Supplementary Online Content

Plasma metabolomics of autism spectrum disorder and influence of shared components in proband families

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This supplementary material has been provided by the authors to give readers additional information about their work.

Methods S1. Inclusion and exclusion criteria for ASD, controls, proband families

We enrolled a total of 104 individuals (75 cases and 29 controls), who were part of a blood transcriptome study conducted at the Boston Children's Hospital to assess gene expression signature unique to ASD in years 2007–2012.

Inclusion criteria for the ASD group were a clinical diagnosis of ASD by Diagnostic and Statistical Manual of Mental Disorders, Fourth Edition, Text Revision and age of 24 months or older. All patients with ASD were assessed with the Autism Diagnostic Observation Schedule (ADOS) and the Autism Diagnostic Interview-Revised (ADI-R). We excluded individuals with known genetic causes of ASD such as fragile X syndrome, tuberous sclerosis, Landau-Kleffner syndrome, and Klinefelter syndrome. We documented a broad range of phenotypes, such as ASD diagnoses, clinical test records, and allergy history. All individuals in the control group had no abnormal lab test results and did not have any chronic disease, intellectual disability, ASD, or other neurological disorders.

In our family-based analysis, there were 25 trios (parents with one ASD proband), 4 quartets (parents with two ASD probands), 4 father/mother-ASD pairs, 10 families with only father/mother/father and mother, and 38 families with only ASD cases. There were 31 families meeting the minimum requirements for the shared environment analysis (i.e., with at least one ASD proband and at least one parent).

Methods S2. Measurement of the metabolome

Briefly, 50 μL aliquots of plasma were mixed with acetonitrile containing 14 stable isotope internal standards at a 2:1 ratio to precipitate proteins. Samples were then equilibrated on ice for 30 minutes and centrifuged for 10 minutes at 13 400 rpm at 4°C. The supernatant was transferred to autosampler vials and kept in a refrigerated autosampler until untargeted metabolic profiling. Each extract was analyzed in triplicate using a dual column chromatography scheme that includes hydrophilic interaction liquid chromatography (HILIC; XBridge BEH Amide XP HILIC column; Waters, Waltham, MA, 50x2.1mm, 2.5μm) and reversed phase liquid chromatography (RPLC; C18 column; Higgins Analytical, Mountain View, CA, 50x2.1mm, 2.6 μm). The chromatography was coupled with HRMS in positive (HILIC) and negative electrospray ionization (ESI) modes (RPLC) that enabled an increased coverage of the plasma metabolome. Mass spectral data was collected with a 5-minute mobile phase gradient on a Thermo Q-Exactive HF high-resolution mass spectrometer (Thermo Fisher, San Diego, CA) set to collect data from mass-to-charge ratio (m/z) of 85 to 1,275 at a resolution of 120,000. Data were collected on a mobile phase gradient over a 5-minute period. Analyte separation for HILIC was performed with a gradient elution with mobile phases A: LCMS grade water, B: LCMS grade acetonitrile, C: 2% formic acid. The initial 1.5 min period consisted of 22.5% A, 75% B, and 2.5% C, followed by a linear increase to 75% A, 22.5% B, and 2.5% C at 4 min and a final hold of 1 min. C18 chromatography was performed on an end capped C18 column with mobile phases A: water, B: acetonitrile, C: 10 mM ammonium acetate. The initial 1 min period consisted of 60% A, 35% B, and 5% C followed by a linear increase to 0% A, 95% B, and 5% C at 3 min and held for the remaining 2 min. For both methods, the mobile phase flow rate was 0.35 mL/min for the first min and increased to 0.4 mL/min for the final 4 min. Tune parameters for sheath gas were 45 for ESI+ and 30 for ESI-. Auxiliary gas was set at 25 for ESI+ and 5 for ESI-. Spray voltage was set at 3.5 kV for ESI+ and -3.0 kV for ESI-.

Methods S3. Data acquisition and QAQC

Prior to analysis, probands, controls and parental samples were randomized into 5 batches. Samples were analyzed in triplicate in batches of 40 study samples, with each batch including 6 separate analyses of two different QAQC samples. The QAQC samples (identified as QSTD_plasma and CHEAR_plasma) were designed to include a wide distribution of donor ages, sex and races to be as representative as possible. To verify the quality of the untargeted metabolomics data, QA/QC is completed using the pooled reference samples, labeled internal standards and triplicate analysis for each sample. For all samples, labeled internal standards ([$^{13}C_6$]-D-glucose, [^{15}N,$^{13}C_5$]-L-methionine, [$^{13}C_5$]-L-glutamic acid, [^{15}N]-L-tyrosine, [3,3-$^{13}C_2$]-cystine, [trimethyl-$^{13}C_3$]-caffeine and [$^{13}C_5$, $^{15}N_2$]-L-glutamine) were added at levels reflecting normal physiological concentrations. Data is qualified using a five-step procedure that includes record keeping for study information (name, PI information, date samples received, number of samples, number of batches, length, internal study ID, species, matrix, preservative, freeze/thaws prior to arrival), sample preparation record keeping (technician, time samples were removed from storage, sample preparation workflow, pooled sample batch, internal standards, number of QC samples), chromatographic QA/QC (method information, solvents, run length, column and identifier information, injection volume, evaluation of representative peak extracted ion chromatograms, retention time and deviation); mass spectrometry QA/QC (instrument name, tune file, polarity and resolution, coefficient of variation (CV) for metabolites in pooled QAQC samples and internals standards, median CV for all metabolites); and overall study QA/QC (PCA clustering to evaluate batch effects and outliers, distribution of the sum of feature intensity across all samples and batch).

QA/QC analysis is completed daily for each batch using an automated workflow and is verified by at least two different individuals. Final study QAQC is completed upon completion of all sample analyses. Batches not meeting acceptance criteria are discarded and re-analyzed (if applicable). Post-instrument acquisition, data extraction and alignment contain additional levels of QA/QC. Using xMSanalyzer, replicate injections are first tested for correlation coefficient, samples with $r < 0.7$ and p-value > 0.05 are discarded. Feature median triplicate RSD, peak score, number of non-detects, samples with detected values in two of three injections and Q-score (a combination of RSD and non-detected values) are also evaluated for the finalized data.

A summary of key QAQC metrics is provided. PCA was performed to evaluate potential differences in QAQC pooled samples and study samples (Figure S1A-B), batch effects (Figure S1C-D) and any global differences among parental, control and proband samples (Figure 1E-F). Although PCA suggest global differences between QAQC and study samples, this can be expected since the population and collection protocols may have differed from those used to collect study samples. No differences among batches or sample types were observed. Summary statistics for both analytical modes, including triplicate CVs, average peak intensity ranges, and number of missing values are provided in Figure S2A-B. Triplicate CVs for HILIC and RPLC were 30.2% and 28.6%, respectively, while average peak intensities ranged over 7 orders of magnitude and the majority of features were detected in >50% of samples. To assess inter-sample variation, we used pooled QC samples, CHEAR_plasma, for variation assessment because it has the closest matrix effects to the actual samples. We selected a total of 30 pooled QC measurements and removed features that contained > 80% zero intensity. We estimated the CVs for each of the log2 transformed features because most of the features were right-skewed. Features in the highest 20% of the CVs were considered low quality and were excluded from further downstream analysis. The median CVs were 27.3% (HILIC) and 3.9% (RPLC) (Figure S3). Analytical variation was further evaluated by determining internal standard CVs across all samples, as well as within parental, control and proband groups (Table S3). The average CV for all sample groups was 7.9%, with the majority under 10%. Average CV for [3,3-$^{13}C_2$]-cystine was the only standard with an average CV >20%.

Methods S4. Pathway enrichment analysis

To discover the perturbed molecular pathways in ASD, we ran Mummichog (a web version through www.metaboanalyst.ca) with the accurate masses of all features, the *P* values and *Z* scores from MWAS as input. We used FDR equivalent *P* value as the cut off threshold and matched with the pathways in the Homo sapiens library (KEGG Oct 29, 2019 version). Significant pathway enrichment was determined through the gamma *P* value.

We show the ASD-associated molecular pathways in Table S4. We found 31 enriched pathways (RPLC: 19) and only listed 10 of them (RPLC: 5) that had a marginal *P* value of < 0.1. Glutathione (GSH) is a tripeptide antioxidant to protect damages caused by reactive oxygen species such as free radicals and various kinds of peroxides [1]. Catalyzed by GSH peroxidase, GSH reacts oxidative species and reduced glutathione disulfide (GSSG). The recycling of GSSG back to GSH is catalyzed by GSH reductase. This is a continuous process and the ratio of GSH/GSSG in an organism can be used as a measure of oxidative stress [2]. Meta-analysis of GSH peroxidase in red blood cells had concluded that reduction of its activities is associated with ASD [3], which is in line with the dysregulation of glutathione metabolism found. It is not clear the causes of reduced function of GSH enzyme but could be related to genetic polymorphisms in glutaredoxin and cystathionine gamma-lyase genes [4]and selenium deficiency in diet because GSH peroxidase is a selenium dependent enzyme [5].

Methods S5. Chemical annotation

For each of the putatively identified chemicals, we further annotated their source, generation activity, route of exposure, and biological functions. We synthesized the annotations through querying the HMDB, PubChem, KEGG, Chemical Entities of Biological Interest, and the Comparative Toxicogenomics Database.

Further annotation regarding the sources and roles of the putatively identified chemicals is shown in Table S5. For the HILIC data, we found that over half of the identified (12/21) could have a man-made origin, such as pharmaceuticals and pesticides. Fourteen percent of them (3/21) were the compounds participated in human metabolic pathways and 24% of them (5/21) were natural chemicals found in food. For RPLC data, all of them have an exogenous origin. Half of the chemicals (5/10) were pharmaceuticals and 20% (2/10) were dietary chemicals.

Table S1. Putatively identified metabolites from the metabolome-wide association study using HILIC analytical platform

Please see the end of the Supplementary Information.

Table S2. Putatively identified metabolites from the metabolome-wide association study using RPLC analytical platform

Please see the end of the Supplementary Information.

Table S3. Summary of labelled internal standard CVs

Internal Standard	All samples	Probands	Controls	Father	Mother
[trimethyl-$^{13}C_3$]-caffeine	1.8%	1.8%	1.4%	1.4%	1.7%
[^{15}N,$^{13}C_5$]-L-methionine	6.7%	2.3%	19.4%	2.2%	2.6%
[$^{13}C_5$]-L-glutamic acid	3.9%	3.7%	4.7%	3.3%	5.1%
[$^{13}C_5$, $15N_2$]-L-glutamine	14.3%	11.4%	2.9%	15.6%	16.0%
[3,3-$^{13}C_2$]-cystine	22.4%	16.3%	19.5%	27.6%	23.1%
[^{15}N]-L-tyrosine	6.7%	2.2%	19.3%	1.9%	2.2%
[$^{13}C_6$]-D-glucose,	2.4%	2.2%	3.0%	1.9%	2.5%

Table S4. Summary of the pathway enrichment analysis using *Mummichog*

Platform	Pathway	Total metabolites in pathway	No. of significant metabolites	Gamma *p* value
HILIC				
	Glutathione metabolism	28	5	0.048
	Lysine degradation	25	4	0.051
	Aminoacyl-tRNA biosynthesis	48	5	0.053
	Alanine, aspartate and glutamate metabolism	28	4	0.061
	D-Glutamine and D-glutamate metabolism	6	2	0.063
	Arachidonic acid metabolism	36	3	0.072
	Valine, leucine and isoleucine biosynthesis	8	2	0.075
	Valine, leucine and isoleucine degradation	40	3	0.077
	Arginine and proline metabolism	38	3	0.077
	Pyrimidine metabolism	39	4	0.082
RP				
	Caffeine metabolism	10	2	0.070
	Fatty acid biosynthesis	47	2	0.072
	Amino sugar and nucleotide sugar metabolism	37	3	0.075
	Fructose and mannose metabolism	20	2	0.080
	Steroid hormone biosynthesis	85	3	0.097

Only pathways with gamma *P* value < 0.1 are shown.

HILIC: Hydrophilic interaction liquid chromatography.

RP: Reversed phase liquid chromatography.

Table S5. Exposure and functional annotation of the putatively identified metabolites from the metabolome-wide association study

Platform	Name	Source	Process [a]	Route of exposure	Role
HILIC					
	Lamivudine-triphosphate	Endogenous	Biological	NA	Drug metabolite; waste product
	Nornitrogen mustard	Endogenous	Biological	NA	Drug metabolite; waste product
	4R-Hydroxy solifenacin	Endogenous	Biological	NA	Drug metabolite; waste product
	desbutyl-lumefantrine	Endogenous	Biological	NA	Drug metabolite; waste product
	Thiodiacetic acid	Endogenous	Biological	NA	Drug metabolite; waste product
	2-Oxo-3-hydroxy-4-phosphobutanoic acid	Endogenous	Biological	NA	Participated in host metabolic pathway
	O-Phosphotyrosine	Endogenous	Biological	NA	Participated in host metabolic pathway
	2-Oxophytanate;2-Oxophytanic acid	Endogenous	Biological	NA	Participated in host metabolic pathway
	N-Methylpelletierine	Exogenous	Agricultural	Ingestion	Dietary molecule; participated in host metabolic pathway
	Piperidine	Exogenous	Agricultural	Ingestion	Dietary molecule
	Apigenin 7-sulfate	Exogenous	Agricultural	Ingestion	Dietary molecule
	N-(14-Methylhexadecanoyl)pyrrolidine	Exogenous	Agricultural	Ingestion	Dietary molecule
	Toxoflavine	Exogenous	Biological	Ingestion, contact	Bacterial toxin
	Tulobuterol	Exogenous	Biological	Contact	Pharmaceuticals
	5-Hydroxy-734-trimethoxy-8-methylisoflavone 5-O-neohesperidoside	Exogenous	Biological	Ingestion	Dietary molecule; participated in host metabolic pathway
	Octylamine;N-Octylamine;Monoctylamine	Exogenous	Industrial	Ingestion, contact	Lubricants and greases; industrial intermediate
	Carbophenothion	Exogenous	Industrial	Ingestion, contact	Pesticide
	Silver sulfadiazine	Exogenous	Industrial	Ingestion	Pharmaceuticals
	3beta-Hydroxylanostane-711-dione acetate	Exogenous	Industrial	Ingestion	Pharmaceuticals
	Saccharin sodium anhydrous	Exogenous	Industrial	Ingestion	Sweetening Agents
	2-(2-Chloro-phenyl)-5-(5-methylthiophen-2-yl)-134oxadiazole	NA	NA	NA	NA
RP					
	(3b6b8a12a)-812-Epoxy-7(11)-eremophilene-6812-trimethoxy-3-ol	Exogenous	Agricultural	Ingestion	Dietary molecule
	Visnagin	Exogenous	Agricultural	Ingestion	Pharmaceuticals
	Oseltamivir phosphate	Exogenous	Biological	Ingestion	Pharmaceuticals
	Captopril	Exogenous	Biological	Ingestion	Pharmaceuticals
	8-Hydroxyalanylclavam	Exogenous	Biological	Ingestion	Pharmaceuticals (related to biosynthesis of antibiotics)
	N-(Ethoxycarbonyl)methyl)-p-menthane-3-carboxamide	Exogenous	Biological	Ingestion	Food additive
	Zeranol	Exogenous	Agricultural	Ingestion	Growth promoter for food animals
	Oleandolide	Exogenous	Biological	Ingestion	Pharmaceuticals (related to biosynthesis of antibiotics)
	Floionolic acid	Exogenous	Agricultural	Ingestion	Dietary molecule
	1-Dodecanoyl-sn-glycerol	NA	NA	NA	NA

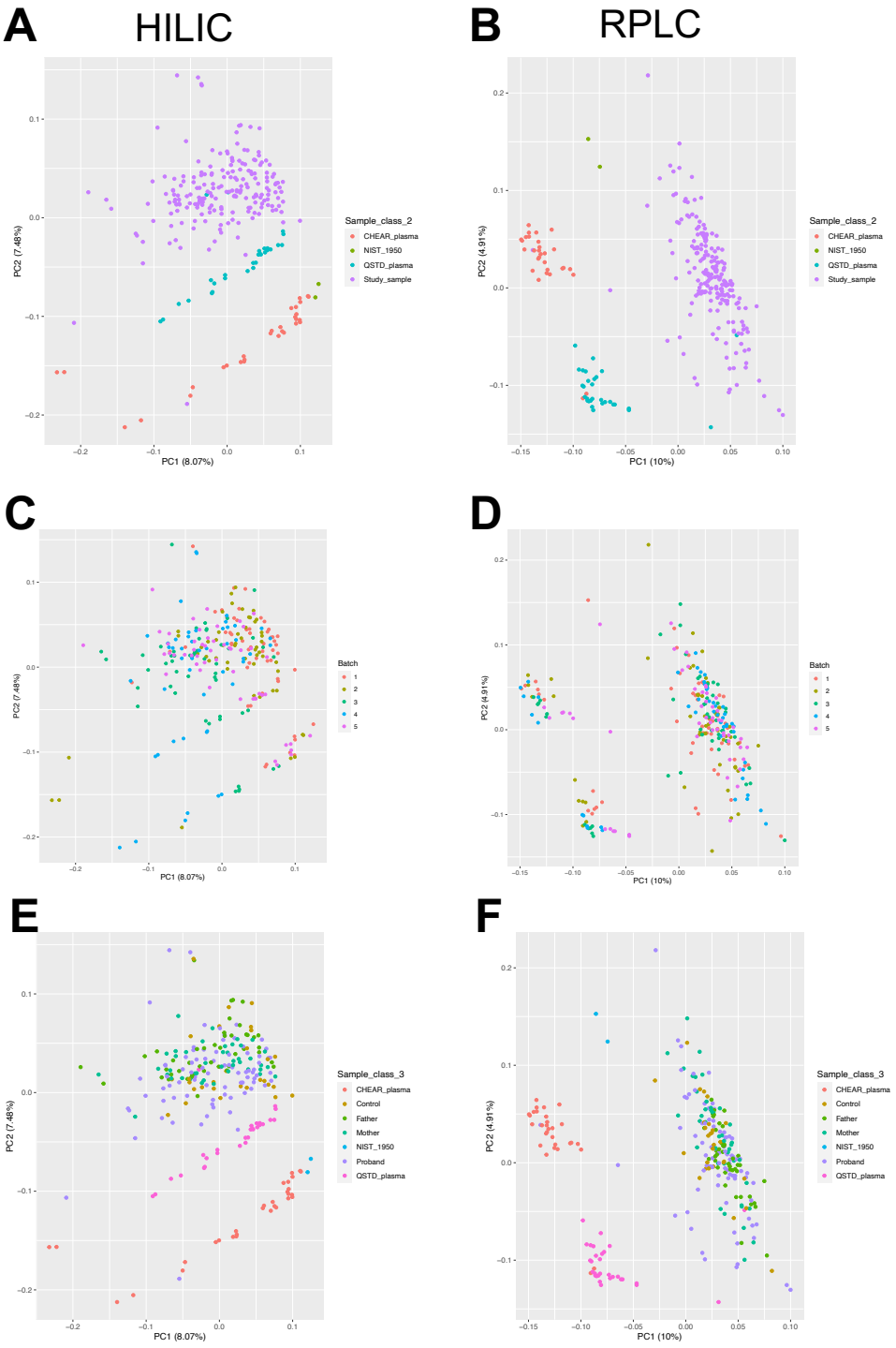
NA: Not available.

HILIC: Hydrophilic interaction liquid chromatography.

RP: Reversed phase liquid chromatography.

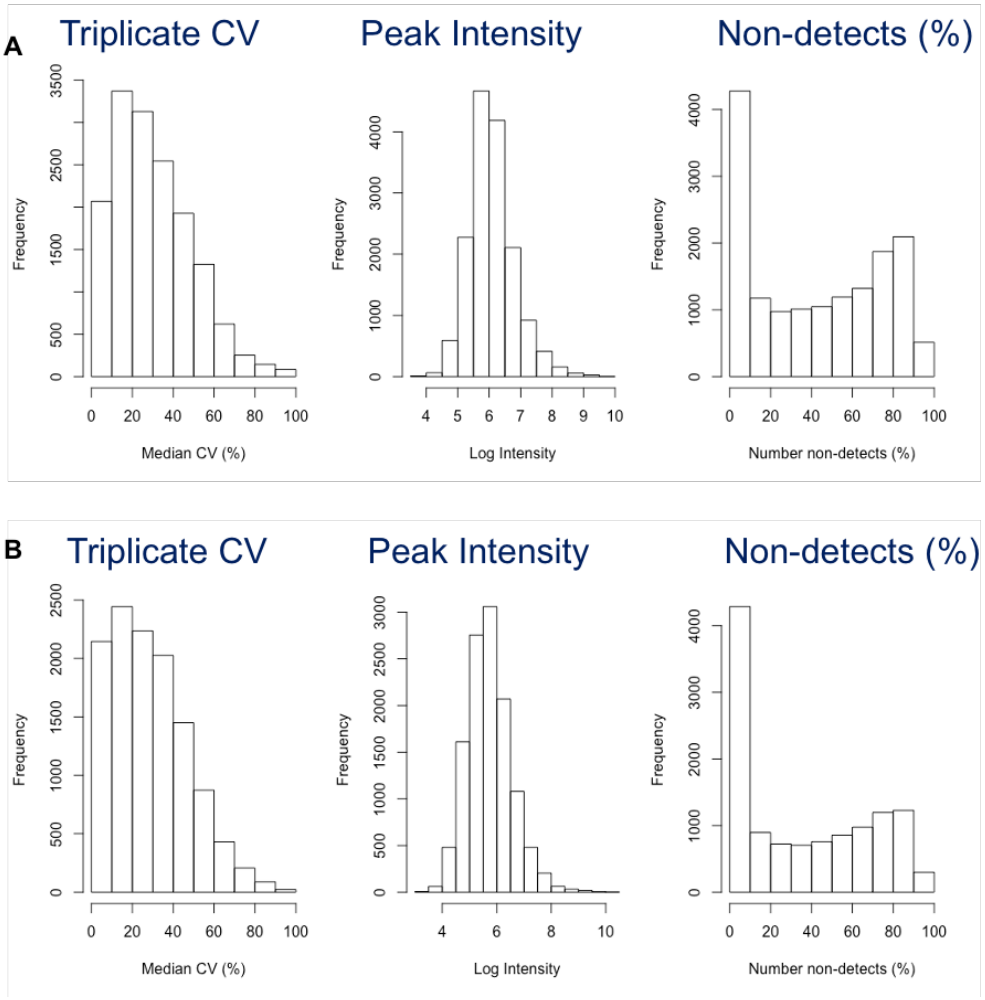
[a] The main activity source associated with the metabolite.

Figure S1. Principal component analysis for all samples measured using HILIC and RPLC



Score plots were colored based upon A-B) QAQC or study samples; C-D) Batch number; E-F) Sample case.

Figure S2. Data extraction QAQC metrics



A) HILIC and B) RPLC

Figure S3. Empirical cumulative distribution of the coefficient of variation of features in quality control samples

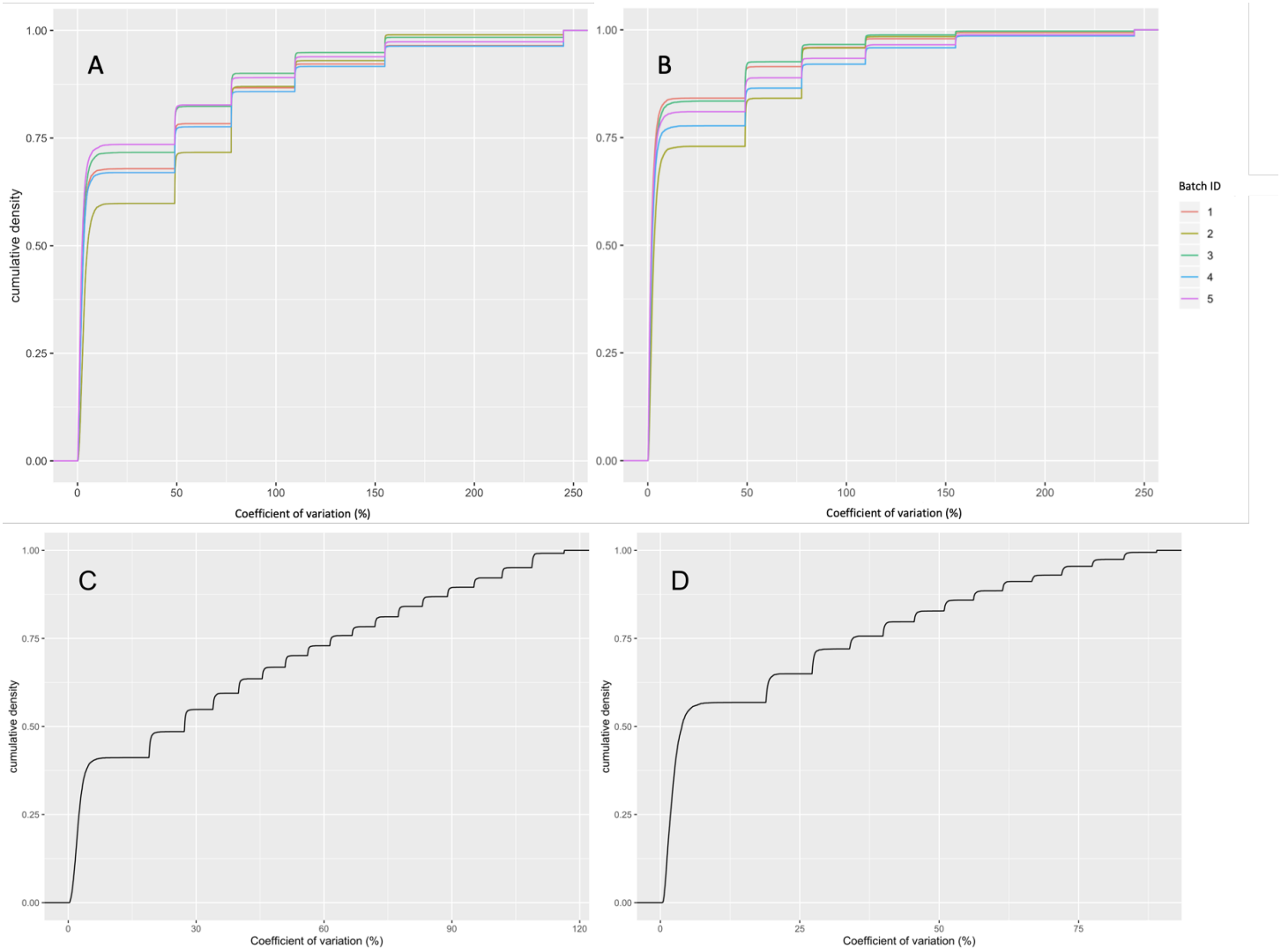


Figure S1. Empirical cumulative distribution of the coefficient of variation of the features found in quality control samples. A & B) Analytical batch 1 to 5 are shown. Each batch contains 6 QC measurements. C&D) Batches are combined and CV is estimated with 30 QC measurements. A & C) HILIC platform. B & D) RPLC platform.

Figure S4. Volcano plots showing the estimates from metabolome-wide association study

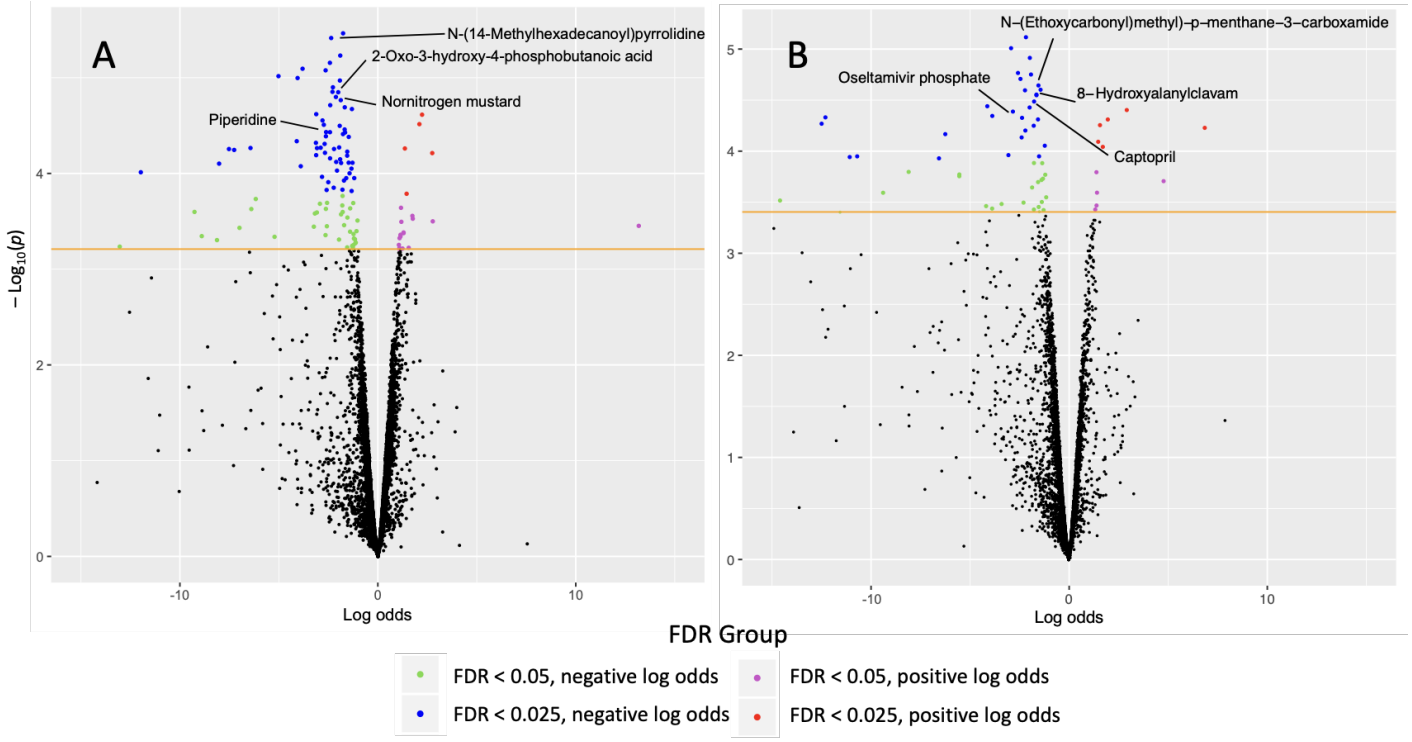
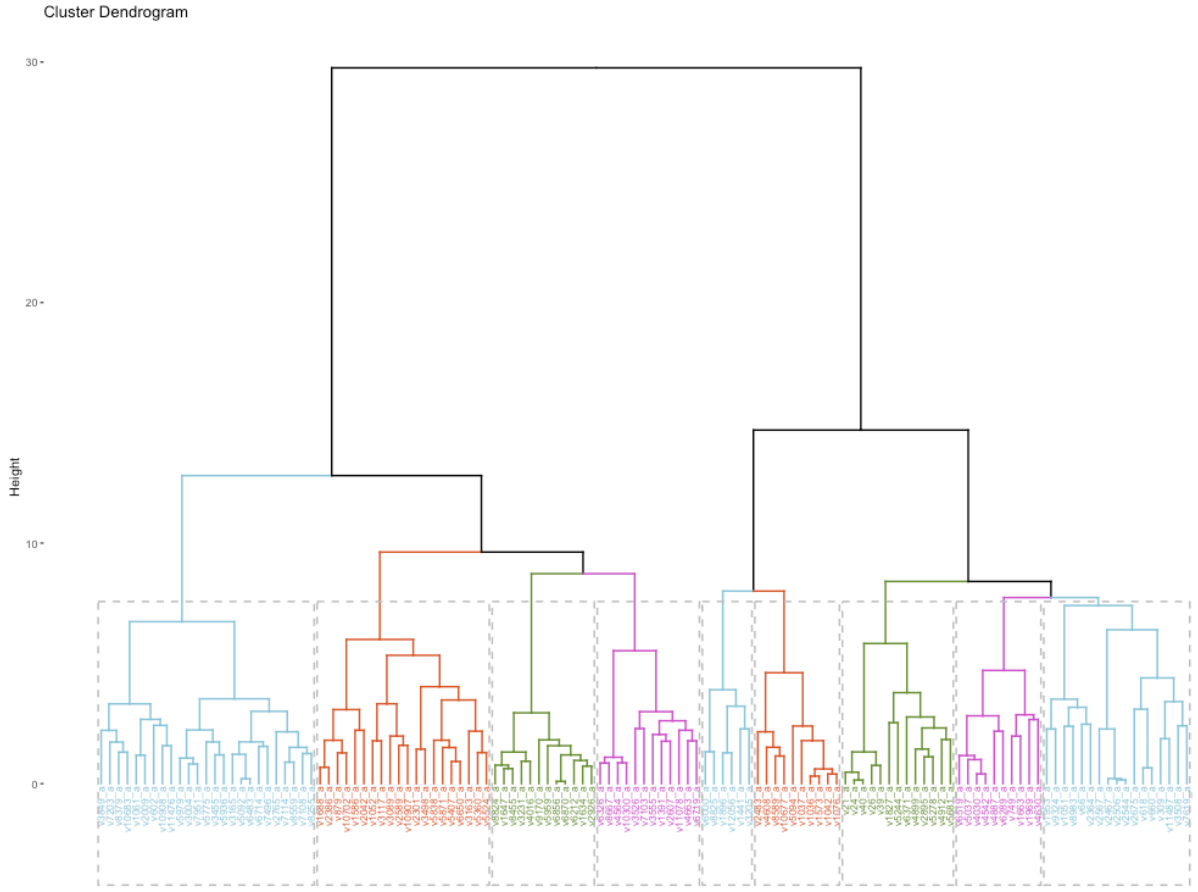


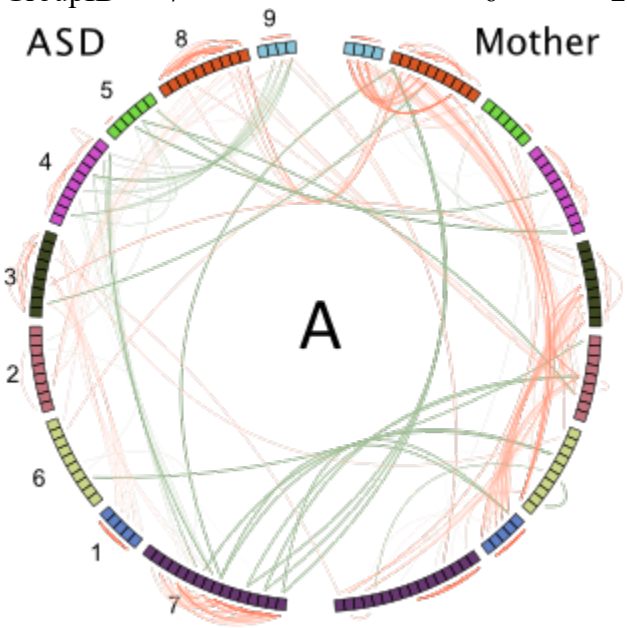
Figure S4. Volcano plots showing the estimates from metabolome-wide association study. A) hydrophilic interaction liquid chromatography platform; B) reversed phase chromatography platform. Minus $\log_{10}$ of the p values are shown on the vertical axis, and log odds of autism spectrum disorder (per two fold increase of the feature intensity, scaled to have unit variance for comparisons) are shown on the horizontal axis. X axis is restricted to show a numerical range between -15 to 15. Orange horizontal line denotes a false discovery rate (FDR) threshold at 0.05. FDR significant features are colored into 4 groups as shown in the legend. Four putatively identified features with lowest p values were labeled.

Figure S5. Dendrograms of the hierarchical clustering of the MWAS significant features

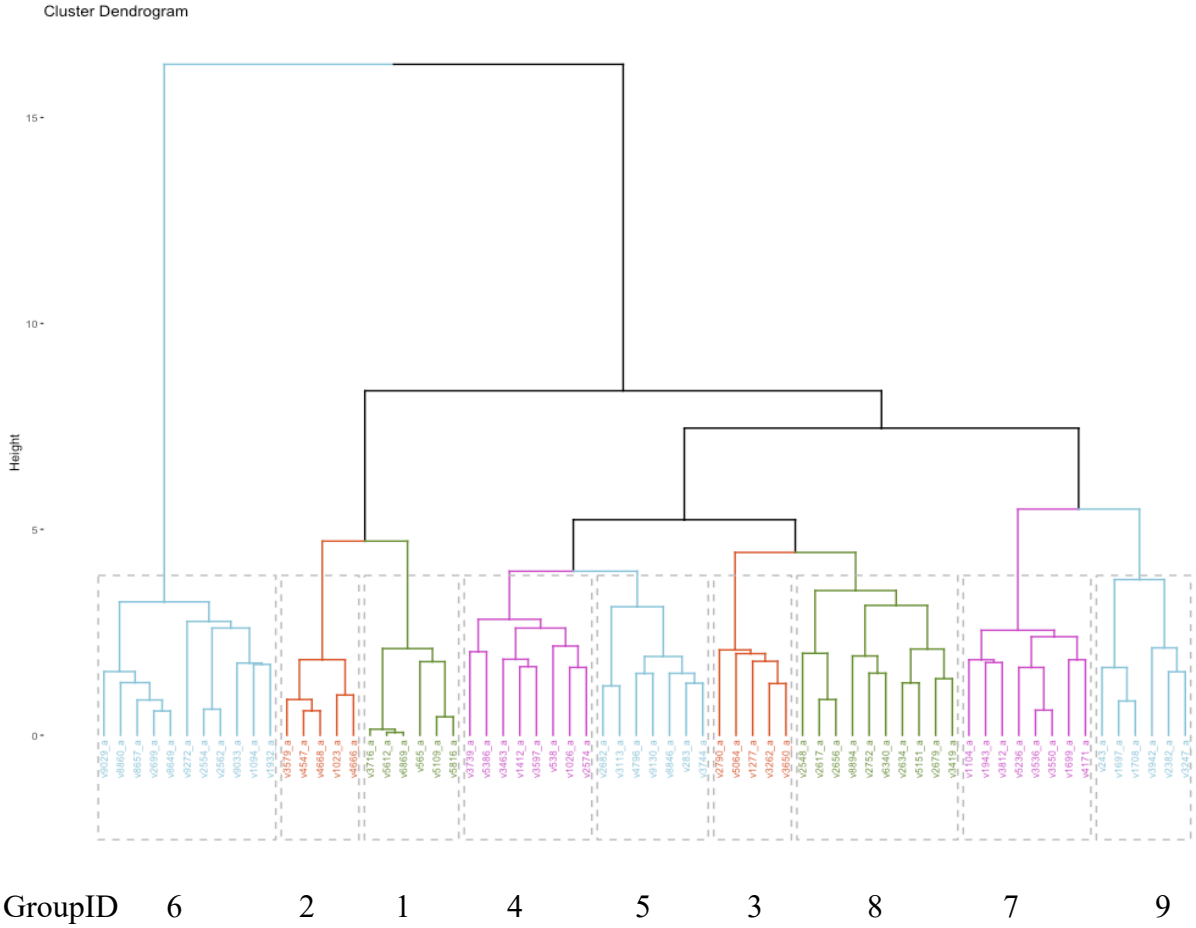
HILIC:



GroupID 7 6 2 3 9 1 8 5 4



RPLC



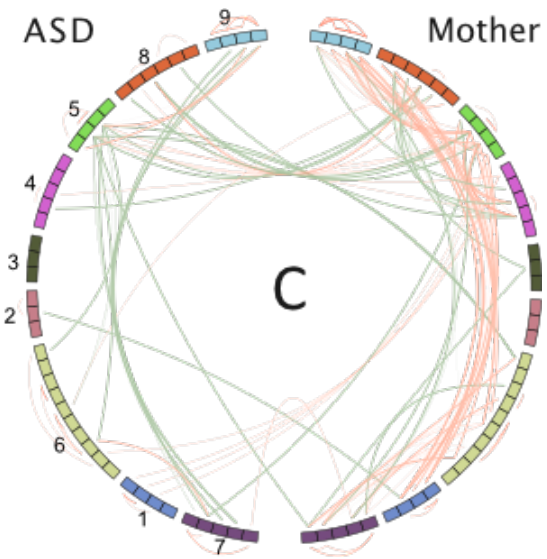


Figure S5. Dendrograms of the hierarchical clustering of the MWAS significant features of the comparison between ASD cases and controls (HILIC: 125; RPLC: 66). We used Euclidean distance as the metric for closeness and arbitrarily set to create 9 feature groups to aid pattern inspection in Figure 3. The Y axis denotes the closeness, and the X axis shows the internal IDs of the features. We only show the features that were detected both in ASD and their parents in Figure 3 (i.e., on the circular tract), therefore the number of features in Figure 3 is smaller than the features shown in the dendrograms. We labelled the corresponding groups in dendrograms and correlation globes for easier comparison.

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Table S1. Putatively identified metabolites from the metabolome-wide association study of autism cases and controls using HILIC analytical platform. Both uniquely and multiply matched annotations are shown.

mzid	Monoisotopic Mass	Time (s)	Odds ratio	OR lower CI	OR higher CI	p value	q value	dbID	Name
v2364	174.1004	66.4	530763.5	2022.41	8.3E+09	0.000353	0.038789	C00437	N-Acetylornithine;N2-Acetyl-L-ornithine
v2042	163.0494	122.8	0	0	0.001	9.72E-05	0.017272	C00715	Pterin;2-Amino-4-oxopteridine;2-Amino-4-hydroxypteridine
v6212	336.2301	28.4	0.32	0.157	0.583	0.000536	0.04761	C00959	Prostaglandin B1;PGB1
v1969	160.0848	70.8	9.335	3.821	31.837	2.43E-05	0.012975	C00993	D-Alanyl-D-alanine;D-Ala-D-Ala
v2364	174.1004	66.4	530763.5	2022.41	8.3E+09	0.000353	0.038789	C01047	N5-Ethyl-L-glutamine;L-Theanine
v5278	292.2038	24.6	0	0	0.01	7.90E-05	0.015103	C01226	12-OPDA;(15Z)-12-Oxophyto-1015-dienoate;(15Z)-12-Oxophyto-1015-dienoic acid;9(S)13(S)-12-Oxo-PDA;12-Oxo-1015(Z)-phytodienoic acid
v1051	129.1518	28	0.001	0	0.027	0.00037	0.039469	C01740	Octylamine;N-Octylamine;Monoctylamine
v24	85.0891	44.2	0.061	0.013	0.188	2.80E-05	0.014011	C01746	Piperidine;Azacyclohexane;Hexahydropyridine
v1036	129.0426	81.1	3.281	1.802	6.691	0.00032	0.036032	C01877	4-Oxoproline;4-Oxo-L-proline
v1036	129.0426	81.1	3.281	1.802	6.691	0.00032	0.036032	C01879	Pidolic acid;5-Oxoproline;Pyroglutamic acid;5-Pyrrolidone-2-carboxylic acid;Pyroglutamate;5-Oxo-L-proline;L-Pyroglutamic acid;L-5-Pyrrolidone-2-carboxylic acid
v6000	326.2821	25.5	4.275	2.164	10.106	0.000163	0.024299	C02117	2-Oxophytanate;2-Oxophytanic acid
v6212	336.2301	28.4	0.32	0.157	0.583	0.000536	0.04761	C02165	Leukotriene B4;(6Z8E10E14Z)-(5S12R)-512-Dihydroxyeicosa-681014-tetraenoate;(6Z8E10E14Z)-(5S12R)-512-Dihydroxyicosa-681014-tetraenoate;LTB4
v1036	129.0426	81.1	3.281	1.802	6.691	0.00032	0.036032	C02237	5-Oxo-D-proline;D-Pyroglutamic acid;D-5-Pyrrolidone-2-carboxylic acid
v2042	163.0481	122.8	0	0	0.001	9.72E-05	0.017272	C03066	3-Hydroxy-L-glutamate;3-Hydroxy-L-glutamic acid
v2042	163.0481	122.8	0	0	0.001	9.72E-05	0.017272	C03079	4-Hydroxy-L-glutamate;4-Hydroxy-L-glutamic acid
v1969	160.0848	70.8	9.335	3.821	31.837	2.43E-05	0.012975	C03153	N5-Methyl-L-glutamine
v1036	129.0426	81.1	3.281	1.802	6.691	0.00032	0.036032	C04281	L-1-Pyrroline-3-hydroxy-5-carboxylate;3-Hydroxy-L-1-pyrroline-5-carboxylate;(3R5S)-1-Pyrroline-3-hydroxy-5-carboxylate
v1036	129.0426	81.1	3.281	1.802	6.691	0.00032	0.036032	C04282	1-Pyrroline-4-hydroxy-2-carboxylate
v5278	292.2038	24.6	0	0	0.01	7.90E-05	0.015103	C04672	(9Z15Z)-(13S)-1213-Epoxyoctadeca-91115-trienoic acid;(9Z15Z)-(13S)-1213-Epoxyoctadeca-91115-trienoate;(9Z)-(13S)-1213-Epoxyoctadeca-91115-trienoate;1213(S)-EOT;1213(S)-EOTrE
v6212	336.2301	28.4	0.32	0.157	0.583	0.000536	0.04761	C04685	(13E)-(15S)-15-Hydroxy-9-oxoprosta-1013-dienoate;Prostaglandin A1;PGA1
v6212	336.2301	28.4	0.32	0.157	0.583	0.000536	0.04761	C04686	(13E)-(15S)-15-Hydroxy-9-oxoprosta-1113-dienoate;Prostaglandin C1
v5681	310.2144	24.1	0.001	0	0.014	5.68E-05	0.014039	C04785	13(S)-HPOT;(9Z11E15Z)-(13S)-Hydroperoxyoctadeca-91115-trienoate;(9Z11E15Z)-(13S)-13-Hydroperoxyoctadeca-91115-trienoic acid;13(S)-HpOTrE;13-HPOT
v6212	336.2301	28.4	0.32	0.157	0.583	0.000536	0.04761	C04822	8(R)-HPETE;(5Z9E11Z14Z)-(8R)-8-Hydroperoxyeicosa-591114-tetraenoate;(5Z9E11Z14Z)-(8R)-8-Hydroperoxyicosa-591114-tetraenoate
v6212	336.2301	28.4	0.32	0.157	0.583	0.000536	0.04761	C04849	(5Z9E14Z)-(8xi11R12S)-1112-Epoxy-8-hydroxyicosa-5914-trienoic acid;(5Z9E14Z)-(8xi11R12S)-1112-Epoxy-8-hydroxyicosa-5914-trienoate;Hepoxilin A3
v6212	336.2301	28.4	0.32	0.157	0.583	0.000536	0.04761	C05356	5(S)-HPETE;5(S)-Hydroperoxy-6-trans-81114-cis-eicosatetraenoic acid;(6E8Z11Z14Z)-(5S)-5-Hydroperoxyeicosa-681114-tetraenoate;(6E8Z11Z14Z)-(5S)-5-Hydroperoxyeicosa-681114-tetraenoic acid;(5S6E8Z11Z14Z)-5-Hydroperoxyicosa-681114-tetraenoate
v2042	163.0481	122.8	0	0	0.001	9.72E-05	0.017272	C05947	L-erythro-4-Hydroxyglutamate
v6212	336.2301	28.4	0.32	0.157	0.583	0.000536	0.04761	C05965	12(S)-HPETE;(5Z8Z10E14Z)-(12S)-12-Hydroperoxyicosa-581014-tetraenoic acid;(5Z8Z10E14Z)-(12S)-12-Hydroperoxyicosa-581014-tetraenoate;12-Hydroperoxyeicosatetraenoate;12-Hydroperoxyicosatetraenoate;12-Hydroperoxyeicosatetraenoic acid;12-Hydroperoxyicosatetraenoic acid
v6212	336.2301	28.4	0.32	0.157	0.583	0.000536	0.04761	C05966	15(S)-HPETE;(5Z8Z11Z13E)-(15S)-15-Hydroperoxyicosa-581113-tetraenoic acid;15-Hydroperoxyeicosatetraenoate;15-Hydroperoxyeicosatetraenoic acid;15-Hydroperoxyicosatetraenoic acid;(5Z8Z11Z13E)-(15S)-15-Hydroperoxyicosa-581113-tetraenoate
v3455	213.9879	275.6	0.101	0.03	0.245	1.41E-05	0.011973	C06054	2-Oxo-3-hydroxy-4-phosphobutanoate;alpha-Keto-3-hydroxy-4-phosphobutyrate;(3R)-3-Hydroxy-2-oxo-4-phosphonooxybutanoate
v6483	348.1937	29.3	0.278	0.138	0.502	7.74E-05	0.015103	C06094	Gibberellin A53

v1827	155.131	25.8	0.001	0	0.014	5.56E-05	0.014039	C06184	N-Methylpelletierine
v3004	195.9773	275.1	0.122	0.035	0.297	7.58E-05	0.015103	C06367	1-Carboxyvinyl carboxyphosphonate;Carboxyphosphonoenolpyruvate
v1969	160.0848	70.8	9.335	3.821	31.837	2.43E-05	0.012975	C06442	N(gamma)-Acetyldiaminobutyrate;N4-Acetyl-L-24-diaminobutyrate;N4-Acetyl-L-24-diaminobutanoate
v4564	261.0402	69.3	0.167	0.059	0.385	0.000148	0.022851	C06501	Phosphotyrosine;Phosphonotyrosine
v618	113.0841	32.3	0.042	0.005	0.165	0.000262	0.031993	C06593	epsilon-Caprolactam
v3165	202.0954	78.8	0.142	0.047	0.325	5.35E-05	0.014039	C06658	Proclavaminic acid;Proclavaminate
v3163	202.0742	57.9	0.141	0.038	0.368	0.000491	0.044784	C06732	alphabeta-Didehydrotryptophan
v5681	310.2144	24.1	0.001	0	0.014	5.68E-05	0.014039	C07357	(9Z12Z15Z)-(7S8S)-Dihydroxyoctadeca-91215-trienoic acid;(9Z12Z15Z)-(7S8S)-Dihydroxyoctadeca-91215-trienoate
v3165	202.0954	78.8	0.142	0.047	0.325	5.35E-05	0.014039	C08271	Coprine;N(5)-(1-Hydroxycyclopropyl)-L-glutamine
v5278	292.2038	24.6	0	0	0.01	7.90E-05	0.015103	C08319	alpha-Licanic acid;(9Z11E13E)-4-Oxooctadeca-91113-trienoic acid;4-Oxo-91113-octadecatrienoic acid;4-Oxo-cis-9trans-11trans-13-octadecatrienoic acid
v2675	184.1463	271.8	3.666	1.89	8.141	0.000414	0.042781	C08571	gamma-Undecalactone;2(3H)-Furanone 5-heptyldihydro-
v6212	336.2301	28.4	0.32	0.157	0.583	0.000536	0.04761	C09087	Diterpenoid SP-II
v6483	348.1937	29.3	0.278	0.138	0.502	7.74E-05	0.015103	C09112	Ingenol
v6212	336.2301	28.4	0.32	0.157	0.583	0.000536	0.04761	C09175	Portulal
v2895	192.115	23.6	0.169	0.057	0.395	0.000253	0.031596	C09909	Thymyl acetate
v3163	202.0742	57.9	0.141	0.038	0.368	0.000491	0.044784	C10744	Vasicinone
v1969	160.0848	70.8	9.335	3.821	31.837	2.43E-05	0.012975	C10996	Daminozide
v4887	276.0124	71.5	0.239	0.107	0.463	9.97E-05	0.017412	C11570	2-(2-Chloro-phenyl)-5-(5-methylthiophen-2-yl)-134oxadiazole
v6483	348.1937	29.3	0.278	0.138	0.502	7.74E-05	0.015103	C11858	Gibberellin A14
v6483	348.1937	29.3	0.278	0.138	0.502	7.74E-05	0.015103	C11860	Gibberellin A15 open lactone
v3231	204.981	275	0.264	0.126	0.488	8.91E-05	0.016408	C12284	Saccharin sodium anhydrous
v2675	184.1463	271.8	3.666	1.89	8.141	0.000414	0.042781	C12295	Citronellyl formate
v4608	263.0844	93.3	2.894	1.664	5.726	0.000558	0.049106	C12798	Tulobuterol hydrochloride
v5278	292.2038	24.6	0	0	0.01	7.90E-05	0.015103	C13816	(9R13R)-12-Oxo-phytodienoic acid;(9R13R)-12-Oxo-phyto-10Z15Z-dienoic acid;(10Z15Z)-(9R13R)-12-Oxophyto-1015-dienoic acid
v2675	184.1463	271.8	3.666	1.89	8.141	0.000414	0.042781	C13823	11-Undecanolactone
v2675	184.1463	271.8	3.666	1.89	8.141	0.000414	0.042781	C13910	Undecylenic acid;Undecenoic acid
v3455	213.9871	275.6	0.101	0.03	0.245	1.41E-05	0.011973	C14181	2-Benzothiazolesulfonamide
v6212	336.2301	28.4	0.32	0.157	0.583	0.000536	0.04761	C14781	15H-1112-EETA;15-Hydroxy-1112-epoxyeicosatrienoic acid;(5Z8Z13E)-(15S)-1112-Epoxy-15-hydroxyeicosa-5813-trienoic acid;(5Z8Z13E)-(15S)-1112-Epoxy-15-hydroxyicosa-5813-trienoic acid
v6212	336.2301	28.4	0.32	0.157	0.583	0.000536	0.04761	C14808	Hepoxilin A3;(5Z9E14Z)-(11S12S)-1112-Epoxy-8-hydroxyeicosa-5914-trienoic acid;(5Z9E14Z)-(11S12S)-1112-Epoxy-8-hydroxyicosa-5914-trienoic acid
v6212	336.2301	28.4	0.32	0.157	0.583	0.000536	0.04761	C14810	Hepoxilin B3;(5Z8Z14Z)-(11S12S)-1112-Epoxy-10-hydroxyeicosa-5814-trienoic acid;(5Z8Z14Z)-(11S12S)-1112-Epoxy-10-hydroxyicosa-5814-trienoic acid
v6212	336.2301	28.4	0.32	0.157	0.583	0.000536	0.04761	C14812	12(R)-HPETE;(5Z8Z10E14Z)-(12R)-12-Hydroperoxyeicosa-581014-tetraenoic acid;(5Z8Z10E14Z)-(12R)-12-Hydroperoxyicosa-581014-tetraenoic acid
v6212	336.2301	28.4	0.32	0.157	0.583	0.000536	0.04761	C14813	11H-1415-EETA;11-Hydroxy-1415-EETA;11-Hydroxy-1415-epoxyeicosatrienoic acid;(5Z8Z12E)-1415-Epoxy-11-hydroxyeicosa-5812-trienoic acid;(5Z8Z12E)-1415-Epoxy-11-hydroxyicosa-5812-trienoic acid
v6212	336.2301	28.4	0.32	0.157	0.583	0.000536	0.04761	C14820	11(R)-HPETE;(5Z8Z12E14Z)-(11R)-Hydroperoxyeicosa-581214-tetraenoic acid;(5Z8Z12E14Z)-(11R)-Hydroperoxyicosa-581214-tetraenoic acid
v6212	336.2301	28.4	0.32	0.157	0.583	0.000536	0.04761	C14821	9(S)-HPETE;(5Z7E11Z14Z)-(9S)-9-Hydroperoxyeicosa-571114-tetraenoic acid;(5Z7E11Z14Z)-(9S)-9-Hydroperoxyicosa-571114-tetraenoic acid
v6212	336.2301	28.4	0.32	0.157	0.583	0.000536	0.04761	C14823	8(S)-HPETE;(5Z9E11Z14Z)-(8S)-8-Hydroperoxyeicosa-591114-tetraenoic acid;(5Z9E11Z14Z)-(8S)-8-Hydroperoxyicosa-591114-tetraenoic acid
v1663	149.9987	260.7	0.005	0	0.074	0.000459	0.043897	C14872	Thiodiacetic acid
v5278	292.2038	24.6	0	0	0.01	7.90E-05	0.015103	C14911	17beta-Hydroxy-2-oxa-5alpha-androstan-3-one
v7108	378.1962	69.6	0.304	0.157	0.535	0.000112	0.018593	C14923	12alpha-(Chloromethyl)-12-hydroxy-pregn-4-ene-320-dione
v8983	500.3866	27.5	3.144	1.735	6.367	0.000437	0.043363	C15379	3beta-Hydroxylanostane-711-dione acetate
v5681	310.2144	24.1	0.001	0	0.014	5.68E-05	0.014039	C15753	Dihydroalbocycline

v4899	276.2089	25.1	0.075	0.015	0.229	0.000149	0.022851	C16300	Stearidonic acid;691215-Octadecatetraenoic acid;(6Z9Z12Z15Z)-Octadecatetraenoic acid
v5278	292.2038	24.6	0	0	0.01	7.90E-05	0.015103	C16319	Etherolenic acid;(9Z11E1E3Z)-12-(13-Hexadienyloxy)-911-dodecadienoic acid
v5278	292.2038	24.6	0	0	0.01	7.90E-05	0.015103	C16320	Colnelenic acid;(8E)-9-(1E3Z6Z)-Nona-136-trien-1-yloxynon-8-enoate
v5681	310.2144	24.1	0.001	0	0.014	5.68E-05	0.014039	C16321	9(S)-HPOT;(10E12Z15Z)-(9S)-9-Hydroperoxyoctadeca-101215-trienoic acid;9(S)-HpOTrE; (9S10E12Z15Z)-9-Hydroperoxy-101215-octadecatrienoate
v5278	292.2038	24.6	0	0	0.01	7.90E-05	0.015103	C16324	910-EOT;910-Epoxyoctadecatrienoic acid;(9S)-(10E12Z15Z)-910-Epoxyoctadecatri-101215-enoic acid; 910-EOTrE
v5278	292.2038	24.6	0	0	0.01	7.90E-05	0.015103	C16325	10-OPDA;10-Oxo-1115-phytodienoic acid;(11Z15Z)-10-Oxo-1115-phytodienoic acid
v5681	310.2144	24.1	0.001	0	0.014	5.68E-05	0.014039	C16341	2(R)-HPOT;(2R)-(9Z12Z15Z)-2-Hydroperoxyoctadecatri-91215-enoic acid;2(R)-HpOTrE
v1391	141.0112	273.6	0.12	0.039	0.281	1.59E-05	0.012388	C16552	Nornitrogen mustard
v2926	193.06	115	0.127	0.037	0.309	9.34E-05	0.016906	C16789	Toxoflavine
v2895	192.115	23.6	0.169	0.057	0.395	0.000253	0.031596	C17853	Senkyunolide
v2895	192.115	23.6	0.169	0.057	0.395	0.000253	0.031596	C17875	Sedanonic acid lactone
v3004	195.9773	275.1	0.122	0.035	0.297	7.58E-05	0.015103	C17946	Carboxyphosphonopyruvate
v6326	341.9739	70.7	0.191	0.078	0.388	3.73E-05	0.014011	C18968	Carbophenothion
v4899	276.2089	25.1	0.075	0.015	0.229	0.000149	0.022851	C19042	Kinoprene
v2675	184.1463	271.8	3.666	1.89	8.141	0.000414	0.042781	C19420	2-Ethylhexyl acrylate
v1969	160.0848	70.8	9.335	3.821	31.837	2.43E-05	0.012975	C19929	N-alpha-Acetyl-L-24-diaminobutyrate
v5681	310.2144	24.1	0.001	0	0.014	5.68E-05	0.014039	C19936	(9R10E12Z15Z)-9-Hydroperoxyoctadeca-101215-trienoate
v5681	310.2144	24.1	0.001	0	0.014	5.68E-05	0.014039	C20704	(8E10S12Z15Z)-10-Hydroperoxyoctadeca-81215-trienoate
v24	85.0891	44.2	0.061	0.013	0.188	2.80E-05	0.014011	C20809	(R)-2-Methylpyrrolidine
v3163	202.0742	57.9	0.141	0.038	0.368	0.000491	0.044784	C21124	IPA imine;2-Imino-3-(indol-3-yl)propanoate
v1036	129.0425931	81.1	3.281	1.802	6.691	0.00032	0.036032	HMDB00267	Pyroglutamic acid
v4630	264.0303734	57.9	0.166	0.056	0.385	0.000216	0.029572	HMDB00559	3-Methoxy-4-hydroxyphenylethyleneglycol sulfate
v2301	172.0847923	70.4	0	0	0.01	0.000497	0.044933	HMDB00721	Glycylproline
v2042	163.0494098	122.8	0	0	0.001	9.72E-05	0.017272	HMDB00802	Pterin
v1036	129.0425931	81.1	3.281	1.802	6.691	0.00032	0.036032	HMDB00805	Pyrrolidonecarboxylic acid
v6212	336.2300595	28.4	0.32	0.157	0.583	0.000536	0.04761	HMDB01085	Leukotriene B4
v6212	336.2300595	28.4	0.32	0.157	0.583	0.000536	0.04761	HMDB01193	5(S)-Hydroperoxyeicosatetraenoic acid
v1036	129.0425931	81.1	3.281	1.802	6.691	0.00032	0.036032	HMDB01369	Pyrroline hydroxycarboxylic acid
v1036	129.0425931	81.1	3.281	1.802	6.691	0.00032	0.036032	HMDB01843	N-Acryloylglycine
v1036	129.0425931	81.1	3.281	1.802	6.691	0.00032	0.036032	HMDB02234	1-Pyrroline-4-hydroxy-2-carboxylate
v6212	336.2300595	28.4	0.32	0.157	0.583	0.000536	0.04761	HMDB02236	8-iso-PGA1
v6212	336.2300595	28.4	0.32	0.157	0.583	0.000536	0.04761	HMDB02656	Prostaglandin A1
v4899	276.2089301	25.1	0.075	0.015	0.229	0.000149	0.022851	HMDB02697	19-Norandrosterone
v6212	336.2300595	28.4	0.32	0.157	0.583	0.000536	0.04761	HMDB02982	Prostaglandin B1
v4630	264.0303734	57.9	0.166	0.056	0.385	0.000216	0.029572	HMDB03332	3-Methoxy-4-Hydroxyphenylglycol sulfate
v2364	174.1004423	66.4	530763.5	2022.41	8.3E+09	0.000353	0.038789	HMDB03357	N-Acetylornithine
v1969	160.0847923	70.8	9.335	3.821	31.837	2.43E-05	0.012975	HMDB03459	D-Alanyl-D-alanine
v6212	336.2300595	28.4	0.32	0.157	0.583	0.000536	0.04761	HMDB04243	12(S)-HPETE
v6212	336.2300595	28.4	0.32	0.157	0.583	0.000536	0.04761	HMDB04244	15(S)-HPETE
v4899	276.2089301	25.1	0.075	0.015	0.229	0.000149	0.022851	HMDB04590	19-Nor-5-androstenediol
v6212	336.2300595	28.4	0.32	0.157	0.583	0.000536	0.04761	HMDB04688	Hepoxilin A3
v6212	336.2300595	28.4	0.32	0.157	0.583	0.000536	0.04761	HMDB04690	Hepoxilin B3
v6212	336.2300595	28.4	0.32	0.157	0.583	0.000536	0.04761	HMDB04692	12(R)-HPETE
v6212	336.2300595	28.4	0.32	0.157	0.583	0.000536	0.04761	HMDB04693	11H-1415-EETA
v6212	336.2300595	28.4	0.32	0.157	0.583	0.000536	0.04761	HMDB04696	11(R)-HPETE
v6212	336.2300595	28.4	0.32	0.157	0.583	0.000536	0.04761	HMDB04699	8(S)-HPETE
v6212	336.2300595	28.4	0.32	0.157	0.583	0.000536	0.04761	HMDB05050	15H-1112-EETA
v6212	336.2300595	28.4	0.32	0.157	0.583	0.000536	0.04761	HMDB05087	6-trans-Leukotriene B4
v6212	336.2300595	28.4	0.32	0.157	0.583	0.000536	0.04761	HMDB05088	6-trans-12-epi-Leukotriene B4
v6212	336.2300595	28.4	0.32	0.157	0.583	0.000536	0.04761	HMDB05089	12(S)-Leukotriene B4
v4899	276.2089301	25.1	0.075	0.015	0.229	0.000149	0.022851	HMDB05886	19-Noretiocholanolone
v4564	261.0402236	69.3	0.167	0.059	0.385	0.000148	0.022851	HMDB06049	O-Phosphotyrosine

v4899	276.2089301	25.1	0.075	0.015	0.229	0.000149	0.022851	HMDB06547	Stearidonic acid
v3455	213.9878537	275.6	0.101	0.03	0.245	1.41E-05	0.011973	HMDB06801	2-Oxo-3-hydroxy-4-phosphobutanoic acid
v6212	336.2300595	28.4	0.32	0.157	0.583	0.000536	0.04761	HMDB10204	1415-DiHETE
v6212	336.2300595	28.4	0.32	0.157	0.583	0.000536	0.04761	HMDB10211	1718-DiHETE
v6212	336.2300595	28.4	0.32	0.157	0.583	0.000536	0.04761	HMDB10216	515-DiHETE
v6212	336.2300595	28.4	0.32	0.157	0.583	0.000536	0.04761	HMDB10219	815-DiHETE
v6212	336.2300595	28.4	0.32	0.157	0.583	0.000536	0.04761	HMDB11135	5-HPETE
v2301	172.0847923	70.4	0	0	0.01	0.000497	0.044933	HMDB11178	L-prolyl-L-glycine
v6212	336.2300595	28.4	0.32	0.157	0.583	0.000536	0.04761	HMDB12498	1011-dihydro-12-oxo-LTB4
v6212	336.2300595	28.4	0.32	0.157	0.583	0.000536	0.04761	HMDB12839	67-dihydro-5-oxo-12-epi-LTB4
v5681	310.2144094	24.1	0.001	0	0.014	5.68E-05	0.014039	HMDB13623	12(13)Ep-9-KODE
v6650	355.9497143	72.8	0.314	0.154	0.577	0.000487	0.044784	HMDB15610	Silver sulfadiazine
v1969	160.0847923	70.8	9.335	3.821	31.837	2.43E-05	0.012975	HMDB28680	Alanyl-Alanine
v3165	202.0953569	78.8	0.142	0.047	0.325	5.35E-05	0.014039	HMDB28688	Alanyl-Hydroxyproline
v2364	174.1004423	66.4	530763.5	2022.41	8.3E+09	0.000353	0.038789	HMDB28854	Glycyl-Valine
v3165	202.0953569	78.8	0.142	0.047	0.325	5.35E-05	0.014039	HMDB28856	Hydroxyprolyl-Alanine
v3165	202.0953569	78.8	0.142	0.047	0.325	5.35E-05	0.014039	HMDB29026	Prolyl-Serine
v3165	202.0953569	78.8	0.142	0.047	0.325	5.35E-05	0.014039	HMDB29047	Serinyl-Proline
v2364	174.1004423	66.4	530763.5	2022.41	8.3E+09	0.000353	0.038789	HMDB29127	Valyl-Glycine
v1827	155.1310142	25.8	0.001	0	0.014	5.56E-05	0.014039	HMDB30326	Methylisopelletierine
v2042	163.0480724	122.8	0	0	0.001	9.72E-05	0.017272	HMDB30393	L-N-Carboxymethylserine
v10677	650.2210705	79.3	5.843	2.503	17.473	0.000297	0.034571	HMDB30627	5-Hydroxy-734-trimethoxy-8-methylisoflavone 5-neohesperidoside
v5278	292.2038448	24.6	0	0	0.01	7.90E-05	0.015103	HMDB30996	(2E4Z7Z8E)-Colnelenic acid
v2675	184.1463299	271.8	3.666	1.89	8.141	0.000414	0.042781	HMDB31062	(Z)-3-Methyl-3-decenoic acid
v2675	184.1463299	271.8	3.666	1.89	8.141	0.000414	0.042781	HMDB31063	(Z)-3-Methyl-4-decenoic acid
v2675	184.1463299	271.8	3.666	1.89	8.141	0.000414	0.042781	HMDB31087	trans-2-Hexyl-1-cyclopropaneacetic acid
v1827	155.1310142	25.8	0.001	0	0.014	5.56E-05	0.014039	HMDB31179	2266-Tetramethyl-4-piperidinone
v2042	163.0489408	122.8	0	0	0.001	9.72E-05	0.017272	HMDB31187	Thialdine
v618	113.084064	32.3	0.042	0.005	0.165	0.000262	0.031993	HMDB31199	25-Dihydro-245-trimethyloxazole
v2675	184.1463299	271.8	3.666	1.89	8.141	0.000414	0.042781	HMDB31272	Ethyl (E)-2-nonenoate
v1076	130.0452356	79	3.133	1.733	6.32	0.000455	0.043876	HMDB31370	2-(Methylthio)methyl-2-butenal
v2675	184.1463299	271.8	3.666	1.89	8.141	0.000414	0.042781	HMDB31406	Ethyl 3-cyclohexylpropionate
v1969	160.0847923	70.8	9.335	3.821	31.837	2.43E-05	0.012975	HMDB31411	4-Acetamido-2-aminobutanoic acid
v2895	192.1150298	23.6	0.169	0.057	0.395	0.000253	0.031596	HMDB31571	2-Methyl-1-phenyl-2-propanyl acetate
v2895	192.1150298	23.6	0.169	0.057	0.395	0.000253	0.031596	HMDB31614	4-Phenyl-2-butyl acetate
v2895	192.1150298	23.6	0.169	0.057	0.395	0.000253	0.031596	HMDB31618	Ethyl 4-phenylbutanoate
v2675	184.1463299	271.8	3.666	1.89	8.141	0.000414	0.042781	HMDB31691	cis-3-Hexenyl pentanoate
v618	113.084064	32.3	0.042	0.005	0.165	0.000262	0.031993	HMDB31702	1-Piperidinecarboxaldehyde
v2675	184.1463299	271.8	3.666	1.89	8.141	0.000414	0.042781	HMDB31843	23-Undecanedione
v6483	348.193674	29.3	0.278	0.138	0.502	7.74E-05	0.015103	HMDB32010	Gibberellin A110
v6483	348.193674	29.3	0.278	0.138	0.502	7.74E-05	0.015103	HMDB32011	Gibberellin A112
v2895	192.1150298	23.6	0.169	0.057	0.395	0.000253	0.031596	HMDB32043	Benzyl 3-methylbutanoate
v2675	184.1463299	271.8	3.666	1.89	8.141	0.000414	0.042781	HMDB32308	(E)-3-Heptenyl 2-methylpropanoate
v2675	184.1463299	271.8	3.666	1.89	8.141	0.000414	0.042781	HMDB32320	3-Hexenyl 2-methylbutyrate
v2675	184.1463299	271.8	3.666	1.89	8.141	0.000414	0.042781	HMDB32396	Methyl 2-decenoate
v2675	184.1463299	271.8	3.666	1.89	8.141	0.000414	0.042781	HMDB32404	6-Methyl-5-hepten-2-one propyleneglycol acetal
v2675	184.1463299	271.8	3.666	1.89	8.141	0.000414	0.042781	HMDB32453	cis-3-Octenyl propionate
v2675	184.1463299	271.8	3.666	1.89	8.141	0.000414	0.042781	HMDB32461	Pent-2-enyl hexanoate
v4899	276.2089301	25.1	0.075	0.015	0.229	0.000149	0.022851	HMDB32464	Phenethyl decanoate
v2675	184.1463299	271.8	3.666	1.89	8.141	0.000414	0.042781	HMDB32489	Prenyl caproate
v2675	184.1463299	271.8	3.666	1.89	8.141	0.000414	0.042781	HMDB32534	trans-2-Hexenyl 2-methylbutyrate
v4899	276.2089301	25.1	0.075	0.015	0.229	0.000149	0.022851	HMDB32672	481215-Octadecatetraenoic acid
v6483	348.193674	29.3	0.278	0.138	0.502	7.74E-05	0.015103	HMDB32895	3b-Hydroxy-6b-angeloyloxy-7(11)-eremophilen-128b-olide
v6870	366.1889826	284.8	0.284	0.126	0.547	0.000605	0.049793	HMDB33216	(2R6x)-7-Methyl-3-methylene-1267-octanetetrol 2-glucoside
v2675	184.1463299	271.8	3.666	1.89	8.141	0.000414	0.042781	HMDB33371	Citronellyl formate

v2895	192.1150298	23.6	0.169	0.057	0.395	0.000253	0.031596	HMDB33380	3-Methylbutyl benzoate
v5681	310.2144094	24.1	0.001	0	0.014	5.68E-05	0.014039	HMDB33505	(9Z11R12S13S15Z)-1213-Epoxy-11-hydroxy-915-octadecadienoic acid
v2675	184.1463299	271.8	3.666	1.89	8.141	0.000414	0.042781	HMDB33724	Undecylenic acid
v6483	348.193674	29.3	0.278	0.138	0.502	7.74E-05	0.015103	HMDB33981	Cohumulone
v3165	202.0953569	78.8	0.142	0.047	0.325	5.35E-05	0.014039	HMDB34266	L-Coprine
v10677	650.2210705	79.3	5.843	2.503	17.473	0.000297	0.034571	HMDB34281	Egonol gentiobioside
v24	85.08914936	44.2	0.061	0.013	0.188	2.80E-05	0.014011	HMDB34301	Piperidine
v2364	174.1004423	66.4	530763.5	2022.41	8.3E+09	0.000353	0.038789	HMDB34365	L-Theanine
v5936	323.3188149	26.6	0.095	0.028	0.222	3.85E-06	0.011973	HMDB34373	N-(14-Methylhexadecanoyl)pyrrolidine
v4899	276.2089301	25.1	0.075	0.015	0.229	0.000149	0.022851	HMDB34382	(EE)-1113-Octadecadien-9-ynoic acid
v2675	184.1463299	271.8	3.666	1.89	8.141	0.000414	0.042781	HMDB34428	Cyclohexyl 3-methylbutanoate
v2675	184.1463299	271.8	3.666	1.89	8.141	0.000414	0.042781	HMDB34429	Cyclohexyl pentanoate
v6212	336.2300595	28.4	0.32	0.157	0.583	0.000536	0.04761	HMDB34686	(14S)-1415-Dihydroxy-8(17)13(16)-labdadien-19-oic acid
v6483	348.193674	29.3	0.278	0.138	0.502	7.74E-05	0.015103	HMDB34999	Bakkenolide C
v2895	192.1150298	23.6	0.169	0.057	0.395	0.000253	0.031596	HMDB35010	2-Methylpropyl phenylacetate
v2895	192.1150298	23.6	0.169	0.057	0.395	0.000253	0.031596	HMDB35014	2-Phenylethyl butanoate
v2895	192.1150298	23.6	0.169	0.057	0.395	0.000253	0.031596	HMDB35015	2-Phenylethyl 2-methylpropanoate
v5681	310.2144094	24.1	0.001	0	0.014	5.68E-05	0.014039	HMDB35337	Sterebin A
v2895	192.1150298	23.6	0.169	0.057	0.395	0.000253	0.031596	HMDB35447	5-Isopropyl-2-methylphenol acetate
v2675	184.1463299	271.8	3.666	1.89	8.141	0.000414	0.042781	HMDB36140	5-Hexyldihydro-5-methyl-2(3H)-furanone
v2895	192.1150298	23.6	0.169	0.057	0.395	0.000253	0.031596	HMDB36388	3-Phenylpropyl propanoate
v2895	192.1150298	23.6	0.169	0.057	0.395	0.000253	0.031596	HMDB36734	111213-Trinor-1(10)-spirovetivene-27-dione
v2675	184.1463299	271.8	3.666	1.89	8.141	0.000414	0.042781	HMDB36784	6-Hexyltetrahydro-2H-pyran-2-one
v6483	348.193674	29.3	0.278	0.138	0.502	7.74E-05	0.015103	HMDB36895	Gibberellin A53
v2675	184.1463299	271.8	3.666	1.89	8.141	0.000414	0.042781	HMDB37106	(x)-1-Nonen-3-yl acetate
v2895	192.1150298	23.6	0.169	0.057	0.395	0.000253	0.031596	HMDB37165	4-Methyl-2-(1-phenylethyl)-13-dioxolane 9Cl
v2675	184.1463299	271.8	3.666	1.89	8.141	0.000414	0.042781	HMDB37185	Rhodinyl formate
v2675	184.1463299	271.8	3.666	1.89	8.141	0.000414	0.042781	HMDB37225	Methyl citronellate
v618	113.084064	32.3	0.042	0.005	0.165	0.000262	0.031993	HMDB37293	2-Acetylpyrrolidine
v2675	184.1463299	271.8	3.666	1.89	8.141	0.000414	0.042781	HMDB37309	5-Hexyldihydro-4-methyl-2(3H)-furanone
v1076	130.0452356	79	3.133	1.733	6.32	0.000455	0.043876	HMDB37493	S-2-Propenyl propanethioate
v2895	192.1150298	23.6	0.169	0.057	0.395	0.000253	0.031596	HMDB37709	4-Methylphenyl 3-methylbutanoate
v2895	192.1150298	23.6	0.169	0.057	0.395	0.000253	0.031596	HMDB37716	1-Phenylethyl isobutyrate
v2895	192.1150298	23.6	0.169	0.057	0.395	0.000253	0.031596	HMDB37717	1-Phenylethyl butyrate
v2895	192.1150298	23.6	0.169	0.057	0.395	0.000253	0.031596	HMDB37792	1-Ethoxy-2-methoxy-4-(1-propenyl)benzene
v6519	350.009638	68	0.149	0.051	0.344	7.12E-05	0.01502	HMDB37851	Apigenin 7-sulfate
v5278	292.2038448	24.6	0	0	0.01	7.90E-05	0.015103	HMDB38035	Panaquinquecol 1
v2895	192.1150298	23.6	0.169	0.057	0.395	0.000253	0.031596	HMDB38180	2-(2-Hydroxy-4-methylphenyl)-3-pentanone
v2675	184.1463299	271.8	3.666	1.89	8.141	0.000414	0.042781	HMDB38273	2-Hexenyl valerate
v2675	184.1463299	271.8	3.666	1.89	8.141	0.000414	0.042781	HMDB38274	2-Hexenyl isovalerate
v2675	184.1463299	271.8	3.666	1.89	8.141	0.000414	0.042781	HMDB38277	cis-3-Hexenyl 2-methylbutanoate
v2675	184.1463299	271.8	3.666	1.89	8.141	0.000414	0.042781	HMDB38278	cis-3-Hexenyl 3-methylbutanoate
v2675	184.1463299	271.8	3.666	1.89	8.141	0.000414	0.042781	HMDB38311	xi-gamma-Undecalactone
v5681	310.2144094	24.1	0.001	0	0.014	5.68E-05	0.014039	HMDB38484	Auxin b
v2675	184.1463299	271.8	3.666	1.89	8.141	0.000414	0.042781	HMDB38906	5-Octenyl propanoate
v6212	336.2300595	28.4	0.32	0.157	0.583	0.000536	0.04761	HMDB39171	9alpha-(3-Methylbutanoyloxy)-4S-hydroxy-10(14)-oplopen-3-one
v6212	336.2300595	28.4	0.32	0.157	0.583	0.000536	0.04761	HMDB39441	ent-1(10)-Halimene-1519-dioic acid
v2895	192.1150298	23.6	0.169	0.057	0.395	0.000253	0.031596	HMDB39496	2-Ethoxy-1-methoxy-4-(1-propenyl)benzene
v2895	192.1150298	23.6	0.169	0.057	0.395	0.000253	0.031596	HMDB39643	111213-Trinor-135-bisabolatrien-10-oic acid
v1827	155.1310142	25.8	0.001	0	0.014	5.56E-05	0.014039	HMDB39833	3-(1-Pyrrolidinyl)-2-pentanone
v1827	155.1310142	25.8	0.001	0	0.014	5.56E-05	0.014039	HMDB39834	2-(1-Pyrrolidinyl)-3-pentanone
v2895	192.1150298	23.6	0.169	0.057	0.395	0.000253	0.031596	HMDB39841	2-Benzyl-45-dimethyl-13-dioxolane

v6870	366.1889826	284.8	0.284	0.126	0.547	0.000605	0.049793	HMDB39975	(1S2S4R8S)-p-Menthane-1289-tetrol 2-glucoside
v6870	366.1889826	284.8	0.284	0.126	0.547	0.000605	0.049793	HMDB39976	(1R2R4R8S)-p-Menthane-1289-tetrol 9-glucoside
v1076	130.0452356	79	3.133	1.733	6.32	0.000455	0.043876	HMDB40238	2-Ethyldihydro-3(2H)-thiophenone
v2895	192.1150298	23.6	0.169	0.057	0.395	0.000253	0.031596	HMDB40427	Butyl phenylacetate
v2675	184.1463299	271.8	3.666	1.89	8.141	0.000414	0.042781	HMDB40593	2-Propenyl octanoate
v5278	292.2038448	24.6	0	0	0.01	7.90E-05	0.015103	HMDB40806	7-Paradol
v6483	348.193674	29.3	0.278	0.138	0.502	7.74E-05	0.015103	HMDB40989	3b-Hydroxy-6b-tigloyloxy-7(11)-eremophilen-128b-olide
v1663	149.9986794	260.7	0.005	0	0.074	0.000459	0.043897	HMDB42032	Thiodiacetic acid
v4608	263.0843696	93.3	2.894	1.664	5.726	0.000558	0.049106	HMDB42056	Tulobuterol
v12056	830.7727264	67.1	0.266	0.123	0.498	0.000153	0.023067	HMDB42540	TG(14:018:2(9Z12Z)o-18:0)
v12056	830.7727264	67.1	0.266	0.123	0.498	0.000153	0.023067	HMDB42600	TG(14:020:2n6o-18:0)
v12056	830.7727264	67.1	0.266	0.123	0.498	0.000153	0.023067	HMDB42946	TG(14:0o-18:018:2(9Z12Z))
v12056	830.7727264	67.1	0.266	0.123	0.498	0.000153	0.023067	HMDB42948	TG(14:0o-18:020:2n6)
v12056	830.7727264	67.1	0.266	0.123	0.498	0.000153	0.023067	HMDB52410	TG(18:2(9Z12Z)14:0o-18:0)
v12056	830.7727264	67.1	0.266	0.123	0.498	0.000153	0.023067	HMDB53276	TG(20:2n614:0o-18:0)
v6483	348.193674	29.3	0.278	0.138	0.502	7.74E-05	0.015103	HMDB60094	1220-Dioxo-leukotriene B4
v6212	336.2300595	28.4	0.32	0.157	0.583	0.000536	0.04761	HMDB60103	9-Deoxy-delta12-PGD2
v6212	336.2300595	28.4	0.32	0.157	0.583	0.000536	0.04761	HMDB60104	Prostaglandin C1
v6212	336.2300595	28.4	0.32	0.157	0.583	0.000536	0.04761	HMDB60105	1220-DiHETE
v1036	129.0425931	81.1	3.281	1.802	6.691	0.00032	0.036032	HMDB60262	5-Oxoprolinate
v8559	468.9511032	274.3	0.044	0.007	0.149	4.79E-05	0.014039	HMDB60640	Lamivudine-triphosphate
v1391	141.0112047	273.6	0.12	0.039	0.281	1.59E-05	0.012388	HMDB60688	Nornitrogen mustard
v8589	471.0923475	89.5	3.486	1.817	7.794	0.000609	0.049793	HMDB61083	desbutyl-lumefantrine
v1036	129.0425931	81.1	3.281	1.802	6.691	0.00032	0.036032	HMDB61093	dimethadione
v7108	378.1943427	69.6	0.304	0.157	0.535	0.000112	0.018593	HMDB61127	4R-Hydroxy solifenacin
v2675	184.14633	271.8	3.666	1.89	8.141	0.000414	0.042781	LMFA01020130	27-dimethyl-6-nonenoic acid
v2675	184.14633	271.8	3.666	1.89	8.141	0.000414	0.042781	LMFA01020131	4-ethyl-2-methyl-2-octenoic acid
v2675	184.14633	271.8	3.666	1.89	8.141	0.000414	0.042781	LMFA01030034	2-undecenoic acid
v2675	184.14633	271.8	3.666	1.89	8.141	0.000414	0.042781	LMFA01030035	9-undecenoic acid
v2675	184.14633	271.8	3.666	1.89	8.141	0.000414	0.042781	LMFA01030036	10-undecenoic acid
v4899	276.20893	25.1	0.075	0.015	0.229	0.000149	0.022851	LMFA01030167	3E9Z12Z15Z-octadecatetraenoic acid
v4899	276.20893	25.1	0.075	0.015	0.229	0.000149	0.022851	LMFA01030169	691215-octadecatetraenoic acid
v4899	276.20893	25.1	0.075	0.015	0.229	0.000149	0.022851	LMFA01030171	9E11E13E15E-octadecatetraenoic acid
v4899	276.20893	25.1	0.075	0.015	0.229	0.000149	0.022851	LMFA01030172	9121517-octadecatetraenoic acid
v2675	184.14633	271.8	3.666	1.89	8.141	0.000414	0.042781	LMFA01030217	2Z-undecenoic acid
v2675	184.14633	271.8	3.666	1.89	8.141	0.000414	0.042781	LMFA01030218	3E-undecenoic acid
v2675	184.14633	271.8	3.666	1.89	8.141	0.000414	0.042781	LMFA01030219	6Z-undecenoic acid
v2675	184.14633	271.8	3.666	1.89	8.141	0.000414	0.042781	LMFA01030220	8Z-undecenoic acid
v2675	184.14633	271.8	3.666	1.89	8.141	0.000414	0.042781	LMFA01030221	9Z-undecenoic acid
v2895	192.11503	23.6	0.169	0.057	0.395	0.000253	0.031596	LMFA01030240	2E4E8Z10E-dodecatetraenoic acid
v2895	192.11503	23.6	0.169	0.057	0.395	0.000253	0.031596	LMFA01030241	2E6E8E10E-dodecatetraenoic acid
v2895	192.11503	23.6	0.169	0.057	0.395	0.000253	0.031596	LMFA01030242	2E6E8Z10E-dodecatetraenoic acid
v4899	276.20893	25.1	0.075	0.015	0.229	0.000149	0.022851	LMFA01030354	581114-octadecatetraenoic acid
v4899	276.20893	25.1	0.075	0.015	0.229	0.000149	0.022851	LMFA01030355	591215-octadecatetraenoic acid
v4899	276.20893	25.1	0.075	0.015	0.229	0.000149	0.022851	LMFA01030356	5Z8Z11Z14Z-octadecatetraenoic acid
v4899	276.20893	25.1	0.075	0.015	0.229	0.000149	0.022851	LMFA01030357	6Z9Z12Z15Z-octadecatetraenoic acid
v4899	276.20893	25.1	0.075	0.015	0.229	0.000149	0.022851	LMFA01030358	9Z11Z13E15E-octadecatetraenoic acid
v2895	192.11503	23.6	0.169	0.057	0.395	0.000253	0.031596	LMFA01030464	511-dodecadiynoic acid
v4899	276.20893	25.1	0.075	0.015	0.229	0.000149	0.022851	LMFA01030511	11E13E-octadecadien-9-ynoic acid
v4899	276.20893	25.1	0.075	0.015	0.229	0.000149	0.022851	LMFA01030512	25-octadecadiynoic acid
v4899	276.20893	25.1	0.075	0.015	0.229	0.000149	0.022851	LMFA01030513	26-octadecadiynoic acid

v4899	276.20893	25.1	0.075	0.015	0.229	0.000149	0.022851	LMFA01030514	27-octadecadiynoic acid
v4899	276.20893	25.1	0.075	0.015	0.229	0.000149	0.022851	LMFA01030515	36-octadecadiynoic acid
v4899	276.20893	25.1	0.075	0.015	0.229	0.000149	0.022851	LMFA01030516	37-octadecadiynoic acid
v4899	276.20893	25.1	0.075	0.015	0.229	0.000149	0.022851	LMFA01030517	38-octadecadiynoic acid
v4899	276.20893	25.1	0.075	0.015	0.229	0.000149	0.022851	LMFA01030518	46-octadecadiynoic acid
v4899	276.20893	25.1	0.075	0.015	0.229	0.000149	0.022851	LMFA01030519	47-octadecadiynoic acid
v4899	276.20893	25.1	0.075	0.015	0.229	0.000149	0.022851	LMFA01030520	48-octadecadiynoic acid
v4899	276.20893	25.1	0.075	0.015	0.229	0.000149	0.022851	LMFA01030521	49-octadecadiynoic acid
v4899	276.20893	25.1	0.075	0.015	0.229	0.000149	0.022851	LMFA01030522	57-octadecadiynoic acid
v4899	276.20893	25.1	0.075	0.015	0.229	0.000149	0.022851	LMFA01030523	58-octadecadiynoic acid
v4899	276.20893	25.1	0.075	0.015	0.229	0.000149	0.022851	LMFA01030524	59-octadecadiynoic acid
v4899	276.20893	25.1	0.075	0.015	0.229	0.000149	0.022851	LMFA01030525	510-octadecadiynoic acid
v4899	276.20893	25.1	0.075	0.015	0.229	0.000149	0.022851	LMFA01030526	512-octadecadiynoic acid
v4899	276.20893	25.1	0.075	0.015	0.229	0.000149	0.022851	LMFA01030527	68-octadecadiynoic acid
v4899	276.20893	25.1	0.075	0.015	0.229	0.000149	0.022851	LMFA01030528	69-octadecadiynoic acid
v4899	276.20893	25.1	0.075	0.015	0.229	0.000149	0.022851	LMFA01030529	610-octadecadiynoic acid
v4899	276.20893	25.1	0.075	0.015	0.229	0.000149	0.022851	LMFA01030530	611-octadecadiynoic acid
v4899	276.20893	25.1	0.075	0.015	0.229	0.000149	0.022851	LMFA01030531	612-octadecadiynoic acid
v4899	276.20893	25.1	0.075	0.015	0.229	0.000149	0.022851	LMFA01030532	79-octadecadiynoic acid
v4899	276.20893	25.1	0.075	0.015	0.229	0.000149	0.022851	LMFA01030533	710-octadecadiynoic acid
v4899	276.20893	25.1	0.075	0.015	0.229	0.000149	0.022851	LMFA01030534	711-octadecadiynoic acid
v4899	276.20893	25.1	0.075	0.015	0.229	0.000149	0.022851	LMFA01030535	712-octadecadiynoic acid
v4899	276.20893	25.1	0.075	0.015	0.229	0.000149	0.022851	LMFA01030536	810-octadecadiynoic acid
v4899	276.20893	25.1	0.075	0.015	0.229	0.000149	0.022851	LMFA01030537	811-octadecadiynoic acid
v4899	276.20893	25.1	0.075	0.015	0.229	0.000149	0.022851	LMFA01030538	812-octadecadiynoic acid
v4899	276.20893	25.1	0.075	0.015	0.229	0.000149	0.022851	LMFA01030539	911-octadecadiynoic acid
v4899	276.20893	25.1	0.075	0.015	0.229	0.000149	0.022851	LMFA01030540	912-octadecadiynoic acid
v4899	276.20893	25.1	0.075	0.015	0.229	0.000149	0.022851	LMFA01030541	913-octadecadiynoic acid
v4899	276.20893	25.1	0.075	0.015	0.229	0.000149	0.022851	LMFA01030542	1012-octadecadiynoic acid
v4899	276.20893	25.1	0.075	0.015	0.229	0.000149	0.022851	LMFA01030543	1013-octadecadiynoic acid
v4899	276.20893	25.1	0.075	0.015	0.229	0.000149	0.022851	LMFA01030544	1014-octadecadiynoic acid
v4899	276.20893	25.1	0.075	0.015	0.229	0.000149	0.022851	LMFA01030545	1114-octadecadiynoic acid
v4899	276.20893	25.1	0.075	0.015	0.229	0.000149	0.022851	LMFA01030546	1115-octadecadiynoic acid
v4899	276.20893	25.1	0.075	0.015	0.229	0.000149	0.022851	LMFA01030547	1214-octadecadiynoic acid
v4899	276.20893	25.1	0.075	0.015	0.229	0.000149	0.022851	LMFA01030548	1215-octadecadiynoic acid
v4899	276.20893	25.1	0.075	0.015	0.229	0.000149	0.022851	LMFA01030549	1216-octadecadiynoic acid
v4899	276.20893	25.1	0.075	0.015	0.229	0.000149	0.022851	LMFA01030550	1316-octadecadiynoic acid
v4899	276.20893	25.1	0.075	0.015	0.229	0.000149	0.022851	LMFA01030551	1317-octadecadiynoic acid
v4899	276.20893	25.1	0.075	0.015	0.229	0.000149	0.022851	LMFA01030552	1417-octadecadiynoic acid
v2675	184.14633	271.8	3.666	1.89	8.141	0.000414	0.042781	LMFA01030606	4-undecenoic acid
v2675	184.14633	271.8	3.666	1.89	8.141	0.000414	0.042781	LMFA01030608	6-undecenoic acid
v2675	184.14633	271.8	3.666	1.89	8.141	0.000414	0.042781	LMFA01030609	7-undecenoic acid
v4899	276.20893	25.1	0.075	0.015	0.229	0.000149	0.022851	LMFA01030734	9Z12Z-Octadecadien-6-ynoic acid
v4899	276.20893	25.1	0.075	0.015	0.229	0.000149	0.022851	LMFA01030735	9Z14Z-Octadecadien-12-ynoic acid
v4899	276.20893	25.1	0.075	0.015	0.229	0.000149	0.022851	LMFA01030764	9Z11E13E15Z-octadecatetraenoic acid
v2675	184.14633	271.8	3.666	1.89	8.141	0.000414	0.042781	LMFA01030785	5E-undecenoic acid
v2675	184.14633	271.8	3.666	1.89	8.141	0.000414	0.042781	LMFA01030786	5Z-undecenoic acid
v4899	276.20893	25.1	0.075	0.015	0.229	0.000149	0.022851	LMFA01030813	2E4E6E11Z-octadecatetraenoic acid
v6000	326.2821	25.5	4.275	2.164	10.106	0.000163	0.024299	LMFA01050117	14-hydroxy-11Z-eicosenoic acid
v6000	326.2821	25.5	4.275	2.164	10.106	0.000163	0.024299	LMFA01050256	14R-hydroxy-11E-eicosenoic acid
v6000	326.2821	25.5	4.275	2.164	10.106	0.000163	0.024299	LMFA01050257	14R-hydroxy-11Z-eicosenoic acid
v6000	326.2821	25.5	4.275	2.164	10.106	0.000163	0.024299	LMFA01060132	19-oxo-eicosanoic acid
v6000	326.2821	25.5	4.275	2.164	10.106	0.000163	0.024299	LMFA01060133	2-oxo-eicosanoic acid
v6000	326.2821	25.5	4.275	2.164	10.106	0.000163	0.024299	LMFA01060134	3-oxo-eicosanoic acid
v4899	276.20893	25.1	0.075	0.015	0.229	0.000149	0.022851	LMFA01140005	6-3-ladderane-hexanoic acid

v6212	336.23006	28.4	0.32	0.157	0.583	0.000536	0.04761	LMFA01170128	5Z8Z11Z-Eicosatrienedioic acid
v5681	310.21441	24.1	0.001	0	0.014	5.68E-05	0.014039	LMFA02000018	9S-hydroperoxy-10E12Z15Z-octadecatrienoic acid
v5681	310.21441	24.1	0.001	0	0.014	5.68E-05	0.014039	LMFA02000019	9S-hydroxy-10S11S-epoxy-12Z15Z-octadecadienoic acid
v5681	310.21441	24.1	0.001	0	0.014	5.68E-05	0.014039	LMFA02000020	9S-hydroxy-12R13S-epoxy-10E15Z-octadecadienoic acid
v5278	292.20385	24.6	0	0	0.01	7.90E-05	0.015103	LMFA02000028	13-keto-9Z11E15Z-octadecatrienoic acid
v5681	310.21441	24.1	0.001	0	0.014	5.68E-05	0.014039	LMFA02000030	1516-epoxy-13-OH-9Z11E-octadecadienoic acid
v5681	310.21441	24.1	0.001	0	0.014	5.68E-05	0.014039	LMFA02000052	13S-hydroperoxy-9Z11E15Z-octadecatrienoic acid
v5278	292.20385	24.6	0	0	0.01	7.90E-05	0.015103	LMFA02000053	1213S-epoxy-9Z1115Z-octadecatrienoic acid
v5681	310.21441	24.1	0.001	0	0.014	5.68E-05	0.014039	LMFA02000108	9-hydroperoxy-10E1215Z-octadecatrienoic acid
v5681	310.21441	24.1	0.001	0	0.014	5.68E-05	0.014039	LMFA02000109	12-hydroperoxy-9Z13E15-octadecatrienoic acid
v5681	310.21441	24.1	0.001	0	0.014	5.68E-05	0.014039	LMFA02000110	13-hydroperoxy-911E15Z-octadecatrienoic acid
v5681	310.21441	24.1	0.001	0	0.014	5.68E-05	0.014039	LMFA02000111	16-hydroperoxy-9Z1214E-octadecatrienoic acid
v5681	310.21441	24.1	0.001	0	0.014	5.68E-05	0.014039	LMFA02000112	13S-hydroperoxy-6Z9Z11E-octadecatrienoic acid
v5681	310.21441	24.1	0.001	0	0.014	5.68E-05	0.014039	LMFA02000114	13S-hydroperoxy-9Z11E14Z-octadecatrienoic acid
v5278	292.20385	24.6	0	0	0.01	7.90E-05	0.015103	LMFA02000191	(-)-8-hydroxy-11E17-octadecadien-9-ynoic acid
v5278	292.20385	24.6	0	0	0.01	7.90E-05	0.015103	LMFA02000192	9-hydroxy-10E14Z-octadecadien-12-ynoic acid
v5278	292.20385	24.6	0	0	0.01	7.90E-05	0.015103	LMFA02000193	8-hydroxy-911-octadecadiynoic acid
v5278	292.20385	24.6	0	0	0.01	7.90E-05	0.015103	LMFA02000194	8-hydroxy-1012-octadecadiynoic acid
v5681	310.21441	24.1	0.001	0	0.014	5.68E-05	0.014039	LMFA02000226	7S8S-dihydroxy-9Z12Z15Z-octadecatrienoic acid
v5681	310.21441	24.1	0.001	0	0.014	5.68E-05	0.014039	LMFA02000247	9-oxo-1213-epoxy-10-octadecenoic acid
v5278	292.20385	24.6	0	0	0.01	7.90E-05	0.015103	LMFA02000273	4-oxo-9Z11E13E-octadecatrienoic acid
v5681	310.21441	24.1	0.001	0	0.014	5.68E-05	0.014039	LMFA02000279	910-epoxy-13-oxo-11-octadecenoic acid
v5278	292.20385	24.6	0	0	0.01	7.90E-05	0.015103	LMFA02010001	(1S2S)-3-oxo-2-(2Z-pentenyl)cyclopent-4-eneoctanoic acid
v6212	336.23006	28.4	0.32	0.157	0.583	0.000536	0.04761	LMFA03010005	9-oxo-15S-hydroxy-10Z13E-prostadienoic acid
v6212	336.23006	28.4	0.32	0.157	0.583	0.000536	0.04761	LMFA03010047	9-oxo-15R-hydroxy-10Z13E-prostadienoic acid
v6212	336.23006	28.4	0.32	0.157	0.583	0.000536	0.04761	LMFA03010061	9-oxo-15S-hydroxy-5Z13E-prostadienoic acid
v6212	336.23006	28.4	0.32	0.157	0.583	0.000536	0.04761	LMFA03010071	9S15S-dihydroxy-5Z13E-prostadienoic acid-111R-lactone
v6212	336.23006	28.4	0.32	0.157	0.583	0.000536	0.04761	LMFA03010072	9S11R-dihydroxy-5Z13E-prostadienoic acid-115S-lactone
v6212	336.23006	28.4	0.32	0.157	0.583	0.000536	0.04761	LMFA03010131	9-oxo-15S-hydroxy-8(12)13E-prostadienoic acid
v6212	336.23006	28.4	0.32	0.157	0.583	0.000536	0.04761	LMFA03010160	9-oxo-15S-hydroxy-11Z13E-prostadienoic acid
v6212	336.23006	28.4	0.32	0.157	0.583	0.000536	0.04761	LMFA03010196	11R15S-dihydroxy-5Z13E-prostadienoic acid-19S-lactone
v6212	336.23006	28.4	0.32	0.157	0.583	0.000536	0.04761	LMFA03020001	5S12R-dihydroxy-6Z8E10E14Z-eicosatetraenoic acid
v6212	336.23006	28.4	0.32	0.157	0.583	0.000536	0.04761	LMFA03020013	5S12R-dihydroxy-6E8E10E14Z-eicosatetraenoic acid
v6212	336.23006	28.4	0.32	0.157	0.583	0.000536	0.04761	LMFA03020014	5S12S-dihydroxy-6E8E10E14Z-eicosatetraenoic acid
v6212	336.23006	28.4	0.32	0.157	0.583	0.000536	0.04761	LMFA03020015	5S12S-dihydroxy-6Z8E10E14Z-eicosatetraenoic acid
v6212	336.23006	28.4	0.32	0.157	0.583	0.000536	0.04761	LMFA03020041	(5R6Z8E14Z)-5-hydroxy-12-oxoicosa-6814-trienoic acid
v6212	336.23006	28.4	0.32	0.157	0.583	0.000536	0.04761	LMFA03020071	(8E10E12R14Z)-12-hydroxy-5-oxoicosa-81014-trienoic acid
v6212	336.23006	28.4	0.32	0.157	0.583	0.000536	0.04761	LMFA03020072	(5S6E8Z10E12R14Z)-512-dihydroxyicosa-681014-tetraenoic acid
v6212	336.23006	28.4	0.32	0.157	0.583	0.000536	0.04761	LMFA03060010	5S15S-dihydroxy-6E8Z11Z13E-eicosatetraenoic acid
v6212	336.23006	28.4	0.32	0.157	0.583	0.000536	0.04761	LMFA03060012	5S-hydroperoxy-6E8Z11Z14Z-eicosatetraenoic acid
v6212	336.23006	28.4	0.32	0.157	0.583	0.000536	0.04761	LMFA03060013	12S-hydroperoxy-5Z8Z10E14Z-eicosatetraenoic acid
v6212	336.23006	28.4	0.32	0.157	0.583	0.000536	0.04761	LMFA03060014	15S-hydroperoxy-5Z8Z11Z13E-eicosatetraenoic acid
v6212	336.23006	28.4	0.32	0.157	0.583	0.000536	0.04761	LMFA03060017	5S6R-dihydroxy-7E9E11Z14Z-eicosatetraenoic acid
v6212	336.23006	28.4	0.32	0.157	0.583	0.000536	0.04761	LMFA03060018	5S6S-dihydroxy-7E9E11Z14Z-eicosatetraenoic acid
v6212	336.23006	28.4	0.32	0.157	0.583	0.000536	0.04761	LMFA03060037	8R-hydroperoxy-5Z9E11Z14Z-eicosatetraenoic acid
v6212	336.23006	28.4	0.32	0.157	0.583	0.000536	0.04761	LMFA03060040	9-hydroperoxy-57E11Z14Z-eicosatetraenoic acid
v6212	336.23006	28.4	0.32	0.157	0.583	0.000536	0.04761	LMFA03060041	11-hydroperoxy-5Z8Z12E14-eicosatetraenoic acid
v6212	336.23006	28.4	0.32	0.157	0.583	0.000536	0.04761	LMFA03060044	6-hydroperoxy-4E8Z11Z14Z-eicosatetraenoic acid
v6212	336.23006	28.4	0.32	0.157	0.583	0.000536	0.04761	LMFA03060045	14-hydroperoxy-5Z8Z11Z15E-eicosatetraenoic acid
v6212	336.23006	28.4	0.32	0.157	0.583	0.000536	0.04761	LMFA03060050	8S15S-dihydroxy-5Z9E11Z13E-eicosatetraenoic acid
v6212	336.23006	28.4	0.32	0.157	0.583	0.000536	0.04761	LMFA03060052	512-dihydroxy-681014-eicosatetraenoic acid
v6212	336.23006	28.4	0.32	0.157	0.583	0.000536	0.04761	LMFA03060053	815-dihydroxy-591113-eicosatetraenoic acid
v6212	336.23006	28.4	0.32	0.157	0.583	0.000536	0.04761	LMFA03060070	12R-hydroperoxy-5Z8Z10E14Z-eicosatetraenoic acid
v6212	336.23006	28.4	0.32	0.157	0.583	0.000536	0.04761	LMFA03060071	11R-hydroperoxy-5Z8Z12E14Z-eicosatetraenoic acid
v6212	336.23006	28.4	0.32	0.157	0.583	0.000536	0.04761	LMFA03060072	9S-hydroperoxy-5Z7E11Z14Z-eicosatetraenoic acid

v6212	336.23006	28.4	0.32	0.157	0.583	0.000536	0.04761	LMFA03060073	8S-hydoperoxy-5Z9E11Z14Z-eicosatetraenoic acid
v6212	336.23006	28.4	0.32	0.157	0.583	0.000536	0.04761	LMFA03060076	(-)-89-dihydroxy-5Z11Z14Z17Z-eicosatetraenoic acid
v6212	336.23006	28.4	0.32	0.157	0.583	0.000536	0.04761	LMFA03060077	(-)-1415-dihydroxy-5Z8Z11Z17Z-eicosatetraenoic acid
v6212	336.23006	28.4	0.32	0.157	0.583	0.000536	0.04761	LMFA03060078	(-)-1718-dihydroxy-5Z8Z11Z14Z-eicosatetraenoic acid
v6212	336.23006	28.4	0.32	0.157	0.583	0.000536	0.04761	LMFA03060079	(-)-1112-dihydroxy-5Z8Z14Z17Z-eicosatetraenoic acid
v6212	336.23006	28.4	0.32	0.157	0.583	0.000536	0.04761	LMFA03060090	1415-dihydroxy-581012-eicosatetraenoic acid
v6212	336.23006	28.4	0.32	0.157	0.583	0.000536	0.04761	LMFA03060095	5S11R-dihydroxy-6E8Z12E14Z-eicosatetraenoic acid
v6212	336.23006	28.4	0.32	0.157	0.583	0.000536	0.04761	LMFA03060096	5S15R-dihydroxy-6E8Z11Z13E-eicosatetraenoic acid
v6212	336.23006	28.4	0.32	0.157	0.583	0.000536	0.04761	LMFA03060101	5S12S-dihydroxy-6E8Z10E14Z-eicosatetraenoic acid
v6212	336.23	28.4	0.32	0.157	0.583	0.000536	0.04761	LMFA03060102	(5Z8Z11Z13E)-15-hydroperoxyeicosa-581113-tetraenoic acid
v6212	336.23006	28.4	0.32	0.157	0.583	0.000536	0.04761	LMFA03060107	(6E8Z11Z13E)-515-dihydroxyicosa-681113-tetraenoic acid
v6212	336.23006	28.4	0.32	0.157	0.583	0.000536	0.04761	LMFA03060108	-
v6212	336.23006	28.4	0.32	0.157	0.583	0.000536	0.04761	LMFA03060109	(5Z9E11Z13E)-815-dihydroxyicosa-591113-tetraenoic acid
v6483	348.19368	29.3	0.278	0.138	0.502	7.74E-05	0.015103	LMFA03070044	18-oxo-5S12R-dihydroxy-6Z8E10E14Z16E-eicosapentaenoic acid
v6483	348.19368	29.3	0.278	0.138	0.502	7.74E-05	0.015103	LMFA03070047	12-oxo-5S18S-dihydroxy-6Z8E10E14Z16E-eicosapentaenoic acid
v6212	336.23006	28.4	0.32	0.157	0.583	0.000536	0.04761	LMFA03080007	1112-epoxy-15S-hydroxy-5Z8Z13E-eicosatrienoic acid
v6212	336.23006	28.4	0.32	0.157	0.583	0.000536	0.04761	LMFA03080008	11-hydroxy-1415-epoxy-5Z8Z12E-eicosatrienoic acid
v6212	336.23006	28.4	0.32	0.157	0.583	0.000536	0.04761	LMFA03080012	11R12S-epoxy-8-hydroxy-5Z9E14Z-eicosatrienoic acid
v6212	336.23006	28.4	0.32	0.157	0.583	0.000536	0.04761	LMFA03090003	10-hydroxy-11S12S-epoxy-5Z8Z14Z-eicosatrienoic acid
v6212	336.23006	28.4	0.32	0.157	0.583	0.000536	0.04761	LMFA03090005	8-hydroxy-11S12S-epoxy-5Z14Z9E-eicosatrienoic acid
v6212	336.23006	28.4	0.32	0.157	0.583	0.000536	0.04761	LMFA03090006	13R-hydroxy-14S15S-epoxy-5Z8Z11Z-eicosatrienoic acid
v6212	336.23006	28.4	0.32	0.157	0.583	0.000536	0.04761	LMFA03090007	11S-hydroxy-14S15S-epoxy-5Z8Z12E-eicosatrienoic acid
v6212	336.23006	28.4	0.32	0.157	0.583	0.000536	0.04761	LMFA03110008	9-oxo-15S-hydroxy-10Z13E-prostadienoic acid-cyclo8S12S
v5278	292.20385	24.6	0	0	0.01	7.90E-05	0.015103	LMFA05000686	10-methoxyheptadec-1-en-46-diyne-39-diol
v2675	184.14633	271.8	3.666	1.89	8.141	0.000414	0.042781	LMFA07010198	6E-Nonenyl acetate
v2675	184.14633	271.8	3.666	1.89	8.141	0.000414	0.042781	LMFA07010199	2-Nonenyl acetate
v2675	184.14633	271.8	3.666	1.89	8.141	0.000414	0.042781	LMFA07010477	formyl 4Z-decenoate
v2675	184.14633	271.8	3.666	1.89	8.141	0.000414	0.042781	LMFA07010524	formyl 37-dimethyl-6E-octenoate
v2675	184.14633	271.8	3.666	1.89	8.141	0.000414	0.042781	LMFA07010592	(Z)-3-Hexenyl 3-methylbutanoate
v2675	184.14633	271.8	3.666	1.89	8.141	0.000414	0.042781	LMFA07010717	(2E)-hex-2-en-1-yl 3-methylbutanoate
v2675	184.14633	271.8	3.666	1.89	8.141	0.000414	0.042781	LMFA07010719	(2E)-hex-2-en-1-yl pentanoate
v2675	184.14633	271.8	3.666	1.89	8.141	0.000414	0.042781	LMFA07010748	prop-2-en-1-yl octanoate
v2675	184.14633	271.8	3.666	1.89	8.141	0.000414	0.042781	LMFA07010752	hex-3-en-1-yl 2-methylbutanoate
v2675	184.14633	271.8	3.666	1.89	8.141	0.000414	0.042781	LMFA07010767	(5Z)-oct-5-en-1-yl propanoate
v2675	184.14633	271.8	3.666	1.89	8.141	0.000414	0.042781	LMFA07010804	(3Z)-hex-3-en-1-yl 2-methylbutanoate
v2675	184.14633	271.8	3.666	1.89	8.141	0.000414	0.042781	LMFA07010807	(3Z)-hex-3-en-1-yl pentanoate
v2675	184.14633	271.8	3.666	1.89	8.141	0.000414	0.042781	LMFA07010810	(3Z)-oct-3-en-1-yl propanoate
v2675	184.14633	271.8	3.666	1.89	8.141	0.000414	0.042781	LMFA07010823	cyclohexyl 3-methylbutanoate
v2675	184.14633	271.8	3.666	1.89	8.141	0.000414	0.042781	LMFA07010825	cyclohexyl pentanoate
v2675	184.14633	271.8	3.666	1.89	8.141	0.000414	0.042781	LMFA07010862	ethyl 3-cyclohexylpropanoate
v2895	192.11503	23.6	0.169	0.057	0.395	0.000253	0.031596	LMFA07010871	ethyl 4-phenylbutanoate
v6483	348.19367	29.3	0.278	0.138	0.502	7.74E-05	0.015103	LMFA07010888	(1S2E10R)-10-acetyl-3-methyl-7-methylidene-6-oxocyclodec-2-en-1-yl (2E)-4-hydroxy-4-methylpent-2-enoate
v2675	184.14633	271.8	3.666	1.89	8.141	0.000414	0.042781	LMFA07010939	methyl dec-2-enoate
v2675	184.14633	271.8	3.666	1.89	8.141	0.000414	0.042781	LMFA07010987	(2Z)-pent-2-en-1-yl hexanoate
v2675	184.14633	271.8	3.666	1.89	8.141	0.000414	0.042781	LMFA07011028	(2E)-hex-2-en-1-yl 2-methylbutanoate
v2675	184.14633	271.8	3.666	1.89	8.141	0.000414	0.042781	LMFA07040001	11-undecanolactone
v2675	184.14633	271.8	3.666	1.89	8.141	0.000414	0.042781	LMFA07040030	4-Undecanolide
v5278	292.20385	24.6	0	0	0.01	7.90E-05	0.015103	LMFA10000002	9-1E3Z6Z-trien-1-yloxy-non-8E-enoic acid
v5278	292.20385	24.6	0	0	0.01	7.90E-05	0.015103	LMFA10000003	12-(1E3Z-Hexadienyloxy)-9Z11E-dodecadienoic acid
v2675	184.14633	271.8	3.666	1.89	8.141	0.000414	0.042781	LMPK09000018	(2S6R8S)-28-Dimethyl-17-dioxaspiro55undecane
v2675	184.14633	271.8	3.666	1.89	8.141	0.000414	0.042781	LMPK09000020	2-Ethyl-17-dioxaspiro55undecane
v2675	184.14633	271.8	3.666	1.89	8.141	0.000414	0.042781	LMPK09000021	2-Methyl-17-dioxaspiro56dodecane
v2675	184.14633	271.8	3.666	1.89	8.141	0.000414	0.042781	LMPK09000022	2-Ethyl-7-methyl-16-dioxaspiro45decane
v2675	184.14633	271.8	3.666	1.89	8.141	0.000414	0.042781	LMPK09000023	7-Ethyl-2R-methyl-16-dioxaspiro45decane

v2675	184.14633	271.8	3.666	1.89	8.141	0.000414	0.042781	LMPK09000024	27-Diethyl-16-dioxaspiro44nonane
v2675	184.14633	271.8	3.666	1.89	8.141	0.000414	0.042781	LMPK09000025	(2S6S8S)-28-Dimethyl-17-dioxaspiro55undecane
v2675	184.14633	271.8	3.666	1.89	8.141	0.000414	0.042781	LMPK09000026	2S-Ethyl-7-methyl-16-dioxaspiro45decane
v2675	184.14633	271.8	3.666	1.89	8.141	0.000414	0.042781	LMPK09000027	27-Dimethyl-16-dioxaspiro46undecane
v2675	184.14633	271.8	3.666	1.89	8.141	0.000414	0.042781	LMPK09000028	2-Methyl-7-propyl-16-dioxaspiro44nonane
v10702	653.17178	49.3	0.146	0.051	0.324	3.18E-05	0.014011	LMPK12010152	Cyanidin 3-(6-acetylglucoside)-5-glucoside
v10702	653.17178	49.3	0.146	0.051	0.324	3.18E-05	0.014011	LMPK12010226	Cyanidin 3-glucoside-5-(6-acetylglucoside)
v10702	653.17178	49.3	0.146	0.051	0.324	3.18E-05	0.014011	LMPK12010321	Delphinidin 3-6-(2-acetylrhamnosyl)glucoside
v10702	653.17178	49.3	0.146	0.051	0.324	3.18E-05	0.014011	LMPK12010322	Delphinidin 3-6-(3-acetylrhamnosyl)glucoside
v10677	650.22108	79.3	5.843	2.503	17.473	0.000297	0.034571	LMPK12050358	5-Hydroxy-734-trimethoxy-8-methylisoflavone 5-O-neohesperidoside
v6519	350.00964	68	0.149	0.051	0.344	7.12E-05	0.01502	LMPK12110431	-
v2675	184.14633	271.8	3.666	1.89	8.141	0.000414	0.042781	LMPR0102010014	-
v6000	326.2821	25.5	4.275	2.164	10.106	0.000163	0.024299	LMPR0104010016	371115-tetramethyl-2-oxohexadecanoic acid
v6212	336.23006	28.4	0.32	0.157	0.583	0.000536	0.04761	LMPR0104130006	(5beta8alpha9beta10alpha)-1617-dihydroxykauran-18-oic acid
v6483	348.19368	29.3	0.278	0.138	0.502	7.74E-05	0.015103	LMPR0104170007	-
v6483	348.19368	29.3	0.278	0.138	0.502	7.74E-05	0.015103	LMPR0104170015	-
v6483	348.19368	29.3	0.278	0.138	0.502	7.74E-05	0.015103	LMPR0104170017	-
v6212	336.23006	28.4	0.32	0.157	0.583	0.000536	0.04761	LMPR0104240003	(-)-78:1011-diepoxy-4(16)-dolabellene-1718-diol
v6483	348.19368	29.3	0.278	0.138	0.502	7.74E-05	0.015103	LMPR0104420001	-
v4899	276.20893	25.1	0.075	0.015	0.229	0.000149	0.022851	LMST02010042	3alpha-hydroxy-5alpha-estran-17-one
v4899	276.20893	25.1	0.075	0.015	0.229	0.000149	0.022851	LMST02010050	19-Nor-5-androstenediol

Table S2. Putatively identified metabolites from the metabolome-wide association study of autism cases and controls using RPLC analytical platform. Both uniquely and multiply matched annotations are shown.

mzid	Monoisotopic Mass	Time (s)	Odds ratio	OR lower CI	OR higher CI	p value	q value	dbID	Name
v1277	298.2508	44.2	0.204	0.079	0.433	1.94E-04	0.032	C00869	2-Oxooctadecanoic acid;2-Oxostearate
v3536	272.1776	130.1	0.287	0.145	0.514	8.54E-05	0.023	C00951	Estradiol-17beta;Estradiol;beta-Estradiol
v3536	116.0837	130.1	0.052	0.011	0.159	9.46E-06	0.018	C01585	Hexanoic acid;Hexanoate;Hexylic acid;n-Caproic acid
v3536	272.1776	130.1	0.287	0.145	0.514	8.54E-05	0.023	C02537	Estradiol-17alpha;17alpha-Estradiol
v3536	188.1412	130.1	0.247	0.106	0.493	3.04E-04	0.044	C02774	10-Hydroxydecanoic acid;10-Hydroxydecanoate
v3536	116.0837	130.1	0.052	0.011	0.159	9.46E-06	0.018	C02948	4-Hydroxyhexan-3-one;4-Hydroxy-3-hexanone;Propioin
v3262	116.0837	202.1	0.052	0.011	0.159	9.46E-06	0.018	C03739	trans-12-Cyclohexanediol;trans-Cyclohexane-12-diol
v3536	116.0837	130.1	0.052	0.011	0.159	9.46E-06	0.018	C03739	trans-12-Cyclohexanediol;trans-Cyclohexane-12-diol
v283	312.2301	47.8	0.004	0	0.048	1.70E-04	0.030	C04717	(9Z11E)-(13S)-13-Hydroperoxyoctadeca-911-dienoic acid;(9Z11E)-(13S)-13-Hydroperoxyoctadeca-911-dienoate;13(S)-HPODE;13S-Hydroperoxy-9Z11E-octadecadienoic acid
v283	230.0579	47.8	0	0	0.002	1.10E-04	0.024	C06356	246-Trihydroxybenzophenone;Phenyl(246-trihydroxyphenyl)-methanone
v283	312.2301	47.8	0.004	0	0.048	1.70E-04	0.030	C07338	(9Z12Z)-(11S)-11-Hydroperoxyoctadeca-912-dienoic acid;(9Z12Z)-(11S)-11-Hydroperoxyoctadeca-912-dienoate
v283	312.2301	47.8	0.004	0	0.048	1.70E-04	0.030	C07354	(7S8S)-DiHODE;(9Z12Z)-(7S8S)-Dihydroxyoctadeca-912-dienoic acid;(7S8S9Z12Z)-78-Dihydroxyoctadeca-912-dienoate
v283	230.0579	47.8	0	0	0.002	1.10E-04	0.024	C07718	2-Hydroxy-4-(1-oxo-13-dihydro-2H-inden-2-ylidene)-but-2-enoic acid
v283	230.0579	47.8	0	0	0.002	1.10E-04	0.024	C07725	2-Hydroxy-4-(2-oxo-13-dihydro-2H-inden-1-ylidene)but-2-enoic acid
v283	410.1818	47.8	0.057	0.011	0.178	3.95E-05	0.018	C08093	Oseltamivir phosphate
v1277	298.2508	44.2	0.204	0.079	0.433	1.94E-04	0.032	C08365	Ricinoleic acid;(9Z)-(12R)-Hydroxyoctadecenoic acid;12-Hydroxy-9-octadecenoic acid;12-Hydroxy-cis-9-octadecenoic acid
v283	230.0579	47.8	0	0	0.002	1.10E-04	0.024	C09049	Visnagin
v3536	386.2305	130.1	0.252	0.114	0.478	1.27E-04	0.026	C11990	Oleandolide
v283	230.0579	47.8	0	0	0.002	1.10E-04	0.024	C12085	Bis-noryangonin
v3262	116.0837	202.1	0.052	0.011	0.159	9.46E-06	0.018	C12293	Isoamyl formate
v3262	116.0837	202.1	0.052	0.011	0.159	9.46E-06	0.018	C12304	Butyl acetate;n-Butyl acetate
v2752	116.0837	188.2	0.052	0.011	0.159	9.46E-06	0.018	C12313	cis-12-Cyclohexanediol;cis-Cyclohexane-12-diol
v3942	263.0844	169.5	115.208	13.977	2191.49	1.90E-04	0.032	C12798	Tulobuterol hydrochloride
v1277	298.2508	44.2	0.204	0.079	0.433	1.94E-04	0.032	C13791	(6R7S)-67-Epoxyoctadecanoic acid;6R7S-Epoxy-octadecanoic acid;6R7S-Epoxy-octadecanoate
v283	274.2144	47.8	0.107	0.03	0.276	6.06E-05	0.019	C13854	1-Dodecanoyl-sn-glycerol
v283	198.1045	47.8	0.089	0.022	0.248	7.08E-05	0.020	C14340	4-Phenethylphenol;4-(2-Phenylethyl)phenol
v3536	272.1776	130.1	0.287	0.145	0.514	8.54E-05	0.023	C14500	19-Norandrostenedione;delta4-Estrene-317-dione
v3262	322.1780	202.1	0.242	0.106	0.478	1.85E-04	0.031	C14752	alpha-Zearalanol;Zeranol
v3262	322.1780	202.1	0.242	0.106	0.478	1.85E-04	0.031	C14753	beta-Zearalanol;Taleranol
v283	326.2093	47.8	0	0	0.002	3.94E-04	0.048	C14794	23-Dinor-8-iso prostaglandin F2alpha;23-Dinor-8-iso PGF2alpha
v283	312.2301	47.8	0.004	0	0.048	1.70E-04	0.030	C14827	9(S)-HPODE;9(S)-HPOD;(10E12Z)-(9S)-9-Hydroperoxyoctadeca-1012-dienoic acid;(9S10E12Z)-9-Hydroperoxy-1012-octadecadienoate
v283	312.2301	47.8	0.004	0	0.048	1.70E-04	0.030	C14831	8(R)-HPODE;(9Z12Z)-(8R)-8-Hydroperoxyoctadeca-912-dienoic acid;(8R9Z12Z)-8-Hydroperoxyoctadeca-912-dienoate
v283	312.2301	47.8	0.004	0	0.048	1.70E-04	0.030	C14832	1213-Epoxy-9-hydroxy-10-octadecenoate;12(R)13(S)-Epoxy-9(S)-hydroxy-10(E)-octadecenoic acid;(10E)-(9S12R13S)-1213-Epoxy-9-hydroxyoctadec-10-enoic acid
v283	312.2301	47.8	0.004	0	0.048	1.70E-04	0.030	C14834	910-Epoxy-13-hydroxy-11-octadecenoate;(11E)-910-Epoxyoctadecenoic acid
v283	312.2301	47.8	0.004	0	0.048	1.70E-04	0.030	C14836	910-1213-Diepoxyoctadecanoate;910-1213-Diepoxyoctadecanoic acid
v3536	272.1776	130.1	0.287	0.145	0.514	8.54E-05	0.023	C15129	Estra-135(10)-triene-217beta-diol;2-Hydroxy-3-deoxyestradiol
v3536	272.1776	130.1	0.287	0.145	0.514	8.54E-05	0.023	C15261	Estra-135(10)-triene-316beta-diol;16beta-Estradiol
v283	230.0579	47.8	0	0	0.002	1.10E-04	0.024	C16263	23-Dihydroxy-2-carboxybiphenyl
v1277	216.0746	44.2	0.188	0.078	0.381	2.69E-05	0.018	C17359	8-Hydroxyalanylclavam
v3536	188.1412	130.1	0.247	0.106	0.493	3.04E-04	0.044	C18067	6-Hydroxy-37-dimethyloctanoate

v283	230.0579	47.8	0	0	0.002	1.10E-04	0.024	C18216	4-Hydroxyphenyl-4-hydroxybenzoate
v1277	298.2508	44.2	0.204	0.079	0.433	1.94E-04	0.032	C19418	cis-910-Epoxystearic acid
v1277	298.2508	44.2	0.204	0.079	0.433	1.94E-04	0.032	C19616	18-Hydroxyoleate
v283	312.2301	47.8	0.004	0	0.048	1.70E-04	0.030	C19618	Octadec-9-ene-118-dioic-acid
v3812	332.2563	75	0.294	0.145	0.531	1.64E-04	0.030	C19621	91018-Trihydroxystearate
v283	312.2301	47.8	0.004	0	0.048	1.70E-04	0.030	C19937	(8E10R12Z)-10-Hydroperoxy-812-octadecadienoate
v283	312.2301	47.8	0.004	0	0.048	1.70E-04	0.030	C20186	5S8R-DiHODE;(5S8R)-DiHODE;(5S8R9Z12Z)-58-Dihydroxyoctadeca-912-dienoate
v283	312.2301	47.8	0.004	0	0.048	1.70E-04	0.030	C20703	(8E10S12Z)-10-Hydroperoxyoctadeca-812-dienoate
v3536	272.1776	130.1	0.287	0.145	0.514	8.54E-05	0.023	HMDB00151	Estradiol
v3536	272.1776	130.1	0.287	0.145	0.514	8.54E-05	0.023	HMDB00429	17a-Estradiol
v2752	116.0837	188.2	0.052	0.011	0.159	9.46E-06	0.018	HMDB00535	Caproic acid
v2562	116.0837	22.2	0.052	0.011	0.159	9.46E-06	0.018	HMDB00689	Isocaproic acid
v2752	116.0837	188.2	0.052	0.011	0.159	9.46E-06	0.018	HMDB00689	Isocaproic acid
v3536	216.1362	130.1	0.02	0.002	0.105	4.36E-05	0.018	HMDB00888	Undecanedioic acid
v3536	188.1412	130.1	0.247	0.106	0.493	3.04E-04	0.044	HMDB02203	3-Hydroxycapric acid
v283	312.2301	47.8	0.004	0	0.048	1.70E-04	0.030	HMDB03871	13-L-Hydroperoxylinoleic acid
v283	312.2301	47.8	0.004	0	0.048	1.70E-04	0.030	HMDB04706	8(R)-Hydroperoxylinoleic acid
v283	312.2301	47.8	0.004	0	0.048	1.70E-04	0.030	HMDB06940	9(S)-HPODE
v283	312.2301	47.8	0.004	0	0.048	1.70E-04	0.030	HMDB10201	1213-DiHODE
v283	312.2301	47.8	0.004	0	0.048	1.70E-04	0.030	HMDB10208	1516-DiHODE
v283	312.2301	47.8	0.004	0	0.048	1.70E-04	0.030	HMDB10221	910-DiHODE
v3262	188.1412	202.1	0.247	0.106	0.493	3.04E-04	0.044	HMDB10725	(R)-3-Hydroxydecanoic acid
v1277	298.2508	44.2	0.204	0.079	0.433	1.94E-04	0.032	HMDB10736	3-Oxooctadecanoic acid
v6340	262.0801	167.5	919.538	61.53	57168.7	5.70E-05	0.018	HMDB11164	L-beta-aspartyl-L-glutamic acid
v1277	217.0773	44.2	0.167	0.064	0.355	3.15E-05	0.018	HMDB15328	Captopril
v1943	116.0837	35.1	0.052	0.011	0.159	9.46E-06	0.018	HMDB29762	Methyl (S)-2-Methylbutanoate
v1943	116.0837	35.1	0.052	0.011	0.159	9.46E-06	0.018	HMDB30027	Methyl 3-methylbutanoate
v1943	116.0837	35.1	0.052	0.011	0.159	9.46E-06	0.018	HMDB30056	Isopropyl propionate
v1412	116.0837	182.5	0.052	0.011	0.159	9.46E-06	0.018	HMDB30059	Propyl propionate
v1943	116.0837	35.1	0.052	0.011	0.159	9.46E-06	0.018	HMDB30059	Propyl propionate
v6340	262.0801	167.5	919.538	61.53	57168.7	5.70E-05	0.018	HMDB30413	Na-L-Glutamyl-L-aspartic acid
v4171	262.0801	201.3	919.538	61.53	57168.7	5.70E-05	0.018	HMDB30419	Ng-L-Glutamyl-L-aspartic acid
v3812	332.2563	75	0.294	0.145	0.531	1.64E-04	0.030	HMDB30935	91013-Trihydroxystearic acid
v1277	298.2508	44.2	0.204	0.079	0.433	1.94E-04	0.032	HMDB30979	9-Oxooctadecanoic acid
v1277	298.2508	44.2	0.204	0.079	0.433	1.94E-04	0.032	HMDB30980	10-Oxooctadecanoic acid
v1277	298.2508	44.2	0.204	0.079	0.433	1.94E-04	0.032	HMDB30981	11-Oxooctadecanoic acid
v1277	298.2508	44.2	0.204	0.079	0.433	1.94E-04	0.032	HMDB31127	5-Hexyltetrahydro-2-furanoctanoic acid
v1277	116.0837	44.2	0.052	0.011	0.159	9.46E-06	0.018	HMDB31207	Methyl pentanoate
v1412	116.0837	182.5	0.052	0.011	0.159	9.46E-06	0.018	HMDB31207	Methyl pentanoate
v283	116.0837	47.8	0.052	0.011	0.159	9.46E-06	0.018	HMDB31221	2-Ethylbutanoic acid
v1277	116.0837	44.2	0.052	0.011	0.159	9.46E-06	0.018	HMDB31221	2-Ethylbutanoic acid
v283	116.0837	47.8	0.052	0.011	0.159	9.46E-06	0.018	HMDB31246	2-Methylpropyl acetate
v283	116.0837	47.8	0.052	0.011	0.159	9.46E-06	0.018	HMDB31248	Ethyl 2-methylpropanoate
v283	116.0837	47.8	0.052	0.011	0.159	9.46E-06	0.018	HMDB31325	n-Butyl acetate
v283	116.0837	47.8	0.052	0.011	0.159	9.46E-06	0.018	HMDB31511	Diacetone alcohol
v283	116.0837	47.8	0.052	0.011	0.159	9.46E-06	0.018	HMDB31580	()-2-Methylpentanoic acid
v1708	326.2093	27.3	0	0	0.002	3.94E-04	0.048	HMDB31963	(3b6b8a12a)-812-Epoxy-7(11)-eremophilene-6812-trimethoxy-3-ol
v283	198.1045	47.8	0.089	0.022	0.248	7.08E-05	0.020	HMDB32078	Dibenzyl ether
v3262	269.1991	202.1	0.208	0.09	0.401	2.19E-05	0.018	HMDB32255	N-(Ethoxycarbonyl)methyl)-p-menthane-3-carboxamide
v3262	322.1780	202.1	0.242	0.106	0.478	1.85E-04	0.031	HMDB32702	Zeranol
v3262	188.1412	202.1	0.247	0.106	0.493	3.04E-04	0.044	HMDB33201	9-Hydroxydecanoic acid
v3812	230.0579	75	0	0	0.002	1.10E-04	0.024	HMDB33329	Coriandrin

v3262	188.1412	202.1	0.247	0.106	0.493	3.04E-04	0.044	HMDB33574	(1R2R4R8R)-p-Menthane-289-triol
v3262	188.1412	202.1	0.247	0.106	0.493	3.04E-04	0.044	HMDB33640	7-Methyl-3-methylene-167-octanetriol
v5612	116.0837	77.5	0.052	0.011	0.159	9.46E-06	0.018	HMDB33774	3-Methylpentanoic acid
v283	116.0837	47.8	0.052	0.011	0.159	9.46E-06	0.018	HMDB33774	3-Methylpentanoic acid
v3942	116.0837	169.5	0.052	0.011	0.159	9.46E-06	0.018	HMDB33889	Ethyl butyrate
v5109	116.0837	41.6	0.052	0.011	0.159	9.46E-06	0.018	HMDB33889	Ethyl butyrate
v1277	298.2508	44.2	0.204	0.079	0.433	1.94E-04	0.032	HMDB34074	5-Oxooctadecanoic acid
v2790	116.0837	88.3	0.052	0.011	0.159	9.46E-06	0.018	HMDB34163	3-Methylbutyl formate
v3812	116.0837	75	0.052	0.011	0.159	9.46E-06	0.018	HMDB34163	3-Methylbutyl formate
v3812	332.2563	75	0.294	0.145	0.531	1.64E-04	0.030	HMDB34295	Floionolic acid
v1277	298.2508	44.2	0.204	0.079	0.433	1.94E-04	0.032	HMDB34297	Ricinoleic acid
v3262	188.1412	202.1	0.247	0.106	0.493	3.04E-04	0.044	HMDB34783	cis-p-Menthane-178-triol
v3536	216.1362	130.1	0.02	0.002	0.105	4.36E-05	0.018	HMDB37137	Butyl butyryllactate
v3536	272.1776	130.1	0.287	0.145	0.514	8.54E-05	0.023	HMDB37216	Linalyl phenylacetate
v5612	116.0837	77.5	0.052	0.011	0.159	9.46E-06	0.018	HMDB37266	224-Trimethyl-13-dioxolane
v1697	116.0837	26.5	0.052	0.011	0.159	9.46E-06	0.018	HMDB37266	224-Trimethyl-13-dioxolane
v3262	188.1412	202.1	0.247	0.106	0.493	3.04E-04	0.044	HMDB38186	26-Dimethyl-7-octene-236-triol
v3536	272.1776	130.1	0.287	0.145	0.514	8.54E-05	0.023	HMDB38257	Geranyl phenylacetate
v3744	230.0579	62.9	0	0	0.002	1.10E-04	0.024	HMDB39141	Wyeronic acid
v2679	230.0579	61.8	0	0	0.002	1.10E-04	0.024	HMDB39209	24-Dihydroxy-2-biphenylcarboxylic acid
v3262	188.1412	202.1	0.247	0.106	0.493	3.04E-04	0.044	HMDB39470	(1S2S4R8R)-p-Menthane-129-triol
v3262	188.1412	202.1	0.247	0.106	0.493	3.04E-04	0.044	HMDB39668	2-Hexyl-13-dioxan-5-ol
v3262	188.1412	202.1	0.247	0.106	0.493	3.04E-04	0.044	HMDB39669	2-Hexyl-13-dioxolane-4-methanol
v3262	188.1412	202.1	0.247	0.106	0.493	3.04E-04	0.044	HMDB39893	(1R2R4S)-p-Menthane-128-triol
v3942	116.0837	169.5	0.052	0.011	0.159	9.46E-06	0.018	HMDB40279	245-Trimethyl-13-dioxolane
v3536	116.0837	130.1	0.052	0.011	0.159	9.46E-06	0.018	HMDB40327	Pentyl formate
v3262	188.1412	202.1	0.247	0.106	0.493	3.04E-04	0.044	HMDB40329	xi-5-Hydroxydecanoic acid
v283	312.2301	47.8	0.004	0	0.048	1.70E-04	0.030	HMDB40900	()-(E)-13-Hydroxy-10-oxo-11-octadecenoic acid
v3262	188.1412	202.1	0.247	0.106	0.493	3.04E-04	0.044	HMDB41600	Ethyl ()-3-hydroxyoctanoate
v283	410.1842	47.8	0.057	0.011	0.178	3.95E-05	0.018	HMDB42005	Quinaprilat
v3942	263.0844	169.5	115.208	13.977	2191.49	1.90E-04	0.032	HMDB42056	Tulobuterol
v283	116.0837	47.8	0.052	0.011	0.159	9.46E-06	0.018	LMFA01010006	Hexanoic acid
v283	116.0837	47.8	0.052	0.011	0.159	9.46E-06	0.018	LMFA01020074	2-methyl-pentanoic acid
v283	116.0837	47.8	0.052	0.011	0.159	9.46E-06	0.018	LMFA01020075	3-methyl-pentanoic acid
v283	116.0837	47.8	0.052	0.011	0.159	9.46E-06	0.018	LMFA01020076	4-methyl-pentanoic acid
v283	116.0837	47.8	0.052	0.011	0.159	9.46E-06	0.018	LMFA01020077	2-ethyl-butanoic acid
v283	116.0837	47.8	0.052	0.011	0.159	9.46E-06	0.018	LMFA01020078	22-dimethyl-butanoic acid
v283	116.0837	47.8	0.052	0.011	0.159	9.46E-06	0.018	LMFA01020079	33-dimethyl-butanoic acid
v3812	272.1776	75	0.287	0.145	0.514	8.54E-05	0.023	LMFA01030510	13Z17-Octadecadiene-911-diynoic acid
v3536	272.1776	130.1	0.287	0.145	0.514	8.54E-05	0.023	LMFA01030553	5811-octadecatriynoic acid
v3536	272.1776	130.1	0.287	0.145	0.514	8.54E-05	0.023	LMFA01030554	6912-octadecatriynoic acid
v3536	272.1776	130.1	0.287	0.145	0.514	8.54E-05	0.023	LMFA01030555	81114-octadecatriynoic acid
v3536	188.1412	130.1	0.247	0.106	0.493	3.04E-04	0.044	LMFA01050029	2-hydroxy-decanoic acid
v3536	188.1412	130.1	0.247	0.106	0.493	3.04E-04	0.044	LMFA01050031	4-hydroxy-decanoic acid
v3536	188.1412	130.1	0.247	0.106	0.493	3.04E-04	0.044	LMFA01050032	5-hydroxy-decanoic acid
v3536	188.1412	130.1	0.247	0.106	0.493	3.04E-04	0.044	LMFA01050033	10-hydroxy-decanoic acid
v1277	274.2144	44.2	0.107	0.03	0.276	6.06E-05	0.019	LMFA01050082	215-dihydroxy-pentadecanoic acid
v3536	188.1412	130.1	0.247	0.106	0.493	3.04E-04	0.044	LMFA01050153	3-hydroxy-decanoic acid
v3536	188.1412	130.1	0.247	0.106	0.493	3.04E-04	0.044	LMFA01050154	6-hydroxy-decanoic acid
v3536	188.1412	130.1	0.247	0.106	0.493	3.04E-04	0.044	LMFA01050155	7-hydroxy-decanoic acid
v3536	188.1412	130.1	0.247	0.106	0.493	3.04E-04	0.044	LMFA01050156	9-hydroxy-decanoic acid
v283	274.2144	47.8	0.107	0.03	0.276	6.06E-05	0.019	LMFA01050184	312-dihydroxy-pentadecanoic acid

v283	274.2144	47.8	0.107	0.03	0.276	6.06E-05	0.019	LMFA01050186	412-dihydroxy-pentadecanoic acid
v3536	188.1412	130.1	0.247	0.106	0.493	3.04E-04	0.044	LMFA01050244	2S-hydroxy-decanoic acid
v3536	188.1412	130.1	0.247	0.106	0.493	3.04E-04	0.044	LMFA01050245	3R-hydroxy-decanoic acid
v3536	188.1412	130.1	0.247	0.106	0.493	3.04E-04	0.044	LMFA01050246	3S-hydroxy-decanoic acid
v3536	188.1412	130.1	0.247	0.106	0.493	3.04E-04	0.044	LMFA01050247	9R-hydroxy-decanoic acid
v3536	188.1412	130.1	0.247	0.106	0.493	3.04E-04	0.044	LMFA01050248	9S-hydroxy-decanoic acid
v3536	188.1412	130.1	0.247	0.106	0.493	3.04E-04	0.044	LMFA01050370	6-hydroxy-37-dimethyloctanoic acid
v3262	298.2508	202.1	0.204	0.079	0.433	1.94E-04	0.032	LMFA01050421	8Z-decen-46-diynoic acid
v3536	344.2563	130.1	0.016	0.002	0.09	3.50E-05	0.018	LMFA01080006	1213-dihydroxy-11-methoxy-9-octadecenoic acid
v3536	216.1362	130.1	0.02	0.002	0.105	4.36E-05	0.018	LMFA01170007	Undecanedioic acid
v3262	312.2301	202.1	0.004	0	0.048	1.70E-04	0.030	LMFA01170055	9Z-Octadecenedioic acid
v3262	298.2508	202.1	0.204	0.079	0.433	1.94E-04	0.032	LMFA02000001	9S10R-epoxy-octadecanoic acid
v3262	298.2508	202.1	0.204	0.079	0.433	1.94E-04	0.032	LMFA02000002	9R10S-epoxy-octadecanoic acid
v3942	332.2563	169.5	0.294	0.145	0.531	1.64E-04	0.030	LMFA02000005	18-hydroxy-9S10R-dihydroxy-octadecanoic acid
v3812	332.2563	75	0.294	0.145	0.531	1.64E-04	0.030	LMFA02000006	9R10S18-trihydroxy-octadecanoic acid
v3262	312.2301	202.1	0.004	0	0.048	1.70E-04	0.030	LMFA02000009	9-hydroxy-10-oxo-12Z-octadecenoic acid
v3262	312.2301	202.1	0.004	0	0.048	1.70E-04	0.030	LMFA02000010	10S11S-epoxy-9S-hydroxy-12Z-octadecenoic acid
v3262	312.2301	202.1	0.004	0	0.048	1.70E-04	0.030	LMFA02000012	9S-hydroperoxy-10E12Z-octadecadienoic acid
v3262	312.2301	202.1	0.004	0	0.048	1.70E-04	0.030	LMFA02000013	12R13S-epoxy-9S-hydroxy-10E-octadecenoic acid
v3262	312.2301	202.1	0.004	0	0.048	1.70E-04	0.030	LMFA02000017	12-oxo13-hydroxy-9Z-octadecenoic acid
v283	326.2093	47.8	0	0	0.002	3.94E-04	0.048	LMFA02000031	2R-hydroperoxy-9Z12Z15Z-octadecatrienoic acid
v3262	312.2301	202.1	0.004	0	0.048	1.70E-04	0.030	LMFA02000034	13S-hydroperoxy-9Z11E-octadecadienoic acid
v2752	312.2301	188.2	0.004	0	0.048	1.70E-04	0.030	LMFA02000045	(-)-910-dihydroxy-12Z15Z-octadecadienoic acid
v2752	312.2301	188.2	0.004	0	0.048	1.70E-04	0.030	LMFA02000046	(-)-1213-dihydroxy-9Z15Z-octadecadienoic acid
v2752	312.2301	188.2	0.004	0	0.048	1.70E-04	0.030	LMFA02000047	(-)-1516-dihydroxy-9Z12Z-octadecadienoic acid
v2752	312.2301	188.2	0.004	0	0.048	1.70E-04	0.030	LMFA02000048	(-)-67-dihydroxy-9Z12Z-octadecadienoic acid
v2562	312.2301	22.2	0.004	0	0.048	1.70E-04	0.030	LMFA02000049	(-)-910-dihydroxy-6Z12Z-octadecadienoic acid
v2554	312.2301	30.5	0.004	0	0.048	1.70E-04	0.030	LMFA02000050	(-)-1213-dihydroxy-6Z9Z-octadecadienoic acid
v3262	298.2508	202.1	0.204	0.079	0.433	1.94E-04	0.032	LMFA02000056	2R-hydroxy-9Z-octadecenoic acid
v283	326.2093	47.8	0	0	0.002	3.94E-04	0.048	LMFA02000058	9-oxo-1213-dihydroxy-10E15Z-octadecadienoic acid
v2554	312.2301	30.5	0.004	0	0.048	1.70E-04	0.030	LMFA02000064	8R11S-dihydroxy-9Z12Z-octadecadienoic acid
v3262	298.2508	202.1	0.204	0.079	0.433	1.94E-04	0.032	LMFA02000083	10R-hydroxy11Z-octadecenoic acid
v3262	298.2508	202.1	0.204	0.079	0.433	1.94E-04	0.032	LMFA02000084	10S-hydroxy11Z-octadecenoic acid
v3262	298.2508	202.1	0.204	0.079	0.433	1.94E-04	0.032	LMFA02000085	12R-hydroxy13Z-octadecenoic acid
v3262	298.2508	202.1	0.204	0.079	0.433	1.94E-04	0.032	LMFA02000086	12S-hydroxy13Z-octadecenoic acid
v3262	298.2508	202.1	0.204	0.079	0.433	1.94E-04	0.032	LMFA02000087	11R-hydroxy12Z-octadecenoic acid
v3262	298.2508	202.1	0.204	0.079	0.433	1.94E-04	0.032	LMFA02000088	11S-hydroxy12Z-octadecenoic acid
v3262	298.2508	202.1	0.204	0.079	0.433	1.94E-04	0.032	LMFA02000089	12R-hydroxy10E-octadecenoic acid
v3262	298.2508	202.1	0.204	0.079	0.433	1.94E-04	0.032	LMFA02000090	12S-hydroxy10E-octadecenoic acid
v3262	298.2508	202.1	0.204	0.079	0.433	1.94E-04	0.032	LMFA02000091	12R-hydroxy13E-octadecenoic acid
v3262	298.2508	202.1	0.204	0.079	0.433	1.94E-04	0.032	LMFA02000092	12S-hydroxy13E-octadecenoic acid
v3262	298.2508	202.1	0.204	0.079	0.433	1.94E-04	0.032	LMFA02000093	13R-hydroxy11E-octadecenoic acid
v3262	298.2508	202.1	0.204	0.079	0.433	1.94E-04	0.032	LMFA02000094	13S-hydroxy11E-octadecenoic acid
v3262	298.2508	202.1	0.204	0.079	0.433	1.94E-04	0.032	LMFA02000095	11R-hydroxy12E-octadecenoic acid
v3262	298.2508	202.1	0.204	0.079	0.433	1.94E-04	0.032	LMFA02000096	11S-hydroxy12E-octadecenoic acid
v3262	298.2508	202.1	0.204	0.079	0.433	1.94E-04	0.032	LMFA02000098	13-hydroperoxy-14E-octadecenoic acid
v2554	312.2301	30.5	0.004	0	0.048	1.70E-04	0.030	LMFA02000099	9-hydroperoxy-9E11E-octadecadienoic acid
v1943	312.2301	35.1	0.004	0	0.048	1.70E-04	0.030	LMFA02000100	9-hydroperoxy-10E12E-octadecadienoic acid
v1943	312.2301	35.1	0.004	0	0.048	1.70E-04	0.030	LMFA02000101	10-hydroperoxy-8E12Z-octadecadienoic acid
v1943	312.2301	35.1	0.004	0	0.048	1.70E-04	0.030	LMFA02000102	12-hydroperoxy-9Z13E-octadecadienoic acid
v1699	312.2301	62.3	0.004	0	0.048	1.70E-04	0.030	LMFA02000103	8-hydroperoxy-912-octadecadienoic acid
v1699	312.2301	62.3	0.004	0	0.048	1.70E-04	0.030	LMFA02000104	14-hydroperoxy-912-octadecadienoic acid

v1412	312.2301	182.5	0.004	0	0.048	1.70E-04	0.030	LMFA02000113	8R-hydroperoxy-9Z12Z-octadecadienoic acid
v1412	312.2301	182.5	0.004	0	0.048	1.70E-04	0.030	LMFA02000115	11S-hydroperoxy-9Z12Z-octadecadienoic acid
v3812	332.2563	75	0.294	0.145	0.531	1.64E-04	0.030	LMFA02000147	91018-trihydroxy-octadecanoic acid
v3262	298.2508	202.1	0.204	0.079	0.433	1.94E-04	0.032	LMFA02000149	9-hydroxy-12Z-octadecenoic acid
v3262	298.2508	202.1	0.204	0.079	0.433	1.94E-04	0.032	LMFA02000150	12-hydroxy-9E-octadecenoic acid
v1277	312.2301	44.2	0.004	0	0.048	1.70E-04	0.030	LMFA02000158	9-hydroxy-1213-epoxy-10-octadecenoic acid
v1277	312.2301	44.2	0.004	0	0.048	1.70E-04	0.030	LMFA02000159	1213-epoxy-11-hydroxy-9-octadecenoic acid
v1277	312.2301	44.2	0.004	0	0.048	1.70E-04	0.030	LMFA02000166	813-dihydroxy-911-octadecadienoic acid
v1277	312.2301	44.2	0.004	0	0.048	1.70E-04	0.030	LMFA02000167	914-dihydroxy-1012-octadecadienoic acid
v1277	312.2301	44.2	0.004	0	0.048	1.70E-04	0.030	LMFA02000170	9-hydroxy-10-oxo-12-octadecenoic acid
v1277	312.2301	44.2	0.004	0	0.048	1.70E-04	0.030	LMFA02000171	9-hydroxy-12-oxo-10-octadecenoic acid
v1277	312.2301	44.2	0.004	0	0.048	1.70E-04	0.030	LMFA02000172	9-hydroxy-13-oxo-10-octadecenoic acid
v3262	298.2508	202.1	0.204	0.079	0.433	1.94E-04	0.032	LMFA02000177	12-hydroxy-10E-octadecenoic acid
v3262	298.2508	202.1	0.204	0.079	0.433	1.94E-04	0.032	LMFA02000178	9-hydroxy-10Z-octadecenoic acid
v3262	298.2508	202.1	0.204	0.079	0.433	1.94E-04	0.032	LMFA02000179	9-hydroxy-12-octadecenoic acid
v3262	298.2508	202.1	0.204	0.079	0.433	1.94E-04	0.032	LMFA02000180	17-hydroxy-9Z-octadecenoic acid
v3262	298.2508	202.1	0.204	0.079	0.433	1.94E-04	0.032	LMFA02000181	18-hydroxy-9Z-octadecenoic acid
v3262	298.2508	202.1	0.204	0.079	0.433	1.94E-04	0.032	LMFA02000184	12R-hydroxy-9Z-octadecenoic acid
v3262	298.2508	202.1	0.204	0.079	0.433	1.94E-04	0.032	LMFA02000202	5-hydroxy-2-octadecenoic acid
v3262	298.2508	202.1	0.204	0.079	0.433	1.94E-04	0.032	LMFA02000203	8-hydroxy-9-octadecenoic acid
v3262	298.2508	202.1	0.204	0.079	0.433	1.94E-04	0.032	LMFA02000204	8R-hydroxy-9Z-octadecenoic acid
v3262	298.2508	202.1	0.204	0.079	0.433	1.94E-04	0.032	LMFA02000205	9R-hydroxy-10E-octadecenoic acid
v3262	298.2508	202.1	0.204	0.079	0.433	1.94E-04	0.032	LMFA02000206	9-hydroxy-10E-octadecenoic acid
v3262	298.2508	202.1	0.204	0.079	0.433	1.94E-04	0.032	LMFA02000207	9R-hydroxy-12E-octadecenoic acid
v3262	298.2508	202.1	0.204	0.079	0.433	1.94E-04	0.032	LMFA02000208	9R-hydroxy-12Z-octadecenoic acid
v3262	298.2508	202.1	0.204	0.079	0.433	1.94E-04	0.032	LMFA02000209	10-hydroxy-8-octadecenoic acid
v3262	298.2508	202.1	0.204	0.079	0.433	1.94E-04	0.032	LMFA02000210	10R-hydroxy-8E-octadecenoic acid
v3262	298.2508	202.1	0.204	0.079	0.433	1.94E-04	0.032	LMFA02000211	11-hydroxy-9-octadecenoic acid
v3262	298.2508	202.1	0.204	0.079	0.433	1.94E-04	0.032	LMFA02000212	12R-hydroxy-9E-octadecenoic acid
v3262	298.2508	202.1	0.204	0.079	0.433	1.94E-04	0.032	LMFA02000213	12S-hydroxy-9E-octadecenoic acid
v3262	298.2508	202.1	0.204	0.079	0.433	1.94E-04	0.032	LMFA02000214	12S-hydroxy-9Z-octadecenoic acid
v1277	312.2301	44.2	0.004	0	0.048	1.70E-04	0.030	LMFA02000224	7S8S-dihydroxy-9Z12Z-octadecadienoic acid
v3262	298.2508	202.1	0.204	0.079	0.433	1.94E-04	0.032	LMFA02000240	3-oxo-octadecanoic acid
v3262	298.2508	202.1	0.204	0.079	0.433	1.94E-04	0.032	LMFA02000241	4-oxo-octadecanoic acid
v3262	298.2508	202.1	0.204	0.079	0.433	1.94E-04	0.032	LMFA02000242	5-oxo-octadecanoic acid
v2790	298.2508	88.3	0.204	0.079	0.433	1.94E-04	0.032	LMFA02000243	6-oxo-octadecanoic acid
v2790	298.2508	88.3	0.204	0.079	0.433	1.94E-04	0.032	LMFA02000244	7-oxo-octadecanoic acid
v2790	298.2508	88.3	0.204	0.079	0.433	1.94E-04	0.032	LMFA02000245	9-oxo-octadecanoic acid
v2790	298.2508	88.3	0.204	0.079	0.433	1.94E-04	0.032	LMFA02000246	10-oxo-octadecanoic acid
v1277	312.2301	44.2	0.004	0	0.048	1.70E-04	0.030	LMFA02000248	9-oxo-13-hydroxy-11-octadecenoic acid
v1277	312.2301	44.2	0.004	0	0.048	1.70E-04	0.030	LMFA02000249	10-oxo-13-hydroxy-11-octadecenoic acid
v1277	312.2301	44.2	0.004	0	0.048	1.70E-04	0.030	LMFA02000250	12-oxo-13-hydroxy-9-octadecenoic acid
v2752	298.2508	188.2	0.204	0.079	0.433	1.94E-04	0.032	LMFA02000253	16-methyl-10-oxo-heptadecanoic acid
v2752	298.2508	188.2	0.204	0.079	0.433	1.94E-04	0.032	LMFA02000254	2-methyl-4-oxo-heptadecanoic acid
v2752	298.2508	188.2	0.204	0.079	0.433	1.94E-04	0.032	LMFA02000255	11-oxo-octadecanoic acid
v2752	298.2508	188.2	0.204	0.079	0.433	1.94E-04	0.032	LMFA02000256	12-oxo-octadecanoic acid
v2752	298.2508	188.2	0.204	0.079	0.433	1.94E-04	0.032	LMFA02000257	13-oxo-octadecanoic acid
v2752	298.2508	188.2	0.204	0.079	0.433	1.94E-04	0.032	LMFA02000258	14-oxo-octadecanoic acid
v2752	298.2508	188.2	0.204	0.079	0.433	1.94E-04	0.032	LMFA02000259	15-oxo-octadecanoic acid
v2752	298.2508	188.2	0.204	0.079	0.433	1.94E-04	0.032	LMFA02000260	16-oxo-octadecanoic acid
v2752	298.2508	188.2	0.204	0.079	0.433	1.94E-04	0.032	LMFA02000261	17-oxo-octadecanoic acid
v1699	298.2508	62.3	0.204	0.079	0.433	1.94E-04	0.032	LMFA02000262	2-oxo-octadecanoic acid

v1699	298.2508	62.3	0.204	0.079	0.433	1.94E-04	0.032	LMFA02000263	8-oxo-octadecanoic acid
v1277	312.2301	44.2	0.004	0	0.048	1.70E-04	0.030	LMFA02000264	910-dioxo-octadecanoic acid
v1277	298.2508	44.2	0.204	0.079	0.433	1.94E-04	0.032	LMFA02000275	6R7S-epoxy-octadecanoic acid
v1277	312.2301	44.2	0.004	0	0.048	1.70E-04	0.030	LMFA02000277	910-epoxy-11-hydroxy-12-octadecenoic acid
v283	312.2301	47.8	0.004	0	0.048	1.70E-04	0.030	LMFA02000278	910-epoxy-13-hydroxy-11-octadecenoic acid
v283	312.2301	47.8	0.004	0	0.048	1.70E-04	0.030	LMFA02000284	5S8R-dihydroxy-9Z12Z-octadecadienoic acid
v283	312.2301	47.8	0.004	0	0.048	1.70E-04	0.030	LMFA02000285	10R-hydroperoxy-8E12Z-octadecadienoic acid
v283	312.2301	47.8	0.004	0	0.048	1.70E-04	0.030	LMFA02000286	10S-hydroperoxy-8E12Z-octadecadienoic acid
v283	326.2093	47.8	0	0	0.002	3.94E-04	0.048	LMFA03010011	9S11S15S-trihydroxy-23-dinor-5Z13E-prostadienoic acid
v283	326.2093	47.8	0	0	0.002	3.94E-04	0.048	LMFA03010169	9-oxo-11R15S-dihydroxy-23-dinor-13E-prostenoic acid
v283	326.2093	47.8	0	0	0.002	3.94E-04	0.048	LMFA03010212	23-dinor-9S11R15S-trihydroxy-5Z13E-prostadienoic acid
v283	326.2093	47.8	0	0	0.002	3.94E-04	0.048	LMFA03110010	9S11R15S-trihydroxy-23-dinor-5Z13E-prostadienoic acid-cyclo8S12R
v3536	188.1412	130.1	0.247	0.106	0.493	3.04E-04	0.044	LMFA05000610	26-dimethyloct-7-ene-236-triol
v3536	188.1412	130.1	0.247	0.106	0.493	3.04E-04	0.044	LMFA05000635	7-methyl-3-methylideneoctane-167-triol
v3536	188.1412	130.1	0.247	0.106	0.493	3.04E-04	0.044	LMFA05000657	ethyl 3-hydroxyoctanoate
v283	116.0837	47.8	0.052	0.011	0.159	9.46E-06	0.018	LMFA06000012	2-hydroxy-hexanal
v283	116.0837	47.8	0.052	0.011	0.159	9.46E-06	0.018	LMFA06000013	4-hydroxy-hexanal
v283	116.0837	47.8	0.052	0.011	0.159	9.46E-06	0.018	LMFA06000014	5-hydroxy-hexanal
v283	116.0837	47.8	0.052	0.011	0.159	9.46E-06	0.018	LMFA06000015	6-hydroxy-hexanal
v283	116.0837	47.8	0.052	0.011	0.159	9.46E-06	0.018	LMFA06000125	3-Hydroxyhexanal
v283	116.0837	47.8	0.052	0.011	0.159	9.46E-06	0.018	LMFA07010412	propyl propionate
v283	116.0837	47.8	0.052	0.011	0.159	9.46E-06	0.018	LMFA07010503	ethyl 2-methyl-propionyl
v283	116.0837	47.8	0.052	0.011	0.159	9.46E-06	0.018	LMFA07010575	3-Methyl-2-butenyl formate
v3536	188.1412	130.1	0.247	0.106	0.493	3.04E-04	0.044	LMFA07010583	Hexyl (R)-3-hydroxybutyrate
v3536	216.1362	130.1	0.02	0.002	0.105	4.36E-05	0.018	LMFA07010792	1-butoxy-1-oxopropan-2-yl butanoate
v283	116.0837	47.8	0.052	0.011	0.159	9.46E-06	0.018	LMFA07010874	ethyl butanoate
v283	116.0837	47.8	0.052	0.011	0.159	9.46E-06	0.018	LMFA07010934	methyl 2-methylbutanoate
v283	116.0837	47.8	0.052	0.011	0.159	9.46E-06	0.018	LMFA07010950	methyl 3-methylbutanoate
v283	116.0837	47.8	0.052	0.011	0.159	9.46E-06	0.018	LMFA07010966	methyl pentanoate
v283	116.0837	47.8	0.052	0.011	0.159	9.46E-06	0.018	LMFA12000029	4-Hydroxyhexan-3-one
v3744	116.0837	62.9	0.052	0.011	0.159	9.46E-06	0.018	LMFA12000071	4-Hydroxy-4-methylpentan-2-one
v1943	116.0837	35.1	0.052	0.011	0.159	9.46E-06	0.018	LMFA12000071	4-Hydroxy-4-methylpentan-2-one
v3536	116.0837	130.1	0.052	0.011	0.159	9.46E-06	0.018	LMFA12000076	2S-Hydroxyhexan-3-one
v3744	116.0837	62.9	0.052	0.011	0.159	9.46E-06	0.018	LMFA12000076	2S-Hydroxyhexan-3-one
v3536	116.0837	130.1	0.052	0.011	0.159	9.46E-06	0.018	LMFA12000077	3R-Hydroxyhexan-2-one
v3536	116.0837	130.1	0.052	0.011	0.159	9.46E-06	0.018	LMFA12000078	3S-Hydroxyhexan-2-one
v3536	116.0837	130.1	0.052	0.011	0.159	9.46E-06	0.018	LMFA12000082	2-Hydroxyhexan-3-one
v283	274.2144	47.8	0.107	0.03	0.276	6.06E-05	0.019	LMGL01010008	1-dodecanoyl-sn-glycerol
v1277	448.1733	44.2	0.165	0.051	0.388	3.60E-04	0.046	LMPK12020272	-
v1277	448.1733	44.2	0.165	0.051	0.388	3.60E-04	0.046	LMPK12120352	23452346-Octamethoxychalcone
v283	230.0579	47.8	0	0	0.002	1.10E-04	0.024	LMPK13110003	-
v3536	272.1776	130.1	0.287	0.145	0.514	8.54E-05	0.023	LMST02010001	estra-135(10)-triene-317beta-diol
v3536	272.1776	130.1	0.287	0.145	0.514	8.54E-05	0.023	LMST02010012	estra-579-triene-3beta17beta-diol
v3536	272.1776	130.1	0.287	0.145	0.514	8.54E-05	0.023	LMST02010013	8alpha-estra-135(10)-trien-317beta-diol
v3536	272.1776	130.1	0.287	0.145	0.514	8.54E-05	0.023	LMST02010017	estra-579-triene-3alpha17alpha-diol
v3536	272.1776	130.1	0.287	0.145	0.514	8.54E-05	0.023	LMST02010029	estra-135(10)-triene-317alpha-diol