	10939336	13196830	7999511		552094	1305546	3898388
Dihydro Isorescinnamine Esi+1.4379998	636.3037	1.438	HILICpos	342994	440263	1118244	244657	654286	501006		388442	248689	227302
Dihydrocapsiate	308.2023	12.686	Rpneg	145271	88297	75472	82623	75406	63841	74095	75476	94020	63914
Dihydroergocristine	611.3083	12.659	Rpneg	1	8294	8225	10382	3729	1869	1654	1207	2669	3396
Dihydrogeranylgeranyl diphosphate	512.2301	11.265	Rpneg	3978	2362	1793	2429	1957	1	2221	1400	1500	1543
Dihydroisolysergic acid II	270.1382	11.187	Rpneg	3622	2297	3182	2852	2199	1450	3294	2877	1725	1304
Dihydrojasmonic Acid, Methyl Ester	208.1462	7.911	Rppos	590928	614724	625460	659126	573277	618988	641979	601713	627251	636444
Dihydromenaquinone-8	700.5574	21.319	Rppos	1362248	1251204	1282076	1227251	1494573	1912653	1365941	1485783	1729997	1448343
Dihydroretrofractamide B	357.2262	5.247001	HILICneg	6680	33176	49262	34112	21012	21218	28195	15164	22117	25329
Diisobutyl phthalate	278.152	10.894	Rpneg	27432	52012	46008	56946	82739	27730	28974	49546	76535	42688
Diisobutyl phthalate Esi-11.268999	278.1515	11.269	Rpneg	8353	8889	9681	7305	8871	7865	7918	9926	10131	8196
Diisobutyl phthalate Esi-11.663001	278.1523	11.663	Rpneg	3969	6684	4182	5771	7815	3218	5078	6947	6351	5003
Dimethamine	472.2695	1.255	HILICneg	228762	288671	155351	170126	351968	1	178398	179801	123200	193461
Dimethylaminoethyl reserpilinate	529.2819	5.370999	HILICneg	300790	194945	157230	212333	231168	225642	205359	314239	375210	244600
Dimethylaminoethyl reserpilinate	529.2827	13.134	Rpneg	1	8077	5986	10637	16174	16053	18974	16610	16705	12492
Dimethylethanolamine	89.0843	5.939	HILICpos	1951416	1365263	1696128	3282154	2855744	2233157		2318289	1623762	2734070
Diminazene	622.2969	1.179	HILICneg	17109	114334	60340	77849	96645	1	57408	43580	40355	51523
Dinitramine	644.1768	12.927	Rppos	292087	280251	324993	306550	201403	278126	251686	209872	203761	189542
Dioctyl hexanedioate	370.3081	16.17	Rppos	1108426	1039819	1103557	1018703	1043079	975741	1147082	1106525	1136847	1057632
Dioctyl hexanedioate	370.3082	13.202	Rpneg	116852	43882	38159	48577	29540	37983	32276	24487	33159	21200
Dioctyl hexanedioate Esi-11.781999	370.3072	11.782	Rpneg	14579	11597	9752	41301	28342	8441	9160	10158	9040	8316
Dioctyl hexanedioate Esi-13.337	370.3076	13.337	Rpneg	24840	13968	17983	20149	14329	16795	19383	10626	13084	15826
Diphenylmethylphosphine	222.0565	7.609	Rppos	258839	332107	177650	218855	153005	197851	224319	91911	331957	294745
Dipiperamide E	570.2708	8.214999	Rpneg	13547	11686	15138	10751	15596	17681	13141	11926	9127	8572
Dipropyl hexanedioate	230.152	6.643001	Rpneg	8209	17319	7402	16980	24701	10270	7268	13670	24170	11765
Dipropyl hexanedioate	230.1527	7.853	Rppos	71119	176321	168707	125961	63082	160372	83404	148939	184589	122567
Dipyridamole	521.3478	5.483	HILICpos	1469024	1467738	1360371	1156415	241820	1455842		489622	1129776	262215
Dipyridamole	550.3192	13.706	Rpneg	1	1849	1362	1370	3535	3754	2133	3993	3742	3807
Dirithromycin	851.5737	27.022	Rppos	436846	449410	538825	542718	486472	626979	617521	587052	547408	531538
Dithianon	295.9695	0.992	Rpneg	6528	6064	6065	6562	6652	6534	6451	5433	5562	5858
Dithiocarbamate	288.0103	1.259	HILICneg	48750	56984	35544	41882	70994	1	47089	43263	32464	56879
Divinylchlorophyll a	889.5293	25.073	Rppos	882758	916179	776338	900638	939142	604028	668458	708868	720988	944904
Divinylchlorophyll a	936.5219	1.281	HILICneg	74152	109861	145290	119575	57956	8323	55722	66786	86601	91106
DL-10-hydroxy stearic acid	300.267	12.938	Rpneg	97882	49953	55458	72889	40517	48064	50426	49562	63238	59659
DL-Glyceraldehyde 2-Phosphate	169.9962	5.91	Rpneg	1692435	937322	623950	841400	2581557	2804674	2633486	465248	1097044	672110
DL-Glyceraldehyde 2-Phosphate Esi-0.7799999	169.9977	0.78	Rpneg	478885	394026	455673	412446	172033	426930	318779	460078	292363	341828
DL-Glyceraldehyde 2-Phosphate Esi-1.1680001	169.997	1.168	Rpneg	354493	153812	529509	187499	362985	1	65696	284574	235656	262256
DL-Glycerol 1-phosphate	172.0135	0.78	Rpneg	48740	33215	50140	50295	105988	65995	66050	69761	55569	74316
DL-Glycerol 1-phosphate	172.0158	5.312	HILICneg	275211	237683	238482	227004	202836	130408	147106	159609	159790	186656
DMABA-d6 NHS ester	267.1505	7.484	Rppos	620148	678297	698783	650724	585605	680110	723134	657869	675289	721536
D-Mycinose	401.2258	5.517	Rppos	84270	140294	90517	131976	152707	82637	85216	112226	151471	111909
Docosanedioic acid	416.3136	13.79	Rpneg	28740	29137	29504	30509	37039	39299	49067	49589	42088	36988
Docosanedioic acid Esi-13.789999	416.3134	13.79	Rpneg	28740	29137	29504	30509	37039	39299	49067	49589	42088	36988
Docusate	422.2335	12.344	Rpneg	76830	107917	82336	133445	101742	45767	70971	98451	95724	66297
Dodecan-2R-ol	185.2142	6.173	Rppos	1052490	1009383	974861	1008361	1018461	1022296	1035770	1027342	1069858	999033
Dodecan-2R-ol	186.1984	12.049	Rpneg	8858	11716	10098	9976	9436	13791	8150	13551	15815	11099
Dodecan-2R-ol Esi+7.4779997	185.2146	7.478	Rppos	504223	493531	511162	559809	478025	481293	513456	550624	580668	621007
dodecanamide	199.1934	9.277	Rppos	884488	1038395	1240319	1504427	1075203	1241401	1273353	1404231	1507882	1589498
dodecanamide Esi+8.334	199.1929	8.334	Rppos	352475	302071	308072	295329	313726	282818	286410	277403	291201	275581
Dodecanoic acid, 3,7,11-trimethyl-; 3,7,11-Trimethyldodec	242.2244	12.482	Rpneg	1089678	804806	339901	693174	675396	473097	545563	637238	550943	401046
Dodecanoic acid, 3,7,11-trimethyl-; 3,7,11-Trimethyldodec	242.2241	12.482	Rpneg	1087617	804650	339870	693175	677573	473195	547051	636155	551613	400955

Dodecanoic acid, 3,7,11-trimethyl-; 3,7,11-Trimethyldodec	242.2244	12.561 Rpneg	918490	701246	418316	608232	582495	504135	475282	419622	512250	358471
Dodecanoic acid, 3,7,11-trimethyl-; 3,7,11-Trimethyldodec	242.2245	12.565 Rpneg	913283	703097	418399	608838	582046	506432	11089	13340	512435	358138
Dolastatin 16	938.5346	1.283 HILICneg	254942	213045	281862	248113	76817	19533	103778	71224	101267	103290
Dolichotheline	407.3017	15.662 Rppos	372860	190256	493831	226834	163066	114572	289562	198064	193035	73313
dolichyl diphosphate	566.2786	12.269 Rpneg	13719	14283	10532	13017	17760	8965	15044	10455	8829	13765
dolichyl diphosphate Esi-12.375	566.2802	12.375 Rpneg	5999	4398	4466	4365	4708	3316	5193	4532	4127	6543
Donepezil	378.2332	11.142 Rppos	242464	214323	228564	167836	178463	131161	181744	165964	173388	141968
D-Pantetheine 4'-phosphate	358.0962	1.577 Rpneg	99188	85139	64559	77604	50471	42171	83823	54278	52903	71800
dTMP	382.0754	6.364999 HILICneg	308756	400128	354478	389389	346724	262614	307887	347401	302031	308020
D-Xylono-1,5-lactone	147.0537	0.879 Rppos	715759	872021	948885	933010	981387	980621	1429079	1232831	883254	927203
E-64d	342.2136	1.041 HILICneg	299421	414508	319481	245784	209999	1	259012	238441	1	1
eicosapentaenoic Acid ethyl ester	104.0475	0.898 Rpneg	19746	10089	6727	7361	58836	142329	133426	91460	196594	88460
Eicosapentaenoic Acid ethyl ester	330.255	12.716 Rpneg	2239971	2157647	1657469	2312015	1278328	917999	1346983	1542813	1197219	1112624
Eicosapentaenoic Acid ethyl ester	330.2569	1.014 HILICneg	10139130	12564972	8170257	11686295	5567307	775744	4737301	4115264	3172023	3021497
Eicosapentaenoic Acid ethyl ester Esi-12.809	330.2558	12.809 Rpneg	318621	317296	242233	357143	148207	81004	118456	147371	102876	84676
Eicosapentaenoic Acid ethyl ester Esi-12.811998	330.2559	12.812 Rpneg	26663	322823	240677	27921	148815	84721	117565	146499	86703	92010
Eicosapentaenoyl Serotonin	520.3314	1.133 HILICneg	47860	211933	202256	88818	152473	1	240409	208802	342509	233112
Elaidic carnitine	425.3514	1.923 HILICpos	5203296	3838617	3702040	2592238	3592715	3507857		4437264	5966683	4191241
Emopamil	334.239	12.591 Rpneg	4242	3939	3274	4099	3171	2373	4031	4929	4569	4164
Enigmol	283.2868	16 Rppos	654790	416028	564460	320814	304396	420127	372720	370715	334162	417147
Enniatin B	621.3998	15.347 Rppos	8064328	2009913	1701277	1644475	990581	1758393	2812089	1552931	1876320	1921647
Enoximone sulfoxide	574.1187	6.370999 HILICneg	1122709	1519498	1487288	1502522	1458432	1261019	1294720	1392867	1289522	1346181
Epiandrostanediol	292.239	12.668 Rpneg	5644	4947	4127	3733	4109	1	4106	4975	4204	5705
Epicainide	338.203	1.417 HILICpos	894178	484819	172884	195970	379958	192773		163164	368468	1
Epididydrophaseic acid	282.1492	11.317 Rpneg	20373	1	12300	18998	53013	5239	5467	12911	19287	12809
epi-dihydrophaseic acid	282.1501	10.018 Rpneg	18638	4516	11318	43127	73106	5633	4994	18904	34904	25084
Epijasminoside A	376.1722	5.926 Rpneg	12150	3192	7557	3543	3060	7535	1080	2455	3497	2411
Epimetendiol	318.2562	12.742 Rpneg	7172	5955	10458	11497	5801	3814	3775	4322	8055	3747
Epioxylubimin	234.1619	8.468001 Rppos	1073419	1242406	1487673	1431038	1163215	1274478	1319919	1489003	1478054	1555712
Equilin sulfate	394.1088	10.129 Rpneg	3201	2224	2981	1880	2912	3355	3052	1983	1527	1467
ergosta-3beta,5alpha,6beta,25-tetrol	496.3762	13.415 Rpneg	8742	3868	6261	9907	7259	5728	8586	4637	4536	6138
Erinapyrone C	140.0455	0.911 Rpneg	7337	2259	1164	1869	11740	32838	21128	27640	51933	21616
Erythrinasinate A	586.4935	12.856 Rpneg	30877	24698	18702	20254	30084	32659	32904	37707	38121	36734
Erythrinasinate A	650.5179	0.91 HILICneg	593446	608392	549375	544142	850102	806995	1167754	532306	1328227	896213
Erythrinasinate A Esi-12.507001	586.4972	12.507 Rpneg	11371	7657	1473	5968	6194	3489	4435	6327	6402	4231
erythro-6,8-Nonacosanediol	486.4669	12.764 Rpneg	231857	192462	145573	201281	207325	87862	266659	193585	376046	267769
Erythromycin ethylsuccinate	861.5075	22.926 Rppos	685933	1919646	563275	530014	2626655	1538033	1926561	2281179	1999676	1632018
Erythromycin ethylsuccinate Esi+22.186998	861.5069	22.187 Rppos	68721	242800	177394	100268	437305	1108463	910450	977586	1061260	991376
Eseramine	300.1583	7.524001 Rppos	818391	889618	970434	987518	648045	954672	1002886	1020522	1023212	1096251
Estradiol disulfate	864.1801	6.385001 HILICneg	342127	427495	426888	429639	419706	365829	381374	401412	411487	410468
etamiphylline	261.1635	2.736 Rppos	755782	845714	806814	753336	365751	252775	408697	528416	265953	195652
ETF	100.0138	9.558 HILICneg	248746	160155	149261	205576	179239	197524	220438	276662	250916	216283
ETF	100.0142	1.017 Rpneg	115020	116783	104728	117065	109522	112048	91345	110796	120026	104496
Ethiin	211.0514	4.824 HILICneg	7723	1	10286	3154	119414	407343	173123	230862	467142	400839
Ethiin Esi-2.0739996	211.0514	2.074 HILICneg	25720	38901	34658	30243	316534	303002	331142	398342	358883	300622
Ethyl 2-benzylacetoacetate	220.1106	11.631 Rpneg	4583	3894	3152	3218	2806	2672	4708	3767	6324	3692
Ethyl 3-(N-butylacetamido)propionate	215.1525	7.182 Rpneg	11614	11706	10498	10001	8493	5584	5962	7054	8477	6927
Ethyl 3-(N-butylacetamido)propionate	215.1527	4.886001 HILICneg	133536	8666	8597	19402	26147	70256	18317	12251	148484	13386
Ethyl 3,4,5-trimethoxybenzoate	222.0894	7.369 Rppos	489550	3284697	2417529	1284616	1268357	2872276	634318	604198	1877236	892419
Ethyl aconitate	202.0457	0.888 Rpneg	134157	121664	137188	125762	53384	52786	47578	66187	57323	60445
Ethyl aconitate Esi-0.882	202.0482	0.882 Rpneg	134514	124824	137313	125807	53574	1	1267	5040	57689	4997
Ethyl aconitate Esi-1.0419999	202.0461	1.042 Rpneg	12168	14042	15283	11530	5195	3614	4576	7544	8629	7955
Ethyl butyrylacetate	158.0942	12.537 Rpneg	25480	1965	1934	1437	1519	7525	1080	1967	1098	1078
Ethyl decanoate	200.1781	1.199 HILICneg	3240425	2074103	1099692	2678026	5273827	655695	1603390	2037685	2249044	2524058
Ethyl formate	74.0367	0.737 Rpneg	1	47020	30140	41070	37349	19580	1	23720	52877	44781
Ethyl formate Esi-0.901	74.0368	0.901 Rpneg	1	1389	5229	4418	7253	6729	3761	4891	5732	5631
Ethyl hydrogen sulfate	125.9985	2.423 HILICneg	1016424	1475465	1596406	1450020	1342364	887039	1135503	831791	1189674	1191208
Ethyl menthane carboxamide	271.215	10.177 Rpneg	5185	4365	6586	6671	3466	3605	3576	3335	3500	3303
Ethyl menthane carboxamide	271.2165	2.179 HILICneg	265652	10774	8314	13457	21966	34859	21508	7522	261475	14319
Ethyl menthane carboxamide Esi-11.59	271.2189	11.59 Rpneg	1	4296	5174	5088	5020	3745	5769	7264	1	4411
Ethyl nonanoate	186.1622	11.216 Rpneg	15241	16802	13284	15161	18131	14244	12003	15033	17083	13148
Ethyl nonanoate Esi-11.060999	186.1618	11.061 Rpneg	6650	6237	4836	5131	6151	5331	4304	5378	6628	4491
Ethylene brassylate	287.2135	2.776 HILICpos	642589	271883	247835	179216	217893	204560		173641	147373	360864
Etorphine	410.2598	15.405 Rppos	343913	572914	328058	447663	444651	264384	325422	288467	460280	361016
Etorphine Esi+15.188002	410.2593	15.188 Rppos	308158	493720	283533	378410	385081	215911	279856	234174	384279	297402
Etretinate	354.2223	12.591 Rpneg	11294	9240	10143	7914	7289	6027	7690	3690	8763	6941
Euchrenone a4	970.4637	22.197 Rppos	216702	304672	186456	73499	840676	977884	725397	906678	953202	787683
Euchrenone a4 Esi+22.897999	970.464	22.898 Rppos	225365	262883	154385	211912	377598	261338	281456	307231	265800	274104
Euchrenone a4 Esi+23.093	970.4642	23.093 Rppos	450683	450594	346260	365755	530281	366321	323093	332499	340652	345981
Eudesobovatol A	521.3475	5.599999 HILICpos	2879616	2697550	2818093	2410440	843210	2568282		1656224	1918642	1495881
Eujambolin	520.1259	0.692 HILICpos	7252725	3914236	1	6864091	3692908	8746101		6853517	6527715	9544971
Fagomine	147.0893	8.551001 HILICneg	59876	52777	53785	45746	52871	45258	56864	59415	54701	63558
Famotidine sulfoxide	752.0875	7.638 HILICneg	39204	31885	35070	33088	39193	38890	39076	38606	34714	33909
Famphur	385.0441	0.817 Rpneg	1	3096	7052	4922	5104	7439	12246	8958	9572	8281
Faradiol myristate	670.5858	13.394 Rpneg	4228	4625	6046	10484	2439	1	2508	32401	1	24759
Fasciculol F	801.5046	0.886 HILICneg	1751813	1348019	1	1406499	2032194	1	1	1486532	1145560	1
Fentanyl	336.2214	12.085 Rpneg	7776	5986	4388	5248	4531	1	4466	1	3363	1
Fexofenadine	501.2879	11.429 Rppos	479448	600927	551351	547072	401556	717247	688067	593550	634150	613479
F-Honaucin A	188.0492	6.638 HILICneg	104573	194395	176836	140338	79672	98656	145072	71286	87917	109758
F-Honaucin A	188.0497	0.86 Rpneg	7196	6008	8033	14469	5628	5550	7068	5234	49730	23394
Firocoxib	672.2082	15.314 Rppos	551018	550892	677839	613643	467693	653107	651170	582455	613891	526280
Flavin adenine dinucleotide (FAD)	785.1569	5.841 Rpneg	111559	75198	91475	112584	90427	77214	84021	112351	80401	85149
Sultamicillin tosilate	611.1747	0.659 HILICpos	35955796	13128857	45813380	23057184	15601053	54172868		41683432	41981356	47282248
Flavine mononucleotide (FMN)	456.1046	5.691001 Rpneg	4518	3838	5079	4241	2655	4579	4544	5269	4051	4244
Flaviolin	270.0378	0.839 Rpneg	2586	3405	2885	1	6043	3885	3910	3072	4469	3333
Flumazenil	623.2282	21.963 Rppos	973745	811918	867597	874677	855597	737558	724039	660286	810669	750574
Flutamide	322.0773	5.964 HILICneg	129288	360849	307763	400908	296231	229296	291767	291311	253718	239726
Fortimicin A	870.5326	0.802 HILICneg	414783	490793	427029	485715	101065	135954	211141	195444	79512	215873
Fortimicin AP	380.2252	11.742 Rpneg	2685	3091	2284	2839	2293	4143	2597	2760	2898	5356
Fosinoprilat	553.2797	13.115 Rpneg	9558	7902	8103	12817	13449	14758	18093	14830	14407	10611
Fosinoprilat	553.2814	5.354 HILICneg	491955	268977	321931	378537	331022	313195	264379	356293	394437	336073
Fosmethilan	367.0217	5.117 Rpneg	32125	22588	26395	25170	19499	22252	19323	20751	13191	14632

fragment of acetylcarnitine	84.0215	5.669 HILICpos	2460581	2343853	2304351	2247901	570202	818841		892585	1531520	656012
Fructoselysine 6-phosphate	448.1436	1.213 HILICneg	230273	346547	175629	309471	375865	431683	618218	399579	771900	338994
Fructoselysine 6-phosphate Esi-1.318	448.1434	1.318 HILICneg	177579	301046	187499	293328	317514	666491	533688	316066	786458	315486
FTY720 phenoxy-biotin	596.3258	12.982 Rpneg	91416	270396	277840	434733	193611	119603	112865	129723	109699	150464
FTY720 phenoxy-biotin Esi-12.981001	596.324	12.981 Rpneg	1	270731	276622	434527	193427	119663	112878	28749	26694	21940
FTY720 phenoxy-biotin Esi-12.982	596.3255	12.982 Rpneg	55656	269024	278291	435262	193764	119571	113660	129624	109284	149923
Fumonisin A2	747.4096	13.426 Rpneg	1471	1707	2030	2857	959	1	2618	1656	1976	1
Fumonisin B1	767.3922	0.913 HILICneg	604365	394537	1	301612	1100557	252369	266892	1	453437	373804
Furamizole	598.0832	2.672 Rppos	1810447	1669405	1860478	1231721	1630851	2159086	1638495	1418173	1212322	2094680
Furcatin	428.1677	12.597 Rpneg	4840	3183	1770	2911	1472	1	1	907	1	1
Furfuryl thioacetate	202.0303	7.742 Rpneg	196823	113123	102499	114891	62935	84687	87467	87744	44747	60955
Furmecyclox	251.1525	10.543 Rpneg	34315	34519	33956	30176	38500	37459	32401	33491	30130	29683
Furmecyclox	251.1526	0.678 HILICneg	1250420	958554	277902	791759	3282308	198193	324010	621487	621884	957528
Gabunine	694.3512	12.089 Rppos	429992	451114	770413	579514	515372	635814	629953	590046	767925	614635
GalCer(d18:2/20:1)	773.5782	1.534 HILICpos	4049260	4601234	3726461	4529310	4152084	4275508		4329383	4365783	3948150
Gallagic acid	650.0147	0.982 Rpneg	10172	5127	4368	6724	4166	6551	1914	6951	6132	5332
gamma-L-Glutamyl-butirosin B	684.3187	12.647 Rpneg	6938	4803	2726	5433	2537	2188	4305	5162	3978	6087
gamma-Taraxastane-3,20-diol	426.3868	21.359 Rppos	1649126	777737	577571	1051174	1265134	785934	866447	1142307	535661	396769
Ganodosterone	408.3034	13.131 Rpneg	19737	26082	17291	25851	19240	10449	18658	23420	16583	16391
Gentamicin C1a	431.2729	5.64 Rppos	531326	1233441	558943	1070748	1417193	651067	518726	1049730	1452438	875607
Gentamicin C1a	449.2826	1.405 HILICpos	1	1	121761	268376	185479	297845		133176	197697	228506
Gentianaine	141.0428	1.31 Rpneg	4834	6547	6808	6567	5014	6461	6979	3371	4205	4169
Geranylfarnesyl diphosphate	564.2609	12.285 Rpneg	1	992	1477	1181	1894	1198	5650	1468	1605	2384
Gibberellin A105	312.1369	8.872001 Rppos	610850	736797	1121000	875113	731658	812299	875562	884221	908390	973731
Gibberellin A53 aldehyde	314.1881	9.160001 Rppos	133603	244865	207332	231363	290375	202943	194407	241957	238779	183061
GlcCer(d14:2(4E,6E)/16:0)	701.5086	14.486 Rpneg	16694	86235	25979	60162	51876	65945	69207	60680	1	29751
GlcCer(d15:2(4E,6E)/22:0(2OH))	777.5714	26.133 Rppos	1961978	1438381	2571339	2137905	1066973	1721556	1590382	1245659	1269385	1296141
GlcCer(d16:1/20:0)	727.5971	25.833 Rppos	1698751	1851751	2024601	2852080	1627021	1766728	1343984	2474889	2055175	1652289
Gln Leu Asp	374.1762	11.639 Rpneg	1	3920	1	2853	3948	1	1309	2453	5596	2142
Gln Lys His	822.4412	0.929 HILICneg	292069	1	1	1	314225	54870	1	128586	191493	170600
Gln Lys Ile	387.2454	0.8 HILICneg	152287	267794	284589	233794	1144923	412012	994538	1025636	773555	961310
Gln Pro Ile	402.2091	0.961 HILICneg	109169	174895	217773	173509	147838	24220	161931	143576	88533	146518
Glu Ala His	401.1546	12.853 Rpneg	2966	1466	1	1	4265	2878	2951	3851	3117	2529
Glu Arg Pro	446.2082	1.072 HILICneg	1258771	465373	215662	474482	1715572	598049	367727	625442	799351	637316
Glu Arg Trp	549.2536	1.086 HILICneg	98226	1	76438	107319	74568	108598	72383	120249	121870	93066
Glu Arg Trp Esi-0.93200004	549.2518	0.932 HILICneg	112330	62386	77337	77188	92797	152218	71196	67559	87569	75896
Glu Asn Tyr	424.16	11.881 Rpneg	24405	34360	11931	12176	4786	19182	24319	17961	12080	16347
Glu Gln Gln	403.1688	13.122 Rpneg	3114	2070	1763	1416	2014	1054	1382	1594	1260	958
Gluconic acid	98.0294	0.825 Rpneg	7338	11406	6614	14117	19742	11837	8335	13678	23047	13022
Glucosyl (2E,6E,10x)-10,11-dihydroxy-2,6-farnesadienoate	432.2355	8.211999 Rpneg	53223	56057	55252	59649	74717	52532	54458	56850	64967	54258
Glucosyl (2E,6E,10x)-10,11-dihydroxy-2,6-farnesadienoate E	432.2354	8.114999 Rpneg	18487	19462	17148	24113	25886	17278	17480	19398	26939	18386
Glucosyl sphingosine	443.3226	9.935999 Rppos	122246	99225	177020	137056	543262	101788	113311	125144	130206	105392
Glutamyl-Asparagine	243.0861	1.201 Rppos	275462	302717	311357	340722	447394	526258	508886	554393	554968	513094
Glutathione, oxidized	612.1494	0.816 Rpneg	65716	25079	29212	42660	19175	35848	30607	34704	18748	23126
Gly Cys Glu	307.0835	0.833 Rpneg	181681	152437	278662	191507	150085	261632	236749	187085	128115	172708
Gly His Val	311.1584	5.586999 Rppos	362022	378597	358913	365350	373461	369713	356086	344959	339059	336454
Gly Phe Gln	367.1863	5.92 HILICpos	2190580	1961860	1956193	2018349	2331068	2315735		2355643	2343147	2024603
Glycerol 1-(5-hydroxydodecanoate)	272.2011	9.699999 Rppos	122253	145876	156835	161723	162782	164953	155449	167069	202952	187768
Glycerol 1,3-didodecanoate 2-decanoate	609.5332	25.474 Rppos	4056984	4238339	5523909	4437610	5647405	7359999	6707411	7389771	5387505	6149491
Glycerol 1,3-didodecanoate 2-decanoate Esi+21.096003	609.5386	21.096 Rppos	504673	783146	1201393	1095466	507528	447219	284755	550370	982866	739886
Glycerol 1,3-didodecanoate 2-decanoate Esi+25.11	609.5366	25.11 Rppos	210003	205159	69547	145050	207907	413905	220303	144711	316671	249374
Glycerol 1,3-didodecanoate 2-decanoate Esi+25.485	614.4893	25.485 Rppos	4545706	4568574	5484954	4749354	5509836	6119104	5962903	6364180	4615746	5587178
Glycerol 1-dodecanoate 2-tetradecanoate 3-octanoate	627.5458	23.502 Rppos	781368	816673	865237	1037648	459857	387135	635865	597692	435477	684637
Glycerol 1-dodecanoate 2-tetradecanoate 3-octanoate Esi+2	627.5427	23.164 Rppos	172538	207978	147324	177969	171027	132739	129667	106991	229604	158987
Glycerol trihexanoate	386.2662	10.633 Rpneg	11968	7698	7158	6596	7296	7441	6883	6650	6899	6121
Glycerol trihexanoate Esi-10.791	386.266	10.791 Rpneg	3871	2929	2505	2764	3222	2631	2441	3759	3002	2769
Glycerophosphocholine	257.1032	0.85 Rppos	1451133	1485475	1659657	1808281	1348279	2065128	2247815	1675960	1855957	1728692
Glyceryl 5-hydroxydecanoate	541.382	8.016 Rppos	1	266757	30251	214495	307570	23370	32613	193670	403326	187029
Glyceryl behenate	396.3603	21.336 Rppos	170226	216637	211601	205836	226506	219717	220970	220124	259461	350659
Glyceryl lactooleate	428.316	11.64 Rpneg	3410	4892	1	8734	5365	2744	4656	5112	5014	1
Glyceryl lactooleate Esi-11.524001	368.2903	11.524 Rpneg	6237	2757	1635	3200	1556	2592	1573	2464	3081	2159
Glycidyl oleate	338.2808	13.121 Rpneg	4493	3597	4806	3951	3924	4044	3910	3293	4013	4289
Glycidyl oleate	338.2809	1.425 HILICpos	483323	502969	538996	550195	637871	686337		569300	744877	529505
Glycidyl oleate Esi+0.8909999	338.2819	0.891 HILICpos	428853	376606	430350	392504	491436	325988		302131	493061	455021
Glycolaldehyde	60.0215	9.560999 HILICneg	1010696	479024	467273	827502	668284	690928	905280	1161237	1088638	860344
Glycolaldehyde Esi-6.580001	60.0213	6.580001 HILICneg	115568	125215	80102	45428	180358	299170	371710	334920	773066	248640
Glycolic acid	76.0164	13.277 Rpneg	140606	107828	129629	100322	58019	86464	81189	84187	82490	77787
Glycosides	584.2844	8.214999 Rpneg	4949	4553	3509	3126	5728	4007	3409	3233	3025	2214
Glycosyl-4,4'-diaponeurosporenoate	593.3685	13.056 Rpneg	3050712	997937	734296	776113	332215	606358	974266	527592	483776	588743
Glyoxylic acid	74.0022	0.785 Rpneg	36892	34734	36988	40502	35373	42613	45161	47645	1	43325
Glyuranolide	512.3126	13.067 Rpneg	144618	35167	36907	51278	24408	20229	33400	28527	42971	36150
GN25	322.0511	8.082 Rpneg	3957	4098	1704	2284	2396	2337	5125	7325	4715	6122
Goyaglycoside a	694.4365	12.596 Rpneg	5122	3641	2942	4484	1277	1	1220	1976	1420	898
GPInsP[5']{17:0/20:4(5Z,8Z,11Z,14Z)}	952.5084	1.27 HILICneg	158219	94984	131778	131172	63253	72408	106041	77023	111949	103081
Graveolone	244.0721	6.845 HILICneg	93821	89624	61900	77852	63181	51094	50722	53944	45996	40087
Grayanotoxin I	412.2468	12.576 Rpneg	13566	9839	6184	9625	9392	2919	9298	5525	8746	4944
Grevilline A	648.1256	0.991 HILICneg	48193	55757	49037	52775	59700	1	60558	67894	70818	44411
Guaiol acetate	264.2084	12.09 Rpneg	8120	4789	1769	4893	3939	1964	3343	4604	3671	2329
Guanosine	283.0919	2.122 Rpneg	42181	22924	23370	37818	30128	51753	17474	58005	49175	49535
GW 842166X	448.069	12.914 Rpneg	1140	3055	2668	983	2704	12108	1112	6117	15260	21693
GW 842166X Esi-13.015	448.0698	13.015 Rpneg	923	1825	1525	1	1962	9387	1112	4555	11376	13045
Gynosaponin S	928.5336	26.998 Rppos	3221655	3333156	3630243	3028774	3513834	4041313	3672812	3141651	3404281	3196388
Haplophytine	712.3132	13.277 Rpneg	313599	253752	338387	328228	186559	188581	280381	219206	299382	268334
Haplophytine Esi-13.079001	712.3128	13.079 Rpneg	1873	2698	4695	4572	1	1404	4542	2212	4764	3867
Haplophytine Esi-13.223	652.2923	13.223 Rpneg	5743	3813	1321	4753	2001	1511	3841	3870	3312	4674
Harderoporphyrin	590.2554	23.226 Rppos	977098	984465	909123	907459	979107	481722	846813	841046	805631	840442
Harderoporphyrin Esi+22.64	590.2551	22.64 Rppos	831205	712260	781776	716135	626285	634599	572950	495499	398958	494522
Harderoporphyrin Esi+24.685	590.2557	24.685 Rppos	671935	753427	578063	567178	732328	673218	602789	561214	597747	572184
Hebevinoside XIII	919.5299	21.68 Rppos	419554	365837	490070	409238	392546	512209	436121	491717	436279	412265
Hebevinoside XIV	878.5046	0.907 HILICneg	783708	285610	191901	297101	701934	36007	187893	238732	316826	279776
Heneicosanol	311.3543	13.024 Rppos	627091	552822	308025	443346	532007	416540	438785	397667	427852	403954
Heptanoylcholine	215.1881	7.266999 Rppos	237067	208644	430455	234522	213645	233391	283863	310272	248683	213847

Heptyl heptanoate	228.2101	1.156 HILICneg	3.50E+07	1.95E+07	8109149	1.82E+07	4.88E+07	4961528	1.03E+07	1.61E+07	1.93E+07	3.22E+07
Heptylene-bis(tacrine)	509.3555	5.619 HILICpos	515887	605287	526512	432833	332848	380242		267327	271946	250116
Heptylmalonic acid	184.1097	5.702 Rppos	371805	705048	712513	598281	581957	568675	608140	478822	280361	414853
Heptylmalonic acid Esi+6.3440003	184.1098	6.344 Rppos	304697	395141	192506	281913	221388	198142	191560	384942	165052	148295
Hexacosanedioic acid	426.3707	13.608 Rpneg	131177	36736	34927	41063	30229	31378	26716	20427	27005	12058
Hexacosanedioic acid	426.3728	1.103 HILICneg	155778	62498	35732	85054	127933	1	100446	93339	1	69141
Hexacosanedioic acid Esi-12.541	426.368	12.541 Rpneg	1265	3741	2878	3671	2933	1019	2459	2349	2434	1994
Hexacosanedioic acid Esi-13.412001	426.3714	13.412 Rpneg	50406	19255	18587	20130	12800	17506	14236	9607	14921	7507
Hexadecanoic acid, 2-amino-, (1)-	270.267	8.28 Rppos	1049718	1225778	1380654	1508640	1119056	1285769	1430021	1560881	1613508	1685637
Hexadecanoic acid, 2-amino-, (1)-	271.2523	13.195 Rpneg	8018	5764	6110	7090	5014	5085	4491	1	6802	4661
hexadecyl butyrate	312.3023	13.372 Rpneg	714906	417338	292615	419440	398079	285376	395697	452678	447505	416061
hexamethylene bisacetamide	200.1528	8.453001 Rpneg	14720	59611	11741	16590	5457	31256	12276	7608	37810	38959
hexamethylene bisacetamide	200.1552	0.926 HILICneg	130970	421196	101139	118961	76427	58265	123371	86743	356816	298936
hexanoylcarnitine	259.1778	3.307 HILICpos	1562506	553516	496877	573581	564565	502045		478850	441677	606716
Hexyl glucoside	281.1834	1.425 HILICpos	421891	111448	1	72283	90193	42529		172179	128642	90207
hexyl hexadecanoate	340.3339	0.986 HILICneg	511848	414579	273146	351623	518143	655452	312277	338926	456996	326763
Hexylamine	101.1205	1.16 Rppos	3973146	6674465	7156213	8804523	8208870	8894669	9887553	8974090	9335154	9449942
Hippuric acid	179.0584	4.25 Rpneg	114277	74487	66507	72473	67438	61039	64893	85743	47245	60600
Hippuric acid	179.0584	5.463 HILICneg	171470	72996	60604	77831	91280	74539	101101	103215	60524	85515
His Arg Arg	513.2734	10.065 Rpneg	5649	6758	2470	4198	1	4774	1	1116	4115	7870
His Gly Pro	618.2861	25.173 Rppos	1557069	651273	1462217	2160792	1481809	1318264	1341810	680177	1208413	1338597
His Gly Pro Esi+20.289	618.2873	20.289 Rppos	698636	461791	417788	454908	546252	322564	541548	352752	389540	333900
His Gly Pro Esi+24.406002	618.2863	24.406 Rppos	730665	621224	520898	613351	640357	607764	582160	566770	568475	581204
His Gly Pro Esi+27.009998	618.286	27.01 Rppos	1008118	1011504	1236718	1022555	1047064	1545255	1380872	1237557	1275229	1170977
His His Asn	452.1781	11.627 Rpneg	3046	3359	2026	2443	1506	2270	5198	2986	5294	3937
His Met Lys	474.2254	11.849 Rpneg	2403	1825	978	1004	1672	915	2784	1598	2003	1517
His Phe Gln	490.2199	9.046999 Rpneg	1529	6427	2390	2563	1715	2996	3167	1736	5677	5283
His-HoPhe-OH	498.1725	11.018 Rpneg	10768	7419	8252	7946	9049	6593	6447	6550	6346	5697
Histidinyl-Alanine	226.1043	1.042 Rpneg	3491	3685	1	2610	4934	1404	1507	4436	6648	4263
Histidylproline diketopiperazine	247.143	1.359 Rppos	8325931	1899007	1162434	808528	2804625	6980067	4618094	5300942	12851243	2863915
HMMF	89.0481	1 Rppos	1404550	792336	1360836	700552	688903	688962	1344064	739557	760730	745021
Hodgkinsine	578.3356	13.807 Rpneg	1	2164	3287	2966	5685	6469	3185	8569	5717	8699
Hoduloside VIII	898.4952	23.23 Rppos	3164921	3385385	1806000	2119592	2426677	1758917	2788729	3177619	1795988	3020666
Homoarecoline	169.1099	6.126 Rpneg	11436	7724	17829	6842	10421	17700	6488	7868	7956	13843
Hovenidulcigenin A	561.3568	1.445 HILICpos	260711	465401	173697	211490	295852	237090		148043	107928	181435
Hydroquinidine	326.1998	11.99 Rpneg	6598	2562	4728	10756	12476	5301	6205	5065	4696	4591
Hydrous benzoyl peroxide	302.079	7.816001 Rpneg	1	12369	1993	15339	19814	3090	2194	14685	19635	8744
Hydroxy (3?)Isoallospirost-9 (11)-Ene	828.6265	0.888 HILICneg	1395315	2222161	3887311	2306622	1378641	483866	2304562	1702480	1356088	2219663
hydroxybutyrate	104.0473	6.581 HILICneg	307891	159020	70048	53896	1297670	2551516	2196508	2068484	4343770	1601940
Hydroxycitric acid	208.0236	0.778 Rpneg	19848	44525	31409	47552	46054	32123	37236	41396	55805	40142
Hydroxymethylphosphonate	157.9981	0.999 Rpneg	234562	282707	275666	240255	283483	221634	375369	220073	202704	251375
Hydroxymethylphosphonate	157.9983	8.951999 HILICneg	1609444	1710782	1719764	1698545	1715243	1708584	1648954	1829383	1681386	1626162
Hydroxyminaline	145.0378	7.338 HILICneg	48242	38574	41446	29745	44570	58794	17807	37414	114009	68331
Hydroxypentobarbital	242.1276	1.511 HILICneg	1214906	2429610	1832776	2783088	2927968	552436	3998192	2284901	1297173	1451100
Hydroxyprolyl-Asparagine	227.0906	1.269 Rppos	1644817	1236384	1236144	986053	714499	755325	957865	867202	496375	683605
Hydroxysintaxanthin 5,6-epoxide	479.3416	5.474 HILICpos	189126	240559	222147	258710	229277	271544		212205	319122	165168
Hypercalin B	564.3041	10.428 Rpneg	4070	2819	2668	3247	2514	6692	6692	2776	2733	3244
Hypercalin B Esi-10.306	564.3065	10.306 Rpneg	2461	2212	2399	2777	1695	6235	6325	2425	2589	2650
Hypoxanthine	136.0383	2.648 Rppos	16263721	14118209	15200868	15971868	13948223	17827828	12995253	17343408	16527301	16165406
Hypoxanthine	136.0386	5.928001 HILICpos	22095924	19319226	18601580	20380112	23014124	22801374		23867208	23552688	19899016
hypoxanthine	136.0389	5.312 HILICneg	1.73E+07	1.70E+07	1.47E+07	1.62E+07	1.70E+07	9220594	1.04E+07	1.11E+07	9352868	1.06E+07
Ibandronate	655.2183	19.504 Rppos	753156	1174666	1054498	798484	682327	856364	518090	639229	834188	1463913
ibopamine	307.1787	9.654 Rpneg	7403	7491	8029	7165	6069	7532	7709	7853	7736	7793
Ibutilide	384.2429	1.113 HILICneg	378694	145697	101082	139453	267542	1	115523	141944	1	199720
Idebenone Metabolite (Benzenebutanoic acid, 2-hydroxy-3,	396.0738	6.510001 HILICneg	62145	127994	112136	108383	60792	84635	96931	64848	79647	85886
Idoxanthin	598.4015	13.05 Rpneg	22781	7987	1	12117	6049	3061	4044	3718	5683	3024
Ifosfamide mustard	219.9941	8.598 Rpneg	90647	89722	78024	84481	87594	88090	86121	84932	84689	82990
Ikarisoside D	542.1791	5.11 Rpneg	21770	8945	20700	15127	6470	15375	13929	15640	7060	12801
Ile Arg Tyr	917.5462	25.186 Rppos	892351	570260	871789	919537	486599	394912	460457	394400	348305	445731
Ile Arg Tyr Esi+25.436003	917.5468	25.436 Rppos	906703	412737	1	1	603134	563206	553105	565525	521029	538615
Ile Trp Gly	374.1955	1.255 HILICneg	68256	39032	23500	43513	89924	1	32584	61683	35146	45609
Ile Trp Leu	430.2577	1.255 HILICneg	262174	262531	142510	180481	339542	299433	116568	152881	102131	170709
Ile Trp Val	415.2564	6.882 Rppos	184555	157866	149040	137654	164534	146246	117620	128434	114790	89343
Imatinib	539.2657	0.905 HILICneg	389636	267334	145983	181421	852636	97640	207065	142065	576797	447104
Imatinib Esi-0.80100006	539.266	0.801 HILICneg	150969	75853	51104	66475	157135	1	41382	71321	136096	92716
Iminoerythrose 4-phosphate	199.0256	2.438 HILICneg	66563	95449	102366	140376	57937	79980	98664	113009	112257	133317
Indecainide Esi+1.097	325.2174	1.097 HILICpos	208831	442626	153803	71688	429910	221091		116887	1	51202
Indolelactic acid	187.064	4.909 Rppos	370635	360553	329916	354962	365606	340479	293661	403898	384155	401577
Indomethacin N-octyl amide	528.2405	11.058 Rpneg	3884	2480	1	1345	1774	4547	1426	1627	3553	4208
Inosine	268.081	1.013 Rpneg	20862	5750	49706	1	2076	49735	1	35711	35336	34465
inosine	268.0812	5.928001 HILICpos	39568568	33608108	32219880	34911808	40943796	40307652		42446736	42736500	34884380
inosine	268.0825	6.363999 HILICneg	1.10E+07	1.96E+07	1.62E+07	1.82E+07	1.66E+07	1.41E+07	1.36E+07	1.46E+07	1.30E+07	1.41E+07
Inosine	314.0885	0.889 HILICneg	133215	115404	332403	142848	170412	84381	207655	439296	200721	168511
Inosine Esi+6.02	290.0632	6.02 HILICpos	980822	964351	941823	961732	970692	980646		1020809	1051141	988807
Ipecac (Emetamine)	974.5186	24.414 Rppos	1143063	1090345	1063695	1080860	1196550	1052852	1044181	925146	1076835	961565
Ipecac (Psychotrine)	950.519	25.046 Rppos	1537356	1339410	1192136	1211865	1266855	1050711	1109410	1040313	1114749	1142366
Iproniazid	179.1075	10.268 Rpneg	4382	5262	2758	2237	5618	5322	2280	7721	5428	5650
Iprovalicarb	366.216	12.597 Rpneg	9745	8112	4860	8950	4423	2666	5300	7401	6117	5494
iso-1,2-octadecanediol	285.3026	11.288 Rppos	435543	292226	170882	282615	344703	229735	233041	270910	273288	180964
Isoamyl nitrite	117.0794	1.002 Rpneg	48756	47383	32634	41484	89116	62884	70490	107552	103351	91477
Isoamyl nitrite Esi-1.002	117.0791	1.002 Rpneg	48756	47110	32634	41484	86092	63023	74693	105890	106241	95129
Isobutylglycine	267.1326	5.364999 Rppos	332791	304595	298844	342602	337424	307594	293683	333786	324879	313399
Isoduartin	314.1189	7.914001 Rppos	261921	734728	574582	712353	882676	484478	597138	737089	808004	604684
Isoferulic acid 3-sulfate	274.0167	4.124 HILICneg	38775	56063	40718	38941	59317	98518	19160	35125	33936	72483
Isognaphalin 8-butyrate	384.1203	4.734001 Rpneg	17698	12229	12787	15130	8176	9353	8736	11000	8770	11345
Isolariciresinol 4'-O-beta-D-glucoside	522.2116	1.511 HILICneg	1	90045	85065	127225	140925	11977	177239	90743	31322	52576
Isolinderanolide	336.266	1.425 HILICpos	251182	277378	351457	288890	366123	387301		413617	417985	309302
Isoorientin 2'',6''-diacetate	532.125	11.007 Rpneg	2621	2202	3250	1644	1846	1923	2796	2340	2339	2272
Isopentenyl pyrophosphate	538.0156	7.689 HILICneg	72787	67839	70875	67595	71204	70160	74216	71866	79105	73783
Isopersin	397.3197	2.039 HILICpos	1953584	996145	871812	695471	1000950	1011649		890523	1205348	1051491
Isoprothiolane sulfoxide	306.0574	6.362999 HILICneg	165034	189011	208821	224497	241522	194301	209979	225139	194103	247338
Isoprothiolane sulfoxide	366.0835	11.924 Rpneg	16324	1	19317	8767	28546	6143	1	6536	7888	4835

Isosilychristin	981.2696	24.722 Rppos	11212992	12659410	9991050	10816852	8152618	6845442	7570055	8890615	12312844	9561605
Istamycin C1	431.2746	1.675 HILICpos	475095	859271	369225	734152	980933	1140335		993763	805049	720494
Istamycin C1	879.5771	21.629 Rppos	414671	382268	487700	479520	393414	437991	351462	455286	448623	407494
Janthitrem C	569.3522	5.411 HILICpos	478584	606089	663201	606396	405380	437882		377727	379192	350421
Janthitrem E	603.3555	1.199 HILICneg	112130	281206	242827	282859	223519	1	266225	212824	184539	256549
Jasmolone glucoside	342.1697	10.784 Rpneg	1455	3482	1129	2479	3779	1758	1	3044	4570	2858
Jatrophatrione	314.1898	11.153 Rpneg	1338	6075	3777	5679	9497	2523	3519	6059	7315	4439
JP104	466.2457	11.057 Rpneg	3474	2811	1	1598	2250	5089	1796	2555	3508	3962
JTE-013 Esi+24.606	831.2317	24.606 Rppos	788932	689909	563934	567725	977484	812818	878747	669534	920065	698830
JWH 018 N-(4,5-epoxypentyl) analog	355.1567	12.547 Rpneg	6671	3607	3194	2680	3146	2640	2102	1844	2484	1725
JWH 122 8-methylnaphthyl isomer	354.2083	7.79 Rppos	118238	112896	144100	145967	170685	135469	162773	137921	134425	162535
JWH 210-d9	378.265	12.29 Rpneg	2252	2863	1508	2826	4248	2397	1	2427	3924	1944
Kaempferol 7-methyl ether 3-apiosyl-(1-5)-apiosyl-(1-2)-[rha	872.2596	19.811 Rppos	3152313	3729562	3441249	3590253	2732683	2951369	2791059	3076736	3726339	3326367
Kalihinol A	392.2223	11.632 Rpneg	1	4445	1	4249	5531	1	864	5967	6561	2874
Kalkitoxin	366.2718	13.122 Rpneg	6638	5592	4710	6309	5592	6478	4922	6150	4739	5000
Kamahine C	250.1211	7.749 Rppos	1621128	1862705	1984858	2084448	1708419	1945206	2043080	1949248	1945048	1991586
KAPA	187.121	4.46 Rpneg	20265	17678	15754	9000	10627	1	1	5607	11089	5085
Kojic Acid	142.024	0.99 Rpneg	2793901	2368650	2264597	2523900	2174747	2335281	1903982	2467341	2285190	2246745
Kojic Acid	142.0244	9.565001 HILICneg	2506587	1786897	2322706	1992205	2341282	2661958	2240413	2889444	2666697	2142710
Kojic Acid Esi-0.69299996	142.0238	0.693 HILICneg	19934	33175	1	60490	76722	2652	65254	5203	14187	45855
Kojic Acid Esi-0.908	142.0246	0.908 HILICneg	98137	109624	46918	65990	82470	18529	105130	79906	145991	209052
Kolanone	519.3329	5.511001 HILICpos	4074356	1372687	3172552	2789890	3674563	3824351		3796494	3413552	2541288
Koryoginsenoside R1	868.525	13.623 Rpneg	138748	157678	93788	177894	28809	18653	23207	29213	26312	24314
Kukoamine D	530.3123	12.426 Rpneg	3335	2160	1734	2324	3598	1817	2045	3057	6031	1413
Kukoamine D	547.3377	6.998 Rppos	176632	176335	202585	189358	171337	178972	189685	189108	191783	191625
L-(+)-Arabinose	215.0768	0.925 Rpneg	9537	11282	7570	8726	10307	7555	6542	8427	9245	8921
L-2-Amino-3-(1-pyrazolyl)propanoic acid Esi-1.1669999	155.0695	1.167 Rpneg	80094	95375	92308	88486	34955	51668	33073	29136	49727	49324
Labriformidin	577.2562	5.656 HILICpos	617716	662754	683421	540626	540959	589038		398532	367084	404337
LacCer(d14:0/18:0)	817.5916	20.428 Rppos	1	1281309	847028	1153252	656895	1756040	1979237	1318882	1835117	1039968
LacCer(d14:0/18:0)	853.5987	14.6338 Rpneg	24359	29771	20390	29731	24153	32922	32690	43016	30284	30468
LacCer(d18:1/14:0)	833.5876	12.707 Rpneg	1378	2734	1	33731	8643	9276	20707	13763	4885	3200
Lactapiperanol C	281.1955	7.486 Rppos	441067	381695	671619	473038	410884	421877	658764	521604	430343	442238
Lactapiperanol C	328.1888	10.171 Rpneg	40092	42652	42369	46190	42388	41904	42655	46739	47195	46722
Lactapiperanol C Esi-10.376	328.1882	10.376 Rpneg	24160	22818	23135	24668	21536	23029	23329	26324	22691	24446
Lactapiperanol C Esi-9.305	328.1887	9.305 Rpneg	4659	4740	5086	5056	4498	4722	5357	5027	4113	4661
Lactapiperanol C Esi-9.628999	328.1891	9.628999 Rpneg	22961	21940	25445	22368	19199	23789	25162	26279	24963	25577
Lactapiperanol C Esi-9.778	328.1891	9.778 Rpneg	21866	21265	22276	23253	20971	21843	21032	22334	23627	22361
Lactic acid	90.0317	14.325 Rpneg	9774	1178	8431	22054	1	11465	1540	6193	18834	15932
Lactic acid	90.0319	6.521 HILICneg	8605886	1.83E+07	2.13E+07	1.28E+07	8138219	1.03E+07	1.18E+07	2862724	8709950	1.04E+07
Lactic acid Esi-13.505999	90.0321	13.506 Rpneg	15029	22490	76663	25901	11943	1	61016	1	2734	1
Lactone of PGF-MUM	278.1521	8.974 Rppos	3146438	3768699	3958328	4283893	3709793	3942667	4377886	4548682	4597495	4650778
Lactone of PGF-MUM Esi+8.832	278.1523	8.832 Rppos	1513448	1975307	1996400	2120884	1834655	1866860	1953872	2004931	2433022	1932397
L-Agaridoxin	300.0972	0.913 Rpneg	8094	8915	10704	8527	8539	5891	11144	6919	8001	7479
lambda Isostearic acid	284.2713	13.123 Rpneg	4876436	4602041	4642046	4833137	4671573	4412532	4534924	4889555	4957237	4774970
lambda Isostearic acid	284.2735	1.074 HILICneg	3.62E+07	2.38E+07	1.76E+07	2.36E+07	4.32E+07	7.48E+07	2.21E+07	2.61E+07	1.87E+07	2.25E+07
lambda Isostearic acid Esi-13.122999	284.2711	13.123 Rpneg	4876239	4598624	4629748	4834820	4671113	4412212	4536658	4889555	4953056	4780669
lambda Isostearic acid Esi-14.079001	284.2716	14.079 Rpneg	11005	2978	10061	4228	1	16757	3573	14057	3565	4860
lambda Isostearic acid Esi-14.3220005	284.2716	14.322 Rpneg	123680	27978	142145	77038	23424	99314	40857	126825	64863	69484
Lasiodine A	681.3556	12.089 Rppos	185340	192017	319794	252693	208974	287898	284035	270270	356599	281272
Latanoprost ethyl amide	463.2911	10.05 Rpneg	6989	12075	1031	2943	1	5396	1	1	3612	6992
Latanoprost ethyl amide-d4	443.2973	1.38 HILICpos	1	668992	152817	103794	486471	281982		105824	208800	95726
Lauroyl diethanolamide	287.2459	9.039001 Rppos	1399838	1336392	1413339	1610206	1454068	1500153	1465115	1569538	1502325	1462551
Lauryl hydrogen sulfate	266.1551	11.924 Rpneg	3222657	801602	4474225	3141774	5716896	1649907	2174947	2788654	3358796	2804926
Lauryl hydrogen sulfate	284.1686	1.092 HILICneg	87266	203755	176518	216035	177720	278993	224323	291509	146276	95295
Lauryl hydrogen sulfate Esi-12.593001	266.1555	12.593 Rpneg	2332	969	3459	1662	3852	1	1251	2229	1492	1574
Lentiginosine	157.1097	1.399 HILICneg	100121	199553	175338	193600	108226	78572	142749	257698	84154	249200
Lentiginosine	157.1101	7.02 HILICpos	2424655	2495003	2687725	2142082	1650630	2679682		1588701	3163510	1986588
Lentiginosine	157.1104	0.782 Rppos	310799	335141	240041	1269785	423387	125390	275423	275098	129611	303122
Lepidine C	342.1496	8.647001 Rppos	223559	460996	420322	417465	494450	338348	403253	420863	427182	376969
Lepidiumterpenyl ester	442.3275	11.765 Rpneg	3908	1410	794	1847	1013	1186	1283	1199	1251	1104
Leucyl-Hydroxyproline	244.1424	1.019 Rppos	2678039	2573582	2941284	2388767	3134832	3458846	3412175	3043156	10007759	3167125
Leucyl-Hydroxyproline	244.1429	7.711999 HILICpos	7626746	7352780	8006275	7380831	10294105	10824286		7616353	7264990	7837014
Leucyl-Hydroxyproline Esi+1.524	244.1438	1.524 Rppos	3334053	8341569	3903204	7777358	3642494	4072693	4041341	3621123	3935475	3820946
L-Glutamic acid n-butyl ester	203.1157	5.693 Rpneg	6172	15303	1312	13249	20827	3215	2656	16217	27489	11798
L-Glutamic acid n-butyl ester	203.1157	5.071 HILICneg	51403	78793	61996	59779	60803	57608	53360	46599	48770	48152
L-Glutamine	146.0686	0.859 Rpneg	186640	169169	156136	181221	149041	246314	175472	183781	303287	241903
L-Glutamine	146.0688	8.97 HILICneg	559117	351142	388234	319772	452039	520243	328182	384513	880066	501479
L-Glutamine Esi-1.094	146.0693	1.094 Rpneg	1	1	74309	1	67821	100532	120254	79769	96907	121432
L-Glyceric acid	106.0255	0.823 Rpneg	30515	45893	29990	45179	57528	32441	26441	42968	62034	42122
L-Iditol	182.0782	0.909 Rpneg	12910	15878	9360	15027	14656	13018	11982	12282	17549	11846
Liensinine	610.305	12.117 Rpneg	6376	4474	4488	3821	5423	3248	8625	5194	3694	5484
Linoleoyl Ethanolamide	323.2825	13.457 Rpneg	16492	11936	15172	17218	12829	10142	11121	10202	13882	12655
Linoleyl arachidonate	612.5126	12.598 Rpneg	9605	7398	6198	5833	11880	10312	10548	12724	10191	10448
Linoleyl carnitine	423.336	1.98 HILICpos	2745881	1954512	1545758	966217	1971715	1719305		2846007	3341821	2623876
Lipiferolide	306.1482	11.932 Rpneg	20308	8470	29813	25046	29892	15689	19717	19540	24231	21982
Lipiferolide Esi-11.932	306.1479	11.932 Rpneg	20308	8470	29813	25046	29892	15689	19717	19540	24231	21982
L-isoleucyl-L-proline	228.1474	1.101 Rppos	5140543	5646907	6237969	5446828	8178984	6738856	7105156	7954047	6656027	9059152
L-isoleucyl-L-proline	228.1479	7.685 HILICpos	10873411	11860139	10757354	8763848	13723018	13658480		11779936	11901824	14695257
L-isoleucyl-L-proline Esi+2.028	228.1475	2.028 Rppos	3840568	4091635	4473345	3704461	5866580	4667915	5906664	5111748	5585971	5939975
Lisuride	338.2131	12.651 Rpneg	115273	47591	35938	50515	60372	31374	43812	50476	92757	32956
Lisuride Esi-12.050001	384.2199	12.05 Rpneg	2207	1512	994	1	1816	1180	1534	1917	11979	1
Lisuride Esi-12.333	398.2335	12.333 Rpneg	40412	22324	18312	22661	37508	20156	23698	28016	54353	15361
L-Lyxose	150.0525	0.827 Rpneg	10296	20794	9624	23425	28641	14069	14228	21953	29373	19906
L-Menthyl acetoacetate	240.1727	11.099 Rpneg	76098	33318	23038	24897	25509	17079	40478	35181	28489	37360
L-Menthyl acetoacetate	240.1747	1.24 HILICneg	106740	111277	94153	108194	113228	1	121326	82310	281831	96151
L-Menthyl acetoacetate Esi-11.649001	240.17	11.649 Rpneg	1	2490	2898	2107	5174	2622	3283	3921	2873	4079
L-Menthyl acetoacetate Esi-9.544999	286.1793	9.544999 Rpneg	4485	2306	1	2396	1585	3261	1283	2254	2505	1
L-Norleucine	113.084	5.058 Rppos	445964	1404764	1031998	923592	993329	1153315	506105	492862	1127242	448601
LPA(0:0/16:0)	410.2431	13.554 Rpneg	56864	36804	43198	44854	22562	22019	27001	12013	22003	21144
LPA(0:0/16:0)	410.2447	5.795 HILICneg	64760	71287	60356	61836	40943	101787	38998	35037	32799	32052
LPA(0:0/16:0) Esi-12.673999	410.2419	12.674 Rpneg	7489	11200	10207	14806	9900	7321	11688	12227	11066	13229
LPA(0:0/16:0) Esi-13.553999	410.2436	13.554 Rpneg	56864	37565	42225	45589	22562	22019	27001	6433	22003	21134

LPA(0:0/18:0)	438.2738	13.973 Rpneg	37219	21603	27906	26785	20841	21865	21816	17622	19100	18472
LPA(0:0/18:0) Esi-13.973	438.2737	13.973 Rpneg	37219	21519	27906	26615	20841	21980	22098	17622	19100	18472
L-Rhamnulose	164.0686	6.109 HILICneg	47422	50029	48902	48380	1	1	1	1	1	1
L-threo-3-Methylaspartate	129.0427	0.858 Rppos	1414621	1415737	1634325	1374273	1906297	2596463	2168516	1952628	3489857	2520903
L-threo-3-Methylaspartate Esi+1.028	129.0427	1.028 Rppos	1409444	1056833	898320	1077995	1256121	1969108	915184	1505657	2406326	1719396
L-threo-3-Methylaspartate Esi+1.1590002	129.0425	1.159 Rppos	761185	855073	547156	777841	1014662	1482050	660548	1253195	2096686	1495612
Lucidenic acid M	462.2976	0.971 HILICneg	852026	1017028	525307	708779	653766	185891	249662	236898	383871	256343
Luciduline	207.1627	9.013 Rpneg	16040	14892	15545	13813	15466	15093	15112	14275	14578	14628
Luciduline Esi-10.526	225.1734	10.526 Rpneg	10194	9285	10014	9189	9228	10044	10062	10032	9408	10100
Luciduline Esi-9.669	207.1629	9.669 Rpneg	5291	5213	5904	4988	5837	6033	5487	6027	5373	5501
Lupan-3beta,20-diol	426.3862	20.369 Rppos	1011768	1514244	1532714	1420447	1268389	1610503	1067756	1673871	830587	401006
Lupan-3beta,20-diol Esi+20.134	426.3871	20.134 Rppos	155313	334478	290356	432593	188771	329247	282649	566476	579555	531039
L-Urobilin	640.3513	12.861 Rpneg	1	2019	2648	3151	2462	1345	5653	3028	3020	4113
Lycaconitine	668.3225	13.075 Rpneg	989	3915	6363	5689	1521	2390	5813	2364	5566	4721
Lyciumoside I	630.359	9.398001 Rpneg	3453	2236	2122	2363	2664	1747	1591	2189	2835	1950
Lyciumoside IV	776.4217	0.921 HILICneg	1	1	1	1	309360	70558	1	110217	205289	160592
Lyciumoside IV	776.4202	13.276 Rpneg	4267	1764	3332	2041	1174	1546	1779	1058	1956	1428
Lyngbyatoxin	459.2854	6.927001 Rppos	199953	194492	196358	177763	193851	182709	179024	167981	165960	177718
Lys Ala Lys	707.5043	21.998 Rppos	7428415	7631088	7688167	8579130	5718221	5444176	5719808	5608977	6071032	6135657
Lys Glu Arg	431.2486	8.955001 Rpneg	3221	1	2186	2323	5241	1	2068	1111	3820	2859
Lys Glu Leu	370.2202	5.501999 Rppos	636906	1468292	678761	1233151	1735905	789778	659295	1232691	1661805	957655
Lys His Lys	868.5221	0.796 HILICneg	611516	1673624	1264442	1445266	91343	238483	383648	213439	189911	214881
Lys Thr Gln	357.2024	5.352001 Rppos	105001	155223	100911	149779	185080	106953	102826	132134	176428	129078
LysoPC(18:2(9Z,12Z))	519.3328	5.631 HILICpos	5056132	4343589	4211776	3563591	4045030	4816472		3102282	3140631	2461536
LysoPC(22:6(4Z,7Z,10Z,13Z,16Z,19Z))	567.3321	11.29 Rppos	1706232	1458841	2181100	2191513	1149667	1674943	1501002	1505220	1116186	1253739
LysoPE(0:0/16:0)	453.2851	13.378 Rpneg	125514	136591	81846	127852	79785	64609	75722	85321	71108	71766
LysoPE(0:0/16:0) Esi-13.378	453.285	13.378 Rpneg	125514	136591	81846	127852	79785	64609	75722	85321	71108	71766
LysoPE(18:1(11Z)/0:0)	479.3019	13.434 Rpneg	36369	41406	29118	38497	42256	41104	41965	52002	50361	50670
LysoPE(18:1(11Z)/0:0)	479.3019	5.836999 HILICneg	45550	42713	30350	25941	30252	23149	22779	21710	19424	18960
LysoPE(18:1(11Z)/0:0) Esi-13.434	479.3016	13.434 Rpneg	34318	37372	32667	38158	42176	41261	13591	52179	48079	48436
LysoPE(20:4(8Z,11Z,14Z,17Z)/0:0)	501.2871	5.7 HILICneg	750848	686769	527283	542590	458109	299695	331387	377677	278694	258437
LysoPE(20:4(8Z,11Z,14Z,17Z)/0:0)	501.2862	13.058 Rpneg	67428	56362	55065	64772	46923	51901	69806	86771	83966	59140
LysoPE(20:4(8Z,11Z,14Z,17Z)/0:0) Esi-13.056	501.2845	13.056 Rpneg	50131	42507	42112	49564	36193	40178	54467	5701	5801	46104
LysoPE(20:4(8Z,11Z,14Z,17Z)/0:0) Esi-13.141001	501.2849	13.141 Rpneg	29266	21080	17824	22857	22055	16222	18770	86771	83966	21608
LysoPE(22:5(7Z,10Z,13Z,16Z,19Z)/0:0)	527.2997	13.156 Rpneg	13876	11696	10984	22255	10149	8358	18815	12248	15061	11324
LysoPE(22:5(7Z,10Z,13Z,16Z,19Z)/0:0) Esi-13.247	527.3002	13.247 Rpneg	8020	7492	5875	37445	7475	4524	6324	8240	5429	7697
LysoPE(24:6(6Z,9Z,12Z,15Z,18Z,21Z)/0:0)	553.3203	5.612999 HILICneg	73659	85218	68088	75100	48351	25786	29623	22804	18042	20551
LysoPE(24:6(6Z,9Z,12Z,15Z,18Z,21Z)/0:0)	613.3327	11.754 Rpneg	2061	1163	1	2094	1371	915	1978	2446	1725	4199
Lysyl-Tyrosyl-Lysine	437.2631	12.605 Rpneg	3996	3109	2330	4874	1824	1	1	2313	1	1
Macaridine	490.2134	0.785 HILICneg	11265	14115	6994	13215	89717	1	87498	102942	86070	92010
Magnoshinin	414.2041	12.096 Rpneg	5002	3771	3974	6459	6278	4581	7612	7062	8632	4439
Magnoshinin Esi-11.974	414.2031	11.974 Rpneg	1755	1769	1625	2014	2066	1784	2263	2194	2688	2187
Maleic Anhydrides	144.005	1.053 Rpneg	6532	6249	8246	3946	1	1732	5043	3248	3407	6542
Maleic hydrazide	112.0276	1.306 Rpneg	27900	30291	32818	39463	1	31833	33334	23780	23536	1
Maleic hydrazide Esi-1.1000001	112.027	1.1 Rpneg	33212	23646	25344	26003	21802	17152	22709	10965	22498	24165
Maleic hydrazide Esi-1.101	112.0273	1.101 Rpneg	32682	23805	24886	25716	19756	17621	21837	9292	14086	11063
Maleic hydrazide Esi-5.1889997	112.0274	5.189 HILICneg	252564	686133	800823	653345	482939	416137	479126	421977	467758	470528
Malic acid	134.0215	0.756 Rpneg	3507001	1792065	1356969	1694758	2205281	2442203	1685905	2904758	2234987	2554505
Malic acid Esi-1.139	134.0211	1.139 Rpneg	105394	22121	18202	15703	52209	55573	40903	79540	37873	51547
Malic acid Esi-1.1420001	152.0326	1.142 Rpneg	48190	24056	1	21195	27155	26228	31214	47629	25135	34458
Malonaldehyde	72.0208	1.291 HILICneg	143970	378797	161590	230741	250464	84660	202695	176932	156045	88048
Malonaldehyde	72.021	0.756 Rpneg	121233	204997	64414	157757	226266	89905	81589	155077	262970	171186
Malonaldehyde Esi-0.91620004	72.0206	0.9162 Rpneg	25456	30665	31987	31489	42101	53676	51603	37947	34780	43604
Malyngamide J	606.3843	21.976 Rppos	844758	828806	871832	914439	775284	778262	830414	822775	850625	901980
MEDICA 16	342.2774	12.913 Rpneg	58274	21778	21832	25718	18925	21690	17616	13916	17251	8476
MEDICA 16 Esi-11.252	342.2762	11.252 Rpneg	12443	9219	8379	13760	13855	7646	7794	7891	8627	8460
MEDICA 16 Esi-11.655999	388.2794	11.656 Rpneg	5352	3303	1506	4373	4688	2918	3200	2447	1	1913
MEDICA 16 Esi-12.456	360.2884	12.456 Rpneg	1	9688	4942	4463	5504	4831	4615	6713	5808	5276
MEDICA 16 Esi-13.196	342.2779	13.196 Rpneg	8817	21435	1	10813	4518	2548	8249	5310	9647	12820
MeIQ	212.1052	5.658001 Rpneg	11277	23821	17025	9096	21739	31679	6989	46286	12813	15299
MeIQ	212.1057	1.074 HILICneg	880738	655296	449475	559655	1443629	173475	347925	616385	702012	749411
Melleolide B	414.2047	7.966001 Rppos	2410718	4072126	3088439	2955949	3051708	4941808	8592958	3328356	5679223	3697868
Melleolide B Esi+8.438001	414.2061	8.438001 Rppos	170177	134602	535522	156355	365832	332436	454692	336396	342704	239624
Melongoside G	885.5027	21.937 Rppos	256606	307349	328053	321977	357796	400829	489365	466164	513524	472172
Memantine	225.1729	8.508001 Rpneg	571101	488812	710155	535582	470900	659189	721049	615666	500510	645981
Memantine	225.1731	7.547999 HILICneg	46983	74115	21182	33005	32211	26107	16779	26779	21940	48604
Memantine Esi-8.780999	225.1731	8.780999 Rpneg	128111	110646	181461	117384	104479	151358	185298	159276	109494	173147
Mepanipyrim	492.225	0.782 HILICneg	71008	58792	49218	78787	134359	1	119905	141543	82444	105766
Mesobilirubinogen	638.3367	12.583 Rpneg	34632	30604	31709	34539	34369	20963	52181	47501	30414	47294
Met Thr Met	427.1463	0.674 HILICneg	39195	53310	9148	29150	58153	11291	28336	26741	30478	19663
Met-Abu-OH	701.2059	16.659 Rppos	265145	246175	252282	268860	253653	252392	254938	264905	274702	273339
Met-Asn-OH	370.0949	10.962 Rppos	132892	143527	155615	147997	137854	223734	149947	148044	173108	153879
Meta-Tyrosine	181.0753	1.318 Rpneg	48493	65496	49732	53950	52593	60451	48586	38432	53293	1
Meteloidine	255.1473	8.596 Rpneg	141385	132215	137375	132253	138299	132094	134479	131430	131787	129900
Meteloidine Esi-9.047	255.1464	9.047 Rpneg	25735	22646	23394	14781	1	4816	17104	1	4228	1
Methacholine	159.126	5.327 HILICpos	7499353	8806958	8809247	8173159	11332469	13512570		11113455	14105411	13109327
Methacholine	159.1255	0.96 Rppos	2686662	3440693	3195077	3546763	4198808	5315828	2585904	4872315	6452732	5756040
Methanesulfonic acid	95.9877	9.052001 Rpneg	1770	3843	3676	2626	2671	4381	1	3118	4432	3728
Methanesulfonic acid	95.9881	4.622001 HILICneg	876655	1026270	915787	756530	677936	363971	793322	473226	704216	812617
Methenamine	140.1061	7.693999 HILICpos	25293618	25958536	25827028	16509661	24510444	23449630		24982678	25573156	24694844
Methimazole	228.0522	6.279 HILICneg	32488	38420	25914	123939	162585	38623	145984	141972	151496	178407
Methional diethyl acetal	238.1237	11.161 Rpneg	7050	4615	6274	6599	14913	2943	3572	6085	8612	5597
Methional diethyl acetal Esi-10.661001	224.1089	10.661 Rpneg	4484	7715	4450	5942	7566	5016	4266	6506	8024	5695
methionine	149.0511	1.26 Rppos	501415	549727	560768	555081	429982	440407	337759	348764	396535	489724
Methionine	149.0508	1.251 Rpneg	22593	1	25637	1	9518	14249	17798	6745	10996	1
Methoxamine	193.1107	7.794 Rppos	446235	450360	542363	552719	464347	483270	522536	545334	552027	574137
methoxyacetic acid	90.0315	0.874 Rpneg	1372376	1652834	2049547	1691846	1677177	1941032	2110561	1629831	1594540	1753664
methoxyacetic acid Esi-1.0550001	90.0319	1.055 Rpneg	904774	886056	865693	1022003	599105	589961	655137	812624	731483	648715
Methyl (3b,11x)-3-Hydroxy-8-oxo-6-eremophilen-12-oate	280.1668	10.269 Rpneg	9144	11859	7006	5595	11512	12739	5862	17641	12317	11530
Methyl 2-benzamidoacetate	193.073	5.308 HILICneg	20762	37831	36173	34722	14956	23910	30016	13647	20436	24282
methyl 8-[3,5-epidioxy-2-(3-hydroperoxy-1-pentenyl)-cyclo	442.2589	12.372 Rpneg	19308	11120	8777	11640	18341	9711	11765	13583	29228	7528
methyl 9,11-epidioxy-12,15-dihydroperoxy-5,7,13-eicosatr	214.1401	9.047 Rpneg	1	10024	4224	5494	4385	4758	3487	3771	9357	6418

Methyl acetyl ricinoleate	354.2774	12.773 Rppos	343342	481108	519879	443449	747357	1045914	1015294	1169107	759247	632734
Methyl acetyl ricinoleate Esi+13.169001	354.2784	13.169 Rppos	149156	173311	217601	155481	290812	321416	411614	523854	307232	302240
Methyl Arachidonyl Fluorophosphonate	370.2427	12.597 Rpneg	12667	8391	8834	10413	4677	4381	1	8163	1	8460
Methyl caffeate	176.0475	7.369 Rppos	329242	2636629	1934014	1010494	855666	2315801	495304	464816	1313964	606598
Methyl hydrogen fumarate	130.0266	0.7 Rpneg	32191	68319	26088	65398	48619	27481	29580	55903	126167	54129
Methyl hydrogen fumarate Esi-1.0439999	130.0269	1.044 Rpneg	8155	14906	22028	12133	20123	8861	4145	10713	13443	16004
Methyl nicotinate	137.0475	7.393 HILICpos	883737	783745	666058	1089982	811146	720039		873352	589804	600774
Methyl nigakinone	280.0846	1.516 HILICneg	54205	103302	107432	104886	92590	1	121817	82663	75027	57681
Methyl oleate	296.2714	1.036 HILICneg	130612	160730	146629	154085	205397	70786	155709	169538	235105	177719
Methyl oleate	296.2717	13.031 Rpneg	336391	269950	134621	238677	222861	195311	228043	290277	304695	256129
methylcitric acid	206.0427	0.697 Rpneg	9224	10167	11835	18166	22886	20762	24700	24427	30057	24804
Methylenediurea	132.065	5.394001 HILICpos	2506201	1429864	303665	4606492	405160	247082		3625338	1810187	2195603
Methylpyrazine	94.0532	0.768 Rppos	890671	721261	734023	1100669	889833	628188	575699	488087	740217	1161244
Methylpyrazine	94.0534	1.222 Rpneg	73429	292500	22629	330064	581532	31297	47140	400179	558774	269026
Methyprylon	183.1259	1.107 HILICneg	374921	702489	467763	636557	636013	425834	336303	354238	400096	709106
TG(12:0/12:0/12:0)	620.5404	27.465 Rppos	8267821	9190843	1.06E+07	7805837	1.81E+07	3.63E+07	2.22E+07	2.43E+07	2.87E+07	2.54E+07
Methyprylon	183.1262	9.048999 Rpneg	21804	58850	31493	31377	24772	32766	32812	25319	55957	47379
Metipranolol	309.1942	9.065001 Rpneg	25533	34435	31593	30920	26181	31687	31487	31425	36125	35560
Metoprolol	327.2048	10.045 Rpneg	5276	5363	5536	5484	4368	5946	5229	5882	5561	6414
Metyrapol	502.2592	1.255 HILICneg	49302	73780	36580	49975	36337	1	24294	33582	1	22917
Metyrosine	195.0898	10.916 Rpneg	3326	4994	4705	2926	3954	8228	1819	5837	5301	2590
MG(0:0/15:0/0:0)	316.2614	11.433 Rpneg	23386	18598	19667	15779	24843	17020	16391	26840	18800	17094
MG(0:0/15:0/0:0) Esi-11.264	316.2611	11.264 Rpneg	12588	9443	11011	9335	12780	8828	9314	12697	10039	10303
MG(0:0/18:0/0:0)	358.3082	16.672 Rpos	4222873	2265835	7472256	3265225	1871898	5547679	2594932	6995753	5079518	4427876
MG(0:0/18:0/0:0) Esi+16.675999	358.3082	16.676 Rpos	4372263	2270525	7447431	73123	283990	649314	2548897	6973600	5104025	4409596
MG(16:0/0:0/0:0)[rac]	312.2664	27.25 Rpos	592012	708753	831941	819208	1040654	2015089	1450165	1562557	1433338	1532345
MG(16:0/0:0/0:0)[rac] Esi+13.864	330.2765	13.864 Rpos	134924	181441	147276	152368	594424	285300	267015	708795	205931	225582
MG(16:0/0:0/0:0)[rac] Esi+14.309	330.2768	14.309 Rpos	1143260	599008	1525324	957795	784489	1604397	1378506	1693055	1377204	2321236
MG(16:0/0:0/0:0)[rac] Esi+25.476	312.2656	25.476 Rpos	208310	231134	381063	263790	310581	447334	527190	431432	276675	453972
MG(18:0e/0:0/0:0)	344.329	14.814 Rpneg	1	2114	3146	4483	5947	4011	3936	7173	4041	4275
MG(18:1(11E)/0:0/0:0)[rac]	338.2826	27.357 Rpos	677651	839867	1019989	829511	1512125	3002479	1955867	2153633	2273305	2180266
MG(18:1(11E)/0:0/0:0)[rac] Esi+25.617	338.283	25.617 Rpos	119940	162284	244465	243486	319363	475690	378903	405314	424004	453010
MG(20:0/0:0/0:0)	386.3391	11.889 Rpneg	4894	4347	1	2423	1151	1634	4642	3114	2290	2381
MG(22:1(13Z)/0:0/0:0)	412.3525	12.384 Rpneg	6350	3029	3043	3785	2280	1793	2563	2116	2734	1714
MG(22:1(13Z)/0:0/0:0)	412.3544	1.107 HILICneg	1	32028	15443	41751	56011	1	106954	83967	1	72018
MG(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/0:0/0:0)	402.2787	12.568 Rpos	1278605	1526801	1441916	1489242	537842	508664	635455	570442	337807	214003
MG(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/0:0/0:0)	402.2764	13.452 Rpneg	133455	153823	116607	161152	1	1	1	1	1	1
MG(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/0:0/0:0) Esi-13.455001	402.2766	13.455 Rpneg	129140	144067	106720	151183	79996	59108	36794	27735	1	1
MG(24:0/0:0/0:0)	424.3912	16.512 Rpos	4339298	5116315	4722930	5010471	3238153	3376648	3387693	3748448	5163937	4016202
MG(24:1(15Z)/0:0/0:0)	440.3839	13.671 Rpneg	69848	18872	18933	22347	6383	16209	15553	10451	15522	1824
MG(24:1(15Z)/0:0/0:0) Esi-13.448999	440.385	13.449 Rpneg	31992	12867	13143	14081	8186	10355	8734	6556	9130	5048
MGDG(16:0/18:2(9Z,12Z))	754.5628	0.923 HILICneg	254715	344768	253143	325812	176390	1	183382	157503	192135	166102
MGDG(18:2(9Z,12Z)/18:2(9Z,12Z))	795.5832	1.525 HILICpos	8507777	12425500	10055000	9798807	4410499	7329727		8675613	7581644	6510089
MGDG(18:2(9Z,12Z)/18:3(9Z,12Z,15Z))	775.5578	24.197 Rppos	1781318	1375985	1879452	1195284	1393752	1913825	1564850	1520711	1273729	1172244
Mintsulfide	236.1614	5.965 Rppos	213038	404510	288507	362265	368913	416380	382180	390248	415190	362742
Momordin IIa	922.4885	22.916 Rppos	1078108	1031993	896166	965188	2780922	1155461	1074474	1412201	2315321	1401800
Momordin IIa Esi+22.19	922.4867	22.19 Rppos	601810	939840	631950	360126	1787907	2446548	1848562	2049160	2366962	1999142
Momordin IIa Esi+23.102999	939.5155	23.103 Rppos	689021	539103	433280	635485	630635	550280	575098	580177	541752	569119
Momordol	500.37	13.032 Rpneg	98847	25263	36171	33255	28715	10693	20548	16110	22131	11013
Momordol Esi-12.989	486.3502	12.989 Rpneg	33014	17227	19476	18604	17109	8668	16238	11657	17724	9424
Momordol Esi-13.0	440.3486	13 Rpneg	124006	39727	43607	46815	38400	16721	29833	24790	36768	19006
Monomenthyl succinate	238.1567	7.301 Rppos	671724	845904	404399	564034	480921	379882	375073	441541	540432	647415
Montecristin	574.496	12.557 Rpneg	2511	1248	1	955	1117	783	795	952	832	1
Mosin C	654.4686	13.239 Rpneg	48922	12290	9946	10193	8026	7463	8279	6430	7191	2597
Mosin C Esi-13.189001	640.4524	13.189 Rpneg	12669	2811	2506	3225	1563	1	1692	999	1462	1
Mosin C Esi-13.239	654.4709	13.239 Rpneg	49339	12457	9898	10435	8324	7961	8416	6188	7509	2817
Mosin C Esi-13.5910015	594.4436	13.591 Rpneg	5302	1052	1676	2662	4351	1530	3771	1	1617	2229
m-Trifluoromethylhippuric acid	307.0661	5.298 HILICneg	682241	1699037	1530387	1703727	1313227	891364	1104172	1053952	902626	885909
Mucocin	698.4945	12.836 Rpneg	6841	1813	4003	2488	2423	892	1589	1677	1522	1
Muconin	682.5066	13.275 Rpneg	26487	10529	9512	8871	6830	1	8516	6166	1	1
Muricatenol	590.4927	27.21 Rppos	1231586	1067493	1274941	1511947	1436686	2387693	1981664	1884929	1641753	2069825
Muricatenol Esi+22.847	590.4912	22.847 Rppos	337017	611681	375030	428765	495325	328841	320636	428577	658667	415873
Muricatenol Esi+23.58	612.4708	23.58 Rppos	486336	447380	388009	375638	490632	804765	566282	562068	902572	777678
Muridienin 2	588.5141	12.79 Rpneg	31148	26188	23580	22839	27180	26745	24578	23467	21644	22318
Musabalbisiane B	498.1762	1.543 HILICneg	221520	198933	1	56347	246696	39118	71010	81509	84641	1
MY-5445	331.0858	1.042 Rpneg	7226	4182	4089	4611	27306	23526	29373	4378	6404	4904
Mycocerosic acid (C26)	396.3963	14.081 Rpneg	118710	44915	27731	41716	49597	32197	42878	39705	35651	22208
Mycocerosic acid (C26)	809.8107	24.916 Rppos	43306200	41092364	45380424	45881772	40684392	41529576	44742724	43489352	42431164	43425664
Myristoleyl linoleate	534.462	12.774 Rpneg	31063	25205	20324	22184	22255	22899	20255	22920	20415	19130
myristoyl acyl carnitine	371.3035	9.686999 Rppos	479715	494372	666010	634980	828589	589690	398230	468206	541614	607747
Myrsinone	294.1834	10.129 Rpneg	73199	72878	76365	78284	69295	75165	77322	81510	78468	80629
Myrsinone Esi-12.082	294.1805	12.082 Rpneg	13203	9611	6152	10198	6608	4581	7870	1	9050	7719
Myrtucommulone A	714.3579	12.354 Rpneg	48994	1560	873	912	809	1	961	748	1489	1
Myxochelin B	449.1815	11.881 Rpneg	2966	4308	1539	1628	1	2915	3555	2049	1695	2574
N-(1-Deoxy-1-fructosyl)valine	261.1223	1.394 Rpos	3300733	3745808	5711182	3639625	4115289	3436328	5094063	4153299	2229345	2940522
N-(2'-(4-benzenesulfonamide)-ethyl) arachidonoyl amine	486.2887	12.763 Rpneg	3304033	3379154	2922525	3417133	3296735	2240315	3654713	3077645	4547714	3555457
N-(2'-(4-benzenesulfonamide)-ethyl) arachidonoyl amine	486.291	0.806 HILICpos	449404	559852	453444	697677	916413	501690		480113	589733	807494
N-(3-(15-methyl-hexadecanoyloxy)-13-methyl-tetradecanoy	607.5212	23.563 Rpos	629602	567242	594190	454872	592621	1095076	798356	863947	1245224	917548
N-(3-(hexadecanoyloxy)-heptadecanoyl)-L-ornithine	660.5413	26.726 Rpos	1346783	1376444	1129309	1141247	904757	1084600	955025	803487	1251368	1027965
N-(3S-hydroxy-butanoyl)-homoserine lactone	187.085	5.832 HILICneg	190348	252668	242197	244492	85847	62071	127715	132170	66088	107346
N-(3S-hydroxy-butanoyl)-homoserine lactone Esi-5.4539995	187.0853	5.454 HILICneg	107883	139789	110097	132327	45511	33455	63125	63573	33896	54557
N-(3S-hydroxydecanoyl)-L-serine	275.1736	5.606 HILICpos	1180021	627140	226933	233412	348588	885614		542000	946007	538287
N-(3S-hydroxydecanoyl)-L-serine Esi+6.381	275.1736	6.381 HILICpos	924026	87511	22435	1	99491	560584		405758	702386	146100
N(alpha)-gamma-L-Glutamylhistamine	240.1225	1.259 Rpneg	19254	16834	16952	14622	17213	16252	30607	12204	13069	14802
N-(Heptan-4-yl)benzo[d][1,3]dioxole-5-carboxamide	543.3328	11.766 Rpos	392958	262828	269484	259467	179650	265724	231186	228375	210675	189903
N-(naphthalen-1-yl)benzamide	229.0884	0.927 Rpos	259299	181977	340434	266327	374962	349284	314194	297420	330635	284378
N-(tetradecanoyl)-sphing-4-enine-1-(2-aminoethylphosphon	616.4991	0.921 HILICneg	709872	1222260	1216887	1267597	985854	262430	980767	1028598	688651	1028893
N,2,3-Trimethyl-2-(1-methylethyl)butanamide	171.1619	8.076999 Rppos	195285	421969	435019	515946	337628	406396	323797	347868	527130	424069
N,N-Didemethylchlorpromazine	290.0625	1.461 Rpneg	17333	13663	14627	14439	6490	17167	1	8703	16483	1
N,N-Didemethylchlorpromazine Esi-1.8419998	290.063	1.842 Rpneg	6724	6229	5795	6781	5413	5212	4118	5986	6049	5739
N,N-Dimethylethanolamine N-oxide	105.0791	6.045 HILICpos	1355078	1178133	1136749	689773	2393212	1240338		1321742	1145167	2105671
N,O-Didesmethylverapamil	912.5296	4.679 HILICneg	77743	70165	80442	67091	74390	62580	85368	74651	81984	84653

N?,N?,N?-Trimethyllysine	188.1523	0.797 Rppos	358219	331253	314695	287598	371786	338913	339225	411349	462135	389690
N-[(4-Hydroxy-3-methoxyphenyl)methyl]octanamide	279.1831	8.773001 Rpneg	4441	4488	5375	4635	3981	5755	5485	5106	4430	5626
N1,N12-Diacetylspermine	308.2194	1.176 HILICpos	334046	565842	81856	309345	471543	1		129159	295077	329117
N17-Dimethylindole-3-carboxaldehyde	196.0736	5.492 Rppos	1	256175	31449	242873	422098	31268	21615	199754	459105	145346
N5-(4-Methoxybenzyl)glutamine	266.1243	9.044999 Rpneg	5125	13758	6568	7266	7114	7308	6990	5765	12589	10671
N6-(1,2-dicarboxyethyl)-AMP	463.0722	0.695 Rpneg	13385	4541	4760	1818	2333	1487	9280	1632	1239	1804
N6,N6-Dimethyladenosine	590.2554	22.923 Rppos	543755	541156	475029	493666	1052559	441377	1031928	544991	939194	934850
N-Acetyl-alpha-D-glucosamine 1-phosphate	347.0625	0.892 Rpneg	1032	1784	2886	1549	1487	1	6299	1	1	1166
N-Acetyl-DL-methionine	191.0615	2.546 Rpneg	31269	26088	34600	38320	24096	31622	30091	25436	30457	31937
N-Acetyl-DL-methionine	191.0617	5.689 HILICneg	34826	55044	43075	59979	47581	43150	48699	38252	39658	37745
n-acetyldopamine	199.0617	0.84 Rppos	563729	637218	582052	509387	621894	539447	649177	605332	650493	670121
N-Acetyl-L-phenylalanyl-L-diiodotyrosine	681.964	0.983 Rpneg	9558	7772	6509	7490	6738	5798	5220	6275	5969	6423
N-Acetylprimaquine	347.1851	0.89 HILICneg	57294	46866	25365	36458	112235	1	40212	29340	45349	56399
N-Acetylprocainamide	294.2045	1.256 HILICpos	270131	296403	164392	188136	324097	217074		208968	187154	180804
Nadolol	309.1937	9.656999 Rpneg	5829	5942	5784	5798	5392	6507	6455	6247	6108	6869
Nadolol Esi-9.386001	309.1931	9.386001 Rpneg	4103	1	4550	4957	4719	4756	4935	5262	5230	5000
Nandrolone phenpropionate	428.2333	6.973 HILICpos	1322387	864577	925061	1206938	906336	865140		948008	881085	1353968
Naphthyl dipeptide	478.2604	1.252 HILICneg	1	182757	87395	99605	146898	1	71376	57271	1	31456
N-arachidonoyl dihydroxypropylamine	359.2854	15.96 Rppos	580298	481692	599067	342002	57349	246987	204859	129754	122621	88296
N-arachidonoyl taurine	411.2421	0.787 HILICneg	32408	27561	27788	36262	62739	50097	51330	45936	47372	52594
N-Caffeoyltryptophan	370.0945	12.929 Rppos	451708	439735	422160	431303	459478	446176	448089	484072	461270	552103
N-Deacetylketoconazole	488.1407	5.189 HILICneg	980058	3017258	2353787	3045650	2048367	1806285	1993483	1845765	1544076	1305860
N-Desmethylmifepristone (RU 42633)	847.5319	23.247 Rppos	1077236	1434558	1062284	1026877	1515349	1458737	1331338	1748977	1461578	1432543
N-docosahexaenoyl GABA	872.5957	4.869 HILICneg	1649483	1754352	1926979	1971833	1789659	1390182	1974499	1968436	1852885	1132350
N-docosanoyl taurine	447.3423	13.473 Rpneg	23272	18154	16223	21663	21891	14476	21048	21033	19187	22652
Nebramycin factor 4	572.2643	11.924 Rpneg	4526	1086	5558	4454	6753	2506	3328	3995	4657	4015
Necatorine	264.0523	3.295 HILICneg	44804	69804	59246	68350	60490	45315	55843	61495	41977	34065
Neoannonin B	652.4846	1.054 HILICneg	282236	269085	213894	230666	318581	356592	267293	295045	1	1
Neoreticulatacin A	609.5334	0.896 HILICpos	1	878766	804262	1	1184399	686407		635981	1032440	805351
Neosakuranin	448.1409	13.277 Rpneg	44258	30043	40611	33364	22169	23804	33070	22101	30743	29533
Neryl glucoside	316.1884	8.175001 Rpneg	77939	64775	43564	72650	95911	57942	44252	60514	88308	54246
Neryl glucoside Esi-7.882001	316.1884	7.882001 Rpneg	4282	5254	2644	1665	7086	2315	3062	3286	6393	4632
Neryl glucoside Esi-8.89	316.1879	8.89 Rpneg	1	1	1826	5885	8409	1544	3067	4610	4654	4376
Netilmicin	475.2994	5.760001 Rppos	445127	863632	437048	804385	1144468	502513	440009	827327	1166503	693765
Netilmicin	475.3017	1.725 HILICpos	449103	824159	342293	606968	797070	1066408		876552	668551	574692
N-Gluconyl ethanolamine	299.1191	0.907 Rpneg	3508	2786	4228	3414	3296	4036	3667	4050	5753	4309
N-Histidyl-2-Aminonaphthalene (?NA)	280.1348	9.64 Rpneg	38626	3153	17442	191954	273896	12571	10087	63984	125770	87608
N-Histidyl-2-Aminonaphthalene (?NA) Esi-10.058999	280.1352	10.059 Rpneg	15545	1	6123	46579	88664	3818	2934	17562	35493	23968
N-Histidyl-2-Aminonaphthalene (?NA) Esi-10.326	280.1355	10.326 Rpneg	1	1	9742	63769	132168	5027	4547	23322	49019	31079
N-Histidyl-2-Aminonaphthalene (?NA) Esi-11.302001	280.135	11.302 Rpneg	96677	1	31016	77729	252861	19413	22205	52366	78169	45492
N-Histidyl-2-Aminonaphthalene (?NA) Esi-9.641999	280.1348	9.641999 Rpneg	9744	924	17442	191602	68457	10085	10087	63984	126225	87608
N-Histidyl-2-Aminonaphthalene (?NA) Esi-9.874	280.1348	9.874 Rpneg	11328	1	5307	42947	76767	3034	2405	15572	29891	21034
N-Hydroxypentobarbital	242.1272	5.33 Rpneg	52204	36249	57825	47309	35973	31930	82059	42605	16333	32107
N-Hydroxypentobarbital Esi-4.7200003	242.1262	4.72 Rpneg	15618	11666	23494	15354	14494	15885	38257	20362	9065	12725
N-Hydroxypentobarbital Esi-5.051	260.1306	5.051 Rpneg	4227	9787	1	9615	13017	1890	1	11056	15559	9006
N-Hydroxypentobarbital Esi-5.4679995	242.1256	5.468 Rpneg	3710	5779	5462	4172	4915	5855	8867	5464	4960	7242
Niacinamide	122.0487	1.608 HILICpos	14352060	16539464	16220634	15140093	16880908	18748344		17552938	18904424	17800556
Nilutamide	317.0624	9.048001 Rpneg	3669	8719	4248	3591	3985	4463	3906	2679	5317	3831
Nitroglycerine	227.0044	1.494 HILICneg	75120	68356	55760	64344	44872	27059	59792	35835	87412	65775
Nitrotyrosine	272.0634	0.702 Rpneg	17028	9311	16275	13758	12418	14703	20569	12994	10627	12197
NKH477	555.3043	13.233 Rpneg	3351	1975	1599	1	2974	2736	3337	2349	3103	2540
N-Lactoyl ethanolamine	133.0739	0.915 Rppos	1025360	1257105	985972	1028892	1089836	926375	834545	1043209	997118	1077648
N-linolenoyl-glutamine	452.2901	11.824 Rpneg	1	1	1	1	888	1058	1	2876	1878	1951
N-linoleoyl taurine	387.2446	12.509 Rpneg	19227	16480	20449	19085	72351	57830	83458	96148	74756	100189
N-linoleoyl taurine Esi-12.509001	387.2437	12.509 Rpneg	23434	22300	1	23614	87856	69702	100444	116744	90826	121872
N-Methyl-1-deoxynojirimycin	223.1064	0.923 Rpneg	4731	1148	5362	6510	2527	10121	3891	11336	2454	4340
N-Methyl-L-alanine	103.0632	0.806 Rpneg	26000	31951	35545	37167	28723	32911	47299	39744	29966	32395
n-Methylnicotinamide	136.0635	6.376 HILICpos	1517606	1596188	1374979	1963837	1594404	1318984		1694789	3943648	1034936
N-methylundec-10-enamide	243.1838	8.968001 Rpneg	137144	166342	160491	216142	130078	109742	105111	111822	129014	109414
N-methylundec-10-enamide	243.184	3.32 HILICneg	2957756	154618	76318	234242	260582	575942	187566	122942	2907024	142116
N-methylundec-10-enamide Esi-14.003999	243.1836	14.004 Rpneg	40155	1295	14075	12820	1	14049	1052	3209	1	1
N'-Nitrosoanabasine	237.1134	10.129 Rpneg	8774	9499	9196	9013	8694	9315	9371	9906	9992	9425
N-Nitrosoguvacine	138.0431	1.185 Rppos	232914	1099401	59566	966887	2419070	156454	128459	1324986	2052915	1026160
Nocodazole	301.0499	4.126 HILICneg	197704	259126	212090	233397	176030	143039	174240	114534	139938	206902
Nocodazole Esi-4.126	301.0494	4.126 HILICneg	134802	226494	166582	166111	157896	128876	153465	123902	128902	182394
N-oleoyl glutamic acid	411.2988	11.99 Rpneg	1	1	1	1	1554	1519	1892	2407	2220	2507
N-oleoyl glutamic acid	411.3005	3.001 HILICpos	1150104	482671	341480	300154	283650	336251		407618	408513	634717
N-oleoyl glutamine	410.3156	4.733 HILICneg	19505	25630	25063	20362	57605	72914	57465	73800	137754	96764
N-oleoyl glutamine	410.3128	12.684 Rpneg	15140	14013	15398	19353	19898	28533	25220	32520	53092	43944
N-oleoyl glutamine Esi-12.683999	410.3113	12.684 Rpneg	8894	9466	10353	12141	16664	23695	19248	25219	45160	34854
N-oleoyl leucine	395.3367	13.056 Rpneg	1	5321	1	3419	4684	2882	3982	5874	6594	4449
N-oleoyl taurine	389.26	12.749 Rpneg	20700	13541	13375	14343	68425	63172	68368	96824	74039	88684
N-oleoyl taurine	389.2608	0.796 HILICneg	1	108968	238037	181841	1799063	552203	1520273	1483908	1718755	1871829
N-Oleoyl-L-Serine	369.2861	8.878999 Rppos	92472	154248	208482	196687	484352	294945	191583	211634	206711	290701
N-Oleoyl-L-Serine	369.2893	2.15 HILICpos	1876750	797931	719435	508236	715044	734136		452710	623448	947986
Nonacosanoic acid	438.4415	14.797 Rpneg	14411	2692	1188	2789	2744	1200	1669	3267	1	1
Norvisnagin	216.0413	0.865 Rpneg	6601	10060	12985	15785	9536	22627	16504	17628	9366	16904
N-palmitoyl alanine	327.2768	12.741 Rpneg	4046	1760	1945	2943	1	1248	1	1	1	1986
N-palmitoyl glutamic acid	385.2849	3.101 HILICpos	1620371	556393	383970	288046	351076	464750		411815	545129	701770
N-palmitoyl glutamine	384.2974	12.584 Rpneg	10387	10810	10141	14279	18099	22578	20903	28771	51750	38902
N-Palmitoyl Glycine	313.2624	12.714 Rpneg	19550	5841	1	13679	18621	15369	15315	17224	12358	7567
N-palmitoyl leucine	369.3235	13.006 Rpneg	1	23745	34304	47551	1	21719	25828	20035	23308	22052
N-palmitoyl serine	325.2625	10.918 Rppos	249830	273169	315494	307324	288664	311004	332346	330107	341269	331087
N-palmitoyl serine	343.2666	2.269 HILICpos	964497	383769	366249	304424	322163	284346		180291	390427	332649
N-palmitoyl serine	343.2737	12.651 Rpneg	13927	11083	8998	12145	10848	4640	10031	11123	12446	8376
N-palmitoyl taurine	363.244	12.683 Rpneg	29691	14659	11649	17846	55117	51349	66875	68272	67939	72889
N-palmitoyl taurine	363.2456	0.819 HILICneg	390103	1025288	741449	793842	392347	440173	400925	418432	869909	1080905
N-palmitoyl tyrosine	419.3076	13.281 Rpneg	5707	4331	4045	5062	7310	5688	8106	8164	8309	9314
N-palmitoyl tyrosine	419.305	0.783 HILICneg	1	42859	35196	38611	79322	42834	69119	69918	71723	74672
N-pentadecanoyl-L-Homoserine lactone	342.2879	4.876999 HILICpos	920327	786328	405445	719303	903042	530849		590940	1280490	414774
N-pentadecanoyl-L-Homoserine lactone Esi+5.5439997	342.2879	5.544 HILICpos	1291022	1347263	1275664	1021768	1077074	1310228		1273354	1324472	1263319
N-stearoyl glutamic acid	413.3141	9.107001 Rppos	346383	472961	702777	436231	1043788	793107	749331	1107168	545799	947559

N-stearoyl glutamic acid	413.3141	2.893 HILICpos	1925434	767727	511681	400170	522521	711735		684400	922626	990950
N-stearoyl glutamic acid Esi+9.235	395.3053	9.235 Rppos	69925	178305	262982	247473	565283	306437	239505	327001	285266	415811
N-stearoyl glutamic acid Esi+9.265	413.3136	9.265 Rppos	253493	243446	368151	222564	514329	524071	537989	653654	452971	597968
N-stearoyl glutamine	412.3298	12.964 Rpneg	1	1736	2170	1	5087	4037	4753	6198	11046	8136
N-stearoyl proline	398.3477	12.426 Rppos	176486	207488	155441	153880	163894	156689	159381	189992	167362	121821
N-stearoyl taurine	391.2762	0.794 HILICneg	200948	153220	204190	195002	853786	330770	814638	757179	780881	864178
N-stearoyl taurine	391.2754	13.03 Rpneg	44805	30141	33432	36430	112136	80845	130117	134737	127845	142171
N-stearoyl tyrosine	447.3375	0.782 HILICneg	60298	49378	63034	52378	67574	31345	72843	69212	65062	69385
N-Succinyl-2-amino-6-oxopimelate	289.0779	5.125 Rpneg	5117	4128	6110	5241	2656	5203	4587	5291	3350	5224
N-tryptophanyl-35-aminobacteriohopane-32,33,34-triol	735.5357	21.986 Rppos	6205981	6612759	6834950	7374022	4906792	4948913	6333318	5168416	5517204	5643162
N-tryptophanyl-35-aminobacteriohopane-32,33,34-triol	777.5634	1.548 HILICneg	134996	156776	121358	129396	239744	163572	159941	235395	149420	170382
NU 7026	444.1438	9.363999 Rpneg	3089	1508	1093	1104	2000	1845	1086	1041	841	1
nuatigenin 3-beta-D-glucopyranoside	652.3875	13.452 Rpneg	26651	4642	2208	4592	5074	2917	4691	6398	5158	5258
N-Undecylbenzenesulfonic acid	312.1768	12.218 Rpneg	160707	104902	517739	110010	112483	68698	86689	99917	96847	73324
N-Undecylbenzenesulfonic acid Esi-12.218001	312.1769	12.218 Rpneg	160707	104902	517719	110010	112483	68698	86689	99917	96507	73324
Oceanalin A	736.5225	14.381 Rpneg	12782	19626	11718	15685	6262	1	1	1	8946	16272
o-Chloroacetanilide	169.028	0.926 Rpneg	21904	24250	27732	21064	22240	18797	32832	18446	15911	19730
Octadecanoic acid-1,2,2,2-tetrafluoro-1-(trifluoromethyl)et	452.2516	11.061 Rpneg	3381	2981	1	2024	2562	3896	2239	2203	4027	3747
Octadecyl fumarate	414.298	13.52 Rpneg	21496	24681	23291	25584	34161	25684	44403	48513	34374	32652
Octadecyl fumarate Esi-11.257001	414.2972	11.257 Rpneg	7755	3699	3040	3769	4728	3355	4238	3808	4090	3171
Octadecyl fumarate Esi-12.600999	386.2992	12.601 Rpneg	1	9873	17112	31391	26563	16089	18721	29890	22863	22339
Octadecyl fumarate Esi-12.703001	368.2892	12.703 Rpneg	1	19266	14940	24484	54412	1	19022	28927	35511	38044
Octamethyltrisiloxane	296.1299	9.882001 Rpneg	6313	2300	3434	12618	19373	2092	1699	5684	9122	5768
octanoic acid	144.1146	1.405 HILICneg	213870	104285	78969	103135	177038	41289	74309	127592	132421	116901
octanoic acid	144.115	9.068 Rpneg	20810	19662	15857	19912	22829	13595	12228	18355	24469	18067
Octanoyl-CoA Esi+0.769	910.2488	0.769 HILICpos	2014948	6482913	11648660	6299730	1	11477759		10926458	10493834	4565044
Octinoxate	272.1778	9.169 Rppos	156917	208655	232635	256857	211513	230417	255989	264210	268990	233771
Octulose-1,8-bisphosphate	400.0167	0.768 Rpneg	117859	75539	106406	88842	23396	81860	57475	62056	35105	47642
Octulose-1,8-bisphosphate Esi-0.7670001	446.0221	0.767 Rpneg	6641	18792	29222	13947	12472	13452	18142	5452	4489	6111
Octylamine	129.1516	2.309 HILICpos	824808	1027510	877669	1701803	2589965	848984		1120381	1660763	1850698
O-Desmethylverapamil	440.2671	12.545 Rpneg	1352	2987	1	1822	1244	1	1516	1014	1533	1410
TG(12:0/17:1/22:0)	862.7802	0.918 HILICpos	6994600	1	1	1	7319532	9721980		9822085	9722177	9050120
OH-Diaponeurosporene glucoside ester	642.4152	13.708 Rpneg	18380	10478	10585	17552	8472	6885	13726	11183	12532	11379
Oleanolic acid 3-[rhamnosyl-(1-4)-glucosyl-(1-6)-glucoside]	926.5237	13.363 Rpneg	5434	1394	4337	6623	821	1	904	1	1	814
Oleoyl Ethanolamide	325.2976	13.724 Rpneg	11643	7518	8971	7586	7059	6120	9758	6114	8938	8459
Oleoyl Ethanolamide	714.6123	0.949 HILICneg	784727	1187740	1073969	1230277	1036170	1	1413579	1191744	1684965	1649571
o-Methoxyhydrocinnamic acid	162.0682	7.29 Rppos	232755	537420	571389	582996	478005	590860	441579	423116	604467	396922
Orotidine	576.1197	6.370999 HILICneg	128214	189181	169644	180606	181742	152790	149362	171819	144930	160503
Orphenadrine N-oxide	285.1696	13.12 Rpneg	1	1	1	1	3922	1	4923	4739	4864	4400
Oscillol diglycoside/ Oacillol bisglycoside/ (Oscillaxanthin)	941.5478	25.074 Rppos	594402	551857	377464	485846	283635	317639	375376	350827	320807	358255
Ovatine	385.2613	13.415 Rpneg	5574	3642	5664	6948	2645	2389	3216	2287	3152	3338
Oxaloglutarate	204.0285	7.741 Rpneg	8630	4678	4434	4982	2942	4185	3952	3951	2592	3196
Oxamate	224.0289	9.565001 HILICneg	54545	22722	37785	37031	45844	52825	40917	66317	64275	38718
Oxfendazole	315.0645	9.048999 Rpneg	8297	20203	9279	7973	8961	10241	8304	5749	11713	8660
Oxprenolol	265.1687	13.038 Rpneg	4081	8282	5938	6769	10148	9182	6228	9721	7254	6232
Oxprenolol	576.3373	1.202 HILICneg	107904	379190	251588	308352	329297	58908	247897	230128	222488	288138
PA(12:0/12:0)	582.3596	1.176 HILICneg	69339	101704	83062	83559	175838	1	64142	51851	42856	69466
PA(12:0/20:0)	630.4698	25.482 Rppos	418301	432482	467115	410862	521367	611312	553756	587012	366751	539476
PA(12:0/20:0)	648.4721	13.459 Rpneg	16061	24421	13821	12364	24326	34016	16738	26940	20356	16362
PA(14:0/18:3(9Z,12Z,15Z))	642.4359	12.451 Rpneg	1	4127	5695	5585	4507	1219	2774	2612	2629	909
PA(15:0/19:1(9Z))	674.4888	14.375 Rpneg	59273	26762	30455	23906	24829	18720	26420	35766	4998	20753
PA(15:0/19:1(9Z)) Esi-13.045375	674.4881	13.04538 Rpneg	1	6886	2766	1	8019	10128	10642	6502	8201	1484
PA(16:0/20:2(11Z,14Z))	718.5157	12.686 Rpneg	3680	3903	2018	2934	4760	3651	9836	3156	6733	6061
PA(16:1(9Z)/18:3(9Z,12Z,15Z))	668.4427	1.078 HILICneg	2396723	1392063	752764	1205862	7899237	94139	1101476	2677708	2072834	3088737
PA(17:0/17:2(9Z,12Z))	672.4722	14.04 Rpneg	11199	5193	5634	5908	8509	7950	9424	10430	6277	10230
PA(17:1(9Z)/17:2(9Z,12Z))	670.457	1.076 HILICneg	4950323	2346763	1502005	2118391	1.09E+07	1041421	970791	2625947	1933995	3007677
PA(18:0/18:3(9Z,12Z,15Z))	698.4843	14.063 Rpneg	5811	2702	2968	2893	5644	5104	6887	10581	3915	7751
PA(18:2(9Z,12Z)/0:0)	434.2434	13.239 Rpneg	9545	6986	7233	7565	6330	6789	8133	7732	9982	8305
PA(18:2(9Z,12Z)/0:0) Esi-13.337999	434.2426	13.338 Rpneg	8556	6373	6018	6119	5387	5590	6652	5873	6217	6447
PA(18:3(9Z,12Z,15Z)/20:1(11Z))	724.5028	12.995 Rpneg	1	6810	7885	1	30059	1496	25544	28620	17733	18412
PA(18:3(9Z,12Z,15Z)/20:1(11Z)) Esi-12.542	724.5033	12.542 Rpneg	1	7008	1	29901	19120	20821	20968	1	6797	20426
PA(18:3(9Z,12Z,15Z)/20:1(11Z)) Esi-12.542 :1	724.5042	12.542 Rpneg	1	7117	1	1453	2825	33032	15547	35659	1402	30811
PA(18:3(9Z,12Z,15Z)/20:1(11Z)) Esi-12.682	724.5039	12.682 Rpneg	1	4491	1	1	6338	2050	11846	13203	4573	1
PA(18:3(9Z,12Z,15Z)/20:1(11Z)) Esi-13.011001	724.5027	13.011 Rpneg	15729	12959	8173	1	23628	1	19154	15254	13245	5720
PA(18:3(9Z,12Z,15Z)/20:1(11Z)) Esi-13.071	724.5037	13.071 Rpneg	6252	7057	8749	6277	1	24007	18688	13693	13842	6728
PA(18:4(6Z,9Z,12Z,15Z)/20:5(5Z,8Z,11Z,14Z,17Z))	714.4329	1.069 HILICneg	4377551	5231203	1224219	3055031	6548537	1	534460	1254618	522023	753358
PA(20:4(5Z,8Z,11Z,14Z)/0:0)	458.2432	13.209 Rpneg	6216	5671	5508	6249	3725	2599	5257	3634	3679	3902
PA(21:0/0:0)	479.3383	13.94 Rppos	294343	322145	359786	399898	367088	507003	345862	402624	456378	334882
PA(21:0/13:0)	658.5063	27.929 Rppos	1	1	267214	1	387984	588980	427741	478183	416744	433342
PA(22:2(13Z,16Z)/0:0)	490.3096	8.214999 Rpneg	8943	8634	8836	9496	7235	7605	7777	9544	8959	9347
PA(22:2(13Z,16Z)/22:0)	794.6157	24.319 Rppos	53050288	20316632	26078754	33149116	51257976	47165844	44345304	41349676	41118920	27834568
PA(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/13:0)	678.4237	24.286 Rppos	3038269	3904143	3201608	3268474	3306551	3408741	3126536	3368317	3769761	3749802
PA(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/19:0)	762.515	1.117 HILICneg	1671717	1079029	1306054	1727493	999213	588830	1449627	1792334	1063008	1277323
PA(O-16:0/14:0)	606.461	12.609 Rpneg	6280	5704	5493	5566	7314	6657	8041	7954	8047	9009
PA(O-20:0/0:0)	512.3465	0.781 HILICneg	83409	42489	44495	60697	62434	20659	78278	96773	50164	50727
PA(P-16:0/0:0)	440.2547	13.451 Rpneg	3156	3548	2791	4503	1	1	1133	1109	1	1
PA(P-16:0/18:3(9Z,12Z,15Z))	654.4616	12.606 Rpneg	15455	11133	10963	11738	5611	4231	6566	8031	7548	6438
PA(P-16:0/20:5(5Z,8Z,11Z,14Z,17Z))	678.4618	12.598 Rpneg	21034	17204	12484	19544	6600	4360	7280	11998	7179	6155
PA(P-18:0/14:1(9Z))	630.4622	12.601 Rpneg	13727	11880	10021	11954	10950	8451	11788	12810	11059	11036
PA(P-18:0/18:3(9Z,12Z,15Z))	682.4927	12.715 Rpneg	4656	3413	1710	3497	756	1	852	1065	1	1
PA(P-20:0/22:0)	772.6337	5.229 HILICpos	1364272	1263753	1411378	946164	1388628	1483981		1582898	1873500	1521711
palmitoylcarnitine	399.3345	1.992 HILICpos	7230577	2968855	3019466	2503980	3126187	2491978		2234778	3038211	2538315
Palmitoyl 3-carbacyclic Phosphatidic Acid	390.2538	13.523 Rpneg	14373	12317	10779	13823	11355	9519	11899	12449	10691	10833
palmitoyl carnitine	399.3347	11.567 Rppos	1442296	3551362	4203956	5316358	5309503	4591645	1895978	3180724	3672538	4228734
Palmitoyl dopamine	373.2996	16.803 Rppos	1	95582	51583	223112	93829	1	38214	92166	1	1
Palmitoyl-EA	299.2823	13.665 Rpneg	25884	8994	12369	11964	11885	9208	12874	9613	12255	9453
Palmityl linolenate	537.512	0.991 HILICpos	1226163	1436798	1121343	1349251	1368290	1288414		1367457	1625520	1063130
Palmityl Trifluoromethyl Ketone	368.2518	12.857 Rpneg	6507	2334	1003	2957	3696	5009	4489	5192	7020	5685
Palmityl Trifluoromethyl Ketone Esi-13.557	368.2479	13.557 Rpneg	45000	1	45046	1	60886	33682	50801	38790	34804	32697
Panaquinquecol 7	276.1753	0.707 HILICneg	130538	75416	1	103722	1	65868	71855	74917	1	30506
Panaxatriol	522.3906	13.49 Rpneg	8287	25915	4406	7809	6253	5063	6373	3054	10914	5004
Panaxydol linoleate	522.3999	1.157 HILICneg	200498	116151	101300	1	238306	1	120526	150539	1	176915

Pangamic acid	226.1575	7.426	Rppos	520153	541013	757569	805080	425893	637014	711465	795174	819139	851809		
Pantetheine	278.1337	1.195	HILICneg	76355	144430	111205	119215	146690	1	85361	1	78250	103853		
Pantothenic Acid	219.111	4.513	Rppos	2780944	2524437	3280942	3273033	1104550	1466811	2160591	2123118	962837	1613083		
Pantothenic Acid	219.1117	1.684	HILICpos	3398557	3195574	3431715	3558126	1575829	1480570		2211383	1014437	1705579		
Pantothenic Acid	219.1107	1.335	Rpneg	2200312	1811309	2360970	2141508	350735	779414	1499303	385334	1	961005		
PC(14:0/18:0)[U]	733.5617	24.661	Rppos	65629072	62591744	60469580	68731160	64457112	72689640	65337224	66784332	66845972	68464992		
PC(14:0/18:0)[U]	733.5628	1.556	HILICpos	59085912	60746144	52051872	64408680	49504864	47086776		48047656	48030608	33298464		
PC(14:0/18:0)[U] Esi+20.03	733.5625	20.03	Rppos	11596885	8120023	10149245	9212718	10862463	9502986	10776810	10213290	9101527	7963435		
PC(14:0/18:0)[U] Esi+25.048998	733.5626	25.049	Rppos	1114354	2052240	1911896	2126518	1721530	1907749	1598569	1682165	1	1697905		
PC(15:1(9Z)/20:2(11Z,14Z))	713.5917	21.611	Rppos	933451	867414	1173174	897456	514926	334454	637824	638075	888622	660602		
PC(15:1(9Z)/22:4(7Z,10Z,13Z,16Z))	775.5632	20.908	Rppos	899530	492687	467336	399159	705716	363224	823539	505903	303113	306880		
PC(16:0/14:0)[U]	705.5389	22.725	Rppos	3955655	4429503	3576782	4241364	2766070	3068982	3042341	3112271	3551378	3190418		
PC(16:0/2:0)	519.3323	11.409	Rppos	2605025	2403054	2309948	2228751	3033132	4490755	3307661	4336191	4121689	3158971		
PC(16:0/2:0) Esi+11.879999	519.3324	11.88	Rppos	3338695	3129393	3083139	2458515	3300368	5003089	4407796	4566960	4209729	3650537		
PC(16:0/20:3(8Z,11Z,14Z))[U]	765.5676	23.718	Rppos	55419112	59561200	69475440	74079184	74865392	87178392	74191056	77580160	84753760	71784280		
PC(16:0/20:4(5Z,8Z,10E,14Z)(12OH[S])) Esi+21.285997	779.5473	21.286	Rppos	705655	904049	910252	689444	889583	887876	1064805	1215065	1003229	1007967		
PC(16:0/20:4(5Z,8Z,10E,14Z)(12OH[S])) Esi+21.587002	779.5479	21.587	Rppos	5406341	5619383	4931895	5395925	3617749	4258348	4688734	3980412	4758919	4018028		
PC(16:0/22:5(7Z,10Z,13Z,16Z,19Z))	809.5895	12.6532	Rpneg	8302	18011	16156	20483	14802	31106	29958	140938	10514	29202		
PC(16:0/22:5(7Z,10Z,13Z,16Z,19Z)) Esi+22.593	789.5664	22.593	Rppos	998545	929993	1076285	958113	1532219	941441	978075	1314802	1494706	1146574		
PC(16:0/22:5(7Z,10Z,13Z,16Z,19Z)) Esi-12.540199	809.5918	12.5402	Rpneg	7802	67087	81802	19282	8997	33439	56524	105369	69230	9219		
PC(16:0/22:5(7Z,10Z,13Z,16Z,19Z)) Esi-12.813002	809.5906	12.813	Rpneg	9162	18171	16156	19156	13531	26488	3474	20643	12849	8206		
PC(16:0/P-18:0)	745.601	26.115	Rppos	2955535	2613851	3034688	3068057	3028018	3454141	2592935	2689137	2740802	2409071		
PC(17:0/14:0)[U]	719.5446	23.626	Rppos	5910694	7422667	7256302	4109526	4393864	6101268	5991438	6393681	6275938	8324942		
PC(17:0/14:0)[U] Esi+25.731998	701.5464	25.732	Rppos	900656	804295	910268	803304	540776	1093730	771348	534215	652057	780430		
PC(17:0/17:0)[U]	761.5933	27.008	Rppos	22785908	18592800	23492760	25102756	20037090	25352032	27136510	26648132	21581144	22730900		
PC(17:1(9Z)/0:0)	509.35	13.973	Rpneg	19075	8948	9506	10630	6742	5710	7893	5603	6238	4093		
PC(17:1(9Z)/20:1(11Z))	799.6152	26.45	Rppos	1316446	1738747	1598917	1097214	4431185	6543652	3762466	4830970	8438292	5852687		
PC(17:1(9Z)/20:1(11Z))	799.6013	1.534	HILICpos	5215540	6120729	5465938	5138705	5993875	6413943		6571773	7217357	6553290		
PC(17:2(9Z,12Z)/16:1(9Z))	723.5198	23.763	Rppos	19427404	21189368	20673648	20198004	19855184	26403880	23128468	22248780	26801614	23730790		
PC(17:2(9Z,12Z)/16:1(9Z)) Esi+17.584	723.5254	17.584	Rppos	3032477	2127604	2104688	1759572	2178841	1596921	685173	468923	1623484	1676233		
PC(17:2(9Z,12Z)/16:1(9Z)) Esi+17.617002	723.5246	17.617	Rppos	3081745	2108519	2216374	1713717	1	1675450	1792817	584842	1714832	1717315		
PC(17:2(9Z,12Z)/20:2(11Z,14Z))	795.5893	26.655	Rppos	1865712	1696870	2018857	2022140	1582070	1524753	1714689	1503113	1677244	1810937		
PC(18:0/20:4(5Z,8Z,10E,14Z)(12OH[S])) Esi+23.705997	807.577	23.706	Rppos	2.41E+07	2.47E+07	2.86E+07	2.59E+07	1.45E+07	1.38E+07	2.10E+07	1.61E+07	1.17E+07	1.33E+07		
PC(18:0/20:4(8Z,11Z,14Z,17Z))	791.5834	23.898	Rppos	17623472	15479859	21603872	22400672	20906622	23938072	18734278	20195984	15864770	17455884		
PC(18:1(17Z)/18:1(17Z))	767.5848	24.147	Rppos	3540609	2705806	3821516	4300237	3143807	4309885	3602268	2731495	3612486	3699847		
PC(18:1(9Z)/22:5(4Z,7Z,10Z,13Z,16Z))	815.5802	23.505	Rppos	2371609	3601051	5593770	5048694	2325371	3283708	2684018	2285256	2019456	2209863		
PC(18:2(9Z,12Z)/15:1(9Z))	743.5437	13.543	Rpneg	1	21935	20710	17307	20683	32198	27496	36445	20202	36742		
PC(18:2(9Z,12Z)/2:0)[U]	543.3323	11.346	Rppos	4614220	4676951	5619928	5582790	4126966	5928138	6656953	6340744	5242785	5071530		
PC(18:4(6Z,9Z,12Z,15Z)/17:1(9Z))	747.5201	23.397	Rppos	22354202	17092542	21971874	23477996	18614952	22053008	19732896	18196028	18458342	17841400		
PC(18:4(6Z,9Z,12Z,15Z)/19:1(9Z))	775.5522	25.381	Rppos	7505887	5531493	9805384	8840195	5170940	5960207	5876167	5225585	3990485	4873892		
PC(18:4(6Z,9Z,12Z,15Z)/19:1(9Z))	795.574	14.357	Rpneg	35412	62003	17701	14426	66658	25221	2865	18712	1	20490		
PC(18:4(9E,11E,13E,15E)/18:2(9Z,12Z))	777.5473	21.183	Rppos	1666231	1185669	1482534	1823887	125289	139855	162337	108753	92180	133533		
PC(19:0/18:4(6Z,9Z,12Z,15Z))	795.5834	23.905	Rppos	20714172	19840120	24185194	22052016	18429490	22677240	21337264	21058048	22231364	21631820		
PC(19:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z))	847.6053	25.52	Rppos	1913876	1222995	2336392	1793312	1831125	2193274	1474694	1946240	1955931	2162496		
PC(2:0/O-16:0)[U]	523.3642	5.458	HILICpos	2325840	2266155	2299571	2173005	1354073	1376075		1	1	1		
PC(2:0/O-16:0)[U] Esi+5.909	523.3654	5.909	HILICpos	827813	761070	678464	806883	561509	553120		651081	581304	389272		
PC(20:3(5Z,8Z,11Z)/20:4(5Z,8Z,11Z,14Z))	831.5759	1.517	HILICpos	20951436	20423224	33791012	30242036	24633310	20751946		26620628	18245156	16775668		
PC(20:3(8Z,11Z,14Z)/13:0)	741.539	23.457	Rppos	1762621	3873371	2582990	1425570	4046283	5682224	4455768	5343169	6564649	4312250		
PC(20:3(8Z,11Z,14Z)/22:5(7Z,10Z,13Z,16Z,19Z))	857.5907	1.517	HILICpos	2094831	850540	794141	952231	609781	565479		842764	1023713	865324		
PC(20:4(5Z,8Z,11Z,14Z)/13:0)	739.5217	22.212	Rppos	1369595	2147670	1303316	1120650	2459647	2553894	2598438	2694254	2262407	3068024		
PC(20:4(5Z,8Z,11Z,14Z)/13:0) Esi+24.130001	699.5261	24.13	Rppos	1619213	1091147	1979998	1015309	1406522	1687975	2374530	1621028	1574868	1437916		
PC(20:4(5Z,8Z,11Z,14Z)/17:2(9Z,12Z))	791.5467	24.516	Rppos	58368020	53768072	58226452	63497284	50291584	56941028	56164120	54843704	55391600	56418172		
PC(20:4(5Z,8Z,11Z,14Z)/17:2(9Z,12Z)) Esi+19.660997	791.5491	19.661	Rppos	13244351	8253320	7799357	7201593	10566064	6857317	12095113	7044854	6424376	4976433		
PC(20:4(5Z,8Z,11Z,14Z)/17:2(9Z,12Z)) Esi+21.883102	791.5701	21.8831	Rppos	2049120	1631269	2234017	1992354	631722	578077	759019	524660	655250	607163		
PC(20:4(5Z,8Z,11Z,14Z)/17:2(9Z,12Z)) Esi+23.546999	773.5399	23.547	Rppos	13285054	11417125	15236863	14738087	11960045	15098519	13394275	11724770	12011131	13097625		
PC(20:4(5Z,8Z,11Z,14Z)/22:2(13Z,16Z))	861.6224	25.9	Rppos	1310852	1866408	1908781	1482860	1587251	2087572	1616393	1447980	1654791	1301245		
PC(20:5(5Z,8Z,11Z,14Z,17Z)/15:1(9Z))	765.5282	13.512	Rpneg	31215	51107	32334	18542	1	1	1	1	1	63707		
PC(20:5(5Z,8Z,11Z,14Z,17Z)/19:0)	821.5923	24.161	Rppos	1545605	1305980	1918389	2191107	1000912	1586725	1228949	1187696	1858841	1308543		
PC(21:0/18:4(6Z,9Z,12Z,15Z))	823.611	26	Rppos	5283674	4454593	6336399	5159207	6514524	7941182	7207400	7581498	8723613	8329860		
PC(21:0/18:4(6Z,9Z,12Z,15Z))	823.6068	1.525	HILICpos	4353109	4379167	4046339	4341485	5014353	4139827		4947844	5436781	6078833		
PC(21:0/18:4(6Z,9Z,12Z,15Z)) Esi+25.514002	823.6061	25.514	Rppos	3762193	2699750	3715560	3324317	3660748	3614264	4033295	4343772	4144448	4558700		
PC(22:4(7Z,10Z,13Z,16Z)/17:2(9Z,12Z))	819.5758	23.53	Rppos	5670036	5113429	8071989	7291041	3406268	3722346	3474382	3298977	2932042	3609098		
PC(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/20:4(8Z,11Z,14Z,17Z))	853.562	21.411	Rppos	3484042	3909320	4031269	4069829	5745910	5268958	6058731	7755754	6426128	6079133		
PC(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/22:6(4Z,7Z,10Z,13Z,16Z,1	877.5636	21.179	Rppos	938562	886296	1159119	1167286	932280	986103	840998	1149047	842316	945208		
PC(7:0/O-8:0)	481.3189	15.386	Rppos	718435	789172	801154	763517	666026	829256	729574	744009	760206	580129		
PC(O-14:0/18:1(9Z))	717.5715	25.608	Rppos	1467370	1475178	1639128	1724111	1412460	1886863	2056475	1432370	2394516	1843483		
PC(O-16:0/2:0)[U]	523.3648	5.581	HILICpos	40499920	39438616	39452824	39216144	29670180	29970324		26654928	26834880	22615664		
PC(O-16:0/2:0)[U]	523.3637	15.314	Rppos	31008900	29494540	33661152	32155388	25590160	35024648	32230840	29975698	30858308	26613488		
PC(O-16:0/2:0)[U] Esi+14.742998	523.3642	14.743	Rppos	1753234	1599258	1744676	1722449	913110	1200485	1169868	915414	995694	882889		
p-Coumaroyl 3-hydroxytyrosine	343.1079	8.968001	Rpneg	6269	5793	6401	6005	5129	4893	4491	4094	3288	2908		
p-Coumaroylagmatine	275.1727	4.213	Rppos	712382	1	1	1	86578	573776	307098	363407	930500	53915		
PE(14:0/22:0)	769.5605	22.595	Rppos	346848	637530	496187	389237	777706	1041277	702606	1025474	1082728	979420		
PE(14:1(9Z)/20:2(11Z,14Z))	731.5098	4.987	HILICneg	44180	89838	36034	42289	47235	53729	46991	57133	75493	68524		
PE(15:0/18:0)	705.5315	1.559	HILICpos	2061884	2483888	1675836	2589921	1161846	1054850		1378241	1432935	1156139		
PE(16:0/19:1(9Z))	731.5462	1.55	HILICpos	4903618	6649676	5144439	6616085	3446943	3466375		2954281	4194976	3418873		
PE(16:0/20:1(11Z))	745.5618	14.785	Rpneg	42629	88978	51913	52969	120247	41909	82101	107180	54835	87297		
PE(16:1(9Z)/20:3(5Z,8Z,11Z))	739.5163	4.947	HILICneg	2675477	3653779	3086979	2900017	3580720	3487036	4471703	4701409	5077973	5112999		
PE(17:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z))	777.5306	4.105	HILICneg	378874	319307	380179	438482	410328	346105	516967	547046	379153	356057		
PE(17:2(9Z,12Z)/20:2(11Z,14Z))	753.5311	4.222	HILICneg	85141	78494	85033	113456	106898	115771	172645	215725	165879	98289		
PE(18:0/0:0)	481.3187	5.804	HILICneg	251513	245042	176884	192801	132461	88067	115812	104903	99231	89905		
PE(18:0/0:0)	481.3163	13.723	Rpneg	249488	232103	100112	119938	137137	102549	94109	98882	102549	91874		
PE(18:0/0:0) Esi-13.723	481.3163	13.723	Rpneg	204243	139609	187561	198393	209402	182822	175140	181849	195534	166837		
PE(18:0/14:0)	690.5279	25.515	Rppos	742280	876793	878825	750876	307214	316519	435560	371144	229927	147881		
PE(18:0/16:1(9Z))	717.529	4.991001	HILICneg	188107	146262	129121	132268	163835	155297	160447	171453	233955	211718		
PE(18:0/17:2(9Z,12Z))	751.5104	1.183	HILICpos	620781	1454279	298333	213133	340830	488462		803323	331068	241219		
PE(18:0/19:1(9Z))	741.5745	24.081	Rppos	1624628	1918321	1894631	1007609	2843312	3355786	2482420	2544391	3920320	2521870		
PE(18:0/20:4(5E,8E,11E,14E))	767.5465	4.870999	HILICneg	5797427	5753761	6670152	6036293	6263697	5972894	6437744	6755466	8231109	6635815		
PE(18:0/20:4(5E,8E,11E,14E)) Esi-1.812	767.535	1.812	HILICneg	108165	200995	160129	192839	217105	185774	177551	291420	87397	191760		
PE(18:0/20:4(5Z,8Z,11Z,13E)(15OH[S]))	765.5319	23.164	Rppos	5938097	7756539	8087568	7062874	4995726	7791317	7923613	7476083	7733183	6951592		
PE(18:0/22:6(4Z,7Z,10Z,12E,16Z,19Z)(14OH))	789.5321	22.829	Rppos	8725999	10725079	12363194	12083204	11521412	14187564	16360483	15679648	13490049	14713857		
PE(18:0/22:6(4Z,7Z,10Z,12E,16Z,19Z)(14OH))	807.5441	5.002999	HILICneg	537766	502962	561034	550657	571974	544477	491452	559161	642379	573313		
PE(18:1(11Z)/18:2(9Z,12Z))	741.529	4.949	HILICneg	923784	1097274	936590	864893	1725138	2140430	1985284	2294916	3110200	2944607		

PE(18:1(6Z)/18:1(6Z))	743.5447	4.958	HILICneg	926801	970991	874237	796777	1394678	1348723	1396422	1516883	2184276	1807285
PE(18:1(9Z)/14:0)	688.5127	23.931	Rppos	806552	631386	611459	663049	1	1	1	1	1	1
PE(18:1(9Z)/17:1(9Z))	729.5324	1.55	HILICpos	822055	580968	579260	599724	201427	235851		422952	267674	213857
PE(18:1(9Z)/18:1(9Z))	725.5345	24.086	Rppos	1057041	1077009	1075885	419176	1501284	2174623	1311642	1545965	1848977	1453586
PE(18:2(9Z,12Z)/0:0)	477.2854	13.183	Rpneg	21078	25323	18347	19758	48003	19548	25669	30649	26964	29982
PE(18:2(9Z,12Z)/0:0) Esi-13.089998	477.2865	13.09	Rpneg	13040	22727	12404	14133	48003	17937	25584	29715	24827	25954
PE(18:2(9Z,12Z)/16:0)	715.517	1.559	HILICpos	215567	309633	137495	165958	707109	236011		348701	459934	835824
PE(18:2(9Z,12Z)/18:3(6Z,9Z,12Z))	737.506	4.975999	HILICneg	157457	219260	169446	168785	503203	599472	606495	658581	689534	676370
PE(18:3(6Z,9Z,12Z)/19:0)	737.5435	24.32	Rppos	282144	342061	278377	458688	212038	251814	311822	310465	311430	281071
PE(18:3(6Z,9Z,12Z)/20:3(8Z,11Z,14Z))	785.4938	21.953	Rppos	579091	800593	1019789	1	959653	1106936	1213910	1293391	1052637	1154230
PE(18:3(6Z,9Z,12Z)/20:3(8Z,11Z,14Z)) Esi-0.8809999	763.5149	0.881	HILICneg	1765255	923642	1030928	1003967	635259	451369	658979	531091	833159	673266
PE(18:3(6Z,9Z,12Z)/20:3(8Z,11Z,14Z)) Esi-0.88600004	763.5132	0.886	HILICneg	1485916	1	993728	1012743	319290	293263	378290	418708	1040416	338353
PE(18:3(6Z,9Z,12Z)/20:3(8Z,11Z,14Z)) Esi-4.139	763.516	4.139	HILICneg	69935	80419	43450	92938	222927	235893	222530	310081	477049	257690
PE(18:4(6Z,9Z,12Z,15Z)/18:0)	739.5178	1.542	HILICpos	1299185	1282561	1147525	1047887	849140	774734		1347501	1343829	1351631
PE(18:4(6Z,9Z,12Z,15Z)/20:3(5Z,8Z,11Z))	761.506	4.892	HILICneg	311706	455162	353901	393336	315112	266983	346014	331864	303093	323764
PE(18:4(6Z,9Z,12Z,15Z)/22:5(4Z,7Z,10Z,13Z,16Z))	785.4983	0.874	HILICneg	2265314	1278369	1303198	1501414	1655770	617323	1603612	1528228	1218561	1521839
PE(18:4(6Z,9Z,12Z,15Z)/22:5(4Z,7Z,10Z,13Z,16Z)) Esi-4.869	785.5044	4.869999	HILICneg	173593	272785	240760	238471	166355	1	218312	212468	1	170284
PE(19:0/0:0)	495.3315	13.555	Rpneg	130472	87389	82813	106365	52281	42099	53073	42733	46503	43834
PE(19:0/0:0)	495.3332	5.541	HILICpos	1787931	1742663	1683579	1566419	1264871	130857		1019056	1030172	893382
PE(19:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z))	805.5649	1.525	HILICpos	1.75E+08	1.51E+08	1.86E+08	1.7E+08	1.03E+08	1.03E+08		1.08E+08	82170752	90642488
PE(19:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z))	805.5618	3.912	HILICneg	1241279	962909	1329554	1521445	1182215	965928	1504189	1523080	1110328	1389412
PE(19:1(9Z)/22:6(4Z,7Z,10Z,13Z,16Z,19Z))	803.5453	3.916	HILICneg	250790	275184	251548	309841	308816	271781	382801	393846	230152	336056
PE(20:0/0:0)	509.349	14.129	Rpos	410322	437129	424300	401959	263337	367324	302924	305215	336326	285972
PE(20:0/0:0)	555.3547	5.792	HILICneg	3088940	4080797	2976542	3059322	2131927	1544704	1769956	1629338	1449992	1409828
PE(20:0/0:0)	555.3519	13.555	Rpneg	115326	81216	75121	100248	48139	39435	48944	42055	43527	44923
PE(20:0/0:0) Esi-13.555	509.3487	13.555	Rpneg	113094	81845	77563	102673	50207	40903	49688	43780	44777	46438
PE(20:1(11Z)/14:1(9Z))	715.5158	4.987999	HILICneg	459346	480612	365230	354025	501541	495328	544747	611502	707287	664691
PE(20:1(11Z)/14:1(9Z))	715.5076	13.755	Rpneg	6414	12730	1	3135	2901	6910	1	5654	14444	14776
PE(20:1(11Z)/20:3(5Z,8Z,11Z))	777.5722	25.817	Rpos	3040646	2659763	3961633	3699386	1883729	2961740	3264805	3281968	2541276	2964367
PE(20:1(11Z)/20:3(8Z,11Z,14Z))	795.5762	12.869	Rpneg	27637	12398	13870	30633	52412	24187	22193	33226	37857	8618
PE(20:1(11Z)/20:3(8Z,11Z,14Z))	795.5769	1.766	HILICneg	283830	256510	295470	345040	261909	91101	300989	299708	256234	272110
PE(20:1(11Z)/20:3(8Z,11Z,14Z)) Esi-12.613999	795.5736	12.614	Rpneg	5925	6577	4328	13529	15708	7237	7486	13318	41766	6475
PE(20:1(11Z)/20:3(8Z,11Z,14Z)) Esi-12.865	795.5752	12.865	Rpneg	26641	8527	24271	25600	49459	24436	32923	34074	32660	22007
PE(20:1(11Z)/20:3(8Z,11Z,14Z)) Esi-13.133001	795.5755	13.133	Rpneg	38548	21613	19398	40930	48843	19065	20870	51363	34514	12122
PE(20:2(11Z,14Z)/0:0)	505.3154	13.237	Rpneg	7480	1659	1236	1258	1216	1356	1533	1699	2202	1
PE(20:2(11Z,14Z)/20:4(5Z,8Z,11Z,14Z))	791.5469	14.366	Rpneg	496887	431101	444910	544784	235332	120321	345297	237846	378206	398215
PE(20:2(11Z,14Z)/20:4(5Z,8Z,11Z,14Z))	791.5474	4.847	HILICneg	1.96E+07	1.97E+07	2.42E+07	2.56E+07	2.16E+07	1.62E+07	2.01E+07	2.18E+07	2.15E+07	2.25E+07
PE(20:2(11Z,14Z)/20:4(5Z,8Z,11Z,14Z)) Esi-1.779	791.5404	1.779	HILICneg	396765	502007	484017	543316	251383	160915	288024	235137	152696	355120
PE(20:2(11Z,14Z)/22:5(7Z,10Z,13Z,16Z,19Z))	817.5682	22.082	Rpos	652159	425778	589602	385177	181294	150284	233784	279427	211819	127931
PE(20:2(11Z,14Z)/22:5(7Z,10Z,13Z,16Z,19Z))	835.5705	4.807	HILICneg	87709	83593	83954	87391	68391	41867	70461	68315	63599	72942
PE(20:3(5Z,8Z,11Z)/18:2(9Z,12Z))	765.5313	4.880001	HILICneg	3288815	3533167	3682120	1	3651088	3664212	3847868	3978394	4124706	4211238
PE(20:3(5Z,8Z,11Z)/20:4(8Z,11Z,14Z,17Z))	789.5307	4.849	HILICneg	6199303	7883625	8003943	7945084	9585549	7293650	1.02E+07	1.04E+07	9047832	1.08E+07
PE(20:3(8Z,11Z,14Z)/20:5(5Z,8Z,11Z,14Z,17Z))	787.516	21.711	Rppos	6937520	8063565	9810212	7644053	9918876	8551338	11378403	11171781	9383393	9877326
PE(20:3(8Z,11Z,14Z)/20:5(5Z,8Z,11Z,14Z,17Z))	787.5164	4.854	HILICneg	4955457	9485654	8505905	7048461	1.19E+07	6787837	1.12E+07	1.12E+07	8732332	1.14E+07
PE(20:3(8Z,11Z,14Z)/20:5(5Z,8Z,11Z,14Z,17Z)) Esi-0.86900	787.5141	0.869	HILICneg	6767879	2976801	4500598	4616835	2812966	1237488	3112154	3417164	3698889	3544219
PE(20:3(8Z,11Z,14Z)/20:5(5Z,8Z,11Z,14Z,17Z)) Esi-4.049	787.5151	4.049	HILICneg	339374	282003	251553	378618	587860	509340	491472	613653	752139	513190
PE(20:3(8Z,11Z,14Z)/22:5(7Z,10Z,13Z,16Z,19Z))	815.5459	4.819	HILICneg	97432	120790	117584	115341	93009	81226	97056	103825	92362	90318
PE(20:4(5Z,8Z,11Z,14Z)/18:1(11Z))	747.5222	22.612	Rpos	1034717	1247672	1234542	781340	1652398	1896180	1798604	1918973	2229418	1877600
PE(20:4(5Z,8Z,11Z,14Z)/20:3(5Z,8Z,11Z))	771.5223	22.337	Rpos	1738821	1334422	2187122	1788052	1510429	2003626	1621350	1209258	1514191	1575463
PE(20:4(5Z,8Z,11Z,14Z)/P-16:0)	723.5214	4.793	HILICneg	3282663	3505510	3001752	3209713	4010286	3795806	3897031	4509206	5484976	4339868
PE(20:4(5Z,8Z,11Z,14Z)/P-18:0)	751.5484	4.739999	HILICneg	1583650	1673922	1562694	2232359	2366069	2162675	2295213	1407848	1724876	2397016
PE(20:4(5Z,8Z,11Z,14Z)/P-18:0) Esi-1.5819999	751.5512	1.582	HILICneg	72085	134848	90454	120064	143166	77150	118990	204129	151948	201500
PE(20:4(8Z,11Z,14Z,17Z)/22:5(4Z,7Z,10Z,13Z,16Z))	813.5276	4.793	HILICneg	81645	129238	106984	104899	78022	51089	84552	84718	62894	73985
PE(20:5(5Z,8Z,11Z,14Z,17Z)/18:3(9Z,12Z,15Z))	759.4876	0.88	HILICneg	4895337	2713071	3137711	3451576	1556034	775787	1794039	2153050	1871137	1134305
PE(20:5(5Z,8Z,11Z,14Z,17Z)/22:0)	821.5983	1.525	HILICpos	6751982	7474423	9323677	9791406	7214536	7727786		7001313	6915755	6383621
PE(20:5(5Z,8Z,11Z,14Z,17Z)/22:1(13Z))	819.5807	1.475	HILICpos	5514433	5068654	6670026	6163453	3666625	3350182		3420142	2956922	3246100
PE(21:0/0:0)	569.3697	5.762001	HILICneg	70120	88412	67062	69616	53813	32116	43429	44777	38997	39738
PE(22:0/0:0)	583.3838	13.973	Rpneg	128720	77287	88637	110151	70332	62829	79949	63927	70492	62519
TG(12:0/20:0/22:5)	897.7812	0.888	HILICpos	82157696	59109364	63151572	57670616	1.33E+08	1.25E+08		1.69E+08	1.34E+08	1.68E+08
PE(22:0/0:0) Esi-13.973	583.3839	13.973	Rpneg	128986	82360	88536	110151	70332	62829	79949	63935	70492	1
PE(22:0/16:0)	779.5784	24.711	Rpos	290587	310804	395253	336830	333762	316613	315579	441533	399413	408122
PE(22:0/20:3(5Z,8Z,11Z))	847.5996	1.517	HILICpos	1964525	497016	2257179	1804102	1449492	1362957		601759	1124938	1437376
PE(22:0/22:5(7Z,10Z,13Z,16Z,19Z))	849.6239	14.401	Rpneg	39158	54440	27768	35963	49765	44761	50900	60697	19805	47670
PE(22:1(11Z)/18:4(6Z,9Z,12Z,15Z))	793.5593	22.376	Rpos	2276085	2328614	2954897	2091426	1179370	1325976	1715843	1488455	1199482	1327836
PE(22:1(11Z)/20:5(5Z,8Z,11Z,14Z,17Z))	819.576	1.633	HILICneg	405658	493871	211590	570632	354970	209398	363872	343959	84837	344650
PE(22:1(11Z)/21:0)	825.6681	24.314	Rpos	2293499	1120630	1903154	2109616	1886844	2121076	2121594	1836511	1547994	1523392
PE(22:1(11Z)/22:0)	839.6833	24.314	Rpos	881122	1052859	2137011	2111420	1759148	2455683	2353839	1827354	1798023	1698901
PE(22:2(13Z,16Z)/16:1(9Z))	751.5516	25.835	Rpos	8887177	8761718	10657379	10197072	9651303	12599721	11893783	10738752	11734159	10410881
PE(22:2(13Z,16Z)/16:1(9Z)) Esi+25.343998	751.5525	25.344	Rpos	1479858	1375365	1638563	1178560	1304484	2275734	1373211	2163073	1893995	2012831
PE(22:2(13Z,16Z)/21:0)	863.6366	1.517	HILICpos	411262	434072	449926	878048	366685	388391		667167	421815	627519
PE(22:4(7Z,10Z,13Z,16Z)/0:0)	529.3178	5.632	HILICneg	152863	192915	138749	166315	146850	90624	102995	100102	74261	83022
PE(22:4(7Z,10Z,13Z,16Z)/0:0)	547.3277	13.36	Rpneg	6881	3769	2630	11620	5024	4687	1	5523	6585	4249
PE(22:4(7Z,10Z,13Z,16Z)/0:0) Esi-13.2109995	529.314	13.211	Rpneg	19853	5216	5447	12239	3382	3035	5583	1	4663	4141
PE(22:4(7Z,10Z,13Z,16Z)/17:0)	781.5616	4.043	HILICneg	1003306	740345	1118343	1146617	914348	763519	1303717	1219555	987179	996013
PE(22:4(7Z,10Z,13Z,16Z)/17:0) Esi-4.9210005	781.5646	4.921001	HILICneg	159611	171900	195745	204501	167859	359981	169698	160942	162583	180550
PE(22:4(7Z,10Z,13Z,16Z)/17:1(9Z))	779.5474	4.08	HILICneg	210247	199742	212136	238672	232616	209481	311723	330976	287353	259643
PE(22:4(7Z,10Z,13Z,16Z)/19:0)	809.5913	13.071	Rpneg	3082	3855	39025	109124	78687	1	1	188475	96440	120498
PE(22:4(7Z,10Z,13Z,16Z)/19:1(9Z))	789.5639	19.411	Rpos	88536	424534	305503	177474	91688	506500	483360	209647	401320	600001
PE(22:4(7Z,10Z,13Z,16Z)/19:1(9Z))	829.562	1.517	HILICpos	26976088	26297238	23156138	24188046	28270208	29820168		27471984	22418496	23819144
PE(22:4(7Z,10Z,13Z,16Z)/21:0)	859.6044	1.517	HILICpos	1216163	698530	1326376	1300977	743310	909644		973928	513604	909751
PE(22:4(7Z,10Z,13Z,16Z)/21:0)	883.6255	14.969	Rpneg	6245	13516	7101	8034	14743	11957	10821	19427	12466	13051
PE(22:4(7Z,10Z,13Z,16Z)/P-18:1(11Z))	777.5625	13.548	Rpneg	1	21086	5633	34830	76792	91854	85615	71619	19981	50433
PE(22:5(4Z,7Z,10Z,13Z,16Z)/P-16:0)	749.5348	4.741001	HILICneg	5766433	5971446	5320344	5394941	6022245	5348511	6218017	6690446	7573754	6478864
PE(22:5(7Z,10Z,13Z,16Z,19Z)/22:4(7Z,10Z,13Z,16Z))	901.5754	14.401	Rpneg	22529	19477	16116	18208	20890	15162	17269	18821	25027	20621
PE(22:5(7Z,10Z,13Z,16Z,19Z)/P-16:0)	749.5367	23.938	Rppos	18188000	19128680	19593816	17912072	18408186	21819162	21581728	20565864	23931824	20708644
PE(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/0:0)	525.2877	5.686	HILICneg	5056458	4419788	3020996	4080776	2148935	958101	1318432	1256654	662882	887530
PE(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/0:0)	525.286	13.12	Rpneg	64278	54399	53363	87802	49086	35967	52303	68762	43981	57512
PE(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/0:0)	525.2862	11.374	Rppos	846297	834648	1012326	1020561	643418	1015396	989057	852063	770352	846584
PE(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/0:0) Esi-0.91100013	525.2833	0.911	HILICneg	540886	339742	260837	219860	950842	266525	277533	197582	545554	472061
PE(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/0:0) Esi-12.609	525.2864	12.609	Rpneg	14808	11979	27067	20954	8734	7817	12270	14537	14507	16034
PE(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/0:0) Esi-5.6860003	525.2876	5.686	HILICneg	4958856	4360365	2932634	4023060	2123163	957512	1309730	1242726	656981	883271
PE(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/19:0)	823.5766	4.812	HILICneg	109108	121446	98222	114576	120032	136030	113191	122231	145924	131957

PE(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/20:4(8Z,11Z,14Z,17Z))	811.5168	4.747001	HILICneg	179192	392260	336158	305658	263921	110319	201434	262627	130914	244818
PE(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/21:0)	878.5876	14.822	Rpneg	9763	7646	7624	7072	1	7896	3225	10755	13542	11549
PE(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/22:2(13Z,16Z))	843.5729	4.935	HILICneg	3983311	2553646	4437050	5493346	2533127	4374750	5828590	4683690	4696444	2538144
PE(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/22:4(7Z,10Z,13Z,16Z))	839.5487	4.758	HILICneg	108073	188948	194711	180870	144638	92576	124637	154866	1	151477
PE(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/22:5(7Z,10Z,13Z,16Z,19Z)	837.5316	4.77	HILICneg	84625	176115	183492	162744	84564	69406	90660	84631	59947	69933
PE(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/22:6(4Z,7Z,10Z,13Z,16Z,1	835.5163	4.705	HILICneg	130586	188441	169945	122425	95564	75236	74928	87127	98394	118436
PE(O-16:0/13:0)	657.466	8.627999	Rppos	1	215675	26328	170490	276406	16482	31972	158902	351081	166937
PE(O-16:0/18:0)	704.5857	23.572	Rppos	1118624	454316	568061	705865	456369	735090	650088	591175	447969	724292
PE(O-18:0/17:0)	719.5839	26.088	Rppos	2238253	2774926	2534963	2125027	1859742	2117413	1800477	1916851	1708492	1751277
PE(O-18:0/20:3(8Z,11Z,14Z))	777.5592	1.467	HILICpos	559814	1005001	716618	618597	610083	1013822		1400510	564247	1299611
PE(P-16:0/0:0)	437.29	13.527	Rpneg	85881	113582	76187	116751	136540	115422	98388	110959	122198	120666
PE(P-16:0/0:0)	454.317	0.883	HILICpos	138803	153573	159765	376496	182642	62163		294219	300438	179276
PE(P-16:0/0:0) Esi-13.527	437.2895	13.527	Rpneg	85713	113582	76187	116903	136664	115282	98936	110821	122195	120671
PE(P-16:0/20:4(8Z,11Z,14Z,17Z))	723.5221	1.533	HILICpos	1576088	1953066	1428264	1461049	1501636	1699834		1940921	1865564	1995889
PE(P-16:0/22:5(7Z,10Z,13Z,16Z,19Z))	749.537	1.533	HILICpos	2073577	1798124	1635092	2029591	1608541	1437529		2118190	1715164	2149046
PE(P-18:1(9Z)/18:0)	751.5507	1.475	HILICpos	1580857	1492699	1556300	1595766	1810505	1371950		1737204	1896988	516729
PE(P-18:1(9Z)/18:4(6Z,9Z,12Z,15Z))	721.5031	4.805	HILICneg	219636	123738	226328	115899	80395	74376	109163	216979	94476	100287
PE(P-18:1(9Z)/20:5(5Z,8Z,11Z,14Z,17Z))	747.5216	4.763	HILICneg	1.05E+07	8720123	1.01E+07	1.06E+07	9553535	9177883	9717835	9983220	1.00E+07	1.05E+07
PE(P-18:1(9Z)/20:5(5Z,8Z,11Z,14Z,17Z)) Esi-4.6139994	747.5207	4.613999	HILICneg	198621	108499	118393	96649	87436	98834	98448	107465	117815	108807
PE(P-18:1(9Z)/22:5(7Z,10Z,13Z,16Z,19Z))	775.549	4.703	HILICneg	4311955	3369175	3996867	4179018	3715723	3190361	3596727	3558412	3636548	3645203
PE(P-18:1(9Z)/22:5(7Z,10Z,13Z,16Z,19Z))	775.5658	1.532	HILICpos	827496	823013	1101972	1	777847	1346273		2049227	1859394	1865484
PE(P-18:1(9Z)/22:5(7Z,10Z,13Z,16Z,19Z)) Esi-1.5599998	775.5496	1.56	HILICneg	83409	159393	112541	248567	120858	73383	108711	119212	182502	129278
PE(P-20:0/15:0)	739.5506	1.064	HILICpos	387776	1	94302	176460	138052	122649		315417	360105	96302
PE(P-20:0/17:1(9Z))	765.5664	1.525	HILICpos	20523452	23358580	23569786	26750080	33544436	33180030		26708328	25916858	21174898
PE(P-20:0/17:2(9Z,12Z))	745.5389	23.748	Rppos	5216237	5738977	5580669	5429908	3912580	4729043	1	1	4977149	1
PE-Cer(d16:1(4E)/20:0)	705.5859	0.882	HILICpos	465115	1	1	1	52673	34175		67425	89410	30926
PE-Cer(d16:1(4E)/21:0)	702.5677	5.319	HILICpos	37228704	32740096	33253904	28157840	34155640	34229960		30067956	31376516	26115968
PE-Cer(d16:1(4E)/22:0)	716.578	5.294	HILICpos	1265760	1327252	1305853	924961	1180026	1066120		1188149	1198447	1086744
PE-Cer(d16:1(4E)/22:0)	762.5886	5.545	HILICneg	420648	253686	307645	407017	306125	163102	366280	445388	529563	462961
PE-Cer(d16:1(4E)/23:0)	730.5984	5.277	HILICpos	17573552	19220680	19501114	14244803	18936040	17576384		16783566	16891196	14655068
PE-Cer(d16:2(4E,6E)/20:0(2OH))	719.5591	1.558	HILICpos	2717428	3304363	2745686	2951267	1708317	1332252		1724294	1549424	1736714
PE-Cer(d16:2(4E,6E)/20:0(2OH))	702.5406	0.923	HILICneg	752096	1571267	1128956	1421138	878295	241668	664853	671838	464815	625197
PE-Cer(d16:2(4E,6E)/20:0(2OH)) Esi-0.9190001	720.5487	0.919	HILICneg	1264345	1572079	1187571	1390859	852296	1	685853	747022	944731	604887
PE-Cer(d16:2(4E,6E)/21:0)	699.5718	22.29	Rppos	1453837	1350350	1613542	1098796	1029186	809423	869539	865347	1183186	997258
PE-Cer(d16:2(4E,6E)/21:0)	700.5524	5.32	HILICpos	3686515	2959825	2425229	3165806	3118037	3328273		2646910	2898733	2405983
PE-Cer(d16:2(4E,6E)/21:0) Esi+21.757002	699.5709	21.757	Rppos	221518	1	288045	617784	137239	1	353176	1	476039	1
PE-Cer(d16:2(4E,6E)/22:0(2OH))	730.5726	0.892	HILICneg	235975	395297	495909	341829	240425	74340	156989	168710	158012	141021
PE-Cer(d16:2(4E,6E)/22:0)	713.5906	23.924	Rppos	1166922	485203	362686	774038	343758	562323	505461	413035	870439	309649
PE-Cer(d16:2(4E,6E)/22:1(13Z))	712.5506	0.883	HILICpos	895399	1111678	777213	1028343	661046	533507		543374	889683	616329
PE-Cer(d16:2(4E,6E)/23:0)	727.6034	23.893	Rppos	319257	704435	609211	401087	810436	632690	826832	743051	1187732	236778
PE-Cer(d16:2(4E,6E)/23:0)	728.5832	5.274	HILICpos	8261243	10202828	7835680	8766127	7413746	8000985		7033708	6869040	5686433
PE-Cer(d16:2(4E,6E)/24:0)	371.3014	5.253	HILICpos	893734	639315	722711	745131	913991	1921931		767394	841441	885557
PE-Cer(d16:2(4E,6E)/24:0)	788.6038	5.515999	HILICneg	98473	94201	87911	112934	99688	110565	120371	119530	115107	120696
Pectenotoxin 1	874.466	14.323	Rpneg	4966	1899	2418	1583	3416	1795	2027	1	761	1
Pederin	503.3112	6.965	Rppos	202643	204797	202563	178311	209034	188288	174576	176605	188980	172547
Pederin	525.2888	5.408001	HILICpos	342395	351859	365175	253812	346383	252879		369415	322149	197759
Peltatol C	626.4326	13.08071	Rpneg	13110	5619	1241	2112	1	1	1154	1032	1691	1
Penazetidine A	368.3735	18.393	Rppos	232058	354121	429785	275433	687047	1	861087	495637	442219	227500
Penciclovir	235.1059	6.022999	Rppos	110389	404779	263750	212131	196673	351635	162773	155534	249651	155691
Penicillic acid	216.06	0.898	Rpneg	8163	1	1	1	14485	30955	26049	26765	48641	23564
PE-NMe(11:0/11:0)	569.3478	11.918	Rppos	267942	256099	380739	382999	216936	330697	325854	280078	257881	286977
TG(12:0/20:3/21:0)	887.7974	0.916	HILICpos	6601942	4645561	4826106	4432677	8554668	9830626		11046503	10955579	11256150
PE-NMe(17:0/17:0)[U]	733.5643	13.551	Rpneg	46842	65401	50687	51192	90859	84111	58473	54654	20020	52910
PE-NMe2(18:0/18:0)[U]	779.57	24.291	Rppos	485175	409539	871475	496472	487086	518790	650064	788842	1215977	902134
PE-NMe2(18:1(9Z)/18:1(9Z))[U]	771.5762	1.542	HILICpos	3495571	4366587	3935751	3588671	5321197	6238400		6195537	7135811	6672814
PE-NMe2(18:1(9Z)/18:1(9Z))[U]	771.5727	14.465	Rpneg	55156	109869	84521	56949	69425	74801	54312	20180	65928	76314
Pentacosanoic acid	382.3792	0.961	HILICneg	121755	86499	39014	85890	129156	67399	126430	94765	306678	66322
Pentacosanoic acid	382.3808	13.871	Rpneg	230424	74130	40077	64241	60659	44187	60172	51313	56205	29903
Pentahomomethionine	265.1333	9.943	Rpneg	7678	3468	3941	4812	3060	3096	4379	3642	2453	3006
Pentamidine	357.2176	8.245001	Rppos	22655	131084	127858	153527	60138	88151	104018	96310	151042	119785
Pentamidine Esi+8.043	357.2189	8.043	Rppos	26671	129155	151626	170225	87280	95254	98260	89167	159614	117583
Peracetic acid	76.0155	0.814	Rpneg	137831	134933	168517	143635	110625	155486	151509	130243	108339	137401
Periandrin V	778.4181	0.919	HILICneg	454783	307788	1	214202	585875	282358	216469	156926	347131	313014
Perindopril lactam	350.2213	12.601	Rpneg	25559	19958	19843	25389	16905	12538	19977	20186	17758	13853
Perlolyrine	264.0887	9.046999	Rpneg	2322	6578	3168	2824	2311	3355	3815	2477	5836	5518
P-Fluorophenylalanine	243.0895	10.058	Rpneg	3377	6220	3577	5278	6667	3286	4540	4137	5548	4231
PG(12:0/17:1(9Z))	677.4645	16.621	Rppos	1468951	282908	194910	193139	374488	578558	641110	526733	777866	562694
PG(14:1(9Z)/13:0)	649.4334	14.513	Rppos	1009540	295809	170352	186941	302989	371268	399235	335559	356246	301613
PG(14:1(9Z)/18:0)	720.4995	21.992	Rppos	1.68E+07	1.75E+07	1.80E+07	1.93E+07	1.25E+07	1.78E+07	1.30E+07	1.28E+07	1.36E+07	1.39E+07
PG(14:1(9Z)/18:0)	720.4942	13.905	Rpneg	85934	70958	63858	94188	16393	19665	20247	14582	27665	24493
PG(14:1(9Z)/18:1(9Z))	718.4765	13.755	Rpneg	14117	14806	8818	12284	2627	2318	3403	2941	5222	4741
PG(15:0/12:0)	698.4352	13.104	Rpneg	72519	5142	3977	7469	2539	1634	5745	4120	5610	2401
PG(15:1(9Z)/18:0)	734.5091	14.038	Rpneg	77456	72519	64552	75400	19039	17092	20281	18785	23781	22371
PG(15:1(9Z)/19:0)	748.5235	14.198	Rpneg	7028820	5930304	3282959	8579506	3342999	3815827	1809606	3480373	2833036	1663852
PG(15:1(9Z)/19:0) Esi-14.185999	748.5232	14.186	Rpneg	7093758	5946971	2927331	8634701	3319998	3844478	2386274	3470983	3777590	3866398
PG(15:1(9Z)/21:0)	793.585	1.525	HILICpos	5402614	6310267	7382061	5437364	5049341	3861786		3992964	4330854	4488384
PG(16:0/0:0)	484.2799	12.736	Rpneg	55549	55941	54744	79840	17849	13826	32409	22957	16228	27685
PG(16:0/0:0) Esi-12.734	484.2796	12.734	Rpneg	55549	55941	54744	79840	17849	5130	32409	22957	8663	27685
PG(16:0/0:0) Esi-12.734 :1	484.2798	12.734	Rpneg	55549	56128	54744	79642	1	5130	32409	22957	24860	27685
PG(16:0/0:0)[U]	484.2815	4.554	HILICneg	533247	633629	425240	453305	86271	47202	88143	43664	38860	53365
PG(16:0/14:0)	694.4756	13.881	Rpneg	8029	6858	4254	6580	1	1182	1	1	1718	1
PG(16:0/17:2(9Z,12Z))	732.4911	13.857	Rpneg	13001	15842	10722	9930	3875	4999	4826	3959	6439	6792
PG(16:0/17:2(9Z,12Z))	732.4933	5.433	HILICneg	306399	193403	256979	268055	80408	189992	181092	152789	173143	151552
PG(16:0/17:2(9Z,12Z)) Esi-5.3349996	732.4933	5.335	HILICneg	186790	103598	133758	168505	43594	1	1	152869	172004	151552
PG(16:1(9Z)/12:0)	664.4302	1.114	HILICneg	259493	197075	132003	158079	264422	152016	159489	208730	1	143428
PG(17:0/18:3(6Z,9Z,12Z))	758.5084	5.399001	HILICneg	62483	42435	56346	58767	46334	90453	75989	33884	58373	101352
PG(17:0/20:0)	792.586	5.502999	HILICneg	94286	72357	74707	82186	77294	48839	80789	81689	89029	94076
PG(17:1(9Z)/18:1(9Z))	760.5232	14.074	Rpneg	36540	38561	43118	39028	28904	32818	28705	30167	23615	42503
PG(17:1(9Z)/18:1(9Z)) Esi-14.011999	759.5047	14.012	Rpneg	31897	34913	26011	38178	22310	29616	23087	29234	35505	36827
PG(17:1(9Z)/18:1(9Z)) Esi-14.073999	760.5205	14.074	Rpneg	41861	53419	24762	30337	29713	26487	30589	28284	14122	1
PG(17:1(9Z)/18:3(9Z,12Z,15Z))	756.4941	12.681	Rpneg	2531	1669	1	1	2427	7097	3238	3728	2540	2577
PG(17:1(9Z)/22:6(4Z,7Z,10Z,13Z,16Z,19Z))	806.5121	5.325	HILICneg	210332	57176	164101	185333	163172	132126	157169	171111	152933	123055

PG(17:2(9Z,12Z)/19:0)	774.539	1.132 HILICneg	1840098	1565811	1908479	1923682	1587400	942174	1729223	1670143	2209658	2184945
PG(17:2(9Z,12Z)/19:0)	774.5398	13.928 Rpneg	188230	227188	195125	86194	274964	287618	287088	282087	271996	225992
PG(17:2(9Z,12Z)/19:1(9Z))	772.5235	0.919 HILICneg	927824	1468757	1255842	1461760	1003377	773519	1520696	1611481	1725296	1564163
PG(18:0/0:0)	512.3108	13.067 Rpneg	26993	28915	33613	47504	22298	18582	30397	25766	38102	32966
PG(18:0/14:0)[U]	722.5093	14.164 Rpneg	55059	28645	23924	33118	19382	23282	28427	25245	5487	12581
PG(18:0/14:0)[U] Esi-14.157999	722.5088	14.158 Rpneg	35191	41133	12682	33118	19662	26229	19362	24725	1911	12581
PG(18:0/17:1(9Z))	762.5414	14.406 Rpneg	217071	256481	197790	348366	58101	46321	77472	64058	49442	97489
PG(18:1(9Z)/0:0)	510.2955	12.726 Rpneg	69871	59289	56086	82599	34459	35376	51704	60834	68249	44389
PG(18:1(9Z)/0:0) Esi-12.604	510.2944	12.604 Rpneg	9099	1	4660	14421	3707	1	5562	60834	68249	5739
PG(18:1(9Z)/0:0) Esi-12.809999	510.2958	12.81 Rpneg	88276	73866	12646	18445	10793	9981	15193	17844	86257	18498
PG(18:1(9Z)/18:1(9Z))	774.5398	14.323 Rpneg	1112187	1255306	1084089	1243930	1134096	882686	1083437	1071213	1574126	1450054
PG(18:1(9Z)/20:5(5Z,8Z,11Z,14Z,17Z))	794.5142	1.107 HILICneg	633101	589575	671745	849925	198967	148131	334297	368323	212616	336759
PG(18:1(9Z)/20:5(5Z,8Z,11Z,14Z,17Z))	794.514	13.648 Rpneg	75206	81484	75259	52490	22663	12929	31981	1	28346	33827
PG(18:1(9Z)/20:5(5Z,8Z,11Z,14Z,17Z)) Esi-0.8920001	794.5051	0.892 HILICneg	486913	377471	162003	452235	1	154413	84907	81916	184061	1
PG(18:2(9Z,12Z)/0:0)	508.2801	12.493 Rpneg	44333	46555	54916	66840	48775	37405	75158	71366	73710	62810
PG(18:2(9Z,12Z)/0:0)	508.2809	4.136 HILICneg	311635	1	791084	485898	454336	1	241355	1	307878	361845
PG(18:2(9Z,12Z)/0:0) Esi-12.573999	508.2801	12.574 Rpneg	28161	17119	21947	32835	17787	11393	24347	30169	31580	25183
PG(18:2(9Z,12Z)/0:0) Esi-4.4910007	508.2817	4.491001 HILICneg	176607	141167	55836	143141	23583	17640	34750	1	29786	32523
PG(18:2(9Z,12Z)/16:1(9Z))	744.4948	13.79 Rpneg	32093	32895	22375	30139	9647	12083	12438	11238	17984	13436
PG(18:2(9Z,12Z)/20:1(11Z))	800.5558	14.448 Rpneg	58165	57329	64813	69119	54617	48518	48470	59227	69103	71994
PG(18:2(9Z,12Z)/22:4(7Z,10Z,13Z,16Z))	822.5398	14.06433 Rpneg	1	32551	24607	25791	54817	54248	24144	43746	38097	63163
PG(18:3(6Z,9Z,12Z)/18:1(11Z))	770.5101	1.127 HILICneg	2142862	1575676	1667415	2032880	890076	448208	1082188	768537	711687	1035841
PG(18:3(6Z,9Z,12Z)/22:5(4Z,7Z,10Z,13Z,16Z))	818.5103	0.813 HILICneg	1293708	1979328	2141181	1996406	707708	210558	627054	572098	481126	580670
PG(18:3(6Z,9Z,12Z)/22:5(4Z,7Z,10Z,13Z,16Z))	818.5099	13.622 Rpneg	280227	304398	270217	342686	101878	48034	87453	94846	85429	83077
PG(18:3(6Z,9Z,12Z)/22:5(4Z,7Z,10Z,13Z,16Z)) Esi-13.774	818.5128	13.774 Rpneg	33452	16241	27120	61497	8613	6101	6786	7558	5973	6002
PG(18:3(9Z,12Z,15Z)/15:0)	730.48	5.428001 HILICneg	74590	77463	151044	66598	45170	96755	87626	83483	150785	114638
PG(18:3(9Z,12Z,15Z)/18:0)	772.5246	13.781 Rpneg	279491	321454	260709	345986	561573	499121	436874	587071	759394	551521
PG(18:3(9Z,12Z,15Z)/18:0) Esi-14.012999	772.5253	14.013 Rpneg	376769	369017	336752	373802	237730	289270	264054	244286	284117	316064
PG(18:3(9Z,12Z,15Z)/18:1(11Z))	770.5101	13.84 Rpneg	329394	249974	280635	360961	149036	106905	154571	132835	186985	149986
PG(18:3(9Z,12Z,15Z)/18:1(11Z))	770.5095	0.849 HILICneg	1410101	1051627	1386533	523637	1399555	771517	615085	484746	660605	608732
PG(18:3(9Z,12Z,15Z)/18:1(11Z)) Esi-13.664	770.5101	13.664 Rpneg	144319	154027	90283	202588	285210	199781	325889	338015	330754	304859
PG(18:3(9Z,12Z,15Z)/18:1(11Z)) Esi-13.940001	770.5098	13.94 Rpneg	141335	103922	88025	148403	45086	34427	51764	36898	30844	1
PG(18:3(9Z,12Z,15Z)/18:1(11Z)) Esi-13.940001 :1	770.5094	13.94 Rpneg	141335	103922	88018	148327	44993	34324	51764	169766	184761	36512
PG(18:3(9Z,12Z,15Z)/20:2(11Z,14Z))	796.5279	1.111 HILICneg	412264	453756	460460	577706	168927	78072	289912	274533	176052	211803
PG(18:3(9Z,12Z,15Z)/20:2(11Z,14Z))	796.5262	13.75 Rpneg	105407	98144	140257	111563	48250	28255	1	53946	1	1
PG(18:3(9Z,12Z,15Z)/20:2(11Z,14Z)) Esi-1.123	796.5287	1.123 HILICneg	409809	369067	1	451227	194509	109445	1	1	1	1
PG(18:4(6Z,9Z,12Z,15Z)/20:0)	798.542	14.273 Rpneg	79821	108342	38200	84748	83816	70628	89177	54021	51069	90240
PG(18:4(6Z,9Z,12Z,15Z)/20:0)	798.5421	1.103 HILICneg	621116	509884	551321	627738	347861	155779	422733	373951	408402	455873
PG(18:4(6Z,9Z,12Z,15Z)/20:0) Esi-13.839998	798.5408	13.84 Rpneg	46693	49027	8322	47572	32572	32838	50100	47577	49565	54396
PG(19:0/17:1(9Z))	776.5558	14.635 Rpneg	1445062	1730112	1401110	2154697	902865	647699	765185	706525	1170124	1228427
PG(19:1(9Z)/15:1(9Z))	746.5084	13.982 Rpneg	1782228	2162123	1567414	1559435	1211322	1445857	1491284	1217472	1523332	1663976
PG(20:3(8Z,11Z,14Z)/16:0)	772.5241	1.131 HILICneg	1723336	1465368	1596258	1575103	873182	628266	1222491	1216470	1380914	1494709
PG(20:3(8Z,11Z,14Z)/22:6(4Z,7Z,10Z,13Z,16Z,19Z))	844.5231	0.803 HILICneg	192829	390146	246999	426721	139582	97840	105188	101279	94388	121692
PG(20:4(5Z,8Z,11Z,14Z)/0:0)	532.2793	12.482 Rpneg	6101	5811	5519	8290	1968	1972	4233	4542	2367	3223
PG(20:4(5Z,8Z,11Z,14Z)/20:3(8Z,11Z,14Z))	820.5234	0.813 HILICneg	1462943	2161029	1912417	1971602	696494	297346	576273	577747	513071	718177
PG(20:4(5Z,8Z,11Z,14Z)/20:3(8Z,11Z,14Z))	820.53	13.729 Rpneg	343748	386502	295364	421276	117952	1	92117	92912	99691	87059
PG(20:5(5Z,8Z,11Z,14Z,17Z)/15:0)	754.4804	5.405 HILICneg	161311	60669	105410	132143	1	20476	65089	67518	64687	80198
PG(22:0/12:0)	750.5402	14.61 Rpneg	270223	298704	214042	433673	115655	85187	109950	140086	110401	124338
PG(22:2(13Z,16Z)/16:0)	802.5712	14.738 Rpneg	90708	88296	81685	123521	21854	42323	46833	68120	55297	75102
PG(22:4(7Z,10Z,13Z,16Z)/15:1(9Z))	782.5145	5.315 HILICneg	254566	150669	175368	198643	125842	139192	1	125540	132908	130807
PG(22:4(7Z,10Z,13Z,16Z)/16:0)	798.5406	14.073 Rpneg	65847	38328	41421	42865	22586	1	1	31494	5319	1
PG(22:4(7Z,10Z,13Z,16Z)/22:6(4Z,7Z,10Z,13Z,16Z,19Z))	870.5396	1.097 HILICneg	1	1	78031	65958	106757	1	182027	66615	124221	148555
PG(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/0:0)	556.2799	12.474 Rpneg	23626	38640	30099	51487	13023	7135	7886	7102	8805	9693
PG(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/0:0) Esi-12.534	556.2792	12.534 Rpneg	37708	38640	30099	51487	13143	1	4369	6665	4118	1
PG(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/18:3(9Z,12Z,15Z))	816.4961	13.533 Rpneg	13465	13134	9206	15193	3347	2023	3032	3637	2529	2880
PG(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/20:4(5Z,8Z,11Z,14Z))	842.5121	0.798 HILICneg	404704	587068	557236	592723	145110	122073	135549	119898	114264	167663
PG(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/22:6(4Z,7Z,10Z,13Z,16Z,1	866.509	0.794 HILICneg	2184779	3702179	2801917	3229530	560620	353340	618794	634441	450175	622405
PG(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/22:6(4Z,7Z,10Z,13Z,16Z,1	866.5109	13.583 Rpneg	366525	440122	268128	481955	84961	50669	59273	68650	75586	65528
PG(O-18:0/18:3(6Z,9Z,12Z))	758.5406	14.455 Rpneg	1	21367	1	9894	14941	15348	7379	7964	23450	25379
TG(13:0/20:1/20:1)	889.8112	1.006 HILICpos	5731341	7600305	7096534	7110061	13446856	13914138		17172168	16117290	17052108
TG(14:0/20:2/20:2)	899.796	0.905 HILICpos	1.25E+08	79695400	84413872	75265480	2.2E+08	2.43E+08		2.78E+08	2.56E+08	3.02E+08
PG(P-18:0/15:1(9Z))	763.5162	13.535 Rpneg	25494	21735	23541	52298	71051	39474	49529	20943	1	63670
PG(P-18:0/15:1(9Z)) Esi-12.766999	764.5108	12.767 Rpneg	2355	1951	2577	3509	2797	1423	2742	6812	7266	2188
PG(P-18:0/17:0)	747.5822	25.801 Rppos	2335479	1928513	2134603	2235549	1581153	2124963	1711367	2313579	1927533	1802988
PG(P-18:0/17:0) Esi+25.218998	747.5782	25.219 Rppos	698926	349648	359697	448326	106591	90565	152293	228740	88488	118019
PG(P-20:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z))	894.5954	0.898 HILICneg	1	114078	117454	118412	1	60744	67152	72764	66881	73317
PGF1?	729.5403	21.645 Rppos	1800425	1946990	1801627	1660902	956065	1216931	1107334	1064716	1571678	1127982
PGF2?-11-acetate methyl ester	474.2841	1.255 HILICneg	145490	208733	129698	128821	280138	1	160723	157857	144137	207436
Phaseoluside A	926.5197	25.419 Rppos	2714771	2776378	2456999	2432868	2156399	2072742	2066162	1790642	1969372	1526029
Phe Gly	222.1021	9.089999 Rpneg	6532	13158	6008	8764	8761	7011	8050	5823	10047	6976
Phe Gly His	381.1423	5.911 HILICpos	589261	439151	341326	800421	428155	390510		746725	563926	539005
Phe Gly Phe Gly	426.1932	1.095 HILICneg	179119	62134	1	84788	204028	1	1	105450	1	123387
Phe Thr Pro	363.1787	9.479999 Rpneg	3767	1911	2349	2908	2455	2963	4495	3459	2936	5733
Phe Trp Lys	980.4888	22.187 Rppos	1	148036	1	1	464128	586059	369555	447820	484457	362508
TG(14:1/14:1/22:0)	847.7648	0.916 HILICpos	1.22E+08	64900852	42751152	54419580	78070608	83900264		96583968	75179368	87825968
Phe4Cl-HoPhe-OH	468.112	1.072 HILICneg	2446236	3079478	986309	2118595	5711117	1	728006	1512571	845557	1613048
Phencyclidine	243.1959	1.984 HILICpos	110709	145987	117269	239078	496344	139082		164892	295160	307480
Phenyl sulfate	173.9988	4.216 Rpneg	66278	113394	53135	50144	39604	54650	77570	41941	28444	44815
phenylalanine	165.079	3.68 Rppos	513360	590440	493549	606327	672343	503946	422820	617222	729372	652763
Phenylamil	627.1868	14.905 Rppos	456521	475959	535500	530447	508468	495804	564717	598166	707655	649965
Pheophorbide a	614.2549	22.181 Rppos	134929	183613	168668	81601	575757	780735	582404	702005	740933	671874
Pheophorbide a Esi+21.686998	614.2551	21.687 Rppos	282914	240368	320755	250514	285252	347908	304658	266048	219566	262963
Pheophorbide a Esi+21.936003	614.2544	21.936 Rppos	221441	259672	250048	191243	359279	421653	432543	439335	359780	376125
Phomenone	264.1374	10.601 Rpneg	1	3759	3707	3087	4780	1054	1234	2771	5340	2217
Phosphatidyl glycerol	246.0498	0.823 Rpneg	18144	16767	23532	23900	1	12893	15867	10517	10785	8994
Phosphatidyl glycerol Esi-0.8249999	264.06	0.825 Rpneg	11709	13776	20893	18342	6402	9275	11385	6912	1769	6138
Phosphoglycolic acid	155.9813	1.041 Rpneg	5889	4152	3853	4131	14732	19563	14909	2379	5193	2905
Phosphoric acid	97.9762	0.773 Rpneg	1089619	694617	881329	809831	437515	594675	1	578637	452052	563080
Phosphorylcholine	183.0664	0.842 Rppos	1532234	1236229	1318194	1365338	910856	880997	1002950	882524	778313	943998
Phytolaccoside I	964.4698	25.469 Rppos	822927	633446	435555	649245	587538	394433	458102	576233	438832	456168
Phytosphingosine	299.2822	10.503 Rppos	1088553	880273	975193	1028145	878783	1112148	1187739	1167540	1233592	1200102
PI(12:0/12:0)	698.3955	11.624 Rpneg	1089	1786	1	1601	921	3178	2590	959	1297	1473

PI(12:0/20:0)	827.5511	20.875 Rppos	519466	554347	656323	615939	281295	216550	373071	384478	281081	319057
PI(13:0/18:1(9Z))	840.4942	0.802 HILICneg	197348	195203	180678	187126	34895	160035	115258	38865	14385	29983
PI(14:0/16:0)	782.4936	21.984 Rppos	468565	646203	738839	737384	454223	1	539279	1	412264	567225
PI(14:0/18:4(6Z,9Z,12Z,15Z))	802.466	12.483 Rpneg	6210	2444	4247	3346	3364	884	2904	1888	4891	1283
PI(14:0/20:2(11Z,14Z))	834.5254	13.96 Rpneg	263227	37999	23436	428681	499951	502887	1	1	50648	39788
PI(14:0/22:2(13Z,16Z))	862.5561	14.298 Rpneg	549566	584672	797665	641828	1685986	1672576	767240	1947117	928776	1233474
PI(14:0/22:2(13Z,16Z)) Esi-14.145002	862.5554	14.145 Rpneg	7458	24477	6437	24347	6374	1	3654	1960036	1070294	858919
PI(15:0/16:0)	796.5124	0.818 HILICneg	644574	964922	615183	531470	169385	281381	162547	159815	409921	194713
PI(15:0/20:5(5Z,8Z,11Z,14Z,17Z))	841.5167	23.264 Rppos	382972	315993	392801	366812	414802	442403	473504	494969	495901	492317
PI(15:1(9Z)/18:1(9Z))	854.5688	1.422 HILICpos	189122	385268	108896	108346	201226	141040		99053	181482	93282
PI(15:1(9Z)/22:4(7Z,10Z,13Z,16Z))	874.498	24.652 Rppos	528031	530163	371376	474963	629357	458165	500121	519469	522125	455502
PI(16:0/0:0)	572.296	12.717 Rpneg	14574	12110	11262	13998	6003	4356	7269	7225	6922	7081
PI(16:0/0:0) Esi-5.0320005	618.2952	5.032001 Rpneg	1778	2420	3266	4210	1029	2159	1593	1688	2235	2558
PI(16:1(9Z)/22:2(13Z,16Z))	934.5846	13.266 Rpneg	25045	11731	8123	12218	9711	7214	11034	10973	14555	10595
PI(16:1(9Z)/22:6(4Z,7Z,10Z,13Z,16Z,19Z))	880.5095	13.682 Rpneg	10979	12066	8091	10290	3697	1	3691	4005	2465	1975
PI(17:1(9Z)/18:0)	850.5578	14.386 Rpneg	46872	45050	72223	50133	46559	33566	51504	32874	49277	38869
PI(17:1(9Z)/18:0) Esi-14.066001	850.5563	14.066 Rpneg	1	12147	1	14315	8869	37154	39322	65939	6456	34573
PI(17:2(9Z,12Z)/20:0)	876.5764	14.452 Rpneg	15904	13897	14076	11634	23508	16982	16517	20247	25569	22247
PI(17:2(9Z,12Z)/20:0) Esi-14.448	876.5751	14.448 Rpneg	15764	13897	14361	11794	23530	16875	15626	19665	25569	22406
PI(18:0/0:0)	600.3266	13.05 Rpneg	135299	116494	134737	149832	104269	83229	146821	142935	182642	152153
PI(18:0/16:0)	838.5543	11.058 Rpneg	7092	4680	1	1	2001	15400	1036	1378	6400	10229
PI(18:0/18:1(9Z))	864.5723	14.559 Rpneg	306991	351485	322830	331337	399513	375783	326580	577025	759770	564102
PI(18:1(9Z)/0:0)	598.3126	12.792 Rpneg	1	23333	16076	18514	15272	14740	29593	23627	25291	24344
PI(18:1(9Z)/0:0) Esi-12.707	598.3121	12.707 Rpneg	1	23042	8394	8956	9170	9996	29585	16788	17972	15612
PI(18:1(9Z)/20:3(8Z,11Z,14Z))	886.5556	14.236 Rpneg	2787049	3016533	750459	758418	7105184	6417370	3704820	7292383	3352239	563691
PI(18:1(9Z)/20:3(8Z,11Z,14Z)) Esi-14.120001	886.5556	14.12 Rpneg	1	3262641	122272	2709501	7098861	6423523	4160937	7298414	4721354	56396
PI(18:2(9Z,12Z)/0:0)	596.2964	12.455 Rpneg	16600	23598	29121	38083	41822	34515	44959	58885	68361	57255
PI(18:2(9Z,12Z)/0:0) Esi-12.538001	596.2984	12.538 Rpneg	7810	1	1	41361	9149	8775	59787	14153	68785	13296
PI(18:2(9Z,12Z)/19:1(9Z))	873.5764	19.392 Rppos	43959	112322	144902	160959	37186	147684	189126	134562	115924	168811
PI(18:2(9Z,12Z)/20:3(8Z,11Z,14Z))	884.5407	13.947 Rpneg	1178056	1165845	1049915	1069130	1316810	904394	1235385	1341649	1233426	1130088
PI(18:2(9Z,12Z)/22:1(11Z))	916.6019	14.877 Rpneg	3643	5042	2352	3360	4830	1	4119	3599	6068	4178
PI(18:2(9Z,12Z)/22:6(4Z,7Z,10Z,13Z,16Z,19Z))	906.5252	13.756 Rpneg	16163	16816	11925	14757	7795	1972	7340	8151	4301	4594
PI(18:2(9Z,12Z)/22:6(4Z,7Z,10Z,13Z,16Z,19Z))	923.5531	24.383 Rppos	268050	233800	229820	237363	272157	237007	172658	212736	182644	189143
PI(18:3(6Z,9Z,12Z)/18:0)	860.5405	13.986 Rpneg	521978	547772	500822	438591	973021	771480	796410	1011289	1183046	1004501
PI(18:3(6Z,9Z,12Z)/18:1(9Z))	875.5595	25.402 Rppos	1418324	1721274	1484869	1358175	1617790	1313748	1391159	1678067	1649841	1541157
PI(18:3(6Z,9Z,12Z)/19:1(9Z))	872.547	14.051 Rpneg	68192	71352	60718	58652	57744	40790	46503	47430	60735	52459
PI(18:3(9Z,12Z,15Z)/18:1(11Z))	858.5256	13.916 Rpneg	701841	636503	532863	622518	329529	305690	446640	242030	232346	202435
PI(18:3(9Z,12Z,15Z)/20:3(8Z,11Z,14Z))	882.5258	13.88 Rpneg	508941	405806	395787	462353	80094	22706	77184	51641	25834	24786
PI(18:3(9Z,12Z,15Z)/20:3(8Z,11Z,14Z)) Esi-13.8029995	882.5256	13.803 Rpneg	508941	405806	395787	462353	87989	46601	95156	106513	79668	79850
PI(18:4(6Z,9Z,12Z,15Z)/18:4(6Z,9Z,12Z,15Z))	850.4646	12.475 Rpneg	3172	1023	1546	1801	1	1	1	1	1	1
PI(19:1(9Z)/18:3(9Z,12Z,15Z))	918.5483	13.276 Rpneg	2615	1314	1	1786	1222	872	2155	2496	3610	2708
PI(20:0/18:2(9Z,12Z))	890.5895	14.698 Rpneg	1	21483	17814	1	32988	25717	32290	9267	34559	1
PI(20:2(11Z,14Z)/18:0)	936.6027	13.043 Rpneg	967	1743	2746	3577	1948	1611	1486	1773	1639	3275
PI(20:3(8Z,11Z,14Z)/18:0)	888.5724	14.406 Rpneg	237544	277839	240630	207972	444303	311549	313913	256562	517694	240847
PI(20:4(5Z,8Z,11Z,14Z)/0:0)	620.2948	12.447 Rpneg	147731	216432	205113	303971	231835	176325	302912	281750	253023	276916
PI(20:4(5Z,8Z,11Z,14Z)/0:0) Esi-12.446	620.2951	12.446 Rpneg	147731	216452	248665	242741	1	176936	303044	284065	253738	277966
PI(20:4(5Z,8Z,11Z,14Z)/0:0) Esi-12.447999	620.2954	12.448 Rpneg	38652	216432	248665	303971	232557	176325	302912	282747	253023	276548
PI(20:5(5Z,8Z,11Z,14Z,17Z)/0:0)	618.2836	15.316 Rpos	423638	382056	431856	389111	322198	450268	410195	370024	385561	327231
PI(20:5(5Z,8Z,11Z,14Z,17Z)/18:3(9Z,12Z,15Z))	895.5242	22.618 Rppos	476408	738921	522337	462687	706550	681021	525903	630875	460222	489800
PI(22:3(10Z,13Z,16Z)/18:3(9Z,12Z,15Z))	910.5568	14.14 Rpneg	554871	463792	679177	607262	500247	324388	633159	457143	378495	382083
PI(22:3(10Z,13Z,16Z)/18:3(9Z,12Z,15Z)) Esi-14.140001	910.5568	14.14 Rpneg	542685	463792	673762	617117	500247	324388	633159	457143	378495	382083
PI(22:4(10Z,13Z,16Z,19Z)/18:0)	914.5882	14.527 Rpneg	114980	100596	105368	116558	121485	64510	100348	88365	131201	88720
PI(22:4(7Z,10Z,13Z,16Z)/17:0)	900.5748	14.4 Rpneg	44965	43286	31941	39116	43541	30050	34292	35392	44557	39014
PI(22:4(7Z,10Z,13Z,16Z)/17:1(9Z))	898.5561	14.08 Rpneg	19252	20350	17259	18383	13632	9897	13712	12012	18263	9418
PI(22:4(7Z,10Z,13Z,16Z)/17:1(9Z)) Esi-14.081999	898.5528	14.082 Rpneg	23040	15308	22749	18590	14820	7471	12762	14236	8921	12178
PI(22:4(7Z,10Z,13Z,16Z)/19:1(9Z))	972.5944	13.255 Rpneg	5190	1813	1142	2767	1207	1	1431	1	1273	785
PI(22:4(7Z,10Z,13Z,16Z)/22:0)	970.6573	1.412 HILICpos	428738	1279066	1	55445	164253	259158		51474	74133	68467
PI(22:5(4Z,7Z,10Z,13Z,16Z)/18:0)	912.5728	14.298 Rpneg	258334	179581	426411	204083	186245	116698	218921	157708	136946	151222
PI(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/0:0)	644.2971	12.441 Rpneg	14345	18046	22915	36416	15723	9572	26008	19855	12514	16683
PI(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/0:0) Esi-12.443	644.3005	12.443 Rpneg	4629	18046	6558	36416	15723	9572	26008	19300	12514	16437
PI(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/17:2(9Z,12Z))	891.5301	24.724 Rppos	502994	522203	380011	401542	585605	423748	442520	452037	491595	478993
PI(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/18:1(9Z))	908.5415	13.907 Rpneg	134474	120885	107674	122621	78224	29275	83527	72202	40527	38911
PI(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/22:6(4Z,7Z,10Z,13Z,16Z,19	976.5104	26.986 Rppos	1141382	1140760	1131288	897069	1250374	1280360	1042240	850402	896076	838339
PI(O-16:0/16:0)	813.5683	22.304 Rppos	313457	285711	620838	607828	531029	435925	392277	458744	227459	283692
TG(14:1/18:0/18:0)	849.7787	0.99 HILICpos	1.37E+08	90004672	63555792	77767960	1.31E+08	1.48E+08		1.57E+08	1.21E+08	1.56E+08
PI(O-16:0/20:1(11Z))	896.5958	12.691 Rpneg	1	1	1	1	1937	1868	2528	1630	5485	2895
PI(P-16:0/20:4(5Z,8Z,11Z,14Z))	902.5556	13.624 Rpneg	16489	4395	7710	5084	3343	3874	3552	6338	7225	5201
PI(P-18:0/20:4(5Z,8Z,11Z,14Z))	916.5664	4.788001 HILICneg	121169	229035	160819	170124	222908	171780	210351	255434	217636	238752
PI(P-18:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z))	940.5708	4.771 HILICneg	55152	90482	77577	89794	78217	58866	59008	77456	59701	83143
PI-Cer(d18:0/18:0)	791.5824	21.893 Rppos	1	1	1	1	568759	653450	606845	610623	1	604902
PI-Cer(d20:0/16:0)	809.5808	14.351 Rpneg	10683	24047	1	9914	8198	6685	7245	8005	4744	4607
Pilocarpic acid	226.1318	9.048999 Rpneg	1760803	3686178	2330000	2355592	1944579	2450102	2407224	2068170	3492691	3177693
Pilocarpic acid	226.1332	1.1 HILICneg	3495030	1.82E+07	1.24E+07	1.10E+07	7071141	3260272	1.46E+07	1.24E+07	2.37E+07	2.01E+07
TG(15:0/15:0/18:2)	819.7342	0.895 HILICpos	22354116	9726310	3287416	5515359	3773724	4608028		5790276	5796161	5018235
PIP(18:1(9Z)/20:4(5Z,8Z,11Z,14Z))	968.4867	26.968 Rppos	685033	784556	663391	655736	783815	384809	671147	589069	611720	591027
PIP2(18:1(9Z)/16:0)	996.4753	23.151 Rppos	341266	251293	318082	274523	317645	218962	217982	294551	261530	275481
PIP2(18:2(9Z,12Z)/16:0)	994.4628	21.921 Rppos	477662	555826	485255	409334	749150	802042	771894	701118	540283	645354
PIP2(18:2(9Z,12Z)/16:0) Esi+22.601	994.4605	22.601 Rppos	318321	288671	274369	214084	541949	349948	377553	351288	322360	385320
Pipercitine	331.3237	9.773001 Rppos	554637	1105594	1228257	1160563	1672048	759256	1003551	1285464	1223094	1120166
Pipericine	335.3175	1.033 HILICpos	898122	466980	363303	563415	1072438	270144		539387	462506	1542980
Pirbuterol	240.1472	7.762 HILICpos	848966	1198982	828797	768544	1026513	1292422		877783	736186	849626
Pirimicarb	238.1418	4.876 Rppos	859611	2212867	1009976	1667965	2129263	986050	895558	1519211	2353698	1386689
Pirimicarb	238.1424	1.575 HILICpos	491173	456565	264260	614701	584135	355115		593218	561058	510089
piritramide	877.575	27.019 Rppos	1309826	1555668	1858028	1440151	1650504	2148614	1946016	1536253	1766858	1635436
Pisumionoside	404.2046	7.178001 Rpneg	15908	19665	15399	21688	25057	15456	15224	17987	23232	18530
Pisumionoside Esi-7.1780005	404.204	7.178001 Rpneg	15908	19665	15399	21688	25057	15456	15224	17987	23236	18530
Pisumionoside Esi-7.1780005 :1	404.2052	7.178001 Rpneg	15908	19665	15399	21688	25057	15456	15224	17987	23232	18530
Pisumionoside Esi-7.6320004	450.2081	7.632 Rpneg	9058	11337	777	1599	1712	1	897	1271	2446	963
Pivampicillin	463.1793	1.322 Rpneg	42084	24920	65847	39344	6579	28707	36650	24250	11907	21565
Poloxalene	164.1046	4.695 Rppos	181953	389551	298879	367410	409515	325576	221756	246918	414274	239146
Polyoxyethylene 40 monostearate	328.2996	13.194 Rpneg	11533	8200	8326	8029	13199	1	7916	9000	1	1
Polyoxyethylene dioleate	590.5268	13.123 Rpneg	18354	13979	15225	14272	13259	12189	12993	14256	14491	13789

poststerone	362.2103	11.424	Rpneg	2630	3569	3311	4031	2740	2382	1138	1996	1907	2776
Pregabalin Esi+5.1860003	159.1256	5.186	HILICpos	1559482	1696823	1118723	2141091	1067715	2579906		2473938	1321414	1721509
Pro Gly Lys	282.1679	5.139	Rppos	799300	1622356	820360	1362604	1809047	861042	815408	1316195	1929397	1167712
Pro Lys Lys	353.2441	7.114999	Rppos	92804	220151	66753	208298	227332	112222	126495	154602	370908	166899
Pro Tyr Val	377.1971	0.915	HILICneg	166167	115150	52764	85976	364512	150908	91269	92665	119651	214108
Proflavine	464.1978	0.796	HILICneg	12333	8990	6026	3085	28160	1	38597	27348	35301	38860
Propane-1,2-diol 1-phosphate	155.0346	0.853	Rppos	383199	459084	405641	469880	259955	451208	232471	264180	403606	337166
Propicillan	378.1215	10.356	Rpneg	3817	3309	3334	3616	3907	3458	3804	3689	4020	3947
propionyl carnitine	217.1317	4.989	HILICpos	10646629	5229570	5463510	4619715	10930791	9334132		9209785	6133410	9376878
propionylcarnitine	217.1314	1.972	Rppos	2427423	955641	1013926	976912	2209735	1904772	1774729	2120938	1317715	1895891
Propyl heptanoate	172.1466	10.684	Rpneg	82137	65383	56895	58771	64283	58128	47522	57686	70958	52947
Propylene glycol mono- and diesters of fats and fatty acids	510.466	21.564	Rppos	3455211	3287931	2451342	2809846	2022914	1512592	2143389	2071025	3134573	2194377
Propylene glycol mono- and diesters of fats and fatty acids Es	510.4654	23.81	Rppos	1088843	1438779	1492064	1559783	1055229	1063279	1068466	1020117	1325455	1127830
Prosafrinine	300.2775	8.309999	Rppos	924926	1167848	1364166	1510710	1050343	1249446	1398500	1593596	1662473	1704992
Prosopinine	287.247	12.475	Rpneg	11635	10801	8699	7476	7158	6585	9306	7513	10046	9508
Prostaglandin D2-1-glyceryl ester	426.2642	12.763	Rpneg	14216	5323	3053	5259	6818	2901	4358	5773	11139	2944
PS(12:0/13:0)	637.39	5.244999	HILICpos	2784215	807115	819307	408687	282197	229223		426693	649037	464092
PS(12:0/16:1(9Z))	677.4281	15.174	Rppos	502478	620183	469577	550467	190853	556183	943063	406083	571256	574063
PS(12:0/16:1(9Z)) Esi+14.824999	677.4285	14.825	Rppos	165629	179286	123938	177354	73973	160819	294306	132901	208883	240424
PS(13:0/12:0)	637.3922	15.124	Rppos	1814031	396509	292109	321766	266357	335342	563532	343936	367612	334000
PS(14:0/22:0)	791.5636	1.533	HILICpos	19944360	20626652	22638724	28108660	18974244	16695342		18125844	16670026	19378702
PS(15:0/12:0)	647.4179	16.041	Rppos	351018	311512	253072	272639	117451	301171	477568	259793	304331	324808
PS(16:1(9Z)/20:1(11Z))	787.5345	13.898	Rpneg	1	62885	17679	27031	27320	75001	22152	24293	44552	41734
PS(17:1(9Z)/19:0)	789.551	14.581	Rpneg	841419	1004014	784627	1036722	513319	529841	640338	781728	806681	824247
PS(17:1(9Z)/19:1(9Z))	787.5365	14.319	Rpneg	116011	105485	84751	83508	155679	172390	139038	153639	196538	202215
PS(17:1(9Z)/19:1(9Z)) Esi-14.319	787.5358	14.319	Rpneg	115904	104750	86523	82837	115122	164604	116604	149618	161009	180741
TG(15:0/16:1/17:0)	821.749	0.921	HILICpos	25114314	15391652	6447705	8919105	6874257	9888820		7475008	11186666	9101323
PS(17:1(9Z)/21:0)	817.5906	1.509	HILICpos	2984649	2815029	3424510	3272098	2531644	2576016		1985170	1783943	2227956
PS(18:0/20:0)	801.5872	20.519	Rppos	62015	95975	55362	32501	75299	271355	122215	121941	211039	209881
PS(18:0/22:2(13Z,16Z))	847.5651	25.046	Rppos	1330736	1374312	1210381	1433022	1504456	1316780	1300392	1413136	1350120	1439147
PS(18:1(9Z)/0:0)[U]	523.29	12.694	Rpneg	5245	2125	1962	3090	1653	1795	1704	2104	3201	2571
PS(18:1(9Z)/18:3(6Z,9Z,12Z))	783.5104	13.895	Rpneg	7927	21014	19194	19052	19257	17694	17649	15744	17810	26793
PS(18:1(9Z)/18:3(6Z,9Z,12Z)) Esi-13.891001	783.5084	13.891	Rpneg	8624	20885	15354	20516	17385	19177	14158	20993	18157	26952
PS(18:1(9Z)/19:1(9Z))	819.5666	14.369	Rpneg	29535	33174	27106	37856	34404	33565	28230	44859	44273	51917
PS(18:2(9Z,12Z)/20:0)	815.5689	19.636	Rppos	1180131	1483361	1284420	1019411	722959	682383	1433092	601732	839210	523995
PS(18:2(9Z,12Z)/22:6(4Z,7Z,10Z,13Z,16Z,19Z))	831.5063	13.757	Rpneg	53091	43705	24352	31564	45510	39547	44134	53618	48512	53084
PS(18:3(6Z,9Z,12Z)/20:0)	813.5514	14.396	Rpneg	206305	261306	179286	218378	166234	111290	171287	173670	151560	192273
PS(18:3(6Z,9Z,12Z)/21:0)	827.5716	4.823	HILICneg	1271623	1442513	1455931	826449	1507404	1165165	1446563	1505123	1491415	1448715
PS(18:3(6Z,9Z,12Z)/22:0)	841.5854	20.691	Rppos	207734	803482	596797	564066	119417	664980	571342	208450	540758	629625
PS(18:3(9Z,12Z,15Z)/22:0)	841.5786	13.06956	Rpneg	5574	16174	1	11081	19624	17953	17485	18153	12516	13608
PS(18:3(9Z,12Z,15Z)/22:0)	841.5819	4.913001	HILICneg	5362489	6376267	5911633	6276945	5537442	4812437	5565358	5569597	4995747	5627422
PS(18:3(9Z,12Z,15Z)/22:0) Esi-12.696	841.5798	12.696	Rpneg	1	1	6864	1	4671	4712	2360	12591	3704	2683
PS(18:4(6Z,9Z,12Z,15Z)/20:0)	811.5377	14.269	Rpneg	244486	249256	226657	127724	264798	148659	248397	320461	147728	332101
PS(18:4(6Z,9Z,12Z,15Z)/20:0) Esi-14.268999	811.5374	14.269	Rpneg	241449	218203	224803	244955	251360	148741	118130	238182	86757	104141
PS(18:4(6Z,9Z,12Z,15Z)/22:2(13Z,16Z))	835.5354	14.14	Rpneg	1622518	1932553	48213	1758423	726041	623094	23041	37294	33879	733094
PS(18:4(6Z,9Z,12Z,15Z)/22:2(13Z,16Z)) Esi-14.069	835.5352	14.069	Rpneg	1328213	1913478	14711	1721858	1659793	1738373	27656	1275241	26987	22660
PS(19:1(9Z)/19:1(9Z))	815.5629	14.702	Rpneg	44511	40650	35446	38941	38274	48208	36740	41331	70216	82334
PS(19:1(9Z)/19:1(9Z)) Esi-14.701998	815.5647	14.702	Rpneg	43567	40611	35718	39216	38303	48315	63526	40263	70581	47272
PS(19:1(9Z)/21:0)	845.6147	14.493	Rpneg	221355	872602	648754	464927	334012	457128	318072	287643	808418	841416
PS(20:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z))	863.5669	4.874	HILICneg	256421	305835	298895	309348	234956	252369	286973	272917	273607	283894
TG(16:0/17:1/22:2)	915.8205	0.997	HILICpos	1347180	1	2291268	1	5740108	6566597		6348382	6953111	7721913
PS(20:2(11Z,14Z)/20:2(11Z,14Z))	839.567	14.519	Rpneg	453250	543128	395912	460802	401747	395145	382907	398102	471133	550520
PS(20:2(11Z,14Z)/20:2(11Z,14Z))	839.57	4.924	HILICneg	292115	330556	198227	271172	252196	267583	193902	450759	396985	244976
PS(20:3(8Z,11Z,14Z)/0:0)	529.2809	11.92	Rppos	618988	879402	723669	761228	922825	978985	934972	808388	998828	767441
PS(20:3(8Z,11Z,14Z)/20:1(11Z))	839.5666	14.519	Rpneg	420711	478842	366675	428719	374051	314852	333943	355684	425797	507633
PS(20:4(5Z,8Z,11Z,14Z)/0:0)	545.2746	12.429	Rpneg	3437	3415	2536	4009	2195	1742	2827	3875	2648	3009
PS(20:4(5Z,8Z,11Z,14Z)/22:6(4Z,7Z,10Z,13Z,16Z,19Z))	855.5055	13.725	Rpneg	36534	30584	20820	27648	21302	14661	20614	18726	17398	20126
PS(20:5(5Z,8Z,11Z,14Z,17Z)/18:1(9Z))	807.508	13.877	Rpneg	63267	78177	48741	61989	55301	41443	50758	63742	49859	51004
PS(20:5(5Z,8Z,11Z,14Z,17Z)/18:3(9Z,12Z,15Z))	849.4821	1.241	HILICneg	177585	107394	199784	186753	61963	1	133794	103602	88656	111659
PS(20:5(5Z,8Z,11Z,14Z,17Z)/18:4(6Z,9Z,12Z,15Z))	801.4622	9.781999	Rpneg	5476	1797	2551	3435	1481	1547	739	1	1050	3113
PS(20:5(5Z,8Z,11Z,14Z,17Z)/22:6(4Z,7Z,10Z,13Z,16Z,19Z))	853.4869	0.906	HILICneg	416979	193824	127628	171791	442961	49733	149727	151400	265387	193279
PS(21:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z))	899.563	20.284	Rppos	1165835	713645	679812	788454	883123	594001	843200	645214	666883	538933
PS(22:0/0:0)	581.3669	5.752999	HILICneg	373552	609560	429260	388375	482381	354179	372052	339307	317226	334585
TG(16:0/18:1/19:0)	891.824	1.039	HILICpos	1	1	1	1	6115425	9274996		6963122	7430764	4983565
PS(22:0/0:0)	581.3689	13.612	Rpneg	9318	5852	14648	7180	11188	4476	5684	11997	14158	5350
PS(22:0/0:0) Esi-13.515001	581.3722	13.515	Rpneg	20219	6975	6669	8612	11060	4305	5112	5535	7013	4633
PS(22:0/18:3(9Z,12Z,15Z))	841.5845	21.5	Rppos	135372	321084	403351	295179	42031	186862	293674	163605	359384	368164
PS(22:1(11Z)/0:0)	579.352	13.24	Rpneg	27024	14129	14288	18005	15297	11278	18777	18568	24180	17377
PS(22:1(11Z)/0:0)	579.3535	12.959	Rppos	1462595	518965	477067	476997	159609	279761	387891	190287	172052	223712
PS(22:1(11Z)/0:0)	579.3553	5.775001	HILICneg	448079	951651	497166	436378	1020604	640510	716976	647243	540040	536800
PS(22:1(11Z)/0:0) Esi-13.234999	579.352	13.235	Rpneg	167775	6856	1747	16130	14983	11028	17451	17142	22733	16809
PS(22:1(11Z)/0:0) Esi-13.339998	579.3523	13.34	Rpneg	94452	15667	14486	16875	13099	12229	14647	16153	41396	15088
PS(22:1(11Z)/16:0)	799.57	20.653	Rppos	57646	95995	50936	1	64064	281356	248876	206770	330378	229658
PS(22:2(13Z,16Z)/20:1(11Z))	869.6107	4.869999	HILICneg	5835972	6037809	6696220	6581200	5797023	4877054	6489105	6302144	6029937	6352012
PS(22:2(13Z,16Z)/20:1(11Z))	869.6141	13.858	Rpneg	137189	542765	279556	250997	506968	522239	647316	1029673	519118	288588
TG(16:0/18:3/22:5)	919.7684	0.873	HILICpos	27534124	29052232	31246520	29916628	24979922	14201351		22393286	12430192	12476719
PS(22:4(7Z,10Z,13Z,16Z)/17:0)	825.557	14.311	Rpneg	23289	32639	27031	35327	39515	35011	34748	42990	25486	31824
PS(22:4(7Z,10Z,13Z,16Z)/17:0) Esi-13.858001	825.5533	13.858	Rpneg	19619	5713	3705	5238	1	1	2735	1	20259	5741
PS(22:4(7Z,10Z,13Z,16Z)/17:1(9Z))	823.5393	24.698	Rppos	411758	304954	371011	450474	360059	510321	366188	376859	373385	380117
PS(22:4(7Z,10Z,13Z,16Z)/19:0)	853.5845	14.552	Rpneg	1	20132	1	1	24795	16974	19118	23674	1	24552
PS(22:4(7Z,10Z,13Z,16Z)/20:1(11Z))	865.582	4.888	HILICneg	2480385	2876494	2921170	2944233	2124110	1711784	2017963	1905351	1537043	1833414
PS(22:4(7Z,10Z,13Z,16Z)/20:1(11Z)) Esi-4.8870006	865.6071	4.887001	HILICneg	3610097	4114828	4267654	4012471	2367769	2052765	2389370	2408528	1203350	2359049
PS(22:4(7Z,10Z,13Z,16Z)/22:1(11Z))	893.6131	4.846	HILICneg	2127699	2106421	2492245	2045497	1746335	1572257	1769661	1616935	1406467	1749644
PS(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/0:0)	569.2747	12.426	Rpneg	1	30640	25414	38853	18297	19717	30566	23113	20626	27860
PS(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/0:0) Esi-12.495001	569.2761	12.495	Rpneg	36743	7821	8416	11361	4993	19340	30566	5527	5055	27860
PS(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/18:1(9Z))	833.5213	0.804	HILICneg	1	59044	22291	102573	1	1	24726	23451	18947	50068
PS(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/20:1(11Z))	861.5517	0.783	HILICneg	8729	51510	92589	102140	62493	1	37247	55102	21767	80200
PS(O-16:0/17:0)	717.533	24.723	Rppos	1328171	1623864	1266066	1122653	1245937	1951243	1574865	1411479	1658191	1866609
PS(O-16:0/18:0)	731.547	22.838	Rppos	6527237	7451439	5017306	5456068	6761053	9269215	6920900	6428092	8431978	7331752
PS(O-16:0/18:0) Esi+23.106	731.547	23.106	Rppos	1060835	2702229	933505	1576041	1	1	1	1	1	1
PS(O-16:0/19:0)	745.5662	27.053	Rppos	2212283	1928078	2179001	2180471	1523807	3048735	2467554	1996185	2467966	2719673
PS(O-16:0/20:0)	759.577	24.706	Rppos	1.54E+08	1.9E+08	1.78E+08	1.55E+08	1.46E+08	1.69E+08	1.47E+08	1.31E+08	1.45E+08	1.34E+08

PS(O-16:0/20:0) Esi+20.070002	759.5781	20.07	Rppos	28388884	19288356	24588056	22234648	25498426	26834500	30969520	24336736	20212768	18874612	
PS(O-16:0/20:1(11Z))	821.5831	14.709	Rpneg	99593	137380	138007	135978	1	95072	75701	73674	114072	131461	
PS(O-16:0/20:2(11Z,14Z))	755.5488	22.354	Rppos	2846626	2830301	3246822	3135716	1867041	3210851	1995530	1789089	2170671	2690295	
PS(O-16:0/22:0) Esi+23.162	787.6068	23.162	Rppos	9471353	7781482	9601678	9615722	5158185	4338704	6279339	6584520	5099139	5630479	
PS(O-18:0/0:0)	571.3477	13.552	Rpneg	3150	1289	1215	1588	1	1	1	1	1	1	
PS(O-18:0/0:0)	557.3258	5.678001	HILICneg	57037	102416	71980	80205	94495	93063	86663	93582	81067	71737	
PS(O-18:0/19:1(9Z))	835.5935	13.307	Rpneg	10446	6547	1	3254	5083	17140	6010	1	6908	5762	
PS(O-20:0/0:0)	521.3482	13.356	Rppos	2274816	2110107	2594768	2242100	1807786	2904666	2380498	1995767	2153324	2193667	
PS(O-20:0/0:0) Esi+12.807001	521.3484	12.807	Rppos	1055429	1152655	1226256	1098333	998417	1496895	1184765	1217980	1299290	961475	
PS(O-20:0/17:0)	773.5909	25.824	Rppos	6092224	7468638	8706451	6985162	5188874	7145266	5652588	5465435	6301962	5500887	
PS(O-20:0/20:0)	837.6213	22.732	Rppos	554853	535999	486322	417802	888563	376074	1058279	830338	780828	667041	
PS(O-20:0/20:3(8Z,11Z,14Z))	809.594	24.408	Rppos	7326892	6706800	5700359	6700688	9683274	6100198	4211672	4571220	8812478	6374095	
PS(O-20:0/22:4(7Z,10Z,13Z,16Z)) Esi+20.686998	835.6094	20.687	Rppos	9389997	5458622	6405391	5513429	7174608	3929525	7968055	5191506	3408368	3161411	
PS(O-20:0/22:4(7Z,10Z,13Z,16Z)) Esi+22.696	857.5887	22.696	Rppos	485720	532479	432304	389305	645713	398822	303724	331396	401255	300907	
PS(O-20:0/22:4(7Z,10Z,13Z,16Z)) Esi+25.824001	835.6088	25.824	Rppos	8369486	8116463	12145696	9167398	9084633	10311411	9421457	8506065	7275517	8070672	
PS(O-20:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z))	831.5764	22.799	Rppos	18380562	16972704	22389812	20519376	22217086	24802576	19854300	17919784	16600086	22303484	
PS(O-20:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z))	849.5862	4.813	HILICneg	514923	613832	624025	687779	610243	526379	509511	512565	504525	520144	
PS(O-20:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z)) Esi+22.17	831.5779	22.17	Rppos	2110596	3862207	1682807	2979156	6373082	9830264	6652960	7678567	2763755	7623335	
PS(P-16:0/12:0)	663.4513	1.126	HILICpos	1304513	2763454	1779148	1778634	1048375	1		1960001	5066101	950772	
PS(P-16:0/21:0)	793.5498	22.813	Rppos	409827	595075	293730	272626	204304	170597	502435	295458	187045	131114	
PS(P-18:0/0:0)	509.3127	13.093	Rpneg	37031	2712	1164	2229	2683	800	1273	1835	2462	1	
PS(P-18:0/15:1(9Z))	777.5116	1.026	HILICneg	349820	121888	470195	1	226485	166951	399216	458457	212371	200264	
PS(P-18:0/17:2(9Z,12Z))	739.5148	23.021	Rppos	6803578	8073493	6872770	6350929	5272033	7662210	6621770	6323208	7145471	6640196	
PS(P-18:0/18:1(9Z))	755.5487	21.803	Rppos	2538639	3033386	2460819	2123433	3757272	6065532	3896809	3638399	6542343	4718122	
PS(P-18:0/18:2(9Z,12Z))	753.5353	21.42	Rppos	2482323	2154170	2224282	2767961	646260	829946	1026233	730071	739539	751846	
PS(P-18:0/20:4(5Z,8Z,11Z,14Z))	777.5326	23.555	Rppos	2248383	2167535	2552182	2412181	1013710	1566803	1743519	1340503	1412365	1619912	
PS(P-18:0/22:4(7Z,10Z,13Z,16Z))	805.5651	25.54	Rppos	247671	353727	351343	314592	319128	553568	346677	361485	603119	661222	
PS(P-20:0/13:0)	715.5161	23.305	Rppos	2947934	3885818	3016616	2014309	2489115	3091038	3155097	2965352	3018332	3323729	
PS(P-20:0/14:0)	747.5407	1.533	HILICpos	3818672	1852552	2431114	3691470	2917178	3086784		3316852	3374505	2885056	
PS(P-20:0/15:0)	743.5476	25.333	Rppos	8021497	10583410	9572217	7265025	7383051	9300395	9144522	8082395	8288206	9318500	
PS(P-20:0/15:0) Esi+22.421001	743.5486	22.421	Rppos	2459420	3117707	2913565	2262256	1662296	2519382	2484945	2785029	2380653	2807924	
PS(P-20:0/17:0) Esi+19.399998	771.5867	19.4	Rppos	851208	760623	997491	663400	348719	610041	526102	334289	957355	1092007	
PS(P-20:0/17:2(9Z,12Z))	767.5467	24.973	Rppos	21970276	27164204	26541680	22529516	20093744	24682138	23288992	22081982	23540256	21301722	
TG(16:0/20:4/22:5)	945.7829	0.871	HILICpos	14606281	16732763	15189886	16878780	12087227	7657257		11555810	6852811	7293556	
PS(P-20:0/17:2(9Z,12Z)) Esi+20.313997	767.5489	20.314	Rppos	6247214	3829990	4430730	4155962	4866444	3878317	6120736	3451490	3735120	3283277	
PS(P-20:0/17:2(9Z,12Z)) Esi+22.166	767.5494	22.166	Rppos	3896077	3472347	3963734	4689874	1836627	2212782	2339296	2725200	1625592	1760015	
PS(P-20:0/18:0) Esi+24.782	785.5918	24.782	Rppos	3922573	5361131	5144064	4287354	6564666	7936116	6350011	6507333	8818311	7400194	
PS(P-20:0/18:1(9Z)) Esi+23.813002	783.5775	23.813	Rppos	14103099	17286040	17032170	14542821	13762459	15313211	15388781	15251711	13711705	12888374	
PS(P-20:0/19:0)	799.6141	25.917	Rppos	1018149	1033295	1168800	920825	2265781	3334383	1871804	2683805	3855307	3255140	
PS(P-20:0/19:1(9Z))	814.6205	1.525	HILICpos	4625175	4274944	5469498	5690271	4700833	4678573		3221240	4188060	3158650	
PS(P-20:0/19:1(9Z))	861.6056	14.735	Rpneg	1	20081	20100	18446	1	18077	16059	16384	27637	32266	
PS(P-20:0/20:0)	813.6293	27.552	Rppos	4313776	4142308	3950846	4411532	4899647	6024221	6294234	5619895	5555678	5444099	
PS(P-20:0/20:1(11Z))	811.6093	25.924	Rppos	15987524	19629432	15867982	15662762	17759036	15797877	16273653	20158176	21576988	17173140	
PS(P-20:0/20:1(11Z)) Esi+25.395002	811.6089	25.395	Rppos	1	1	1	1	4177705	3818293	4566821	4188175	4572353	4655828	
PS(P-20:0/20:2(11Z,14Z))	809.5923	24.913	Rppos	5.09E+08	4.81E+08	5.24E+08	5.42E+08	4.89E+08	4.99E+08	5.31E+08	5.08E+08	5.07E+08	5.15E+08	
TG(16:1/18:0/18:3)	871.7651	0.893	HILICpos	1.05E+08	53190240	46375636	45020704	88033120	80433968		1.16E+08	86950144	1.11E+08	
TG(16:1/18:1/22:4)	923.7954	0.894	HILICpos	53150260	58247396	60045972	61263088	58724712	36124408		53315824	30104110	33838752	
PS(P-20:0/20:2(11Z,14Z))	827.5972	13.13	Rpneg	3101	1763	1495	2086	1026	1	1441	1477	1014	1345	
PS(P-20:0/20:2(11Z,14Z)) Esi+24.823	831.5746	24.823	Rppos	9451048	10553571	10480826	12222032	12110817	10227490	11261964	12306193	11538150	13023692	
PS(P-20:0/20:2(11Z,14Z)) Esi+25.037	831.5739	25.037	Rppos	26498968	23777318	21956220	25989606	23084378	21631514	23719966	22680728	23518466	23554376	
PS(P-20:0/20:3(8Z,11Z,14Z))	871.5976	12.676	Rpneg	8230	3241	4887	2796	1	6138	4239	1	12671	1	
PS(P-20:0/20:3(8Z,11Z,14Z)) Esi-12.5390005	871.5944	12.539	Rpneg	34096	9777	2676	34506	1	69873	1953	5002	2241	1	
PS(P-20:0/20:3(8Z,11Z,14Z)) Esi-12.661001	871.5977	12.661	Rpneg	8224	4166	2512	3659	11365	69817	1	5002	3036	6843	
PS(P-20:0/20:3(8Z,11Z,14Z)) Esi-12.682	871.6	12.682	Rpneg	922	3241	20105	9181	4357	6264	3060	12212	2041	1	
PS(P-20:0/20:5(5Z,8Z,11Z,14Z,17Z))	803.5497	21.35	Rppos	2897698	1742879	1915933	2311385	1184630	1319612	789940	1056868	522795	714357	
PS(P-20:0/20:5(5Z,8Z,11Z,14Z,17Z)) Esi+21.11	803.5502	21.11	Rppos	1665966	1461013	1748232	1604854	1170886	740175	1617408	1522561	743696	1158291	
PS(P-20:0/22:0)	863.6468	27.158	Rppos	854161	752289	1012587	874718	978262	1239219	1164965	1061444	1039274	1145520	
PS(P-20:0/22:1(11Z))	861.622	26.658	Rppos	499351	450457	638727	840077	575803	538735	462678	411798	502897	462594	
PS(P-20:0/22:2(13Z,16Z))	837.6256	26.647	Rppos	11062003	9353570	13106499	13201402	13944285	14404692	11976686	10589203	10682613	12227455	
PS(P-20:0/22:2(13Z,16Z)) Esi+24.541	859.6012	24.541	Rppos	1183302	888118	894148	1027106	756673	807679	952350	920160	777288	1029259	
PS(P-20:0/22:2(13Z,16Z)) Esi+27.182003	837.6265	27.182	Rppos	2211863	1655437	2164403	1860168	1939680	2408730	2632169	1806417	2820904	2720722	
PS(P-20:0/22:4(7Z,10Z,13Z,16Z)) Esi+19.657	833.5922	19.657	Rppos	40212504	25459360	23423072	21045320	36425024	19672134	39079244	24001050	18213496	12723468	
PS(P-20:0/22:4(7Z,10Z,13Z,16Z)) Esi+21.886997	855.5789	21.887	Rppos	176373	176093	175236	204507	354620	321379	350201	361417	306048	475297	
PS(P-20:0/22:4(7Z,10Z,13Z,16Z)) Esi+23.464003	833.5913	23.464	Rppos	4005969	2768312	5669454	7301251	4251005	3661201	4468792	4263043	4036471	5108301	
PS(P-20:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z))	829.5616	21.687	Rppos	61155232	57515936	74178680	58349024	66263776	85124456	71107976	72096360	62337620	67971744	
PS(P-20:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z))	847.5698	4.869999	HILICneg	246744	248523	252671	271877	264793	255798	308728	317509	309650	262822	
Pseudouridine	244.0677	8.154	HILICpos	261952	173711	31645	605291	53826	23657		428725	219416	289127	
Pseudouridine	244.0698	1.309	Rpneg	120804	132976	161155	169616	81459	156053	163600	86120	92735	95670	
Pseudouridine Esi-0.71199995	290.0738	0.712	Rpneg	17932	7176	15782	10495	1	13494	17824	11375	6613	10901	
PtdIns-(5)-P1 (1,2-dioctanoyl)	670.211	15.316	Rppos	1067485	1060778	1272712	1178400	915844	1289939	1235592	1160457	1191905	1053358	
Pterolactam	115.0631	0.923	Rpneg	8045	15483	10023	10916	13173	6844	6770	10378	11320	11162	
Purine	120.0439	12.94	Rpneg	40735	15475	20881	1	63863	38661	39310	34427	37912	33551	
Purine Esi-1.0430001	120.0435	1.043	Rpneg	6453	9207	8986	10062	4033	3615	2757	9661	11640	21561	
Purine Esi-12.671999	120.044	12.672	Rpneg	19935	19713	22025	16332	29938	27369	19055	21448	16805	23408	
Purine Esi-12.93	120.0438	12.93	Rpneg	29005	3998	84070	3486	12758	3037	34787	30771	63847	33551	
Purine Esi-13.176001	120.0438	13.176	Rpneg	30686	1	37751	17280	31067	14866	28356	63130	17839	5105	
Pyridine	79.0432	1.608	HILICpos	400667	452687	452598	412139	466676	409944		483595	554199	497393	
Pyrilamine	289.1559	6.577001	Rppos	120995	349121	297989	316577	238092	370749	187769	158746	351739	178505	
pyroglutamic acid	129.0427	8.73	HILICpos	394708	446192	387423	424022	569217	796373		601169	828362	703693	
Pyro-L-glutaminyl-L-glutamine	257.0996	0.907	Rpneg	5154	3418	4851	3632	7010	10730	9492	7813	14220	9905	
Pyrrhoxanthinol	616.3459	9.083	Rpneg	3118	2857	2553	3332	3105	2730	2705	2759	3546	2812	
pyruvic acid	88.0153	0.827	Rpneg	1	23934	83404	1	1	46445	24589	46463	58911	48644	
Quercetin 3-(2"'-feruloylsophoroside)	848.2051	1.682	Rpneg	35678	26700	25565	31828	25361	34366	18203	35494	34657	31402	
Quillaic acid 3-[xylosyl-(1-3)-[galactosyl-(1-2)]-glucuronide]	960.4408	22.89	Rppos	101272	174141	100909	107921	193404	137211	154495	174077	220167	244085	
QX-314	243.1835	7.469001	Rppos	1553513	1638354	1782394	1866203	1734708	1421116	1489987	1717766	1761886	1535053	
R-1 Methanandamide Phosphate	899.5563	25.064	Rppos	1156684	1074305	858530	1035267	987404	815804	920014	836871	810647	836455	
R-3-(Methylthio)-1-hexanol	194.0973	9.719001	Rpneg	1	15866	109998	15543	22981	3353	4049	18206	22115	10493	
Red chlorophyll catabolite	672.2742	13.278	Rpneg	66788	61394	67821	69503	54789	49988	64925	64881	69545	61451	
Red chlorophyll catabolite	672.2756	0.912	HILICneg	1486066	1347676	1204262	1062830	1987248	658266	3133965	958840	2978821	2073316	
Red chlorophyll catabolite Esi-12.863999	672.2737	12.864	Rpneg	2827	1833	1	1419	1474	790	1959	2769	2415	2484	
Red chlorophyll catabolite Esi-13.134	672.2718	13.134	Rpneg	4148	61394	4286	4863	1	1	64925	1	4947	1	
Resiniferatoxin	674.2741	13.278	Rpneg	24667	22130	25406	24837	19772	17882	22560	22921	24381	21502	

Resiniferatoxin Esi-13.129999	674.2707	13.13 Rpneg	1516	22130	1489	1456	1	1	22560	866	2257	1266	
Retamine	296.21	9.954001 Rpneg	21918	20944	22628	22668	20583	21751	22715	22057	23041	23697	
Retamine	310.2255	0.937 HILICneg	87824	128580	88633	106318	60512	1	49241	51644	1	45127	
Reticulataxanthin	472.341	12.965 Rpneg	23968	7477	8093	1	10125	3438	5073	4921	7282	3401	
Reticulataxanthin Esi-12.964998	472.3348	12.965 Rpneg	25393	10915	10915	9387	10586	3435	1	5342	7446	1	
Retinol phosphate	426.2194	0.954 HILICneg	193977	297797	290819	299989	162743	31904	174294	170375	117887	140565	
Retronecine	201.1006	1.364 HILICneg	71145	157087	191261	233350	290832	84937	158242	337328	155846	387687	
Riboflavine 2',3',4',5'-tetrabutanoate	656.3086	13.277 Rpneg	8911	7335	9393	8834	6442	5654	8307	6431	8293	7666	
Ribosylimidazoleacetic acid	258.0848	0.881 Rpneg	72749	27525	87591	27226	51143	87068	1	33096	52343	31901	
Rivenprost	467.2372	6.576 Rppos	144343	166103	172279	70460	92145	62809	70596	75123	87446	65731	
Roxithromycin	896.545	14.009 Rpneg	24725	21400	22068	24506	7653	2382	7441	4192	4566	4641	
Saccharocin	540.2623	12.048 Rpneg	16272	10200	8243	9996	9689	5511	7546	7204	7129	8781	
S-Acetylphosphopantetheine	400.1062	4.635001 Rpneg	151117	166063	161412	191792	102382	61296	106159	90983	92395	106866	
Sambutoxin	453.2888	13.006 Rppos	339620	360614	290735	306820	206252	265588	262540	227921	222581	186879	
Sandoricin	605.2859	5.581 HILICpos	976985	846717	925631	862838	863855	665445		698099	709814	633607	
Saprisartan	670.067	0.794 Rpneg	5058	1940	1720	2173	2606	2607	2404	1606	857	1	
Sarcostin	382.2394	12.724 Rpneg	30849	14483	10021	13572	15839	8976	11204	12862	22840	9104	
Sarpagine	356.1752	11.89 Rpneg	77770	63769	45525	37809	28963	33337	50634	43117	37212	41697	
Sarpagine Esi-10.919	356.1755	10.919 Rpneg	13575	13800	10180	7405	8064	7146	11636	11613	9567	10189	
SB 939	358.2342	9.844001 Rpneg	10794	7524	7332	8050	7488	6895	7206	7965	7465	7162	
SB 939	656.4858	1.072 HILICneg	3074614	1	1763594	2495365	1	1	1025053	1109730	1117632	1087816	
SC-19220	377.0782	0.934 Rpneg	10131	6882	7680	8188	5448	6917	4256	7328	6394	6453	
S-Carboxymethyl-L-cysteine	225.0306	0.794 Rpneg	14524	10918	17670	13967	13101	26732	17578	17540	12337	23299	
S-Carboxymethyl-L-cysteine Esi-0.8230001	179.0255	0.823 Rpneg	2741	2972	2701	5844	996	6461	4425	10504	6162	6943	
S-Cysteinosuccinic acid	297.0526	7.401 Rpneg	2634	21465	3322	14600	20026	3042	3543	11895	23387	10082	
sebacic acid	202.1208	7.203 Rppos	110906	268176	255171	412660	149811	1028099	250673	270194	632033	500870	
Selenocystathionine	264.0196	0.991 Rpneg	13269	9827	9797	10913	8926	10723	7132	12030	11992	11193	
Ser Arg Lys	435.2427	12.497 Rpneg	4746	4293	3338	5393	1620	1159	2092	1911	1369	2109	
Ser Arg Lys	435.2509	0.781 HILICneg	53201	70175	60942	99444	49139	75732	40401	34383	34129	38614	
Ser Trp Met	422.1625	11.881 Rpneg	78831	115438	37458	40508	14996	63933	78713	58863	39309	54374	
Serratanidine	607.3844	15.268 Rppos	2444192	702267	660451	672964	315482	602595	860585	498300	478348	560572	
Serratine	325.1864	8.455001 Rpneg	13714	15451	13756	14656	14499	15042	12185	15472	18729	14018	
TG(16:1/18:2/22:4)	921.7816	0.88 HILICpos	59129304	66086252	65230032	64479292	56825672	33611064		48918160	29552750	32890380	
Silicic acid	95.9878	1.788 HILICneg	938467	422659	73719	712935	482930	731341	286237	265681	215299	145049	
Silicic acid	95.9879	0.749 Rpneg	2709	27631	1	21669	31292	1	4051	17865	31675	12136	
Silicic acid Esi-5.2270007	95.988	5.227001 HILICneg	450815	390347	322670	302014	396092	225989	304934	340131	194432	310765	
Siphonaxanthin ester/ Siphonaxanthin dodecenoate/ (Sipho	779.5822	27.695 Rppos	478370	383521	485484	403917	367025	701120	561709	393900	527050	375276	
SM(d16:1/20:0)	730.5986	24.739 Rppos	11324428	11693124	11947798	12538064	13020191	13128380	12267482	12177266	12268929	11811117	
SM(d16:1/20:0) Esi+20.149	730.6016	20.149 Rppos	2238007	1839025	1930441	1924444	1989133	1853585	2006263	1935192	1786651	1542760	
SM(d16:1/22:0)	758.6303	27.087 Rppos	12342343	13933354	15134921	14393169	13951101	18172822	16693474	15381058	15782321	15251811	
SM(d16:1/24:0)	786.6618	29.732 Rppos	11235516	9617920	12319627	11636760	9778642	12854931	12774652	11579195	10576553	10653496	
SM(d18:2/18:1)	726.5623	0.883 HILICpos	1973788	2123229	1780916	2584351	1519738	1020221		1191914	1922370	1333873	
SM(d18:2/21:0)	770.6306	25.992 Rppos	952143	994671	1118624	1053677	1107525	1553187	1213259	1267172	1515742	1519761	
SM(d18:2/21:0) Esi+25.992	770.6329	25.992 Rppos	949703	1008631	1297402	1052631	1161989	1597128	1194622	1268141	1550428	1515642	
SM(d18:2/22:0)	784.6419	27.197 Rppos	7090364	6045839	6617705	6575299	6141418	8098079	7160126	7141239	6542559	7125042	
SM(d18:2/22:0)	784.6444	5.177 HILICpos	10031185	13041896	11888780	6521590	14586512	11634119		12892366	9555077	18378976	
SM(d18:2/23:0)	798.6668	28.522 Rppos	2226742	2940737	1640482	2329583	3121912	3057591	2918105	2645110	2773253	2603329	
SM(d18:2/24:0)	812.6783	29.703 Rppos	10218135	8900886	10819304	9781475	8608419	11154835	9505920	8958821	9106325	8523435	
SM(d19:1/16:0)	716.5842	23.711 Rppos	1215905	1436205	1576106	1351845	1488330	1923295	1594090	1375103	1277141	1609658	
SM(d19:1/17:1)	728.5845	22.891 Rppos	1598645	2320259	1994661	1724438	2651946	2818361	2716510	2625046	2800848	2655969	
SM(d19:1/18:0)	744.6134	25.859 Rppos	774808	877266	1044359	655918	939963	1479314	1080041	1092230	1145619	950731	
SM(d20:1/19:0)	772.6485	28.394 Rppos	1777909	1652436	1890186	1833593	1871627	2439864	1951619	2060727	2117644	2026886	
sn-3-O-(geranylgeranyl)glycerol 1-phosphate	444.2636	11.053 Rpneg	10014	5527	1	2074	3457	21811	2641	2959	9766	13892	
Sodium glycocholate	465.308	11.008 Rpneg	13339	14224	1	6283	1568	10870	6516	1	9513	25725	
Sodium Tetradecyl Sulfate	294.1865	12.476 Rpneg	520994	319072	309070	340561	406072	255777	288910	284193	452986	230516	
Sodium Tetradecyl Sulfate Esi-11.772001	294.1872	11.772 Rpneg	2763	3533	1826	1350	2403	3009	1161	4594	1	1829	
Sodium Tetradecyl Sulfate Esi-12.267999	294.1871	12.268 Rpneg	1	26886	25137	1	1	22558	25089	27378	44513	21224	
Sodium Tetradecyl Sulfate Esi-12.475999	294.1866	12.476 Rpneg	517078	328027	317458	348183	412233	259827	295886	291787	450802	234270	
Sodium Tetradecyl Sulfate Esi-12.482001	294.1863	12.482 Rpneg	11591	360770	352991	7646	462297	5696	326694	323045	6989	267207	
Soyasapogenol B 3-O-b-D-glucuronide	680.4197	13.622 Rpneg	11216	4455	2472	5047	3980	2995	5697	4952	2825	4989	
Spectinomycin adenylate	683.1952	21.787 Rppos	13458623	13442432	13162859	13651690	12945835	12310388	12836309	9998685	13649774	12729341	
Spectinomycin adenylate	701.2093	0.687 HILICpos	2E+08	1.04E+08	2.57E+08	1.18E+08	1.04E+08	3.02E+08		1	2.37E+08	2.7E+08	
Sphingofungin F	383.2671	7.825 Rppos	175547	238287	351915	254381	722831	385702	452080	651344	308603	523252	
Sphingosine	281.2698	14.006 Rppos	1290628	1052293	1611480	697327	599336	607894	661069	663751	1397614	575629	
Spinochalcone B	374.187	11.957 Rpneg	2666	3448	2565	3306	2497	3479	3386	3483	2851	3404	
Spiramycin 1	842.5125	13.599 Rpneg	57645	61953	46435	78424	17507	12990	14742	15822	16583	21736	
Spirolide B	693.4634	16.462 Rppos	224875	114583	66136	80401	230264	236376	242111	211847	312763	230196	
Spisulosine	285.3032	1.6 HILICpos	220915	194471	139426	220411	236874	197564		245633	338865	181934	
Spongipregnoloside D	817.4463	22.688 Rppos	610863	601230	488181	542125	454807	414586	449424	360778	329483	357907	
SQDG(16:0/14:0)	780.5015	1.135 HILICneg	718771	490785	624981	850860	374895	42453	503608	602451	400428	563055	
SQDG(22:5(5Z,8Z,11Z,14Z,17Z)/16:1(13Z))	840.5013	13.524 Rpneg	18169	14237	8995	15555	4893	1	1	1	1	4987	
SQMG(0:0/16:1(13Z))	554.2788	12.257 Rpneg	1164	8898	5583	1741	1929	1421	3831	1009	1	2189	
Squalamine	644.4906	0.883 HILICpos	769687	987037	968274	751976	649172	482625		450806	539458	566191	
Stearic Acid ethyl ester	312.3022	14.854 Rpneg	72481	29324	28163	23404	34480	28191	24883	28944	13152	9391	
stearoyl carnitine	427.3661	13.805 Rppos	1991707	1535727	2134070	2375948	2526623	2301760	1606671	1740018	2430510	2325817	
Sterculynic acid	290.2221	12.465 Rpneg	11242	15145	5553	1	8244	3288	5617	7108	6508	5223	
Sterculynic acid Esi-12.662001	290.2235	12.662 Rpneg	4848	2891	1	3509	1	1057	1703	4261	2657	1866	
Sterol 3-beta-D-glucoside	456.2755	12.592 Rpneg	4601	2877	1819	2197	2833	993	2414	2535	2280	1577	
Stigmastanyl glucoside	578.454	13.48 Rpneg	10890	6809	7632	7667	9739	7298	10730	2602	5679	3414	
Stigmatellin Y	484.2811	4.140999 HILICneg	45090	1	27062	38767	21847	1	26218	1	24984	15649	
Stovaine	235.1578	12.465 Rpneg	34638	33611	25382	30813	33910	30265	28921	36087	32151	31535	
Streptidine	262.1389	0.908 Rppos	14895588	17137548	21099772	16872132	16595520	18127864	22405040	17652380	15152976	17230278	
SU 5416	298.1334	13.277 Rpneg	18966	17030	22901	21195	12928	14031	19685	15202	21228	18290	
Succinic acid	118.0261	8.516999 HILICneg	65472	61469	86005	49225	52429	71546	68090	72173	61793	43404	
Succinic acid semialdehyde	84.0211	1.068 Rppos	1034141	1224550	1605693	1539439	787991	745820	804516	844718	763255	669366	
Succinic anhydride	100.0156	0.766 Rpneg	1	18047	1	17799	20987	1	1790	10061	22333	10757	
Succinic anhydride	100.0178	1.261 HILICneg	36723	34359	38798	43070	42388	17071	43420	35324	22149	51246	
Succinylmonocholine Esi+5.632	186.0892	5.632 Rppos	284435	767686	801672	751836	389088	923957	444491	319733	766173	314805	
Succinylproline	215.0801	5.463 HILICneg	300312	344063	344738	418653	119094	93649	169955	193048	95383	137131	
Sulfamethopyrazine	280.0621	2.773 HILICneg	84541	70712	92460	99435	62827	67900	86094	90539	85798	89385	
Sulfamethoxazole N4-hydroxylamine	329.0656	0.879 Rpneg	4490	3697	3634	4242	1774	1585	1393	2437	2069	2139	
Sulfoacetic acid	139.9792	0.755 Rpneg	1	98537	7927	84257	84876	11834	17265	53362	110746	54399	

Sulfur mustard	315.945	4.411	HILICneg	361115	373514	395468	332678	343006	212113	389155	247173	350939	420873
Sumatriptan	612.2528	15.316	Rppos	371057	334013	405145	382399	298694	425373	379854	363666	363024	319108
Synaptolepis factor K1	614.3823	11.64	Rpneg	8433	8284	3917	5724	4745	3590	7930	5901	11072	5991
Tacrolimus metabolite M-IV	879.4953	3.924	HILICneg	230353	180109	231642	246706	233978	192475	295073	306990	209452	245041
Tartronate semialdehyde	104.0113	0.762	Rpneg	21326	43861	30321	48386	47624	31822	36523	41786	55345	39377
Taurine	125.0144	7.604001	HILICpos	860295	915374	990626	824432	1281296	1161449		1003728	835083	1016361
Taurine	125.0149	0.851	Rppos	3305405	3303337	3770438	3173984	3962275	3936435	4294927	3609748	3272922	3577058
Taurine	125.0149	0.848	Rpneg	1169260	1015545	1287353	1062210	1167153	1369311	1420929	1325252	990135	1173910
Taurine	125.015	7.634	HILICneg	3882710	3556740	3664757	3372094	3927923	3733919	3959286	3839855	2954158	3614090
Taurine Esi-1.16	125.015	1.16	Rpneg	164283	132186	261602	155303	168123	259159	479526	186436	236010	208009
Taurine Esi-2.305	125.015	2.305	Rpneg	18641	10828	18023	11280	12247	26211	22737	14357	616	17058
Taurine Esi-5.1149993	125.0149	5.114999	Rpneg	21246	12660	11554	27297	5907	6722	10446	12799	9571	11967
Taurodeoxycholic acid	499.2948	11.59	Rpneg	3762	3062	863	4919	4289	1645	760	2075	2424	1288
Taurodeoxycholic acid Esi-11.59	499.296	11.59	Rpneg	2615	3062	863	1918	4289	1754	1	2075	2424	1288
Tauropine	197.0362	4.139	HILICneg	2345482	1967364	2283558	2139078	3227010	1553299	2831109	2262411	1986336	1944974
Tauroursocholic acid	515.289	10.975	Rpneg	5481	3748	2368	13100	4598	4203	2256	4366	4481	8000
Taxa-4(20),11(12)-dien-5?-acetoxy-10?-ol	346.2502	11.907	Rpneg	5408	6013	3736	3093	994	1801	4187	6891	5670	3392
Tecostanine	229.1659	4.36	HILICneg	1180604	61321	1	105174	145790	203618	161049	119724	1072700	1
Tecostanine	229.1678	8.169999	Rpneg	11094	15682	15550	16823	12275	9243	8763	9487	11920	10162
Tenitramine	462.1223	13.407	Rpneg	6200	4689	4326	2991	4437	5053	3495	3341	3380	3253
Terbinafine	599.4234	8.3	Rppos	1	277493	33006	212332	327508	20017	38816	198900	396161	196553
Termitomycesphin A	743.5502	20.9	Rppos	963456	655282	834098	791637	632799	836729	763391	444500	883465	952990
Termitomycesphin A	743.5597	1.55	HILICpos	2075896	2714613	2246858	1935678	2229783	1937066		2620895	2721583	2512279
Termitomycesphin A	803.5749	4.653	HILICneg	82782	49526	57504	62028	54999	48561	52703	59582	69072	58431
tetracosyl butyrate	424.4282	14.569	Rpneg	63320	24938	19114	20802	28022	22573	22670	25157	4547	11313
tetracosyl butyrate Esi-14.565001	424.4277	14.565	Rpneg	80519	29712	23207	26898	35575	22861	24959	32611	21056	14066
Tetradecyl acetate	256.2402	12.774	Rpneg	5953716	5636785	5047536	5600538	5354264	5063376	5094465	5552615	5358039	5127385
Tetradecyl acetate Esi-12.774001	256.2404	12.774	Rpneg	5955090	5653527	5014239	5588149	5380431	5063700	5093456	5555789	5329186	5139398
tetradecyl hexanoate	312.3033	1.017	HILICneg	675071	524337	339657	430266	1005787	3068810	556775	732220	664006	658867
Tetradecyl sulfate	354.2071	12.273	Rpneg	102982	56933	46552	57292	101489	51082	58629	70008	127428	41435
Tetrahydropersin	384.3202	1.122	HILICneg	452064	70317	43400	81986	134940	1	99066	106971	1	90651
TG(17:0/17:1/17:0)	873.7808	0.908	HILICpos	2.13E+08	1.2E+08	1.05E+08	1.05E+08	2.31E+08	2.48E+08		2.87E+08	2.38E+08	2.79E+08
Tetrahydropersin	384.3209	12.008	Rpneg	9949	6727	5983	8307	6264	4606	5174	6765	7759	4496
Tetranor-PGF1alpha	300.1938	10.103	Rpneg	12622	9497	3795	7586	6212	10745	5477	7367	8527	4364
Tetranor-PGF1alpha Esi-9.874	300.1933	9.874	Rpneg	11344	7743	3757	7613	6990	9049	4272	6155	7652	4823
TG(12:0/12:0/12:0) Esi+23.776	637.5716	23.776	Rppos	724677	648098	351657	753053	1	185635	1	1	680308	1
TG(12:0/12:0/12:0) Esi+27.938	642.5212	27.938	Rppos	3027638	3523885	4172702	3325939	5393957	8315402	6017040	6945635	5934576	6132324
TG(12:0/12:0/12:0) Esi+27.938 :1	637.5656	27.938	Rppos	1635028	2071195	2709336	2106692	3141636	5106225	3753925	4394985	4039779	3782332
TG(12:0/13:0/13:0)[iso3]	688.5609	21.87	Rppos	272948	201181	248039	326073	202403	221521	175624	218653	341426	271341
TG(12:0/13:0/14:1(9Z))[iso6]	660.5702	15.75	Rppos	136898	129486	212579	168373	166102	180604	173102	208135	187441	156945
TG(12:0/14:0/18:2(9Z,12Z))[iso6]	763.6489	0.877	HILICpos	2193276	575700	235862	350750	1	111934		199082	1	1
TG(12:0/14:0/20:2(11Z,14Z))[iso6]	791.6971	0.883	HILICpos	6198606	2318981	966639	1597463	879881	765007		981517	1245972	1081430
TG(12:0/15:0/21:0)[iso6]	823.7636	1.006	HILICpos	17600204	12159317	8086596	8786894	15785723	15957823		14124813	12740560	12158853
TG(12:0/15:1(9Z)/22:0)[iso6]	835.7655	0.925	HILICpos	2750985	2593009	1421712	2003413	1786653	2385859		2754425	2210685	2360585
TG(12:0/16:1(9Z)/19:0)[iso6]	807.731	0.898	HILICpos	1013757	805622	682611	865260	457850	438419		987342	1249187	483959
TG(12:0/16:1(9Z)/19:1(9Z))[iso6]	805.7165	0.886	HILICpos	739495	565815	378687	562579	306061	246641		326526	475936	339527
TG(12:0/17:0/20:2(11Z,14Z))[iso6]	833.751	0.901	HILICpos	3054564	1999758	1594577	1160139	1288123	687730		1	1977395	1901729
TG(12:0/17:0/20:2(11Z,14Z))[iso6] Esi+0.901	833.753	0.901	HILICpos	3054564	1999758	1594577	1292110	1289379	687730		1	2008214	1901729
TG(12:0/17:0/22:2(13Z,16Z))[iso6]	861.7849	0.911	HILICpos	8162730	7507520	6019671	6030551	5828001	9171587		10153171	9837665	9650929
TG(12:0/17:1(9Z)/22:0)[iso6]	863.7963	0.996778	HILICpos	3996800	3957785	4763835	4729568	6440480	7781121		8016734	7312293	7601086
TG(12:0/18:0/20:5(5Z,8Z,11Z,14Z,17Z))[iso6]	841.7213	0.875	HILICpos	2322787	1292430	805165	1019668	630020	643027		805251	917052	789368
TG(12:0/18:2(9Z,12Z)/19:1(9Z))[iso6]	831.731	0.88	HILICpos	1807826	1042328	952085	1035928	1	1		108804	866999	1
TG(12:0/19:0/21:0)[iso6]	879.8201	1.722	HILICpos	733646	625175	481297	739901	1484364	1465278		2019871	1843482	1943508
TG(17:0/17:1/22:1)	931.8541	1.072	HILICpos	9111604	8593492	9233438	8697401	20619968	21660748		29186238	23996706	26784208
TG(12:0/20:0/20:5(5Z,8Z,11Z,14Z,17Z))[iso6]	869.7509	0.878	HILICpos	21099680	10046568	7219508	8117340	9413077	10176277		12117698	11330082	12765738
TG(13:0/16:0/22:4(7Z,10Z,13Z,16Z))[iso6]	857.7605	0.905	HILICpos	11143758	8785867	7557926	7901872	10303910	12071780		12889551	10963804	12765040
TG(13:0/16:0/22:4(7Z,10Z,13Z,16Z))[iso6] Esi+0.8909999	857.7574	0.891	HILICpos	2507793	1639884	1439332	1447456	1889201	2011053		2137930	2020964	2252133
TG(13:0/18:3(6Z,9Z,12Z)/22:1(11Z))[iso6]	885.7854	0.9	HILICpos	4256943	3331763	3325378	2808901	5229827	5190018		6345462	5235619	5968726
TG(13:0/18:3(6Z,9Z,12Z)/22:1(11Z))[iso6] Esi+0.902	885.7853	0.902	HILICpos	4224660	3354443	3430986	3052431	5298319	5455769		1	5610855	6011730
TG(13:0/20:1(11Z)/20:1(11Z))[iso3] Esi+0.981	889.8106	0.981	HILICpos	2085311	5266863	3808867	4607739	1	1		12475288	8123142	1
TG(14:0/16:1(9Z)/22:3(10Z,13Z,16Z))[iso6]	854.7479	0.899	HILICpos	3208808	2843269	2427709	2360076	2675985	2816314		2752891	2257404	2805699
TG(14:0/17:0/18:0)[iso6]	837.7756	1.015	HILICpos	870814	1332907	1426237	1405920	975983	1060194		708675	1712838	1177643
TG(14:1(9Z)/19:0/19:0)[iso3]	877.8053	1.7	HILICpos	363557	569922	399354	892409	1104394	2587954		3795713	673812	3051526
TG(14:1(9Z)/20:3(8Z,11Z,14Z)/20:3(8Z,11Z,14Z))[iso3]	893.7539	0.875	HILICpos	12247898	8781848	6968771	8114103	5894827	4737821		6742060	4793695	4901120
TG(15:0/21:0/21:0)[iso3]	978.8768	0.974	HILICneg	258395	196932	146604	215252	136920	1	112084	128271	155351	112157
TG(16:0/16:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z))[iso3]	895.7663	0.88	HILICpos	54668012	46030992	46366500	46639248	52615100	35637692		58540536	37409552	45838060
TG(16:0/18:1(9Z)/22:0)[iso6]	933.8695	1.717	HILICpos	810120	445988	157760	582801	1426653	1893780		2446810	594773	2074016
TG(16:0/18:1(9Z)/22:4(7Z,10Z,13Z,16Z))[iso6]	925.8092	0.908	HILICpos	37439616	37941672	40133528	37353912	57523720	35451500		55353952	38516876	45556764
TG(16:0/20:3(8Z,11Z,14Z)/22:5(7Z,10Z,13Z,16Z,19Z))[iso6]	947.798	0.88	HILICpos	17823170	20771684	20330258	21214494	21741744	14079584		20648432	12045928	13612629
TG(18:2/19:1/19:1)	927.8276	0.925	HILICpos	6147333	16473109	14625321	16465783	31234518	30064802		38869800	32047366	36541236
TG(16:0/20:5(5Z,8Z,11Z,14Z,17Z)/22:5(7Z,10Z,13Z,16Z,19Z	926.7375	23.61	Rppos	828139	1472378	390982	1329977	320982	113763	135784	611428	1318282	443445
TG(16:0/20:5(5Z,8Z,11Z,14Z,17Z)/22:5(7Z,10Z,13Z,16Z,19Z	943.7671	0.869	HILICpos	9882505	11487737	10323273	12669188	4497669	1		4513170	1	1
TG(16:1(9Z)/18:2(9Z,12Z)/22:0)[iso6]	929.8409	1.015	HILICpos	12422455	12453170	12669308	11824675	28356872	34691596		39291124	34425160	39572312
TG(16:1(9Z)/18:3(9Z,12Z,15Z)/21:0)[iso6]	913.8112	0.908	HILICpos	2453905	2193020	2900355	1597763	3564816	4249241		5061316	4636652	5142491
TG(16:1(9Z)/18:3(9Z,12Z,15Z)/21:0)[iso6] Esi+0.908	913.8193	0.908	HILICpos	2283911	2354155	2917394	1454050	3060574	2996304		4619934	4523697	4367425
TG(16:1(9Z)/18:4(6Z,9Z,12Z,15Z)/22:4(7Z,10Z,13Z,16Z))[iso	900.7239	24.227	Rppos	1273488	1524583	1171457	1187264	4022038	1233514	3803794	5087211	812322	2884179
TG(17:1(9Z)/18:1(9Z)/19:1(9Z))[iso6]	901.8102	0.925	HILICpos	45696880	75935664	73809408	70019712	2.05E+08	2.45E+08		2.6E+08	2.49E+08	2.7E+08
TG(17:1(9Z)/18:1(9Z)/19:1(9Z))[iso6]	901.805	22.408	Rppos	1	1	2238652	1000639	1	1125792	1394134	1942684	3089429	2310914
TG(17:1(9Z)/18:1(9Z)/22:1(13Z))[iso6]	943.8514	1.034	HILICpos	1	1	1	1	2142922	2456841		2594093	2688218	2977997
TG(17:1(9Z)/18:2(9Z,12Z)/22:2(13Z,16Z))[iso6]	939.8267	0.915	HILICpos	1379113	1577646	1485548	1469461	2071438	1623724		1962278	1545885	1477124
TG(18:2(9Z,12Z)/18:4(6Z,9Z,12Z,15Z)/22:4(7Z,10Z,13Z,16Z	926.7356	22.846	Rppos	40558	271683	1	160386	66075	227498	153844	259494	285330	173350
TG(19:1(9Z)/20:5(5Z,8Z,11Z,14Z,17Z)/22:6(4Z,7Z,10Z,13Z,1	1010.751	0.731	HILICneg	72999	59636	65203	78799	47213	53303	46795	40080	42411	52066
TG(8:0/8:0/8:0)	487.39	18.542	Rppos	1079593	733472	887377	880076	633321	610110	865142	889574	812339	879420
TG(8:0/8:0/8:0) Esi+18.540003	492.3412	18.54	Rppos	564369	429022	459783	607039	418418	350150	396384	536409	484740	359831
TG003	309.1006	0.831	Rpneg	17401	14369	28862	19163	1	1	1	12844	1	1
Thalmine	608.2869	11.748	Rpneg	2449	1779	2331	1598	3317	1185	4121	3178	1295	2422
Thelepin	969.6208	5.305	HILICneg	138603	145658	143487	174164	116861	90523	96840	96690	83971	91785
Thiacloprid	252.0234	1.491	HILICneg	58760	52874	51892	42824	33664	7108	50326	30393	41678	57593
Thiamethoxam	337.0225	0.71	Rpneg	7857	5852	16980	3647	34125	4939	3802	2294	1281	6906
Thiobenzamide S-oxide	199.0321	4.136	HILICneg	140279	1	204702	183314	305500	1	201427	1	204681	193084
Thiocyanate	117.9663	8.935999	HILICneg	75127	85269	69871	93915	48912	56673	73691	69280	75478	58303
Thiodiacetic acid sulfoxide	244.0243	0.716	Rpneg	2896	11277	1792	11497	11468	1	2174	4908	12441	7927

Thioguanine	167.0272	4.124 HILICneg	907213	1227124	740525	1001900	881313	672113	855275	676796	994859	936343
Thioperamide	352.1919	11.136 Rpneg	3523	4851	2987	3552	5548	2676	1	3418	4344	3145
Thr Glu Gln	422.1649	1.074 HILICneg	8112182	4957656	2267467	4800698	1.26E+07	690760	2345930	5384185	3630055	5313985
Thr Leu Met	363.1819	1.152 HILICneg	1140162	559484	211992	424187	2374342	45190	151614	572145	343941	328685
Thr Leu Met Esi-1.149	381.1932	1.149 HILICneg	1319139	693914	302943	507619	2670202	1	289417	657064	547901	544256
Thr Phe Pro	363.1785	10.102 Rpneg	2583	1499	1697	2347	1263	1580	2487	2167	1331	2251
Thr-Abu-OH	326.1126	11.88 Rpneg	1927	1	5389	3790	5575	3996	2139	1797	2665	3688
Thromboxanoic acid skeleton	340.2614	12.154 Rpneg	9703	25108	17590	51458	61748	39389	35945	54833	43939	43331
Thromboxanoic acid skeleton Esi-12.227999	340.2601	12.228 Rpneg	7573	20225	20724	1	110626	35093	30664	1	79881	37329
thymidine	242.0903	4.182 Rpneg	26501	16975	19615	21484	21397	18192	18417	19482	18060	15595
Tiopronin	209.0374	1.923 HILICneg	7504	5299	8213	6137	46548	72666	53084	107093	185022	114252
Tokoronin	580.3603	1.185 HILICneg	245180	521702	346829	476733	458048	1	364475	297428	248637	327434
Torvanol A	498.0817	5.791 Rpneg	4462	2783	864	2632	2492	3412	3770	2990	1601	1534
toxisterol3 B1 / (5E)-(10R)-10-ethoxy-10,19-dihydrovitamin	430.3813	0.927 HILICneg	1	135310	153923	165987	146710	37483	123666	114846	1	105568
Tragopogonsaponin L	913.5194	23.076 Rppos	606808	452267	505054	443735	682579	379932	397888	409261	639291	452629
Trans-2,3-dehydrododecanoyl-CoA	946.2788	22.146 Rppos	2279029	2373155	2259303	2455588	1559558	562550	1543044	673025	799818	658324
trans-2-Enoyl-OPC4-CoA	984.2668	24.722 Rppos	1677464	1700191	1350763	1592449	1391267	1173243	1102028	1219605	1670815	1319201
trans-Aconitate	174.0157	1.06 Rpneg	23634	18286	27952	16956	23718	16751	1	10370	7727	20301
trans-Aconitate	174.0173	1.26 HILICneg	252415	218244	105209	143727	281048	118151	177113	166958	113176	234806
trans-Aconitate Esi-0.8979999	174.0166	0.898 Rpneg	3286	3611	5654	4307	3074	5536	6956	3578	4749	5815
trans-Brassidic acid	338.318	13.394 Rpneg	286265	209481	133779	203545	194349	133492	191377	212763	174336	193177
trans-Selacholeic acid	366.3493	13.59 Rpneg	252109	162682	100859	154545	127250	70964	138039	140469	102590	101907
Triacontanedioic acid	482.4348	20.473 Rppos	2765838	3824071	3650024	3682589	2328071	2529660	2244911	2299921	3438254	2840557
Triacontanedioic acid Esi+17.576998	482.4348	17.577 Rppos	3814171	4291157	3652099	4250279	1033393	3118969	2930731	3112033	2334834	3480298
Triamcinolone hexacetonide	532.2824	0.981 HILICneg	369415	79066	74497	80222	268228	386474	118281	122740	420629	158677
Tributyrin	302.173	7.729001 Rpneg	11352	18161	9816	19312	17303	8647	8365	17485	17558	13967
Tributyrin Esi-7.4189997	302.1729	7.419 Rpneg	10913	12708	7210	12950	15786	7575	7623	9529	16292	9539
Tributyrin Esi-7.734	302.1722	7.734 Rpneg	11352	18433	9816	19312	9817	1052	1478	17485	8048	13967
Tridodecylamine	521.589	22.577 Rppos	2650852	2503491	2166703	2412812	2572912	2529101	2439162	2476787	2623420	2334753
Tridodecylamine	521.5902	1.5 HILICpos	1308037	1492878	1179246	1439642	1495855	1354845		1872959	3144938	1256895
Triethyl phosphate	424.1624	1.074 HILICneg	2375858	1587721	801368	1412308	4027093	1	731379	1562670	1136154	1683301
Triethylene glycol diglycidyl ether	262.142	6.408 Rpneg	54256	64031	48940	73397	76879	48989	50927	60686	80438	60353
trifluoroacetic acid	113.9929	1.062 Rpneg	1293462	1350924	1076311	912086	1654909	1500088	1565029	1680100	1450918	1234293
trifluoroacetic acid Esi-0.873	113.9928	0.873 Rpneg	117813	107913	98483	87695	135603	154308	115649	119921	77640	11135
trifluoroacetic acid Esi-12.671999	113.9928	12.672 Rpneg	555208	766675	914464	900328	232298	560450	816587	478283	829793	867894
Trigoneoside XIb	906.4889	23.693 Rppos	973854	1273403	1274653	1244334	2013152	1970235	1260866	1782564	2566140	1781225
Trilauroyl-glycerol	655.5782	26.693 Rppos	1570289	1784136	1624546	1793677	1209472	1263310	1135785	1300017	1724612	1190392
Trimethoprim	289.1538	5.505001 Rppos	590965	260858	269665	547008	645011	666219	530779	421169	575662	651293
Trimethoprim Esi+5.6969995	289.1534	5.697 Rppos	277340	421411	215057	214775	226088	211285	232379	349505	310649	278250
Triphenyl phosphate	326.0711	8.285001 Rppos	257658	354473	654311	318311	280015	289673	335531	313947	334677	339118
Triphenyl phosphate	372.0803	0.902 HILICneg	61116	59409	95792	53789	63464	1	47006	109714	70127	47046
Tris(2-chloroethyl)phosphate	283.9542	6.913001 Rppos	278318	385317	335139	374852	399262	329571	331857	363528	429992	346505
Tris(butoxyethyl)phosphate	398.2448	9.158999 Rppos	146680	183617	1435165	214014	237393	128808	154073	209842	277934	184485
Trolamine	131.0945	1.87 Rppos	867127	780180	659842	726916	1546168	1502168	1410081	2166721	1925548	1648761
Trolamine	149.1048	6.97 HILICpos	371297	305268	113740	753092	171483	132336		570718	416310	394818
Trolamine Esi+1.743	131.0944	1.743 Rppos	438124	423943	294545	385352	804644	680579	645800	1040265	935355	726883
Tromethamine	259.1712	6.028 Rppos	1	1	1	1	315705	231578	1	201688	215125	247664
Trp Arg Glu	535.2362	5.17 HILICneg	61874	26737	21965	39846	36904	9406	14905	20954	11838	13296
Trp His Trp	549.2104	20.752 Rppos	703881	535374	703157	564734	693231	720865	730636	638926	698996	596919
Trp Met Ala	452.1733	12.283 Rpneg	2815	3184	1517	2597	1207	1906	3018	2334	2108	2998
Trp Met Asp	450.1555	11.057 Rpneg	11138	7315	10033	6782	6173	5545	8970	7066	5380	6789
Trp Met Asp Esi-10.849999	450.157	10.85 Rpneg	7501	4679	6859	4742	4259	3073	5956	4839	3533	3954
Trp Met Leu	508.2415	0.996 HILICneg	183377	123422	55604	71810	311077	1	74761	92379	77414	106271
Tuberstemonine	375.2449	12.581 Rpneg	4546	2099	1092	2994	3238	1797	5574	4689	3552	3026
Tumonoic Acid A	369.252	1.077 HILICneg	692139	465369	454313	508106	405888	84348	410526	419747	233612	487960
Tyr Gln His	938.3901	0.994 HILICneg	65165	100140	64322	83355	62957	1	54918	60900	58660	40186
Tyr Glu Asp	425.1433	1.311 Rpneg	22855	30549	22367	31908	24081	28101	32085	14796	18735	23437
Tyr Glu Thr	471.1865	5.094 Rpneg	49025	23755	32782	28314	14134	20701	14645	24481	12427	18058
Tyr Gly Asn	352.1396	4.158001 Rpneg	18053	14397	17357	16659	13127	15443	13410	18546	16670	20002
TyrMe-Phe4Cl-OH	558.1427	1.734 Rpneg	113162	91026	90443	107433	92571	109009	67455	109586	112032	106692
TyrMe-Phe4Cl-OH	558.1446	6.367 HILICneg	318063	403770	385456	392539	391789	330295	363518	363184	368058	377216
U-75302	361.2607	13.444 Rpneg	2207	1401	2449	2557	1408	837	1387	1249	1636	1218
Ubiquinone 8	743.5886	24.497 Rppos	322845	276399	206165	366221	286638	1	208437	233660	195104	187082
Ubisemiquinone	862.6853	22.48 Rppos	990596	3407052	3903486	4565545	3780998	908430	3128790	2819497	2729264	1468229
Ubisemiquinone Esi+22.477999	862.6849	22.478 Rppos	972376	3420186	3896503	4443924	3532388	912102	3241980	2744079	2710013	1270102
UDP-N-acetyl-D-mannosamine	607.0804	0.808 Rpneg	17717	14559	19833	16417	11865	10687	13241	8202	8142	7730
UK 78282	875.5591	25.211 Rppos	1418324	1725268	1484869	1386704	847955	774457	761310	818713	783897	834064
UNC0321	519.3251	5.867 Rppos	431324	721087	414168	646403	884332	463499	389041	653367	881707	531982
Unoprostone isopropyl ester	423.3349	10.696 Rppos	441039	3086594	3932219	3880143	8652452	6431350	3126539	5654783	5174856	7576979
Unoprostone isopropyl ester	441.3459	2.715 HILICpos	3195288	1447942	1051679	787143	977061	1368609		1618726	2271841	2051117
Unoprostone isopropyl ester Esi+10.508001	441.3452	10.508 Rppos	727376	1936908	2731552	2047545	3907976	2978544	2832237	3988292	2326631	3471246
Unoprostone isopropyl ester Esi+10.746001	441.3453	10.746 Rppos	624174	931079	1450314	913266	2017513	1955312	2128484	2651961	1601945	2150746
Unoprostone isopropyl ester Esi+11.374	423.3351	11.374 Rppos	154016	608522	951301	708870	1462825	1139619	1111753	1270936	849261	1092954
uracil	112.0274	2.354 HILICneg	2676912	3168722	3630237	3199015	2607483	1541276	2117921	1826265	2037873	1961363
Uralenol	370.1058	5.11 Rpneg	1	39792	1663	26865	39391	1375	1544	19592	43865	15878
URB937	354.1579	12.287 Rpneg	6607	5534	3042	5103	3320	1297	2951	5155	3596	5288
Ustilagic acid	830.4178	11.922 Rpneg	5681	1027	9553	7311	17773	3202	7307	6455	5482	7697
Val Gln Val	688.4143	1.073 HILICneg	400355	477920	156777	284358	551433	1	130165	255899	160716	159748
Val Leu Asn	326.1942	5.338 Rppos	734693	1506635	710796	1394460	1855528	801678	755723	1353760	1978026	1167817
Val LysLys	763.5647	21.979 Rppos	14909839	15727936	16157763	16706591	14218493	11913477	15086130	14774128	12745433	12898065
Valdiate	310.1781	10.209 Rpneg	53637	52572	55963	55990	51826	54234	56200	59333	56808	60427
Valdiate Esi-7.399001	310.1772	7.399001 Rpneg	10863	8008	10727	11112	7360	9262	10691	10072	9112	11562
Valnemulin	564.3589	13.73 Rpneg	10056	11159	14520	16795	9323	11398	14100	11329	16077	14962
Valnemulin	564.3635	1.185 HILICneg	1	84334	74594	80541	200202	1	84316	105480	93632	101472
Val-Val-OH	370.135	12.213 Rpneg	2610	1880	10519	2096	1957	1271	1485	1052	1834	1
Valyl-Lysine	245.1739	0.823 Rppos	331910	740264	372288	608463	749032	421377	355535	577768	1043257	613848
Valyl-Proline	214.131	5.135 Rpneg	1599	8862	2714	11789	9372	1850	1886	11022	1	1
Verapamil	471.3099	1.417 HILICpos	450101	567823	84014	106672	287328	217176		93887	93268	73272
Vignatic acid A	553.2812	11.838 Rppos	576735	612187	727329	678482	714091	769979	671077	505060	585281	525369
Viniferifuran	452.1272	10.879 Rpneg	2315	3407	2438	1654	2141	1320	2540	2959	2428	2334
Vitisifuran B	921.2729	0.708 HILICpos	1464817	591334	1611859	752090	389528	1810842		866621	1650785	755510
Vogeletin	316.0609	1.51 HILICneg	25306	44935	44017	53392	53550	1	94667	42940	28834	47447

VPGPR Enterostatin	524.3049	13.638 Rpneg	2451	1155	1824	1584	2050	1488	2101	1850	2417	2050
Xanthosine	284.0771	6.33 HILICneg	104154	71739	62645	71337	75224	31023	33521	32012	19681	47736
Xeniasterol-a	538.3827	13.48 Rpneg	5816	15873	3422	5201	4147	3271	4698	2778	8431	4250
Xestoaminol C	229.2405	1.814 HILICpos	909044	593634	425024	472718	562238	462009		557963	1115046	742976
YS121	453.1464	7.782 HILICneg	62530	66847	76443	59735	85345	73530	73459	64678	58556	55686
zeta-Carotene epoxide	602.4677	12.857 Rpneg	6149	5321	3897	4524	5772	6622	6860	7739	7902	7492
Zolazepam	632.2656	4.152 HILICneg	44424	1	39389	31836	1	1	22324	1	1	19367
Zopiclone	434.1123	0.839 Rpneg	2038	1710	3837	2413	1418	3336	3277	1654	1246	1
Zotepine	331.0776	6.363999 HILICneg	496914	658203	671743	677347	632942	504115	555067	609848	561271	656590
Zwittergent 3-14	328.2481	14.099 Rppos	805360	710062	623538	1410422	445625	778286	881313	661807	474884	358428