

Supplementary Methods

Gut microbiome profiling

DNA was extracted using the DNeasy PowerSoil DNA isolation kit (QIAGEN, Hilden, Germany). The V4 hypervariable region of the 16S rRNA gene was amplified on an Illumina MiSeq platform (2 x 300 paired-end mode) by the University of Minnesota Genomics Center¹. Sequences were processed in QIIME 2². Quality filtering, adaptor trimming, and stitching of raw sequences were done using the quality control pipeline SHI7 (trim threshold 32, threshold of Q37)³. Paired ends were merged using FLASH⁴. Operational taxonomic unit (OTU) picking was done using NINJA-OPS (default parameters and 97% similarity threshold) and the Greengenes database; Bowtie2 was used for alignment⁵⁻⁷. OTUs with a frequency <0.01% of the reads were removed, as were those present in fewer than 10 samples. Sequence data were deposited in the Sequence Read Archive of the National Center for Biotechnology's Information (NCBI) under BioProject ID SRP141394. The BIOM table was exported from QIIME into R 3.4 (R Foundation for Statistical Computing, Vienna, Austria), where all downstream analyses were performed.

Serum metabolome profiling

Sample preparation. Serum samples were prepared using the automated MicroLab STAR® system from Hamilton Company. For the metabolomic analysis, a total of 100 µL of sample was extracted under vigorous shaking for 2 min (Glen Mills GenoGrinder 2000) with methanol 80%, containing the following recovery standards: DL-2-fluorophenylglycine, tridecanoic acid, d6-cholesterol, and DL-4-chlorophenylalanine. The resulting extract was divided into 5 fractions: two for analysis by two separate reverse phase (RP)/UPLC-MS/MS methods with positive ion mode electrospray ionization (ESI), one for analysis by RP/UPLC-MS/MS with negative ion mode ESI, and one for analysis by HILIC/UPLC-MS/MS with negative ion mode ESI. The remaining aliquot was reserved for backup. Samples were placed briefly on a TurboVap® (Zymark) to remove the organic solvent. The sample extracts were stored overnight under nitrogen before preparation for analysis.

Mass spectrometry. All methods utilized a Waters ACQUITY UPLC and a Thermo Scientific Q-Exactive high-resolution/accurate mass spectrometer interfaced with a heated electrospray ionization (HESI-II) source and Orbitrap mass analyzer operated at $R = 35,000$ mass resolution. The sample extract was dried then reconstituted in solvents compatible to each of the four methods. For each sample, two aliquots of each sample were reconstituted in 50 µL of 6.5 mM ammonium bicarbonate in water (pH 8) for the negative ion analysis and another two aliquots of each were reconstituted using 50 µL 0.1% formic acid in water (pH ~3.5) for the positive ion method. Each reconstitution solvent contained a series of standards at fixed concentrations to ensure injection and chromatographic consistency. The internal standards consist of a variety of deuterium labeled or halogenated biochemicals specifically designed both to cover the entire chromatographic run and to not interfere with the detection of any endogenous biochemicals. Authentic standards of d7-glucose, d3-leucine, d8-phenylalanine, and d5-tryptophan were purchased from Cambridge Isotope Laboratories (Andover, MA). d5-hippuric acid, d5-indole acetic acid, and d9-progesterone were procured from C/D/N

Isotopes, Inc. (Pointe-Claire, Quebec). Bromophenylalanine was provided by Sigma-Aldrich Co. LLC. (St. Louis, MO) and amitriptyline was from MP Biomedicals, LLC. (Aurora, OH). Recovery standards of DL-2-fluorophenylglycine and DL-4-chlorophenylalanine were from Aldrich Chemical Co. (Milwaukee, WI). Tridecanoic acid was purchased from Sigma-Aldrich (St. Louis, MO) and d6-cholesterol was from Cambridge Isotope Laboratories (Andover, MA). Standards for the HILIC dilution series of alpha-ketoglutarate, ATP, malic acid, NADH, and oxaloacetic acid were purchased from Sigma-Aldrich Co. LLC. (St. Louis, MO) while succinic acid, pyruvic acid and NAD⁺ were purchased from MP Biomedicals, LLC. (Santa Ana, CA). Limit of detection (LOD) for standards analyzed in a dilution series using reverse phase chromatography is available in **Table 1**.

Table 1: Limit of detection (LOD) for standards in a dilution series using reverse-phase chromatography

Standard	HRAM LOD ng/mL	UMR LOD ng/mL
d7-glucose	1.0	50.0
d3-leucine	0.25	5.0
d8-phenylalanine	0.25	3.0
d5-tryptophan	0.25	25.0
d5-hippuric acid	0.25	5.0
Br-phenylalanine	0.25	3.0
d5-indole acetic acid	3.0	25.0
amitriptyline	0.5	3.0
d9-progesterone	1.0	25.0

One aliquot was analyzed using acidic positive ion conditions (LC pos), chromatographically optimized for more hydrophilic compounds. In this method, the extract was gradient eluted from a C18 column (Waters UPLC BEH C18-2.1 × 100 mm, 1.7 µm) using water and methanol, containing 0.05% perfluoropentanoic acid (PFPA) and 0.1% formic acid (FA) at pH = 2.5. Elution was performed at 0.35 mL min⁻¹ in a linear gradient from 5% to 80% of methanol containing 0.1% FA and 0.05% PFPA over 3.35 min. A second aliquot was also analyzed using acidic positive ion conditions; however, it was chromatographically optimized for more hydrophobic compounds. In this method, the extract was gradient eluted from the same aforementioned C18 column using methanol 50%, acetonitrile 50%, water, 0.05 % PFPA, and 0.01 % FA at pH = 2.5 and was operated at an overall higher organic content. Elution was performed at 0.60 mL/min in a linear gradient from 40% to 99.5% over 1 min, hold 2.4 min at 99.5% of methanol 50%, acetonitrile 50%, 0.05% PFPA, and 0.01% FA. A third aliquot was analyzed using basic negative ion-optimized conditions with a separate dedicated C18 column (LC neg). The basic extracts were gradient eluted from the column using methanol 95% and water 5%, with 6.5 mM ammonium bicarbonate at pH 8. Elution was performed at 0.35 mL min⁻¹ with a linear gradient from 0.5% to 70% of methanol 95%, water 5% with 6.5 mM

ammonium bicarbonate over 4 min, followed by a rapid gradient to 99% in 0.5 min. The sample injection volume was 5 μ L and a 2 \times needle loop overfill was used. Separations utilized separate acid and base-dedicated 2.1 mm \times 100 mm Waters BEH C18 1.7 μ m columns held at 40 °C. The fourth aliquot was analyzed via negative ionization following elution from an HILIC column (LC HILIC) (Waters UPLC BEH Amide 2.1 \times 150 mm, 1.7 μ m, held at 40 °C) using a gradient consisting of water (15%), methanol (5%), and acetonitrile (80%) with 10 mM ammonium formate, pH 10.16. Elution flow rate was 0.5 mL/min with a linear gradient from 5% to 50% in 3.5 min, followed by a linear gradient from 50% to 95% in 2 min, of water (50%), acetonitrile (50%) with 10 mM ammonium formate, pH 10.6. The MS analysis alternated between MS and data-dependent MS_n scans using dynamic exclusion. The scan range varied slightly between methods but covered 70–1000 *m/z*.

Quality assurance and quality control (QA/QC). Several types of controls were analyzed in concert with the experimental samples: a pooled matrix sample generated by taking a small volume of each experimental sample served as a technical replicate throughout the platform run; extracted water samples served as process blanks; and a cocktail of QC standards (carefully chosen not to interfere with the measurement of endogenous compounds) spiked into every analyzed sample allowed instrument performance monitoring and aided chromatographic alignment. **Tables 2–4** describe QC samples and standards. Instrument variability was determined by calculating the median relative standard deviation (RSD) for the internal standards that were added to each sample prior to injection into the mass spectrometers (median RSD = 3–4%). Instruments are calibrated at least weekly in the utilized polarity using thermo and mass accuracy is monitored at the batch level for the internal standards. A batch fails QC if any of the internal standards are more than 5 ppm away from the theoretical mass. Overall process variability was determined by calculating the median RSD for all endogenous metabolites (i.e., non-instrument standards) present in 100% of the pooled matrix (MTRX) samples, which are technical replicates created from a large pool of extensively characterized human plasma. The median RSD for MTRX samples was 9–10%. Five MTRX samples and three process blank samples were processed per every batch of 30 samples. Experimental samples were randomized across the platform run with QC samples spaced evenly among the injections, as outlined in **Figure 1** below.

Table 2: Description of metabolon QC samples

Type	Description	Purpose
CMTRX	Pool created by taking a small aliquot from every customer samples.	Assess the effect of a non-plasma matrix on the Metabolon process and distinguish biological variability from process variability.
PRCS	Aliquot of ultra-pure water	Process Blank used to assess the contribution to compound signals from the process.
SOLV	Aliquot of solvents used in extraction.	Solvent Blank used to segregate contamination sources in the extraction.

Table 3: Metabolon QC standards

Type	Description	Purpose
RS	Recovery Standard	Assess variability and verify performance of extraction and instrumentation.
IS	Internal Standard	Assess variability and performance of instrument.

Table 4: Quality control internal standards

Condition	Internal standards
LC neg	d7-glucose d3-methionine d3-leucine d8-phenylalanine d5-tryptophan Br-phenylalanine d15-octanoic acid d19-decanoic acid d27-tetradecanoic acid d35-octadecanoic acid d2-eicosanoic acid
LC HILIC	d35-octadecanoic acid d5-indole acetic acid Br-phenylalanine d5-tryptophan

	d4-tyrosine d3-serine d3-aspartic acid d7-ornithine d4-lysine
LC pos	d7-glucose d3-methionine d3-leucine d8-phenylalanine d5-tryptophan Br-phenylalanine d4-tyrosine d5-indole acetic acid d5-hippuric acid amitriptyline d9-progesterone d4-diethylphthalate

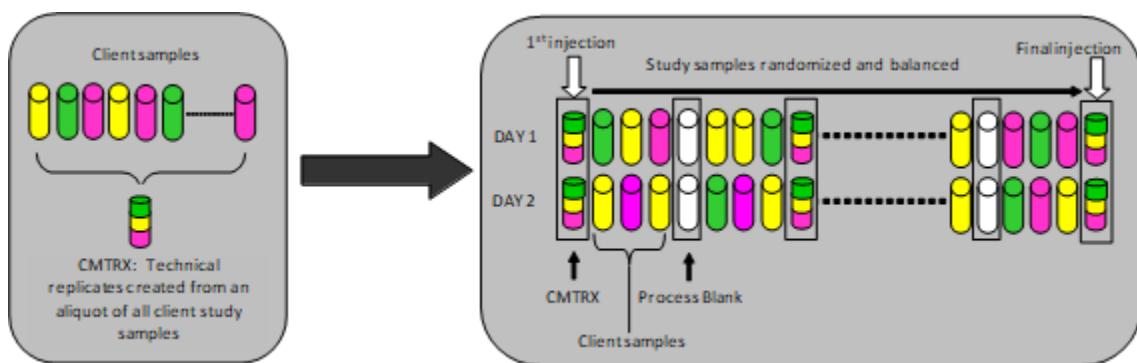


Figure 1. Preparation of client-specific technical replicates. A small aliquot of each client sample (colored cylinders) is pooled to create a CMTRX technical replicate sample (multi-colored cylinder), which is then injected periodically throughout the platform run. Variability among consistently detected biochemicals can be used to calculate an estimate of overall process and platform variability.

All studies include the analysis of a technical replicate of a sample pooled from the experimental samples. This pool was analyzed 16 times over the course of the analysis of the experimental samples in the present study.

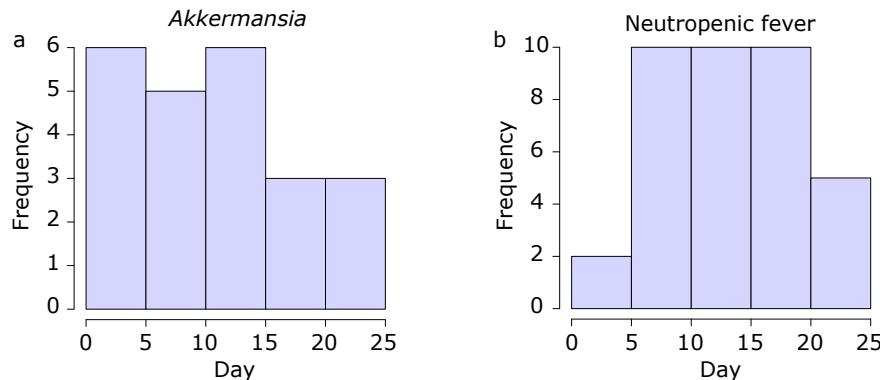
Compound identification and quantification. Raw data were extracted, peak-identified, and QC processed using Metabolon pipelines. Compounds were identified by comparison to library entries of purified standards or recurrent unknown entities^{8,9}. Briefly, Metabolon maintains a library based on authenticated standards (analyzed using the same methodology as the experimental samples) that contains the retention time/index (RI), mass to charge ratio (m/z), and chromatographic data (including MS/MS spectral data) on all molecules present in the library. Furthermore, biochemical identifications are based on three criteria: retention index within a narrow RI window of the proposed

identification (typically within a 5 second window), accurate mass match to the library ± 10 ppm (typically well within a 5 ppm window), and the MS/MS forward and reverse scores between the experimental data and authentic standards. The MS/MS scores are based on a comparison of the ions present in the experimental spectrum to the ions present in the library spectrum. While there may be similarities between these molecules based on one of these factors, the use of all three data points can be utilized to distinguish and differentiate biochemicals. More than 3300 commercially available purified standard compounds have been acquired and registered for analysis on all platforms for determination of their analytical characteristics. Compounds in **supplementary data 1** for which no authentic standards were available for confirmation are marked with an “*” after the compound name to designate these as Metabolomics Standards Initiative level 2/3¹⁰. Most such identifications are based on the experimental signature having the same characteristics as the compound class. For example, sphingomyelins all have a conserved fragmentation spectrum and so have a highly diagnostic pattern in order to permit the identification of the experimental signature as a sphingomyelin. The QC and curation processes were designed to ensure accurate and consistent identification of true chemical entities, and to remove those representing system artifacts, mis-assignments, and background noise. Metabolon data analysts use proprietary visualization and interpretation software to confirm the consistency of peak identification among the various samples. Library matches for each compound were checked for each sample and corrected if necessary. Peaks were quantified using area-under-the-curve. A data normalization step was performed to correct variation resulting from instrument inter-day tuning differences. Essentially, each compound was corrected in run-day blocks by registering the medians to equal 1 and normalizing each data point proportionately. Metabolites were assigned to pathways based on three publicly available key chemical information resources: PubChem, HMDB and KEGG pathway database.

References

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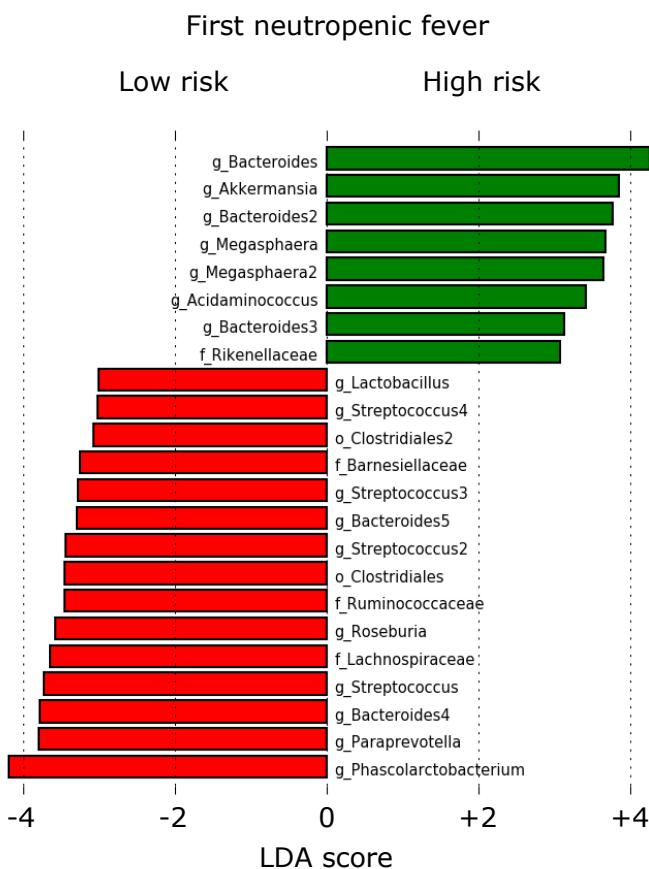
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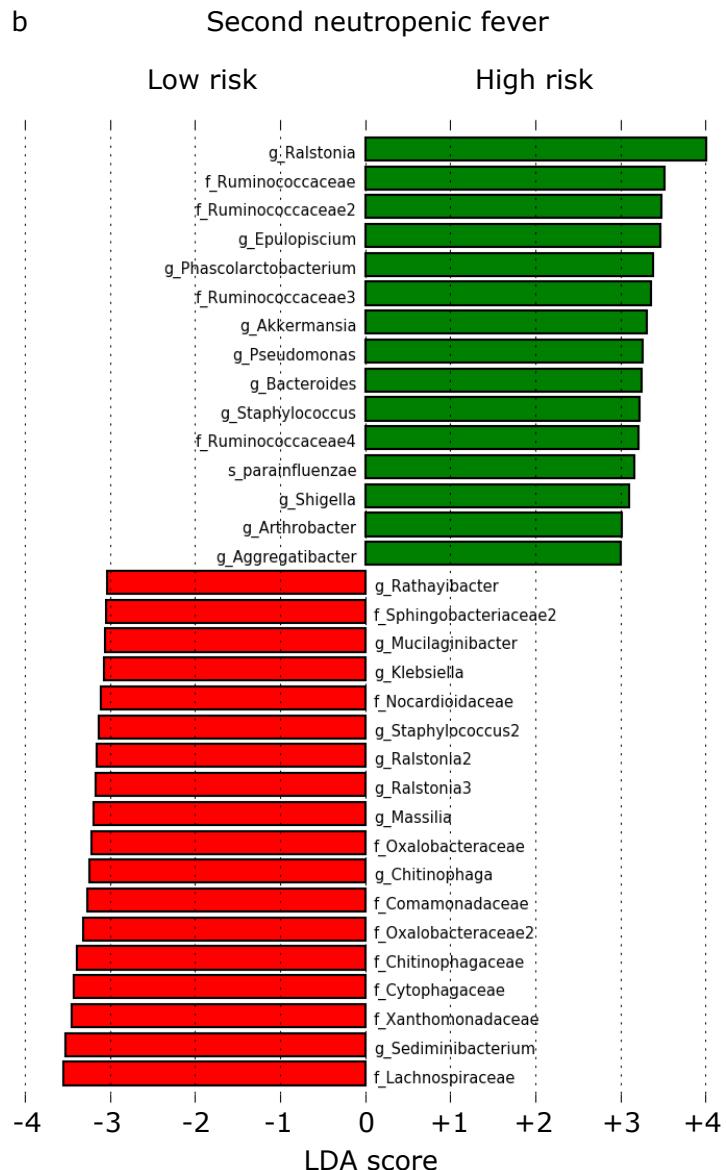
Supplementary Figure S1: Dynamics of *Akkermansia* abundance relative to neutropenic fever

(a) Change point analysis showing changes in *Akkermansia* relative abundance at different time points. The y-axis shows the number of patients who experienced the largest change in gut *Akkermansia* relative abundance on the corresponding day along the x-axis. Analysis was done using the *changepoint* package in R (cpt.mean function, “at most one change” [AMOC] method, and default parameters). **(b)** Histogram of NF frequency relative to time. Time is measured from the first day of chemotherapy.

a

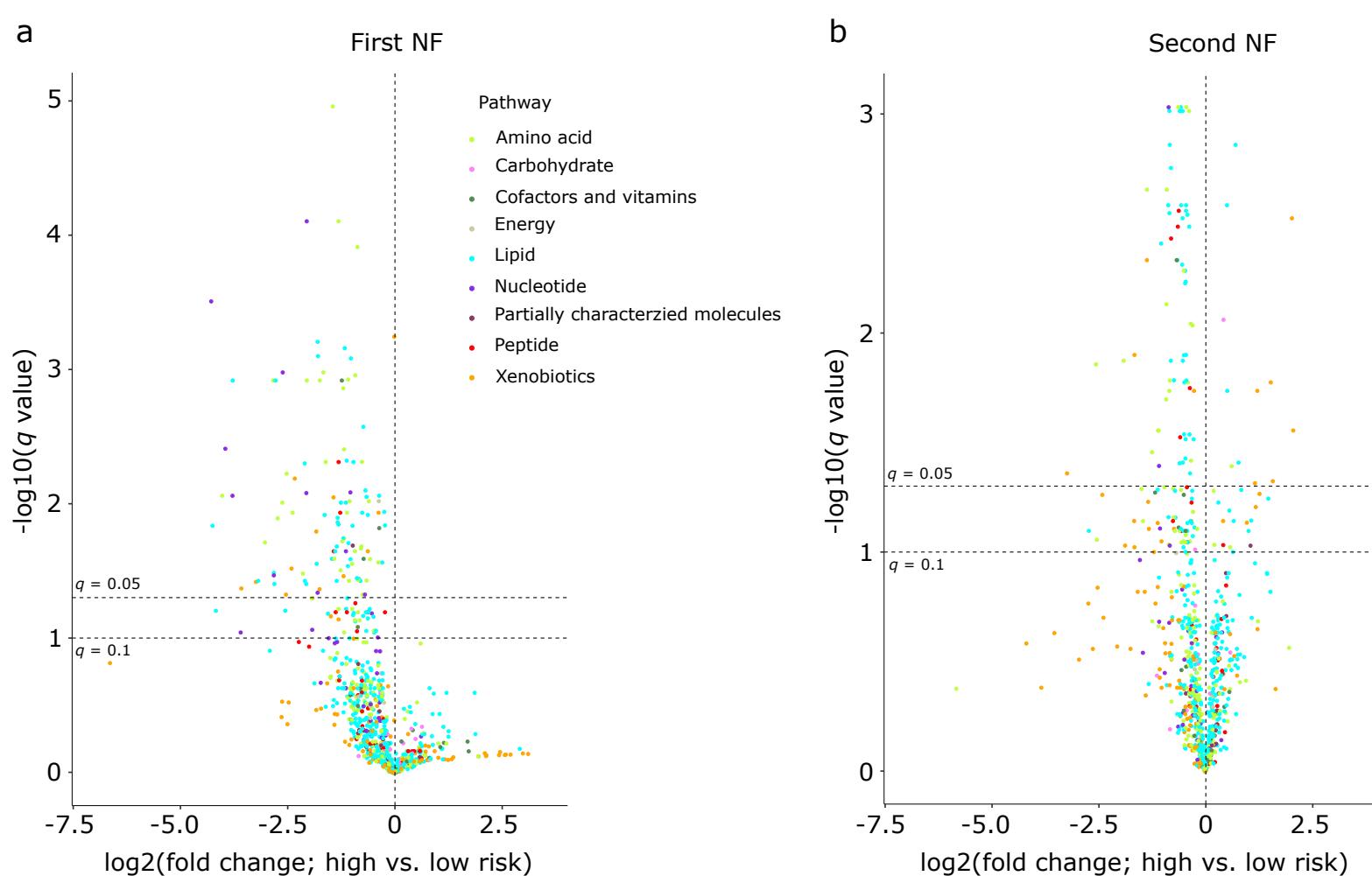


b



Supplementary Figure S2: Differentially abundant taxa in high- vs. low-risk stool samples based on first vs. second episode of neutropenic fever

Linear discriminant analysis (LDA) coupled with effect size measurements (LEfSe) in each subgroup is shown separately. The plot in panel (a) was generated using all samples collected before the first neutropenic fever and the plot in panel (b) was generated using all samples collected between the first and second neutropenic fever episodes. High- and low-risk samples were defined similar to Figure 2b. Differentially abundant OTUs (LDA score >3.0, p<0.05) in high-risk samples are shown as green bars to the right; those more abundant in low-risk samples are shown as red bars to the left. "o", "f" and "g" indicate order, family and genus, respectively.



Supplementary Figure S3. Serum metabolomics associated with first vs. second NF (post-hoc exploratory analysis) Volcano plots showing the magnitude and significance of metabolomic changes within 24 hours before first (**a**) and second (**b**) NF. High-risk (preceding NF within 24 hours) and low-risk samples (not preceding NF within 24 hours) were compared. Points to the right (left) of the vertical line (no change) in each panel represent metabolites that were increased (decreased) before NF. The horizontal lines represent $q=0.05$ and $q=0.1$, above which the metabolites are statistically significant according to the corresponding threshold. *p* values from Welch's t-test were corrected for multiple testing to derive the *q* values. The complete list of metabolites is provided in supplementary data 2-3.

Supplementary data 1: UPLC-MS/MS metabolites in serum

Compounds in column B for which no authentic standards were available for confirmation are marked with * after the compound name to designate these as Metabolomics Standards Initiative level 2/3

Metabolites were assigned to pathways based on three publicly available key chemical information resources: PubChem, HMDB and KEGG. PCM: Partially Characterized Molecules

Fold change and log₂_fold change compared samples preceding vs. not preceding NF within 24 hours

Cells in column B colored in gold indicate metabolites detectable in <50% of samples

Color coding in column G was applied along the fold change gradient, with blue and red representing decreased and increased levels in samples preceding vs. not preceding NF within 24 hours

Color coding in column J was applied along the q value gradient, with darker colors indicating more significant values

p values are from Welch's two-sample t-test, q values are derived after FDR correction for multiple testing

code	metabolite	pathway	sub_pathway	retention index	mass	fold change	log2		p	q
							foldchange	log2foldchange		
M40	asparagine	Amino Acid	Alanine and Aspartate Metabolism	1225	133	0.69	-0.53	0.0000	0.0000	0.0000
M17	threonine	Amino Acid	Glycine, Serine and Threonine Metabolism	1314	120	0.58	-0.79	0.0000	0.0000	0.0000
M4219	uridine	Nucleotide	Pyrimidine Metabolism, Uracil containing	1457.6	243	0.50	-1.00	0.0000	0.0000	0.0000
M527	guanidinoacetate	Amino Acid	Creatine Metabolism	2884	116	0.31	-1.70	0.0000	0.0000	0.0000
M2601	2-palmitoyl-GPC* (16:0)*	Lipid	Lysophospholipid	6215	570	0.61	-0.72	0.0000	0.0000	0.0000
M2834	1-(1-enyl-palmitoyl)-GPE (P-16:0)*	Lipid	Lysoplasmalogen	1558	438	0.63	-0.67	0.0000	0.0000	0.0000
M105	lysine	Amino Acid	Lysine Metabolism	2850	147	0.70	-0.52	0.0000	0.0000	0.0000
M2833	1-(1-enyl-palmitoyl)-GPE (P-16:0)*	Lipid	Lysoplasmalogen	1547	480	0.51	-0.98	0.0000	0.0000	0.0000
M2838	1-(1-enyl-stearoyl)-GPE (P-18:0)*	Lipid	Lysoplasmalogen	1649	466	0.61	-0.71	0.0000	0.0000	0.0000
M2240	glycerophosphoethanolamine	Lipid	Phospholipid Metabolism	659	216	0.72	-0.47	0.0000	0.0000	0.0000
M649	gamma-glutamylcitrulline*	Peptide	Gamma-glutamyl Amino Acid	1644	305	0.50	-1.00	0.0000	0.0000	0.0000
M121	fructosyllysine	Amino Acid	Lysine Metabolism	2784	309	0.51	-0.97	0.0000	0.0000	0.0000
M2673	1-linoleoyl-GPE (18:2)*	Lipid	Lysophospholipid	1482	478	0.53	-0.90	0.0000	0.0000	0.0000
M640	gamma-glutamyl-alpha-lysine	Peptide	Gamma-glutamyl Amino Acid	2784	276	0.59	-0.76	0.0000	0.0000	0.0000
M644	gamma-glutamylthreonine	Peptide	Gamma-glutamyl Amino Acid	1750	249	0.58	-0.79	0.0000	0.0000	0.0000
M2602	1-palmitoleoyl-GPC* (16:1)*	Lipid	Lysophospholipid	1450	494	0.56	-0.83	0.0000	0.0000	0.0000
M48	N-acetylglutamine	Amino Acid	Glutamate Metabolism	771	187	0.46	-1.12	0.0000	0.0000	0.0000
M2600	1-palmitoyl-GPC (16:0)	Lipid	Lysophospholipid	1525	496	0.71	-0.50	0.0000	0.0000	0.0000
M2603	2-palmitoleoyl-GPC* (16:1)*	Lipid	Lysophospholipid	5720	568	0.54	-0.90	0.0000	0.0000	0.0000
M492	citrulline	Amino Acid	Urea cycle; Arginine and Proline Metabolism	1520	176	0.65	-0.63	0.0000	0.0000	0.0000
M45	glutamine	Amino Acid	Glutamate Metabolism	1291	147	0.75	-0.41	0.0000	0.0000	0.0000
M2836	1-(1-enyl-oleoyl)-GPE (P-18:1)*	Lipid	Lysoplasmalogen	6250	462	0.64	-0.65	0.0000	0.0000	0.0000
M3315	cortisone	Lipid	Corticosteroids	4575	359	1.54	0.63	0.0000	0.0000	0.0000
M2613	1-oleoyl-GPC (18:1)	Lipid	Lysophospholipid	1540	522	0.71	-0.49	0.0000	0.0000	0.0000
M29	alanine	Amino Acid	Alanine and Aspartate Metabolism	1700	90	0.74	-0.43	0.0000	0.0000	0.0000
M2616	1-linoleoyl-GPC (18:2)	Lipid	Lysophospholipid	1465	520	0.65	-0.63	0.0000	0.0000	0.0000
M70	histidine	Amino Acid	Histidine Metabolism	755.9	154	0.70	-0.52	0.0000	0.0000	0.0000
M2236	glycerophosphorylcholine (GPC)	Lipid	Phospholipid Metabolism	672	258	0.73	-0.46	0.0000	0.0000	0.0000
M635	gamma-glutamylglutamine	Peptide	Gamma-glutamyl Amino Acid	1430	276	0.71	-0.49	0.0000	0.0000	0.0000
M2708	1-palmitoyl-GPC (16:0)*	Lipid	Lysophospholipid	5570	483	0.71	-0.49	0.0000	0.0000	0.0000
M2365	1-linoleoyl-2-arachidonoyl-GPC (18:2/20:4n6)*	Lipid	Phosphatidylcholine (PC)	2000	807	0.67	-0.57	0.0000	0.0000	0.0000
M2686	1-arachidonoyl-GPE (20:4n5)*	Lipid	Lysophospholipid	1470	502	0.70	-0.51	0.0000	0.0001	0.0001
M493	homoaarginine	Amino Acid	Urea cycle; Arginine and Proline Metabolism	2882	189	0.47	-1.10	0.0000	0.0001	0.0001
M4429	retinol (Vitamin A)	Cofactors and Vitamins	Vitamin A Metabolism	1636	269	0.60	-0.74	0.0000	0.0001	0.0001
M2801	1-(1-enyl-palmitoyl)-2-linoleoyl-GPE (P-16:0/18:2)*	Lipid	Plasmalogen	2400	701	0.62	-0.69	0.0000	0.0001	0.0001
M1894	arachidonoylcarnitine (C20:4)	Lipid	Fatty Acid Metabolism (Acyl Carnitine, Polyunsaturated)	1353	448	0.61	-0.71	0.0000	0.0001	0.0001
M2649	1-lignoceroyl-GPC (24:0)	Lipid	Lysophospholipid	1907	608	0.47	-1.08	0.0000	0.0001	0.0001
M2804	1-(1-enyl-palmitoyl)-2-arachidonoyl-GPE (P-16:0/20:4)*	Lipid	Plasmalogen	2300	725	0.69	-0.53	0.0000	0.0001	0.0001
M4220	uracil	Nucleotide	Pyrimidine Metabolism, Uracil containing	827	113	0.42	-1.25	0.0000	0.0001	0.0001
M2635	1-arachidonoyl-GPC* (20:4)*	Lipid	Lysophospholipid	1460	544	0.70	-0.51	0.0000	0.0001	0.0001
M2616	1-linolenoyl-GPC (18:3)*	Lipid	Lysophospholipid	1410	518	0.56	-0.85	0.0000	0.0001	0.0001
M1890	ximenoylcarnitine (C26:1)*	Lipid	Fatty Acid Metabolism (Acyl Carnitine, Monounsaturated)	1607	538	0.44	-1.17	0.0000	0.0001	0.0001
M2611	1-stearoyl-GPC (18:0)	Lipid	Lysophospholipid	1606	524	0.71	-0.49	0.0000	0.0001	0.0001
M2359	1,2-dilinoleoyl-GPC (18:2/18:2)	Lipid	Phosphatidylcholine (PC)	2100	783	0.67	-0.57	0.0000	0.0001	0.0001
M4231	5,6-dihydroxuracil	Nucleotide	Pyrimidine Metabolism, Uracil containing	1120	113	0.36	-1.46	0.0000	0.0001	0.0001
M4356	oxalate (ethanedioate)	Cofactors and Vitamins	Ascorbate and Aldrate Metabolism	603	89	0.63	-0.66	0.0000	0.0002	0.0002
M5117	pyrrole	Xenobiotics	Food Component/Plant	2304	253	0.38	-1.41	0.0000	0.0002	0.0002
M3078	glycosyl ceramide (d18:1/20:0, d16:1/22:0)*	Lipid	Hexosylceramides (HCKER)	3414	757	0.67	-0.59	0.0000	0.0002	0.0002
M438	S-methylmethionine	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	2555	164	0.19	-2.43	0.0000	0.0002	0.0002
M2671	1-oleoyl-GPE (18:1)	Lipid	Lysophospholipid	1554	480	0.69	-0.53	0.0000	0.0003	0.0003
M429	2,3-dihydroxy-2-methylbutyrate	Amino Acid	Leucine, Isoleucine and Valine Metabolism	1318	133	0.24	-2.06	0.0000	0.0003	0.0003
M2182	linoleoyl ethanolamide	Lipid	Endocannabinoid	6150	322	1.63	0.70	0.0000	0.0003	0.0003
M504	N-acetylcitrulline	Amino Acid	Urea cycle; Arginine and Proline Metabolism	1010	218	0.26	-1.92	0.0000	0.0003	0.0003
M495	proline	Amino Acid	Urea cycle; Arginine and Proline Metabolism	1603	116	0.74	-0.43	0.0000	0.0003	0.0003
M2197	N-stearoylserine*	Lipid	Endocannabinoid	5777	370	0.70	-0.51	0.0000	0.0004	0.0004
M632	gamma-glutamylalanine	Peptide	Gamma-glutamyl Amino Acid	1986	219	0.62	-0.70	0.0000	0.0004	0.0004
M1352	mannose	Carbohydrate	Fructose, Mannose and Galactose Metabolism	2200	225	1.42	0.50	0.0000	0.0004	0.0004
M391	1-carboxyethylsleucine	Amino Acid	Leucine, Isoleucine and Valine Metabolism	2628	202	0.55	-0.87	0.0000	0.0006	0.0006
M2810	1-(1-enyl-stearoyl)-2-linoleoyl-GPE (P-18:0/18:2)*	Lipid	Plasmalogen	2750	729	0.69	-0.54	0.0000	0.0007	0.0007
M2811	1-(1-enyl-stearoyl)-2-arachidonoyl-GPE (P-18:0/20:4)*	Lipid	Plasmalogen	2550	753	0.69	-0.53	0.0000	0.0007	0.0007
M4120	hypoxanthine	Nucleotide	Purine Metabolism, (Hypo)Xanthine/Inosine containing	1291.2	135	0.55	-0.86	0.0001	0.0008	0.0008
M4499	N-acetylarginine	Amino Acid	Urea cycle; Arginine and Proline Metabolism	2245	217	0.59	-0.76	0.0001	0.0008	0.0008
M4353	threonate	Cofactors and Vitamins	Ascorbate and Aldrate Metabolism	2384	135	0.67	-0.58	0.0001	0.0008	0.0008
M5585	dexamethasone	Xenobiotics	Drug - Antiinflammatory, Immunosuppressant	4974	391	0.10	-3.36	0.0001	0.0008	0.0008
M5382	3-(cystein-S-yl)acetaminophen*	Xenobiotics	Drug - Analgesics, Anesthetics	2420	271	4.55	2.19	0.0001	0.0008	0.0008
M641	gamma-glutamyl-epsilon-lysine	Peptide	Gamma-glutamyl Amino Acid	2725	276	0.59	-0.75	0.0001	0.0009	0.0009
M1	glycine	Amino Acid	Glycine, Serine and Threonine Metabolism	1375	76	0.74	-0.43	0.0001	0.0011	0.0011
M4602	7-methylanthine	Xenobiotics	Xanthine Metabolism	1350	167	0.40	-1.31	0.0001	0.0012	0.0012
M5206	tartronate (hydroxy malonate)	Xenobiotics	Food Component/Plant	610	119	0.59	-0.76	0.0001	0.0013	0.0013
M3261	pregnenetriol sulfate*	Lipid	Pregnenolone Steroids	4749	413	1.87	0.91	0.0001	0.0013	0.0013
M4121	xanthine	Nucleotide	Purine Metabolism, (Hypo)Xanthine/Inosine containing	2023	151	0.27	-1.89	0.0001	0.0014	0.0014
M2034	2R,3R-dihydroxybutyrate	Lipid	Fatty Acid, Dihydroxy	1543	119	0.70	-0.51	0.0001	0.0014	0.0014
M2194	N-palmitoylserine	Lipid	Endocannabinoid	5557	342	0.60	-0.74	0.0001	0.0014	0.0014
M4603	5-acetylaminono-6-amino-3-methyluracil	Xenobiotics	Xanthine Metabolism	1710	197	0.37	-1.45	0.0001	0.0016	0.0016
M470	hypotaurine	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	724	110	0.59	-0.76	0.0001	0.0016	0.0016
M3058	glycosyl-N-stearoyl-sphingosine (d18:1/18:0)	Lipid	Hexosylceramides (HCKER)	3053	729	0.70	-0.52	0.0001	0.0017	0.0017
M637	gamma-glutamylhistidine	Peptide	Gamma-glutamyl Amino Acid	2740	285	0.69	-0.53	0.0002	0.0018	0.0018
M2233	dopamine 4-sulfate	Amino Acid	Tyrosine Metabolism	1511	232	0.40	-1.31	0.0002	0.0019	0.0019
M636	gamma-glutamylglycine	Peptide	Gamma-glutamyl Amino Acid	1535	205	0.67	-0.58	0.0002	0.0019	0.0019
M1659	glutarate (C5-DC)	Lipid	Fatty Acid, Dicarboxylate	2900	131	0.45	-1.14	0.0002	0.0019	0.0019
M5044	S-allylcysteine	Xenobiotics	Food Component/Plant	2690	162	0.27	-1.87	0.0002	0.0019	0.0019
M279	8-methoxykynurenamate	Amino Acid	Tryptophan Metabolism	2574	220	0.42	-1.27	0.0002	0.0021	0.0021
M4252	cytosine	Nucleotide	Pyrimidine Metabolism, Cytidine containing	2060	112	0.30	-1.74	0.0002	0.0025	0.0025
M6080	sulfate*	Xenobiotics	Chemical	616	97	0.82	-0.28	0.0002	0.0025	0.0025
M1240	lactate	Carbohydrate	Glycolysis, Gluconeogenesis, and Pyruvate Metabolism	1469	89	0.81	-0.30	0.0002	0.0025	0.0025
M3161	sphingosine 1-phosphate	Lipid	Sphingosines	1375	380	0.80	-0.32	0.0003	0.0027	0.0027
M646	gamma-glutamyltyrosine	Peptide	Gamma-glutamyl Amino Acid	2518	311	0.72	-0.48	0.0003	0.0030	0.0030
M4600	1-methylxanthine	Xenobiotics	Xanthine Metabolism	1568.8	165	0.35	-1.51	0.0003	0.0030	0.0030
M4601	3-methylxanthine	Xenobiotics	Xanthine Metabolism	1700	165	0.41	-1.28	0.0003	0.0	

M162	tyrosine	Amino Acid	Tyrosine Metabolism	2430	182	0.81	-0.31	0.0007	0.0060
M454	alpha-ketobutyrate	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	940	101	1.61	0.68	0.0007	0.0061
M278	xanthureneate	Amino Acid	Tryptophan Metabolism	2236	206	0.60	-0.74	0.0007	0.0061
M4131	urate	Nucleotide	Purine Metabolism, (Hypo)Xanthine/Inosine containing	757.1	167	0.69	-0.53	0.0008	0.0061
M457	S-methylcysteine	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	880	134	0.73	-0.46	0.0008	0.0062
M2713	1-oleoyl-GPC (18:1)*	Lipid	Lysophospholipid	5610	509	0.60	-0.74	0.0008	0.0066
M2159	oleoyl ethanolamide	Lipid	Endocannabinoid	6450	324	1.42	0.50	0.0009	0.0070
M505	N-acetylproline	Amino Acid	Urea cycle; Arginine and Proline Metabolism	1695	158	0.69	-0.53	0.0009	0.0074
M4817	N-acetylallin	Xenobiotics	Food Component/Plant	1348	220	0.31	-1.68	0.0009	0.0074
M4280	5,6-dihydrothymine	Nucleotide	Pyrimidine Metabolism, Thymine containing	1637.8	127	0.35	-1.53	0.0010	0.0076
M92	1-methyl-5-imidazoleacetate	Amino Acid	Histidine Metabolism	1989	141	0.52	-0.96	0.0010	0.0078
M2809	1-(1-enyl-stearoyl)-2-oleoyl-GPE (P-18:0/18:1)	Lipid	Plasmalogen	3100	731	0.80	-0.33	0.0010	0.0079
M6089	O-sulf-L-tyrosine	Xenobiotics	Chemical	990	260	0.75	-0.41	0.0010	0.0079
M5376	3-(N-acetyl-L-cystein-S-yl) acetaminophen	Xenobiotics	Drug - Analgesics, Anesthetics	2094	311	2.87	1.52	0.0011	0.0081
M261	C-glycosylyptophan	Amino Acid	Tryptophan Metabolism	1777	365	0.77	-0.38	0.0011	0.0081
M5386	3-(methylthio)acetaminophen sulfate*	Xenobiotics	Drug - Analgesics, Anesthetics	2265	276	2.51	1.33	0.0011	0.0084
M3243	pregnenolone sulfate	Lipid	Pregnenolone Steroids	5100	395	1.67	0.74	0.0012	0.0088
M117	hydroxy-N6,N6-trimethyllysine*	Amino Acid	Lysine Metabolism	2759	205	0.68	-0.56	0.0013	0.0093
M5214	3-indoleglyoxylic acid	Xenobiotics	Food Component/Plant	2140	188	0.71	-0.49	0.0013	0.0095
M458	S-methylcysteine sulfoxide	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	900	152	0.67	-0.58	0.0014	0.0099
M127	glutaryl carnitine (C5-DC)	Amino Acid	Lysine Metabolism	2393	276	0.69	-0.53	0.0014	0.0100
M947	prolylglycine	Peptide	Dipeptide	2136	173	0.60	-0.74	0.0016	0.0112
M5380	2-methoxyacetaminophen sulfate*	Xenobiotics	Drug - Analgesics, Anesthetics	1949	260	4.40	2.14	0.0016	0.0112
M3386	5alpha-androstan-3beta,17beta-diol disulfate	Lipid	Androgenic Steroids	3880	225	0.60	-0.75	0.0016	0.0112
M1950	stearylcholine*	Lipid	Fatty Acid Metabolism (Acyl Choline)	1520	370	0.58	-0.78	0.0017	0.0116
M2360	1-linoleoyl-2-linolenoyl-GPC (18:2/18:3)*	Lipid	Phosphatidylcholine (PC)	1939	781	0.67	-0.59	0.0017	0.0116
M3064	glycosy-L-habenohydro-sphingadienine (d18:2/22:0)*	Lipid	Hexosylceramides (HCCER)	3420	783	0.73	-0.46	0.0018	0.0120
M2814	1-(1-enyl-palmityl)-2-linoleoyl-GPC (P-16:0/18:2)*	Lipid	Plasmalogen	2300	743	0.83	-0.26	0.0018	0.0122
M46	alpha-ketoglutamate*	Amino Acid	Glutamate Metabolism	1916	144	0.80	-0.32	0.0018	0.0123
M228	vanilllic alcohol sulfate	Amino Acid	Tyrosine Metabolism	1808	233	0.22	-2.21	0.0019	0.0125
M3474	glycochenodeoxycholate 3-sulfate	Lipid	Primary Bile Acid Metabolism	4820	264	2.53	1.34	0.0019	0.0126
M353	isovalerylglycine	Amino Acid	Leucine, Isoleucine and Valine Metabolism	1950	158	0.55	-0.87	0.0020	0.0129
M72	3-methylhistidine	Amino Acid	Histidine Metabolism	2670	170	0.57	-0.80	0.0021	0.0132
M3109	lignoceroyl sphingomyelin (d18:1/24:0)	Lipid	Sphingomyelins	3437	816	0.85	-0.24	0.0020	0.0132
M35	N-carbamoylalanine	Amino Acid	Alanine and Aspartate Metabolism	950	133	0.52	-0.95	0.0021	0.0132
M2715	1-linoleoyl-GPC (18:2)*	Lipid	Lysophospholipid	5516	507	0.82	-0.29	0.0021	0.0133
M3361	androstenediol (3beta,17beta) monosulfate (2)	Lipid	Androgenic Steroids	4500	369	0.54	-0.90	0.0021	0.0134
M2842	glycerol-3-phosphate	Lipid	Glycerolipid Metabolism	580	173	0.71	-0.49	0.0021	0.0134
M3082	glycosy ceramide (d18:2/24:1, d18:1/24:2)*	Lipid	Hexosylceramides (HCCER)	3380	809	0.64	-0.64	0.0022	0.0134
M3389	5alpha-androstan-3beta,17alpha-diol disulfate	Lipid	Androgenic Steroids	4215	225	0.41	-1.30	0.0022	0.0134
M4594	1-methylurate	Xenobiotics	Xanthine Metabolism	1900	181	0.50	-0.99	0.0022	0.0137
M576	cysteinylglycine	Amino Acid	Glutathione Metabolism	2132	179	1.68	0.75	0.0022	0.0137
M1866	stearoylcarnitine (C18)	Lipid	Fatty Acid Metabolism (Acyl Carnitine, Long Chain Saturated)	1485	428	0.71	-0.50	0.0023	0.0141
M175	4-hydroxyphenylpyruvate	Amino Acid	Tyrosine Metabolism	1690	179	0.70	-0.51	0.0025	0.0148
M2905	palmityl-oleoyl-glycerol (16:0/18:1)[2]*	Lipid	Diacylglycerol	3695	613	0.74	-0.43	0.0025	0.0151
M3259	pregnenediol sulfate (C21H34O5S)*	Lipid	Pregnenolone Steroids	5000	397	1.73	0.79	0.0025	0.0151
M5374	4-acetamidophenol	Xenobiotics	Drug - Analgesics, Anesthetics	2173.7	150	3.23	1.69	0.0026	0.0154
M1165	DSGEGDFAEKGGR*	Peptide	Fibrinogen Cleavage Peptide	2535	731	1.41	0.50	0.0026	0.0154
M6435	GlcNAc sulfate conjugate of C21H34O2 steroid	PCM	PCM	4336.7	300	2.59	1.38	0.0026	0.0154
M4604	5-acetylaminino-6-formylamino-3-methyluracil	Xenobiotics	Xanthine Metabolism	1424	225	0.57	-0.82	0.0027	0.0159
M3519	taurosoideoxycholic acid sulfate (1)	Lipid	Secondary Bile Acid Metabolism	4325	289	3.19	1.67	0.0028	0.0161
M462	cystine	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	3424	239	0.86	-0.22	0.0029	0.0161
M2889	diaicylglycerol (16:1/18:2 [2], 16:0/18:3 [1])*	Lipid	Diaicylglycerol	2733	609	0.73	-0.45	0.0028	0.0161
M4206	dihydrotroacetate	Nucleotide	Pyrimidine Metabolism, Orotate containing	1910	157	0.40	-1.32	0.0028	0.0161
M4933	homostachydine*	Xenobiotics	Food Component/Plant	1750	158	0.57	-0.80	0.0029	0.0162
M461	cysteine-sulfate	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	640.9	200	0.88	-0.18	0.0030	0.0168
M2010	16-hydroxypalmitate	Lipid	Fatty Acid, Monohydroxy	5236.2	271	0.77	-0.37	0.0030	0.0169
M93	1-methyl-5-imidazoleacetate	Amino Acid	Histidine Metabolism	1011	169	0.57	-0.80	0.0033	0.0176
M2670	2-stearoyl-GPE (18:0)*	Lipid	Lysophospholipid	6350	480	0.75	-0.42	0.0032	0.0176
M5377	4-acetaminophen sulfate	Xenobiotics	Drug - Analgesics, Anesthetics	1792	230	2.58	1.37	0.0033	0.0176
M1805	hexanoylglycine (C6)	Lipid	Fatty Acid Metabolism (Acyl Glycine)	2900	172	2.25	1.17	0.0032	0.0176
M336	N-acetylleucine	Amino Acid	Leucine, Isoleucine and Valine Metabolism	2400	172	0.73	-0.46	0.0032	0.0176
M2556	1-stearyl-2-arachidonoyl-GPI (18:0/20:4)	Lipid	Phosphatidylinositol (PI)	3000	905	0.84	-0.26	0.0034	0.0177
M4772	2,3-dihydroxyisovalerate	Xenobiotics	Food Component/Plant	1050	133	0.43	-1.21	0.0033	0.0177
M4182	guanosine	Nucleotide	Purine Metabolism, Guanine containing	1728	284	0.48	-1.06	0.0034	0.0177
M471	taurine	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	660	126	0.80	-0.33	0.0033	0.0177
M491	2-oxoarginine*	Amino Acid	Urea cycle; Arginine and Proline Metabolism	1760	174	0.67	-0.58	0.0034	0.0178
M3262	pregnenetriol disulfate*	Lipid	Pregnenolone Steroids	3504	246	1.64	0.71	0.0035	0.0180
M131	picoplate	Amino Acid	Lysine Metabolism	2200	130	0.64	-0.65	0.0035	0.0183
M1166	ADpsEGDFXAEGGGVR*	Peptide	Fibrinogen Cleavage Peptide	2016	807	1.53	0.61	0.0036	0.0186
M3104	hydroxypalmitoyl sphingomyelin (d18:1/16:0(OH))	Lipid	Sphingomyelins	2056	720	1.19	0.25	0.0037	0.0187
M6261	diglycyl sulfosuccinate	Xenobiotics	Chemical	3557	309	0.40	-1.31	0.0039	0.0197
M3063	glycosy-L-nervonoyl-sphingosine (d18:1/24:1)*	Lipid	Hexosylceramides (HCCER)	3990	811	0.56	-0.84	0.0039	0.0197
M307	indoleacetylglutamine	Amino Acid	Tryptophan Metabolism	2185	304	0.47	-1.10	0.0041	0.0204
M3081	glycosy ceramide (d18:1/23:1, d17:1/24:1)*	Lipid	Hexosylceramides (HCCER)	3667	797	0.49	-1.04	0.0041	0.0204
M270	N-acetyltyrosine (2)	Amino Acid	Tryptophan Metabolism	2378	249	0.60	-0.75	0.0042	0.0209
M513	hydroxylproline	Amino Acid	Urea cycle; Arginine and Proline Metabolism	1064	132	0.79	-0.34	0.0048	0.0236
M423	3-methyl-2-oxobutyrate	Amino Acid	Leucine, Isoleucine and Valine Metabolism	1465	115	1.13	0.18	0.0052	0.0255
M123	2-aminoadipate	Amino Acid	Lysine Metabolism	3500	160	0.80	-0.32	0.0055	0.0267
M1781	hexanoylglutamine	Lipid	Fatty Acid Metabolism (Acyl Glutamine)	2780	243	1.50	0.59	0.0055	0.0268
M460	S-carboxymethylcysteine	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	1785	194	0.67	-0.58	0.0057	0.0275
M1702	eicosaneedioate (C20-DC)	Lipid	Fatty Acid, Dicarboxylate	5200.9	341	0.72	-0.48	0.0059	0.0284
M298	indoleactate	Amino Acid	Tryptophan Metabolism	2286	204	0.77	-0.38	0.0060	0.0285
M1880	cis-4-decenoylecarnitine (C10:1)	Amino Acid	Fatty Acid Metabolism (Acyl Carnitine, Monounsaturated)	1057	314	1.66	0.73	0.0061	0.0292
M5961	2,6-dihydroxybenzoic acid	Xenobiotics	Drug - Topical Agents	2575	153	0.47	-1.10	0.0063	0.0297
M1505	10-undecenoate (11:1n)	Lipid	Medium Chain Fatty Acid	5085.8	183	1.50	0.58	0.0065	0.0299
M1811	3-(4-hydroxyphenyl)lactate (HPLA)	Amino Acid	Tyrosine Metabolism	1379	181	0.81	-0.31	0.0065	0.0299
M5378	4-acetamidophenylglucuronide	Xenobiotics	Drug - Analgesics, Anesthetics	1400	326	2.01	1.01	0.0065	0.0299
M639	gamma-glutamylleucine	Peptide	Gamma-glutamyl Amino Acid	1685	259	0.83	-0.26	0.0065	0.0299
M4462	hippurate	Xenobiotics	Benzote Metabolism	2106.9	2106.9	0.72	-0.48	0.0064	0.0299
M1865	margaroylcarnitine (C17)*	Lipid	Fatty Acid Metabolism (Acyl Carnitine, Long Chain Saturated)	1424	414	0.70	-0.51	0.0064	0.0299
M2201	myo-inositol	Lipid	Inositol Metabolism	3506.3	225	0.68	-0.56	0.0067	0.0308
M1881	undecenoylecarnitine (C11:1)	Lipid	Fatty Acid Metabolism (Acyl Carnitine, Monounsaturated)	1069	328	1.57	0.65	0.0070	0.0320
M1277	arabitol/syntol	Carbohydrate	Pentose Metabolism	1932.4	151	0.83	-0.27	0.0071	0.0321
M5381	2-methoxyacetaminophen glucuronide*	Xenobiotics	Drug - Analgesics, Anesthetics	1633	356	2.23	1.16	0.0073	0.0328
M1867	arachidoylcarnitine (C20)*	Lipid	Fatty Acid Metabolism (Acyl Choline)	1512	456	0.64	-0.65	0.0075	0.0331
M3472	glycochenodeoxycholate glucuronide (1)	Lipid	Primary Bile Acid Metabolism	4806	312	1.67	0.74	0.0075	0.0331
M3087	lactosyl-N-palmitoyl-sphingosine (d18:1/16:0)	Lipid	Lactosylceramides (LCCER)	2527	863	0.62	-0.68	0.0074	0.0331
M6154	ectoine	Xenobiotics	Chemical	1980	143	0.65	-0.62	0.0076	0.0336
M2266	1-myristoyl-2-arachidonoyl-GPC (14:0/20:4)*	Lipid	Phosphatidylcholine (PC)	1950	755	0.70	-0.51	0.0077	0.0337
M3541	taurochenodeoxycholic acid 3-sulfate	Lipid	Secondary Bile Acid Metabolism	4809	289	3.63	1.86	0.0077	0.0337
M485	urea	Amino Acid	Urea cycle; Arginine and Proline Metabolism	700	121	0.80	-0.32	0.0082	0.0355
M1944	oleylcholine	Lipid	Fatty Acid Metabolism (Acyl Choline)	1449	368	0.72	-0.48	0.0085	0.0367
M1882	5-dodecenoylcarnitine (C12:1)	Lipid	Fatty Acid Metabolism (Acyl Carnitine, Monounsaturated)	1135	342	1.35	0.43	0.0085	0.0367
M5249	2-acetamidophenol sulfate	Xenobiotics	Food Component/Plant	225					

M494	homocitrulline	Amino Acid	Urea cycle; Arginine and Proline Metabolism	789	188	0.66	-0.59	0.0117	0.0471
M536	taurocholenate sulfate*	Lipid	Secondary Bile Acid Metabolism	4750	280	3.22	1.69	0.0126	0.0505
M4174	N6-succinyladenosine	Nucleotide	Purine Metabolism, Adenine containing	940	382	0.64	-0.64	0.0130	0.0517
M5005	piperine	Xenobiotics	Food Component/Plant	1168	286	0.48	-1.05	0.0130	0.0517
M5088	4-allylphenol sulfate	Xenobiotics	Food Component/Plant	3805	213	0.49	-1.04	0.0135	0.0530
M6423	pentose acid*	PCM	PCM	2180	165	0.59	-0.76	0.0135	0.0530
M2438	1-stearoyl-2-arachidonoyl-GPE (18:0/20:4)	Lipid	Phosphatidylethanolamine (PE)	2475	769	1.21	0.28	0.0137	0.0535
M2442	1-stearoyl-2-docosahexaenoyl-GPE (18:0/22:6)*	Lipid	Phosphatidylethanolamine (PE)	2375	793	1.27	0.35	0.0138	0.0535
M3090	lactosy-N-behenoyl-sphingosine (d18:1/22:0)*	Lipid	Lactosylceramides (LCLR)	3842	947	0.80	-0.32	0.0138	0.0535
M473	N-acetyltaurine	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	800	166	0.68	-0.55	0.0139	0.0536
M3281	Salpha-pregnadiol disulfate	Lipid	Progestin Steroids	4310	239	2.02	1.02	0.0140	0.0539
M6235	6-hydroxyindole sulfate	Xenobiotics	Chemical	2498	212	0.55	-0.88	0.0140	0.0539
M545	spermidine	Amino Acid	Polyamine Metabolism	3235	146	0.53	-0.90	0.0145	0.0552
M3477	glycocholate sulfate	Lipid	Primary Bile Acid Metabolism	4560	272	3.79	1.92	0.0145	0.0553
M3048	ceramide (d18:1/17:0, d17:1/18:0)*	Lipid	Ceramides	3055	553	1.29	0.37	0.0151	0.0570
M3360	androstenediol (3beta,17beta) monosulfate (1)	Lipid	Androgenic Steroids	4535	369	1.61	0.69	0.0153	0.0577
M2418	1-palmitoyl-2-docosahexaenoyl-GPE (16:0/22:6)*	Lipid	Phosphatidylethanolamine (PE)	2160	765	1.25	0.32	0.0156	0.0586
M107	N6-acetylysine	Amino Acid	Lysine Metabolism	1059	187	0.76	-0.39	0.0157	0.0586
M4436	pantothenate (Vitamin B5)	Cofactors and Vitamins	Pantothenate and CoA Metabolism	1498.7	218	0.81	-0.31	0.0158	0.0589
M483	arginine	Amino Acid	Urea cycle; Arginine and Proline Metabolism	2825	175	0.88	-0.18	0.0160	0.0592
M3131	sphingomyelin (d18:1/25:0, d19:0/24:1, d20:1/23:0, d19:1/24:0)*	Lipid	Sphingomyelins	3500	830	0.82	-0.28	0.0165	0.0607
M3107	tricosanoyl sphingomyelin (d18:1/23:0)*	Lipid	Sphingomyelins	3350	802	0.84	-0.25	0.0164	0.0607
M434	methionine	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	2526	150	0.83	-0.28	0.0168	0.0617
M4431	carotene diol (1)	Cofactors and Vitamins	Vitamin A Metabolism	1720	568	0.76	-0.40	0.0172	0.0628
M426	isobutyrylcarnitine (C4)	Amino Acid	Leucine, Isoleucine and Valine Metabolism	2810	232	0.70	-0.51	0.0176	0.0636
M4591	paraxanthine	Xenobiotics	Xanthine Metabolism	2279	179	0.58	-0.80	0.0176	0.0636
M1869	lignoceroylcarnitine (C24)*	Lipid	Fatty Acid Metabolism (Acyl Carnitine, Long Chain Saturated)	1603	512	0.80	-0.31	0.0178	0.0636
M4241	N-acetyl-beta-alanine	Nucleotide	Pyrimidine Metabolism, Uracil containing	773	130	0.71	-0.48	0.0177	0.0636
M163	N-acetyltyrosine	Amino Acid	Tyrosine Metabolism	1680	222	0.78	-0.35	0.0177	0.0636
M2425	1-stearoyl-2-oleoyl-GPE (18:0/18:1)	Lipid	Phosphatidylethanolamine (PE)	2950	747	1.31	0.39	0.0179	0.0638
M322	3-indoxyl sulfate	Amino Acid	Tryptophan Metabolism	2222.2	212	0.55	-0.86	0.0180	0.0638
M5017	sulfate of piperic metabolite C16H19NO3 (2)*	Xenobiotics	Food Component/Plant	4112	352	0.54	-0.88	0.0182	0.0645
M5218	vanillic acid glycine	Xenobiotics	Food Component/Plant	1682	224	0.26	-1.93	0.0185	0.0650
M4636	2-piperidinone	Xenobiotics	Food Component/Plant	1675	100	0.40	-1.34	0.0187	0.0652
M522	argininate*	Amino Acid	Urea cycle; Arginine and Proline Metabolism	2150	176	0.75	-0.42	0.0186	0.0652
M1947	dihomo-linolenoyl-choline	Lipid	Fatty Acid Metabolism (Acyl Choline)	1424	392	0.64	-0.65	0.0187	0.0652
M5505	metronidazole	Xenobiotics	Drug - Antibiotic	2046	172	3.37	1.75	0.0189	0.0657
M3310	tetrahydrocortisol glucuronide	Lipid	Corticosteroids	4666	541	1.58	0.66	0.0193	0.0665
M1948	linoleoylcholine*	Lipid	Fatty Acid Metabolism (Acyl Choline)	1388	366	0.74	-0.43	0.0195	0.0670
M1220	1,5-anhydroglucitol (1,5-AG)	Carbohydrate	Glycolysis, Gluconeogenesis, and Pyruvate Metabolism	802	163	0.75	-0.42	0.0202	0.0688
M4348	ascorbic acid 2-sulfate	Cofactors and Vitamins	Ascorbate and Aldarate Metabolism	3042	255	0.83	-0.27	0.0204	0.0688
M1864	palmitoylcarnitine (C16)	Lipid	Fatty Acid Metabolism (Acyl Carnitine, Long Chain Saturated)	1425	400	0.82	-0.28	0.0202	0.0688
M1943	palmitoylcholine	Xenobiotics	Fatty Acid Metabolism (Acyl Choline)	1482	342	0.76	-0.40	0.0203	0.0688
M6241	perfluorooctanoate (PFOA)	Chemical	Chemical	5130	413	0.79	-0.35	0.0203	0.0688
M3035	cortisol	Lipid	Corticosteroids	4710	361	1.47	0.55	0.0206	0.0691
M1468	phosphate	Energy	Oxidative Phosphorylation	576	99	0.78	-0.35	0.0206	0.0691
M2711	1-stearoyl-GPG (18:0)	Lipid	Lysophospholipid	5816	511	0.33	-1.61	0.0213	0.0711
M1884	myristoleylcarnitine (C14:1)*	Lipid	Fatty Acid Metabolism (Acyl Carnitine, Monounsaturated)	1316	370	1.33	0.41	0.0214	0.0711
M3025	N-stearoyl-sphingosine (d18:1/18:0)*	Lipid	Ceramides	3392	567	1.25	0.33	0.0214	0.0711
M140	phenylalanine	Amino Acid	Phenylalanine Metabolism	2878	166	1.13	0.18	0.0224	0.0740
M1444	succinate	Energy	TCA Cycle	3149	117	0.86	-0.23	0.0226	0.0745
M437	N-formylmethionine	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	1543.8	176	0.85	-0.23	0.0229	0.0751
M11	N-acetylsérine	Amino Acid	Glycine, Serine and Threonine Metabolism	2000	146	0.73	-0.46	0.0235	0.0768
M4597	1,7-dimethylurate	Xenobiotics	Xanthine Metabolism	1578.6	195	0.56	-0.85	0.0239	0.0779
M245	thyroxine	Amino Acid	Tyrosine Metabolism	4808	776	0.85	-0.23	0.0240	0.0779
M2725	1-linoleoyl-GPI* (18:2)*	Lipid	Lysophospholipid	5494	595	1.19	0.25	0.0243	0.0786
M5514	flucnazole	Xenobiotics	Drug - Antibiotic	836	351	0.52	-0.95	0.0247	0.0797
M1161	fibrinopeptide A (3-16)	Peptide	Fibrinogen Cleavage Peptide	2786	674	1.30	0.38	0.0261	0.0836
M351	isovalerate (C5)	Amino Acid	Leucine, Isoleucine and Valine Metabolism	1564	101	0.81	-0.30	0.0261	0.0836
M5	sarcosine	Amino Acid	Glycine, Serine and Threonine Metabolism	1280	90	0.75	-0.42	0.0263	0.0840
M2802	1-(1-enyl-palmitoyl)-2-palmitoyl-GPC (P-16:0/16:0)*	Lipid	Plasmalogens	2550	719	0.73	-0.45	0.0266	0.0846
M1406	glucuronate	Carbohydrate	Aminosugar Metabolism	3233.3	193	1.70	0.76	0.0267	0.0846
M219	gentisate	Amino Acid	Tyrosine Metabolism	905	153	0.50	-1.00	0.0272	0.0859
M80	imidazole propionate	Amino Acid	Histidine Metabolism	2263	141	2.69	1.43	0.0275	0.0863
M1951	docosahexaenoylcholine	Lipid	Fatty Acid Metabolism (Acyl Choline)	1378	414	0.73	-0.46	0.0276	0.0865
M3009	N-palmitoyl-sphinganine (d18:0/16:0)	Lipid	Dihydroceramides	3090	541	1.20	0.27	0.0278	0.0867
M2850	1-pentadecanoylglycerol (15:0)	Lipid	Monoacylglycerol	6200	241	0.58	-0.79	0.0282	0.0868
M2669	1-stearoyl-GPE (18:0)	Lipid	Lysophospholipid	1626	482	0.83	-0.28	0.0279	0.0868
M2871	2-oleyoylglycerol (18:1)	Lipid	Monoacylglycerol	6500	281	0.59	-0.77	0.0281	0.0868
M1936	acetoacetate	Lipid	Ketone Bodies	1062	103	1.72	0.78	0.0282	0.0868
M1283	arabonate/xylose	Carbohydrate	Pentose Metabolism	2700	165	0.76	-0.39	0.0283	0.0870
M2404	1,2-dipalmitoyl-GPE (16:0/16:0)*	Lipid	Phosphatidylethanolamine (PE)	2498	693	1.46	0.55	0.0284	0.0870
M1180	fibrinopeptide B (1-13)	Peptide	Fibrinogen Cleavage Peptide	2482	697	1.25	0.32	0.0286	0.0872
M2841	1-myristoylglycerol (14:0)	Lipid	Monoacylglycerol	6353.3	227	0.51	-0.96	0.0294	0.0879
M1971	2-hydroxystearate	Lipid	Fatty Acid, Monohydroxy	5695	299	1.16	0.21	0.0290	0.0879
M2233	phosphocholine	Lipid	Phospholipid Metabolism	700	184	0.87	-0.20	0.0293	0.0879
M1567	linoleate (18:2n6)	Lipid	Long Chain Polyunsaturated Fatty Acid (n3 and n6)	5535	279	1.18	0.24	0.0294	0.0879
M31	N-acetylalanine	Amino Acid	Alanine and Aspartate Metabolism	1564.8	130	0.85	-0.24	0.0293	0.0879
M4552	p-cresol sulfate	Xenobiotics	Benzene Metabolism	2890	187	0.49	-1.02	0.0291	0.0879
M4357	gulonate*	Cofactors and Vitamins	Ascorbate and Aldarate Metabolism	2750	195	0.62	-0.68	0.0300	0.0894
M75	N-acetyl-3-methylhistidine*	Amino Acid	Histidine Metabolism	2056	212	0.49	-1.03	0.0306	0.0909
M340	1-carboxybutyric acid	Amino Acid	Leucine, Isoleucine and Valine Metabolism	2663	202	0.75	-0.42	0.0313	0.0926
M1543	eicosanoate (20:1n9 or 1n11)	Lipid	Long Chain Monounsaturated Fatty Acid	5950	309	1.28	0.36	0.0323	0.0953
M642	gamma-glutamylmethionine	Peptide	Gamma-glutamyl Amino Acid	2640	279	0.78	-0.36	0.0330	0.0970
M1494	caprate (10:0)	Lipid	Medium Chain Fatty Acid	5090.7	171	0.73	-0.45	0.0336	0.0986
M3404	11beta-hydroxyandrosterone glucuronide	Lipid	Androgenic Steroids	4209	481	1.48	0.57	0.0344	0.1006
M1952	arachidonylcholine	Lipid	Fatty Acid Metabolism (Acyl Choline)	1390	390	0.76	-0.39	0.0355	0.1031
M645	gamma-glutamyltryptophan	Peptide	Gamma-glutamyl Amino Acid	1960	332	0.80	-0.33	0.0354	0.1031
M1915	suberoylcarnitine (C8-D)	Lipid	Fatty Acid Metabolism (Acyl Carnitine, Dicarboxylate)	2964	318	1.86	0.90	0.0365	0.1058
M399	2-methylbutyrylglycerine (C5)	Lipid	Leucine, Isoleucine and Valine Metabolism	1884	158	0.69	-0.53	0.0375	0.1082
M1495	cis-4-decenolate (10:1n6)*	Lipid	Medium Chain Fatty Acid	4890	169	1.26	0.34	0.0381	0.1096
M18	N-acetylthreonine	Amino Acid	Glycine, Serine and Threonine Metabolism	1700	160	0.82	-0.29	0.0384	0.1101
M4235	2'-deoxyuridine	Nucleotide	Pyrimidine Metabolism, Orotate containing	1100	273	0.47	-1.08	0.0391	0.1110
M4417	adenine	Nucleotide	Purine Metabolism, Adenine containing	2221	136	1.23	0.29	0.0389	0.1110
M3102	sphingomyelin (d18:0/20:0, d16:0/22:0)*	Lipid	Dihydrosphingomyelins	2850	762	0.81	-0.30	0.0390	0.1110
M1416	N-acetyleneuraminate	Carbohydrate	Aminosugar Metabolism	660	310	0.88	-0.18	0.0397	0.1125
M1706	hydroxy-CMPF*	Lipid	Fatty Acid, Dicarboxylate	1516	255	0.72	-0.47	0.0404	0.1139
M2924	oleoyl-oleoylglycerol (18:1/18:1) [2]*	Lipid	Diacetyl glycerol	3695	639	0.81	-0.31	0.0405	0.1139
M1157	ADSGEDGDXAEGGVR*	Peptide	Fibrinogen Cleavage Peptide	3350	769	1.44	0.52	0.0412	0.1157
M5224	ethyl beta-glucofuranoside	Xenobiotics	Food Component/Plant	1519	207	0.56	-0.83	0.0416	0.1165
M1490	heptanoate (7:0)	Lipid	Medium Chain Fatty Acid	3670	129	0.88	-0.19	0.0422	0.1176
M3192	cholesterol	Lipid	Sterol	2707	369	0.91	-0.14	0.0425	0.1182
M582	2-hydroxybutyrate/2-hydroxyisobutyrate	Amino Acid	Glutathione Metabolism	1258	103	1.18	0.24	0.0431	0.1193
M2803	1-(1-enyl-palmitoyl)-2-palmitoleyl-GPC (P-16:0/16:1)*	Lipid	Plasmalogens	2218	717	0.78	-0.36	0.0433	0.1197
M2857	1-linolenoylglycerol (18:3)	Lipid	Monoacylglycerol	6214	277	0.68	-0.56	0.0439	0.1210
M2923	oleoyl-oleoylglycerol (18:1/18:1) [1]*	Lipid	Diacetyl glycer						

M3057	glycosyl-N-palmitoyl-sphingosine (d18:1/16:0)	Lipid	Hexosylceramides (HCER)	2623	701	0.83	-0.28	0.0515	0.1360
M47	N-acetylglutamate	Amino Acid	Glutamate Metabolism	1050	190	0.86	-0.22	0.0516	0.1360
M2806	1-(1-enyl-palmitoyl)-2-oleoyl-GPC (P-16:0/18:1)*	Lipid	Plasmalogens	2550	745	0.88	-0.18	0.0524	0.1378
M77	hydantoin-5-propionate	Amino Acid	Histidine Metabolism	2080	171	1.44	0.52	0.0527	0.1380
M10	serine	Amino Acid	Glycine, Serine and Threonine Metabolism	1239	106	0.89	-0.17	0.0530	0.1385
M3021	N-palmitoyl-sphingosine (d18:1/16:0)	Lipid	Ceramides	2893	539	1.16	0.21	0.0532	0.1386
M3326	cortolone glucuronide (1)	Lipid	Corticosteroids	4600	541	1.36	0.45	0.0535	0.1389
M1162	Fibrinopeptide A (16:1)*	Peptide	Fibrinogen Cleavage Peptide	2850	602	1.19	0.25	0.0542	0.1404
M91	1-ribosyl-imidazoleacetate*	Amino Acid	Histidine Metabolism	2006	259	0.81	-0.30	0.0553	0.1424
M4224	5-methyluridine (ribothymidine)	Nucleotide	Pyrimidine Metabolism, Uracil containing	1778.1	257	0.87	-0.20	0.0555	0.1424
M1695	hexadecanedioate (C16)	Lipid	Fatty Acid, Dicarboxylate	4615	285	1.31	0.39	0.0552	0.1424
M254	tryptophan	Amino Acid	Tryptophan Metabolism	2986	205	0.89	-0.17	0.0559	0.1432
M2172	N-oleoyltaurine	Lipid	Endocannabinoid	5610	388	0.73	-0.45	0.0572	0.1461
M498	dimethylarginine (ADMA + SDMA)	Amino Acid	Urea cycle, Arginine and Proline Metabolism	2850	203	0.76	-0.39	0.0574	0.1462
M1462	citraconate/glutaconate	Energy	TCA Cycle	2600	129	0.68	-0.56	0.0581	0.1472
M3342	epiandrosterone sulfate	Lipid	Androgenic Steroids	4855	369	0.68	-0.55	0.0583	0.1472
M3159	sphingosine	Lipid	Sphingosines	1393	300	0.42	-1.26	0.0580	0.1472
M3124	sphingomyelin (d18:1/21:0, d17:1/22:0, d16:1/23:0)*	Lipid	Sphingomyelins	3000	774	0.85	-0.24	0.0585	0.1473
M1540	10-nomadecanoate (19:1n9)	Lipid	Long Chain Monounsaturated Fatty Acid	5780	295	1.21	0.28	0.0590	0.1477
M2238	phosphoethanolamine (PE)	Lipid	Phospholipid Metabolism	700	142	0.51	-0.96	0.0590	0.1477
M417	N-acetylvaline	Amino Acid	Leucine, Isoleucine and Valine Metabolism	1704	158	0.85	-0.23	0.0595	0.1485
M4254	3-methylcytidine	Nucleotide	Pyrimidine Metabolism, Cytidine containing	2176	258	1.26	0.33	0.0609	0.1518
M402	tigloylglycine	Amino Acid	Leucine, Isoleucine and Valine Metabolism	1926	158	0.72	-0.48	0.0619	0.1537
M137	N,N-dimethyl-L-aminovalerate	Amino Acid	Lysine Metabolism	2290	146	0.49	-1.02	0.0624	0.1547
M1533	oleate/vaccenate (18:1)	Lipid	Long Chain Monounsaturated Fatty Acid	5655	281	1.17	0.22	0.0628	0.1551
M2587	1-linoleoyl-GPA (18:2)*	Lipid	Lysophospholipid	1550	435	0.77	-0.38	0.0634	0.1558
M5009	glucuronide of piperine metabolite C17H21NO3 (4)*	Xenobiotics	Food Component/Plant	3992	462	0.61	-0.71	0.0633	0.1558
M3224	campesterol	Lipid	Sterol	2873	383	1.50	0.59	0.0641	0.1568
M1579	dihomololeate (20:2n6)	Lipid	Long Chain Polyunsaturated Fatty Acid (n3 and n6)	5730	307	1.19	0.25	0.0642	0.1568
M1974	2-hydroxybehenate	Lipid	Fatty Acid, Monohydroxy	6384	355	1.13	0.17	0.0645	0.1571
M263	oxindolylalanine	Amino Acid	Tryptophan Metabolism	2756	221	0.82	-0.29	0.0647	0.1571
M2913	palmitoyl-arachidonoyl-glycerol (16:0/20:4) [1]*	Lipid	Diacetyl glycerol	2916	635	0.81	-0.31	0.0648	0.1571
M1547	erucate (22:1n9)	Lipid	Long Chain Monounsaturated Fatty Acid	6355.6	337	1.20	0.26	0.0656	0.1587
M4316	1-methylnicotinamide	Cofactors and Vitamins	Nicotinate and Nicotinamide Metabolism	1940	137	0.73	-0.46	0.0666	0.1605
M2851	1-palmitoylglycerol (16:0)	Lipid	Monacylglycerol	6550	255	0.75	-0.41	0.0670	0.1611
M3123	sphingomyelin (d18:1/20:2, d18:2/20:1, d16:1/22:2)*	Lipid	Sphingomyelins	2200	756	1.13	0.18	0.0674	0.1616
M202	vanillylmandelate (VMA)	Amino Acid	Tyrosine Metabolism	941	197	1.24	0.31	0.0681	0.1629
M4785	3-formylindole	Xenobiotics	Food Component/Plant	2736	146	0.85	-0.24	0.0689	0.1644
M2852	1-palmitoleoylglycerol (16:1)*	Lipid	Monacylglycerol	6094	253	0.56	-0.84	0.0702	0.1671
M4505	4-methylcatechol sulfate	Xenobiotics	Benzoate Metabolism	2665	203	0.56	-0.83	0.0710	0.1680
M5410	celecoxib	Xenobiotics	Drug - Analgesics, Anesthetics	5283	380	1.17	0.23	0.0709	0.1680
M3209	3beta-hydroxy-5-cholestenoate	Lipid	Sterol	5398	415	1.31	0.39	0.0716	0.1691
M2855	1-oleoylglycerol (18:1)	Lipid	Monacylglycerol	6650	281	0.66	-0.60	0.0736	0.1728
M1861	laurylcarnitine (C12)	Lipid	Fatty Acid Metabolism (Acyl Carnitine, Medium Chain)	1235	344	1.23	0.30	0.0735	0.1728
M78	trans-urocanate	Amino Acid	Histidine Metabolism	2285	139	4.47	2.16	0.0748	0.1753
M3337	dehydroepiandrosterone sulfate (DHEA-S)	Lipid	Androgenic Steroids	4745	367	1.36	0.44	0.0752	0.1758
M2869	2-palmitoleoylglycerol (16:1)*	Lipid	Monacylglycerol	6016	253	0.53	-0.91	0.0758	0.1766
M4938	indolin-2-one	Xenobiotics	Food Component/Plant	2575	134	0.67	-0.57	0.0762	0.1772
M4411	biliverdin	Cofactors and Vitamins	Hemoglobin and Porphyrin Metabolism	1016	583	1.33	0.41	0.0769	0.1775
M1489	caproate (6:0)	Lipid	Medium Chain Fatty Acid	2713.7	115	0.89	-0.17	0.0769	0.1775
M4593	theophylline	Xenobiotics	Xanthine Metabolism	1870	181	0.71	-0.50	0.0768	0.1775
M3455	taurocholate	Lipid	Primary Bile Acid Metabolism	5150	514	1.86	0.90	0.0781	0.1797
M1707	3-carboxy-4-methyl-5-pentyl-2-furanpropionate (3-CMPFP)	Lipid	Fatty Acid, Dicarboxylate	4000	267	1.80	-0.33	0.0798	0.1831
M1262	ribitol	Carbohydrate	Pentose Metabolism	1789.6	151	0.90	-0.16	0.0807	0.1843
M2938	stearyl-arachidonoyl-glycerol (18:0/20:4) [2]*	Lipid	Diacetyl glycerol	3522	663	0.82	-0.29	0.0806	0.1843
M5159	N,N,N-trimethyl-alanyl/proline betaine (TMAP)	Amino Acid	Urea cycle; Arginine and Proline Metabolism	2470	229	0.82	-0.29	0.0818	0.1863
M1690	tridecenedioate (C13:1-DC)*	Lipid	Fatty Acid, Dicarboxylate	3051	241	1.27	0.35	0.0821	0.1865
M3517	glycoursoeoxicholic acid sulfate (1)	Lipid	Secondary Bile Acid Metabolism	4309	264	1.89	0.92	0.0824	0.1868
M3043	N-palmitoyl-hepta decapingsine (d17:1/16:0)*	Lipid	Ceramides	2645	525	1.18	0.24	0.0831	0.1880
M81	formimino glutamate	Amino Acid	Histidine Metabolism	1880	175	1.27	0.34	0.0842	0.1888
M638	gamma-glutamylsucine*	Peptide	Gamma-glutamyl Amino Acid	2940	261	0.85	-0.23	0.0837	0.1888
M4191	N2-methylguanosine	Nucleotide	Purine Metabolism, Guanine containing	1988	296	0.82	-0.29	0.0840	0.1888
M2914	palmitoyl-arachidonoyl-glycerol (16:0/20:4) [2]*	Lipid	Diacetyl glycerol	3015	635	0.80	-0.32	0.0843	0.1888
M4244	3-(3-amino-3-carboxypropyl)uridine*	Nucleotide	Pyrimidine Metabolism, Uracil containing	1369	344	0.73	-0.45	0.0848	0.1889
M3103	sphingomyelin (d18:0/18:0, d19:0/17:0)*	Lipid	Dihydro sphingomyelins	2500	734	0.84	-0.25	0.0848	0.1889
M6213	4-hydroxylchlorothalonil	Xenobiotics	Chemical	4427	245	0.86	-0.22	0.0850	0.1890
M1979	3-hydroxyhexanoate	Lipid	Fatty Acid, Monohydroxy	1725	131	1.22	0.28	0.0853	0.1891
M79	cis-urocanate	Amino Acid	Histidine Metabolism	1200	137	2.33	1.22	0.0860	0.1901
M5736	ondansetron	Xenobiotics	Drug - Gastrointestinal	3301	294	1.90	0.93	0.0867	0.1909
M5077	thymol sulfate	Xenobiotics	Food Component/Plant	4410	229	0.32	-1.65	0.0867	0.1909
M3248	17alpha-hydroxy pregnanolone glucuronide	Lipid	Pregnaneolone Steroids	5071.9	509	1.29	0.37	0.0878	0.1928
M299	indoleacetate	Amino Acid	Tryptophan Metabolism	2200	174	0.72	-0.47	0.0889	0.1946
M109	N2-acetyl,N6-methyllysine	Amino Acid	Lysine Metabolism	2168	203	0.60	-0.73	0.0894	0.1953
M2872	2-linoleoylglycerol (18:2)	Lipid	Monacylglycerol	6250	279	0.73	-0.45	0.0904	0.1971
M6416	glycine conjugate of C10H14O2 (1)*	PCM	PCM	4335	222	1.29	0.37	0.0911	0.1982
M6141	dimethylglycine	Amino Acid	Glycine, Serine and Threonine Metabolism	1104	104	0.84	-0.25	0.0931	0.2019
M1887	eicosenoyl carnitine (C20:1)*	Lipid	Fatty Acid Metabolism (Acyl Carnitine, Monounsaturated)	1484	454	0.79	-0.33	0.0936	0.2023
M2940	oleoyl-arachidonoyl-glycerol (18:1/20:4) [2]*	Lipid	Diacetyl glycerol	2990	661	0.83	-0.28	0.0937	0.2023
M1178	Fibrinopeptide B (11-11)	Peptide	Fibrinogen Cleavage Peptide	2389	411	1.26	0.33	0.0943	0.2032
M2931	linoleoyl-linoleoyl-glycerol (18:2/18:2) [1]*	Lipid	Diacetyl glycerol	2720	635	1.58	0.66	0.0959	0.2060
M5090	methyl glucopyranoside (alpha + beta)	Xenobiotics	Food Component/Plant	1070	193	0.68	-0.56	0.0970	0.2075
M3490	taurodeoxycholic acid 3-sulfate	Lipid	Secondary Bile Acid Metabolism	4850	289	1.70	0.77	0.0969	0.2075
M1372	galactonate	Carbohydrate	Fructose, Mannose and Galactose Metabolism	3085	195	0.64	-0.64	0.0997	0.2128
M1938	3-hydroxybutyrate (BHB)	Lipid	Ketone Bodies	1480	103	1.49	0.57	0.1004	0.2138
M387	N-acetylsarcosine	Amino Acid	Leucine, Isoleucine and Valine Metabolism	2325	172	0.82	-0.29	0.1010	0.2146
M3031	N-palmitoyl-sphingadienine (d18:2/16:0)*	Lipid	Ceramides	2490	537	1.12	0.16	0.1030	0.2183
M201	vanillate	Amino Acid	Tryptophan Metabolism	1625	211	0.83	-0.27	0.1034	0.2185
M2821	1-palmitoyl-2-stearoyl-GPC (16:0/18:0)	Lipid	Phosphatidylcholine (PC)	2750	763	0.60	-0.74	0.1046	0.2204
M455	cysteine	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	1475	122	1.16	0.21	0.1047	0.2204
M4780	2-isopropylmalate	Xenobiotics	Food Component/Plant	2605	175	0.64	-0.64	0.1062	0.2229
M1517	arachidate (20:0)	Lipid	Long Chain Saturated Fatty Acid	6240	311	1.16	0.22	0.1072	0.2246
M4376	delta-CEHC	Cofactors and Vitamins	Tocopherol Metabolism	3422	249	1.61	0.68	0.1076	0.2249
M573	cysteine-glutathione disulfide	Amino Acid	Glutathione Metabolism	2465	427	0.56	-0.83	0.1079	0.2249
M4893	ergothioneine	Xenobiotics	Food Component/Plant	850	230	1.57	0.65	0.1086	0.2260
M2856	1-linoleoylglycerol (18:2)	Lipid	Monacylglycerol	6477	279	0.74	-0.43	0.1091	0.2265
M2241	glycerophosphoserine*	Lipid	Phospholipid Metabolism	577	260	0.82	-0.28	0.1109	0.2297
M3112	sphingomyelin (d17:1/14:0, d16:1/15:0)*	Lipid	Sphingomyelins	1950	662	0.84	-0.26	0.1115	0.2304
M6175	2-naphthol sulfate	Xenobiotics	Chemical	3658	223	0.77	-0.37	0.1130	0.2323
M1837	picolinoylglycine	Lipid	Fatty Acid Metabolism (Acyl Glycine)	1945	181	0.82	-0.29	0.1128	0.2323
M5738	diphenoxylate	Xenobiotics	Drug - Gastrointestinal	1093	453	1.43	0.52	0.1133	0.2326
M2293	1-palmitoyl-2-dihydro-linolenoyl-GPC (16:0/20:3n3 or 6)*	Lipid	Phosphatidylcholine (PC)	2285	785	0.94	-0.09	0.1151	0.2356
M3208	3beta,7alpha-dihydroxy-5-cholestenoate	Lipid	Sterol	5275	431	1.12	0.16	0.1159	0.2368
M3221	beta-sitosterol	Lipid	Sterol	3054	397	1.75	0.80	0.1169	0.2382
M1932	carnitine	Lipid	Carnitine Metabolism	1978	162	0.89	-0.17	0.1194	0.2428
M2937	stearyl-arachidonoyl-glycerol (18:0/20:4) [1]*	Lipid	Diacetyl glycerol	3404	663	0.87	-0.20	0.1200	0.2435
M3271									

M375	3-methylglutaryl carnitine (2)	Amino Acid	Leucine, Isoleucine and Valine Metabolism	2687	290	0.79	-0.35	0.1277	0.2509
M4931	histidine betaine (hercynine)*	Xenobiotics	Food Component/Plant	2094	198	1.40	0.48	0.1280	0.2509
M1512	margarate (17:0)	Lipid	Long Chain Saturated Fatty Acid	5731	269	1.15	0.20	0.1271	0.2509
M116	N6,N6,N6-trimethyllysine	Amino Acid	Lysine Metabolism	2825	189	0.86	-0.22	0.1290	0.2521
M2447	1-oleoyl-2-arachidonoyl-GPE (18:1/20:4)*	Lipid	Phosphatidylethanolamine (PE)	2200	767	1.14	0.19	0.1303	0.2537
M3100	behenoyl dihydroxyphosphorylomelin (d18:0/22:0)*	Lipid	Dihydrophosphorylomelins	3300	790	0.87	-0.20	0.1301	0.2537
M2037	3,4-dihydroxybutyrate	Lipid	Fatty Acid, Dihydroxy	2204	119	0.87	-0.20	0.1313	0.2540
M3098	myristoyl dihydroxyphosphorylomelin (d18:0/14:0)*	Lipid	Dihydrophosphorylomelins	2060	678	0.87	-0.21	0.1316	0.2540
M3462	taurochenodeoxycholate	Lipid	Primary Bile Acid Metabolism	5250	498	1.47	0.56	0.1316	0.2540
M226	tyramine O-sulfate	Amino Acid	Tyrosine Metabolism	1565	216	1.85	0.88	0.1316	0.2540
M1472	malonate	Lipid	Fatty Acid Synthesis	3447	103	0.92	-0.12	0.1325	0.2551
M5203	caffeoic acid sulfate	Xenobiotics	Food Component/Plant	1307	259	0.47	-1.09	0.1327	0.2551
M1516	nonadecanoate (19:0)	Lipid	Long Chain Saturated Fatty Acid	6068	297	1.12	0.17	0.1330	0.2551
M327	6-bromotryptophan	Amino Acid	Tryptophan Metabolism	3371	283	0.70	-0.52	0.1336	0.2557
M76	N-acetyl-1-methylhistidine*	Amino Acid	Histidine Metabolism	2100	212	0.65	-0.63	0.1346	0.2570
M139	N-acetyl-2-amino adipate	Amino Acid	Lysine Metabolism	1374	204	0.86	-0.21	0.1348	0.2570
M1772	propionylglycine (C3)	Lipid	Fatty Acid Metabolism (also BCAA Metabolism)	966	130	0.75	-0.42	0.1370	0.2605
M2399	oleoyl-arachidonoyl-glycerol (18:1/20:4) [1]*	Lipid	Diaclyglycerol	2907	661	0.85	-0.23	0.1377	0.2612
M1844	hexanoylcarnitine (C6)	Lipid	Fatty Acid Metabolism (Acyl Carnitine, Medium Chain)	3358	260	1.15	0.20	0.1389	0.2631
M3000	sphinganine	Lipid	Sphingolipid Synthesis	1413	302	0.49	-1.03	0.1394	0.2635
M1709	2-hydroxysebacate	Lipid	Fatty Acid, Dicarboxylate	1324	217	0.78	-0.35	0.1412	0.2663
M3453	cholate	Lipid	Primary Bile Acid Metabolism	5165	407	2.14	1.10	0.1422	0.2675
M6177	2,4-di-tert-butylphenol	Xenobiotics	Chemical	5749	205	0.92	-0.12	0.1427	0.2680
M2310	1-palmitoleyl-2-linolenoyl-GPC (16:1/18:3)*	Lipid	Phosphatidylcholine (PC)	1900	755	0.85	-0.23	0.1467	0.2743
M4300	quinolinate	Cofactors and Vitamins	Nicotinate and Nicotinamide Metabolism	845	168	0.82	-0.29	0.1466	0.2743
M2242	glycerophosphoinositol*	Lipid	Phospholipid Metabolism	516	335	1.13	0.17	0.1470	0.2744
M1684	dodecenodioate (C12:1-OC)*	Lipid	Fatty Acid, Dicarboxylate	2700	227	0.82	-0.29	0.1490	0.2775
M1959	2-hydroxyheptanoate*	Lipid	Fatty Acid, Monohydroxy	925	145	1.19	0.26	0.1502	0.2791
M2031	9,10-DIHOMA	Lipid	Fatty Acid, Dihydroxy	5180	313	1.54	0.63	0.1513	0.2807
M1561	linolenate (18:3n3 or 3n6)	Lipid	Long Chain Polyunsaturated Fatty Acid (n3 and n6)	5450	277	1.14	0.20	0.1526	0.2826
M4470	4-hydroxyhippurate	Xenobiotics	Benzene Metabolism	1475	194	0.70	-0.52	0.1538	0.2836
M272	kyurenate	Amino Acid	Tryptophan Metabolism	2224	188	0.87	-0.20	0.1538	0.2836
M4325	N1-Methyl-4-pyridone-3-carboxamide	Cofactors and Vitamins	Nicotinate and Nicotinamide Metabolism	1260	153	0.66	-0.59	0.1541	0.2836
M3379	Salpha-androstan-3alpha,17beta-diol monosulfate (2)	Lipid	Androgenic Steroids	5080	371	0.73	-0.46	0.1562	0.2869
M1377	Fibrinopeptide B (1-9)	Peptide	Fibrinogen Cleavage Peptide	1669	473	1.39	0.47	0.1589	0.2913
M1671	maleate	Lipid	Fatty Acid, Dicarboxylate	2640	115	1.52	0.61	0.1594	0.2915
M1460	2-methylcitrate/homocitrate	Energy	TCA Cycle	575	205	1.10	0.14	0.1601	0.2919
M2	N-acetylglycine	Amino Acid	Glycine, Serine and Threonine Metabolism	826	118	1.19	0.25	0.1602	0.2919
M4453	cystathione	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	2270	223	1.76	0.82	0.1608	0.2921
M4809	gluconate	Xenobiotics	Food Component/Plant	2922	195	0.62	-0.69	0.1623	0.2921
M1243	glycerate	Carbohydrate	Glycolysis, Gluconeogenesis, and Pyruvate Metabolism	2070.4	105	0.93	-0.11	0.1621	0.2921
M3032	N-stearoyl-sphingadienine (d18:2/18:0)*	Lipid	Ceramides	2846	565	1.12	0.16	0.1623	0.2921
M5959	salicylate	Xenobiotics	Drug - Topical Agents	802	137	0.37	-1.44	0.1611	0.2921
M3113	sphingomyelin (d18:1/14:0, d16:1/16:0)*	Lipid	Sphingomyelins	1998	676	0.91	-0.13	0.1619	0.2921
M5936	diphenhydramine	Xenobiotics	Drug - Respiratory	911	256	3.42	1.77	0.1637	0.2941
M2002	9-hydroxystearate	Lipid	Fatty Acid, Monohydroxy	5384	299	0.83	-0.28	0.1642	0.2943
M1814	cis-3,4-methyleneheptanoylglycine	Lipid	Fatty Acid Metabolism (Acyl Glycine)	3731	198	1.26	0.34	0.1645	0.2943
M3012	N-stearoyl-sphinganine (d18:0/18:0)*	Lipid	Dihydroceramides	3526	569	1.20	0.26	0.1655	0.2955
M6430	branched-chain, straight-chain, or cyclopoly 10:1 fatty acid (1)*	PCM	PCM	4805	169	1.29	0.37	0.1674	0.2983
M180	4-hydroxyphenylacetylglutamine	Amino Acid	Tyrosine Metabolism	2730	296	1.50	0.58	0.1707	0.3030
M2129	N,N-dimethyl-pro-pro	Peptide	Modified Peptides	2500	241	0.85	-0.24	0.1710	0.3030
M4909	quinate	Xenobiotics	Food Component/Plant	2432.9	191	0.65	-0.63	0.1705	0.3030
M1325	sucrose	Carbohydrate	Disaccharides and Oligosaccharides	865	341	0.50	-1.00	0.1765	0.3121
M1519	behenate (22:0)*	Lipid	Long Chain Saturated Fatty Acid	6745	339	0.87	-0.20	0.1772	0.3128
M2429	1-stearoyl-2-linoleoyl-GPE (18:0/18:2)*	Lipid	Phosphatidylethanolamine (PE)	2575	745	1.14	0.19	0.1784	0.3142
M1771	propionylcarnitine (C3)	Lipid	Fatty Acid Metabolism (also BCAA Metabolism)	2590	218	0.86	-0.22	0.1821	0.3202
M5210	(S)-a-amino-omega-caprolactam	Xenobiotics	Food Component/Plant	2378	129	0.91	-0.14	0.1838	0.3225
M354	isovalerylcarnitine (C5)	Amino Acid	Leucine, Isoleucine and Valine Metabolism	3085	246	0.85	-0.23	0.1845	0.3232
M1557	steardionate (18:4n3)	Lipid	Long Chain Polyunsaturated Fatty Acid (n3 and n6)	5395	275	0.82	-0.29	0.1853	0.3240
M71	1-methylhistidine	Amino Acid	Histidine Metabolism	2755	170	0.86	-0.22	0.1871	0.3253
M1679	azetate (C9-OC)	Lipid	Fatty Acid, Dicarboxylate	1276	187	0.82	-0.29	0.1872	0.3253
M4369	gamma-CEHC glucuronide*	Cofactors and Vitamins	Tocopherol Metabolism	2500	439	1.40	0.49	0.1867	0.3253
M580	2-aminobutyrate	Amino Acid	Glutathione Metabolism	2059	104	0.90	-0.15	0.1915	0.3319
M4963	methyl indole-3-acetate	Xenobiotics	Food Component/Plant	3380	190	0.72	-0.48	0.1917	0.3319
M1187	phenylacetylglutamine	Peptide	Acetylated Peptides	2330	263	0.77	-0.38	0.1924	0.3324
M551	acisoga	Amino Acid	Polyamine Metabolism	2297	183	0.66	-0.60	0.1947	0.3357
M2911	palmitoleyl-linoleoyl-glycerol (16:1/18:2) [1]*	Lipid	Diaclyglycerol	2664	609	0.82	-0.29	0.1950	0.3357
M4409	bilirubin (E,E)*	Cofactors and Vitamins	Hemoglobin and Porphyrin Metabolism	1045	585	0.86	-0.22	0.1966	0.3365
M1577	docosadienoate (22:2n6)	Lipid	Long Chain Polyunsaturated Fatty Acid (n3 and n6)	6034	335	1.11	0.15	0.1960	0.3365
M23	O-acetylhomoserine	Amino Acid	Glycine, Serine and Threonine Metabolism	1850	160	0.03	-5.06	0.1963	0.3365
M4139	AMP	Nucleotide	Purine Metabolism, Adenine containing	1013	348	1.05	0.07	0.1972	0.3369
M1907	adipoylcarnitine (C6-DC)	Lipid	Fatty Acid Metabolism (Acyl Carnitine, Dicarboxylate)	2570	290	1.31	0.39	0.1989	0.3388
M4437	retinal	Cofactors and Vitamins	Vitamin A Metabolism	1666	285	0.77	-0.37	0.1990	0.3388
M159	4-hydroxyphenylacetate	Amino Acid	Phenylalanine Metabolism	1361	151	1.48	0.57	0.2010	0.3415
M1447	succinylcarnitine (C4-DC)	Energy	TCA Cycle	2291	262	1.16	0.21	0.2037	0.3454
M1514	stearate (18:0)	Lipid	Long Chain Saturated Fatty Acid	5872	283	1.08	0.12	0.2064	0.3495
M1750	2-aminoheptanoate	Lipid	Fatty Acid, Amino	3160	146	0.87	-0.20	0.2076	0.3508
M1756	N-acetyl-2-aminooctanoate*	Lipid	Fatty Acid, Amino	3943	200	0.78	-0.36	0.2090	0.3525
M1502	laurate (12:0)	Lipid	Medium Chain Fatty Acid	5300	199	0.81	-0.30	0.2099	0.3534
M2416	1-palmitoyl-2-arachidonoyl-GPE (16:0/20:4)*	Lipid	Phosphatidylethanolamine (PE)	2250	741	1.10	0.14	0.2146	0.3606
M3120	sphingomyelin (d18:1/19:0, d19:1/18:0)*	Lipid	Sphingomyelins	2550	746	0.91	-0.13	0.2154	0.3613
M4283	3-aminoisobutyrate	Nucleotide	Pyrimidine Metabolism, Thymine containing	2190	104	0.61	-0.72	0.2173	0.3638
M634	gamma-glutamylglutamate	Peptide	Gamma-glutamyl Amino Acid	1775	277	0.82	-0.29	0.2218	0.3706
M395	2-hydroxy-3-methylvalerate	Amino Acid	Leucine, Isoleucine and Valine Metabolism	1800	131	1.17	0.22	0.2265	0.3764
M1441	aconitate [cis or trans]	Energy	TCA Cycle	580	173	1.10	0.14	0.2262	0.3764
M2162	palmitoyl ethanolamide	Lipid	Endocannabinoid	6300	298	1.07	0.10	0.2262	0.3764
M508	N-delta-acetylornithine	Amino Acid	Urea cycle; Arginine and Proline Metabolism	858	173	0.79	-0.34	0.2269	0.3764
M1966	2-hydroxypropanoate	Lipid	Fatty Acid, Monohydroxy	5511.2	271	1.07	0.10	0.2297	0.3802
M2243	trimethylamine N-oxide	Lipid	Phospholipid Metabolism	2100	76	0.66	-0.59	0.2311	0.3820
M4382	gamma-tocopherol/beta-tocopherol	Cofactors and Vitamins	Tocopherol Metabolism	2384	416	1.17	0.23	0.2320	0.3827
M3129	sphingomyelin (d18:1/24:1, d18:2/24:0)*	Lipid	Sphingomyelins	3200	814	1.06	0.09	0.2334	0.3843
M3037	cortisol 21-sulfate	Lipid	Corticosteroids	4330	441	1.72	0.78	0.2372	0.3898
M2932	linoleoyl-linoleoyl-glycerol (18:2/18:2) [2]*	Lipid	Diaclyglycerol	2790	635	1.25	0.33	0.2378	0.3902
M4559	o-cresol sulfate	Xenobiotics	Benzene Metabolism	2796	187	0.84	-0.25	0.2398	0.3928
M1189	4-hydroxyphenylacetylglutamine	Peptide	Sphingosines	1650	279	1.63	0.70	0.2469	0.4033
M3167	hexadecapsphingosine (d16:1)*	Xenobiotics	Benzene Metabolism	1289	272	0.55	-0.87	0.2471	0.4033
M4525	4-vinylphenol sulfate	Xenobiotics	Benzene Metabolism	3320	199	0.63	-0.67	0.2487	0.4051
M1572	dihomolinolenate (20:3n3 or 3n6)	Lipid	Long Chain Polyunsaturated Fatty Acid (n3 and n6)	5596	305	1.11	0.16	0.2496	0.4052
M3540	glycodeoxycholate 3-sulfate	Lipid	Secondary Bile Acid Metabolism	4875	264	1.39	0.48	0.2493	0.4052
M363	beta-hydroxyisovalerate	Amino Acid	Leucine, Isoleucine and Valine Metabolism	1027	117	1.13	0.18	0.2513	0.4064
M1931	deoxycarnitine	Lipid	Carnitine Metabolism	2052	146	0.90	-0.14	0.2512	0.4064
M1918	octadecenedioylcarnitine (C18:1-DC)*	Lipid	Fatty Acid Metabolism (Acyl Carnitine, Dicarboxylate)	1180	456	1.25	0.33	0.2534	0.4091
M1823	N-palmitoylglycine	Lipid	Fatty Acid Metabolism (Acyl Glycine)	5580	312	0.91	-0.14	0.2549	0.4108
M347	alpha-hydroxyisocaproate	Amino Acid	Leucine, Isoleucine and Valine Metabolism	1840	131	0.92	-0.12	0.2558	0.4115
M1956	alpha-hydroxycaproate	Lipid	Fatty Acid, Monohydroxy	1920	131	1.38	0.47	0.2574	0.4134
M3121	sphingomyelin (d18:1/20:0, d16:1								

M1566	hexadecadienoate (16:2n6)	Lipid	Long Chain Polyunsaturated Fatty Acid (n3 and n6)	5398	251	1.12	0.16	0.2805	0.4397
M2862	1-arachidonoylglycerol (20:4)	Lipid	Monoacylglycerol	6250	303	0.88	-0.19	0.2830	0.4401
M2358	1-oleoyl-2-docosahexaenoyl-GPC (18:1/22:6)*	Lipid	Phosphatidylcholine (PC)	2100	833	0.95	-0.08	0.2832	0.4401
M6443	bilirubin degradation product, C16H18N2O5 (1)	PCM	PCM	3098	317	1.34	0.42	0.2817	0.4401
M4590	caffeine	Xenobiotics	Xanthine Metabolism	2106	195	0.71	-0.49	0.2818	0.4401
M427	isobutyrylglycine (C4)	Amino Acid	Leucine, Isoleucine and Valine Metabolism	1420	144	0.83	-0.27	0.2828	0.4401
M3340	androsterone glucuronide	Lipid	Androgenic Steroids	4953	465	0.78	-0.35	0.2841	0.4407
M364	beta-hydroxyisovalerylcarnitine	Amino Acid	Leucine, Isoleucine and Valine Metabolism	2584	262	0.92	-0.13	0.2846	0.4408
M2808	1-(1-enyl-palmitoyl)-2-oleyl-GPE (P-16:0/18:1)*	Lipid	Plasmalogens	2750	703	0.94	-0.10	0.2876	0.4417
M2534	1-palmitoyl-2-oleyl-GPI (16:0/18:1)*	Lipid	Phosphatidylinositol (PI)	3140	855	0.92	-0.12	0.2879	0.4417
M1164	Fibrinopeptide A (8-16)	Peptide	Fibrinogen Cleavage Peptide	3944	903	0.89	-0.16	0.2881	0.4417
M1443	isocitrate	Energy	TCA Cycle	773	210	1.10	0.13	0.2881	0.4417
M190	phenol sulfate	Amino Acid	Tyrosine Metabolism	2156	173	0.66	-0.59	0.2872	0.4417
M3001	sphinganine-1-phosphate	Lipid	Sphingolipid Synthesis	1431	362	1.08	0.11	0.2878	0.4417
M563	4-guanidinobutanate	Amino Acid	Guanidino and Acetamido Metabolism	2320	146	0.87	-0.21	0.2912	0.4441
M1351	mannitol/sorbitol	Carbohydrate	Fructose, Mannose and Galactose Metabolism	2320	181	0.61	-0.72	0.2910	0.4441
M487	ornithine	Amino Acid	Urea cycle; Arginine and Proline Metabolism	2800	133	0.92	-0.12	0.2910	0.4441
M5129	2-keto-3-deoxy-gluconate	Xenobiotics	Food Component/Plant	1900	177	0.90	-0.15	0.2957	0.4502
M2014	13-HODE + 9-HODE	Lipid	Fatty Acid, Monohydroxy	5275	295	1.12	0.16	0.2970	0.4515
M1431	erythronate*	Carbohydrate	Aminosugar Metabolism	2186	135	0.93	-0.11	0.2990	0.4538
M37	N-acetylspartate (NAAs)	Amino Acid	Alanine and Aspartate Metabolism	3143	174	0.89	-0.16	0.3011	0.4561
M141	N-acetylphenylalanine	Amino Acid	Phenylalanine Metabolism	2597	206	1.14	0.19	0.3027	0.4578
M5064	3-hydroxystachydrine*	Xenobiotics	Food Component/Plant	1049	160	0.68	-0.56	0.3036	0.4584
M3051	ceramide (d16:1/24:1, d18:1/22:1)*	Lipid	Ceramides	3850	621	1.09	0.12	0.3051	0.4593
M867	leucylalanine	Peptide	Dipeptide	2264	201	0.83	-0.26	0.3052	0.4593
M1689	dodecadienoate (12:2)*	Lipid	Fatty Acid, Dicarboxylate	5146	195	1.10	0.13	0.3059	0.4596
M3099	palmityl dihydroxyphingomyelin (d18:0/16:0)*	Lipid	Dihydroxyphingomyelins	2290	706	0.95	-0.07	0.3071	0.4607
M2877	1-heptadecenoylglycerol (17:1)*	Lipid	Monoacylglycerol	6390	267	0.72	-0.48	0.3130	0.4688
M5063	stachydrine	Xenobiotics	Food Component/Plant	1440	144	0.78	-0.36	0.3180	0.4754
M2933	linoleyl-linolenyl-glycerol (18:2/18:3) [1]*	Lipid	Diacylglycerol	2426	633	1.32	0.40	0.3189	0.4760
M3526	glycochoylate	Lipid	Secondary Bile Acid Metabolism	5020	464	1.35	0.43	0.3232	0.4816
M146	1-carboxyethylphenylalanine	Amino Acid	Phenylalanine Metabolism	2844	236	0.87	-0.20	0.3281	0.4881
M2941	linoleyl-arachidonoyl-glycerol (18:2/20:4) [1]*	Lipid	Diacylglycerol	2590	659	0.90	-0.15	0.3290	0.4886
M1451	malate	Energy	TCA Cycle	615.6	133	1.10	0.14	0.3302	0.4896
M16	2-methylserine	Amino Acid	Glycine, Serine and Threonine Metabolism	1652	120	0.84	-0.24	0.3355	0.4959
M60	2-pyrrolidinone	Amino Acid	Glutamate Metabolism	1262	86	0.91	-0.13	0.3353	0.4959
M6450	bilirubin degradation product, C16H18N2O5 (3)	PCM	PCM	3354	317	1.25	0.32	0.3368	0.4969
M6152	dimethyl sulfone	Xenobiotics	Chemical	832	95	0.81	-0.30	0.3377	0.4975
M7	betaine	Amino Acid	Glycine, Serine and Threonine Metabolism	1064	118	0.94	-0.09	0.3413	0.5017
M1694	tetradecadienoate (C14:2-DC)*	Lipid	Fatty Acid, Dicarboxylate	3148	253	1.13	0.18	0.3416	0.5017
M1699	octadecenoate (C18:1-DC)	Lipid	Fatty Acid, Dicarboxylate	4875	311	0.90	-0.15	0.3426	0.5023
M1531	10-heptadecenoate (17:1n7)	Lipid	Long Chain Monounsaturated Fatty Acid	5555	267	1.12	0.16	0.3467	0.5066
M1960	2-hydroxyoctanoate	Lipid	Fatty Acid, Monohydroxy	3736.8	159	1.38	0.47	0.3466	0.5066
M1159	Fibrinopeptide A (3-15)	Peptide	Fibrinogen Cleavage Peptide	2419	596	1.13	0.17	0.3479	0.5077
M2322	1-stearoyl-2-oleoyl-GPC (18:0/18:1)	Lipid	Phosphatidylcholine (PC)	2644	789	1.06	0.08	0.3531	0.5127
M156	2-hydroxyphenylacetate	Amino Acid	Phenylalanine Metabolism	858.6	151	1.19	0.25	0.3523	0.5127
M1491	caprylate (8:0)	Amino Acid	Urea cycle; Arginine and Proline Metabolism	1335	130	0.74	-0.43	0.3527	0.5127
M650	gamma-glutamyl 2-aminobutyrate	Lipid	Medium Chain Fatty Acid	4362	143	0.80	-0.32	0.3543	0.5130
M443	hydroxysparagine	Peptide	Gamma-glutamyl Amino Acid	2380	233	0.91	-0.14	0.3544	0.5130
M3502	taurolicholate 3-sulfate	Amino Acid	Alanine and Aspartate Metabolism	1149	149	0.94	-0.09	0.3572	0.5163
M6452	glutamine_degradant*	Lipid	Secondary Bile Acid Metabolism	5027	281	1.30	0.38	0.3597	0.5190
M86	N-acetylcarnosine	Amino Acid	PCM	1900	129	1.17	0.22	0.3608	0.5198
M2278	1,2-dipalmitoyl-GPC (16:0/16:0)	Lipid	Histidine Metabolism	2141	269	0.90	-0.15	0.3615	0.5200
M2297	1-palmitoyl-2-arachidonoyl-GPC (16:0/20:4n6)	Lipid	Phosphatidylcholine (PC)	2450	735	1.06	0.08	0.3638	0.5210
M1980	3-hydroxyoctanoate	Lipid	Phosphatidylcholine (PC)	2200	783	0.96	-0.06	0.3644	0.5210
M3264	androstenediol (3beta,17beta) disulfate (2)	Lipid	Fatty Acid, Monohydroxy	3446	159	1.10	0.14	0.3653	0.5210
M4433	carotene diol (3)	Cofactors and Vitamins	Androgenic Steroids	4065	224	0.90	-0.14	0.3652	0.5210
M1186	phenylacetylglutamate	Peptide	Vitamin A Metabolism	1948	568	0.88	-0.18	0.3649	0.5210
M2861	1-dihomo-linolenylglycerol (20:3)	Lipid	Acetylated Peptides	1570	264	0.87	-0.20	0.3657	0.5210
M489	3-amino-2-piperidone	Amino Acid	Monacylglycerol	6400	305	0.87	-0.20	0.3678	0.5210
M210	homovanillate (HVA)	Amino Acid	Urea cycle; Arginine and Proline Metabolism	2065	115	0.92	-0.12	0.3667	0.5210
M3311	tetrahydrocortisol sulfate (1)	Lipid	Tyrosine Metabolism	1649	181	1.13	0.18	0.3674	0.5210
M4466	2-hydroxyhippurate (salicylate)	Xenobiotics	Corticosteroids	4276	445	1.53	0.61	0.3680	0.5210
M6259	3,5-dichloro-2,6-dihydroxybenzoic acid	Lipid	Benzene Metabolism	2184	194	0.49	-1.02	0.3717	0.5239
M3175	3-hydroxy-3-methylglutarate	Xenobiotics	Chemical	693	221	0.93	-0.11	0.3716	0.5239
M4264	2'-O-methylcytidine	Nucleotide	Mevalonate Metabolism	2850	161	0.93	-0.11	0.3715	0.5239
M4368	gamma-CEHC	Cofactors and Vitamins	Pyrimidine Metabolism, Cytidine containing	2411	258	1.13	0.17	0.3737	0.5259
M4410	bilirubin (E,Z or Z,E)*	Lipid	Tocopherol Metabolism	3843	263	1.19	0.26	0.3750	0.5269
M2542	1-stearoyl-2-oleoyl-GPI (18:0/18:1)*	Lipid	Hemoglobin and Porphyrin Metabolism	1265	585	0.90	-0.15	0.3769	0.5288
M440	methionine sulfoxide	Amino Acid	Phosphatidylinositol (PI)	3711	883	0.93	-0.10	0.3776	0.5289
M3114	sphingomyelin (d18:2/14:0, d18:3/18:1)*	Lipid	Methionine, Cysteine, SAM and Taurine Metabolism	1272	166	0.91	-0.14	0.3794	0.5306
M2339	1-stearoyl-2-docosahexaenoyl-GPC (18:0/22:6)	Lipid	Sphingomyelins	1860	674	0.91	-0.13	0.3809	0.5319
M5404	salicylic glucuronide*	Xenobiotics	Drug - Analgesics, Anesthetics	2300	835	1.04	0.06	0.3818	0.5323
M204	3-methoxytyrosine	Amino Acid	Pyrimidine Metabolism, Cytidine containing	1463	370	0.55	-0.87	0.3833	0.5336
M2934	linoleyl-linolenyl-glycerol (18:2/18:3) [2]*	Lipid	Tyrosine Metabolism	2555	212	0.90	-0.15	0.3853	0.5355
M2283	1-palmitoyl-2-oleoyl-GPC (16:0/18:1)	Lipid	Diacylglycerol	2478	633	1.21	0.27	0.3881	0.5386
M4284	methylphosphate	Nucleotide	Phosphatidylcholine (PC)	2450	761	1.04	0.05	0.3891	0.5392
M2915	palmityl-oleoyl-arachidonoyl-glycerol (16:1/20:4) [2]*	Lipid	Purine and Pyrimidine Metabolism	544	113	0.92	-0.12	0.3916	0.5409
M400	bijigI carnitine (C5)	Amino Acid	Diacylglycerol	2528	633	0.83	-0.28	0.3912	0.5409
M1613	Fibrinopeptide A (7-16)*	Peptide	Short Chain Fatty Acid	1962	244	0.87	-0.20	0.3921	0.5409
M512	N-methylhydroxyproline	Amino Acid	Long Chain Polyunsaturated Fatty Acid (n3 and n6)	1145	146	0.73	-0.46	0.3953	0.5436
M4349	ascorbic acid 3-sulfate*	Cofactors and Vitamins	Ascorbate and Aldarate Metabolism	2025	255	0.89	-0.16	0.3998	0.5489
M2907	palmitoyl-linoleoyl-glycerol (16:0/18:2) [2]*	Lipid	Diacylglycerol	3197	611	0.92	-0.12	0.4011	0.5499
M1700	octadecadienoate (C18:2-DC)*	Lipid	Fatty Acid, Dicarboxylate	4676	309	0.82	-0.28	0.4041	0.5532
M1487	butyrate/isobutyrate (4:0)	Lipid	Short Chain Fatty Acid	1062	87	0.88	-0.18	0.4060	0.5542
M1560	eicosapentaenoate (EPA; 20:5n3)	Lipid	Long Chain Polyunsaturated Fatty Acid (n3 and n6)	5450	301	1.10	0.14	0.4060	0.5542
M6451	bilirubin degradation product, C16H18N2O5 (4)	PCM	PCM	3428	317	1.21	0.27	0.4067	0.5543
M2410	1-palmitoyl-2-linoleoyl-GPE (16:0/18:2)	Lipid	Phosphatidylethanolamine (PE)	2350	717	1.08	0.11	0.4132	0.5619
M6399	glutamine conjugate of C6H10O2 (1)*	PCM	PCM	2404	241	0.88	-0.19	0.4135	0.5619
M439	methionine sulfone	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	1250	182	0.88	-0.19	0.4188	0.5674
M3283	pregnanediol-3-glucuronide	Lipid	Progester Steroids	5145	495	1.15	0.20	0.4187	0.5674
M578	cys-gly, oxidized	Amino Acid	Glutathione Metabolism	2947	355	1.17	0.23	0.4195	0.5675
M1753	2-aminoocanoate	Lipid	Fatty Acid, Amino	750	160	1.30	0.37	0.4228	0.5693
M1179	Fibrinopeptide B (1-12)	Peptide	Fibrinogen Cleavage Peptide	2366	661	0.90	-0.16	0.4226	0.5693
M255	N-acetyltryptophan	Amino Acid	Tryptophan Metabolism	2630	245	0.91	-0.14	0.4217	0.5693
M274	N-formylanthranilic acid	Amino Acid	Tryptophan Metabolism	2150	164	1.20	0.26	0.4244	0.5707
M1962	2-hydroxydecanoate	Lipid	Fatty Acid, Monohydroxy	4840	187	1.15	0.20	0.4264	0.5726
M1576	docosapentaenoate (n6 DPA; 22:5n6)	Lipid	Long Chain Polyunsaturated Fatty Acid (n3 and n6)	5624.5	329	1.08	0.12	0.4273	0.5729
M385	isoleucine	Amino Acid	Leucine, Isoleucine and Valine Metabolism	2800	132	0.96	-0.06	0.4302	0.5751
M1550	tetradecadienoate (14:2)*	Lipid	Long Chain Polyunsaturated Fatty Acid (n3 and n6)	5292	223	1.10	0.14	0.4300	0.5751
M1648	(16 or 17)-methylsteareate (a19:0 or a19:0)	Lipid	Fatty Acid, Branched	5993	297	1.08	0.10	0.4320	0.5753
M6445	bilirubin degradation product, C17H18N2O4 (1)	PCM	PCM	4633	313	0.90	-0.16	0.4323	0.5753
M1510	palmitate (16:0)	Lipid	Long Chain Saturated Fatty Acid	5618	255	1.06	0.08	0.4318	0.5753
M1703	eicosenedioate (C20:1-DC)*	Lipid	Fatty Acid, Dicarboxylate	5095	339	0.95	-0.08	0.4362	0.5797
M348									

M1973	2-hydroxyarachidate*	Lipid	Fatty Acid, Monohydroxy	5990	327	0.95	-0.07	0.4670	0.6073
M3033	N-benzenoyl-sphingadienine (d18:2/22:0)*	Lipid	Ceramides	3911	621	0.95	-0.07	0.4668	0.6073
M1917	octadecanediolcarnitine (C18-DC)*	Lipid	Fatty Acid Metabolism (Acyl Carnitine, Dicarboxylate)	1227	458	1.14	0.19	0.4702	0.6106
M4352	2-O-methylascorbic acid	Cofactors and Vitamins	Ascorbate and Aldarate Metabolism	1512	189	0.94	-0.09	0.4735	0.6140
M1860	decanoylcarnitine (C10)	Lipid	Fatty Acid Metabolism (Acyl Carnitine, Medium Chain)	1130	316	1.08	0.10	0.4764	0.6169
M4432	carotene diol (2)	Cofactors and Vitamins	Cofactors and Vitamins	1904	568	0.92	-0.11	0.4776	0.6175
M3356	androsterone sulfate	Lipid	Androgenic Steroids	5022	369	0.88	-0.19	0.4789	0.6184
M1526	myristoleate (14:1n5)	Lipid	Long Chain Monounsaturated Fatty Acid	5346.9	225	1.10	0.13	0.4818	0.6212
M3339	16a-hydroxy DHEA 3-sulfate	Lipid	Androgenic Steroids	4240	383	0.85	-0.24	0.4828	0.6216
M3127	sphingomyelin (d18:2/22:2, d18:2/22:1, d16:1/24:2)*	Lipid	Sphingomyelins	2350	784	1.04	0.06	0.4852	0.6238
M4238	3-ureidopropionate	Nucleotide	Pyrimidine Metabolism, Uracil containing	875	133	1.16	0.21	0.4869	0.6252
M6260	3-bromo-5-chloro-2,6-dihydroxybenzoic acid*	Xenobiotics	Chemical	4505	265	0.94	-0.08	0.4904	0.6278
M5073	tartarate	Xenobiotics	Food Component/Plant	615.3	149	0.74	-0.43	0.4901	0.6278
M2539	1-palmitoyl-2-arachidonoyl-GPI (16:0/20:4)*	Lipid	Phosphatidylinositol (PI)	2567	877	0.91	-0.14	0.4914	0.6282
M6401	glutamine conjugate of C7H12O2*	PCM	PCM	3053	255	1.15	0.20	0.4923	0.6285
M6424	carnitine of C10H14O2 (5)*	PCM	PCM	4521	370	1.07	0.10	0.4968	0.6324
M3454	glycocholate	Lipid	Primary Bile Acid Metabolism	5163	464	1.21	0.28	0.4962	0.6324
M529	creatine	Amino Acid	Creatine Metabolism	2055	114	1.03	0.04	0.4993	0.6347
M1774	methylmalonate (MMA)	Lipid	Fatty Acid Metabolism (also BCAA Metabolism)	3078.4	117	0.93	-0.10	0.5056	0.6419
M4999	phytanate	Xenobiotics	Food Component/Plant	5908	311	0.90	-0.15	0.5091	0.6455
M4304	nicotinamide	Cofactors and Vitamins	Nicotinate and Nicotinamide Metabolism	1942	123	0.84	-0.26	0.5121	0.6484
M282	picolinate	Amino Acid	Tryptophan Metabolism	910	124	1.09	0.12	0.5139	0.6497
M394	3-methyl-2-oxovalerate	Amino Acid	Leucine, Isoleucine and Valine Metabolism	2064.2	129	0.95	-0.07	0.5151	0.6503
M3109	sphingomyelin (d18:2/18:1)*	Lipid	Sphingomyelins	2025	728	1.04	0.05	0.5185	0.6537
M6221	3-hydroxypyridine sulfate	Xenobiotics	Chemical	1595.5	174	0.63	-0.66	0.5202	0.6549
M2303	1-palmitoyl-2-docosahexaenoyl-GPC (16:0/22:6)	Lipid	Phosphatidylcholine (PC)	2055	807	0.97	-0.04	0.5215	0.6557
M1921	3-hydroxyhexanoylcarnitine (1)	Lipid	Fatty Acid Metabolism (Acyl Carnitine, Hydroxy)	2918	276	1.10	0.13	0.5287	0.6638
M1430	N-acetylglucosaminylsphingosine	Carbohydrate	Aminosugar Metabolism	1212	336	0.95	-0.08	0.5338	0.6674
M4419	N-carbamoylvaline	Amino Acid	Leucine, Isoleucine and Valine Metabolism	1270	159	0.91	-0.14	0.5338	0.6674
M4451	pyridoxate	Cofactors and Vitamins	Vitamin B6 Metabolism	2185	182	1.09	0.12	0.5334	0.6674
M3206	7-HOCA	Lipid	Sterol	5288.1	429	0.96	-0.06	0.5354	0.6685
M1160	Fibrinopeptide A (4-15)	Peptide	Fibrinogen Cleavage Peptide	2570	552	1.10	0.14	0.5378	0.6706
M2262	1-myristoyl-2-palmitoyl-GPC (14:0/16:0)	Lipid	Phosphatidylcholine (PC)	2250	707	0.92	-0.11	0.5416	0.6713
M2721	1-stearoyl-GPI (18:0)	Lipid	Lysophospholipid	5794	599	0.96	-0.06	0.5435	0.6713
M1966	2-hydroxylaurate	Lipid	Fatty Acid, Monohydroxy	5211	215	0.96	-0.06	0.5422	0.6713
M120	5-(galactosyloxy)-L-lysine	Amino Acid	Lysine Metabolism	2755	325	0.94	-0.09	0.5415	0.6713
M4435	beta-cryptoxanthin	Cofactors and Vitamins	Vitamin A Metabolism	2560	552	0.86	-0.22	0.5393	0.6713
M4164	N6-carbamoylthreonyladenosine	Nucleotide	Purine Metabolism, Adenine containing	2164	411	0.92	-0.12	0.5410	0.6713
M4335	pantoate	Cofactors and Vitamins	Pantothenate and CoA Metabolism	1143	147	1.12	0.17	0.5432	0.6713
M1699	octadecanedioate (C18)	Lipid	Fatty Acid, Dicarboxylate	5043	313	1.07	0.10	0.5458	0.6732
M2873	2-arachidonoylglycerol (20:4)	Lipid	Monacylglycerol	6170	303	0.93	-0.11	0.5490	0.6762
M151	phenylfatty acid (PLA)	Amino Acid	Phenylalanine Metabolism	2208	165	1.09	0.12	0.5539	0.6813
M6417	glycine conjugate of C10H12O2*	PCM	PCM	4005	220	1.10	0.14	0.5562	0.6825
M150	phenylpyruvate	Amino Acid	Phenylalanine Metabolism	2515	163	1.07	0.10	0.5564	0.6825
M2731	1-arachidonoyl-GPI* (20:4)*	Lipid	Lysophospholipid	5482	619	0.96	-0.06	0.5718	0.7005
M643	gamma-glutamylphenylalanine	Peptide	Gamma-glutamyl Amino Acid	1825	293	1.06	0.08	0.5738	0.7020
M4530	4-vinylcatechol sulfate	Xenobiotics	Benzene Metabolism	3060	215	0.70	-0.52	0.5757	0.7033
M554	N1,N12-diacylsperrmine	Amino Acid	Polyamine Metabolism	3105	287	0.76	-0.40	0.5769	0.7039
M564	guanidinoisuccinate	Amino Acid	Guanidino and Acetamido Metabolism	640.2	174	1.13	0.18	0.5788	0.7053
M2444	1-oleoyl-2-linoleoyl-GPE (18:1/18:2)*	Lipid	Phosphatidylethanolamine (PE)	2270	743	1.06	0.09	0.5828	0.7086
M546	N(1')-acetylperrmine	Amino Acid	Polyamine Metabolism	3075	188	0.83	-0.28	0.5831	0.7086
M3130	sphingomyelin (d18:2/24:1, d18:1/24:2)*	Lipid	Sphingomyelins	2750	812	1.02	0.03	0.5862	0.7115
M2286	1-palmitoyl-2-linoleoyl-GPC (16:0/18:2)	Lipid	Phosphatidylcholine (PC)	2160	759	0.98	-0.03	0.5877	0.7122
M2543	1-stearoyl-2-linoleoyl-GPI (18:0/18:2)	Lipid	Phosphatidylinositol (PI)	3185	881	1.05	0.07	0.5899	0.7132
M6190	perfluorooctanesulfonate (PFOS)	Xenobiotics	Chemical	662	499	0.91	-0.13	0.5900	0.7132
M4153	1-methyldenosine	Nucleotide	Purine Metabolism, Adenine containing	2120	282	1.07	0.09	0.5917	0.7143
M829	glycylaline	Peptide	Dipeptide	2734	175	1.40	0.48	0.5941	0.7162
M1986	3-hydroxymyristate	Lipid	Fatty Acid, Monohydroxy	5335	243	1.06	0.09	0.5977	0.7197
M3117	sphingomyelin (d18:2/16:0, d18:1/16:1)*	Lipid	Sphingomyelins	2002	702	1.02	0.04	0.5993	0.7206
M515	prolylhydroxyproline	Amino Acid	Urea cycle; Arginine and Proline Metabolism	2128	229	0.94	-0.09	0.6009	0.7215
M6239	thioproline	Xenobiotics	Chemical	1250	134	1.04	0.06	0.6043	0.7246
M91	1-methyl-4-imidazoleacetate	Amino Acid	Histidine Metabolism	2064	141	0.84	-0.24	0.6120	0.7319
M4523	4-ethylphenyl sulfate	Xenobiotics	Benzene Metabolism	3580	201	0.75	-0.41	0.6119	0.7319
M2279	1-palmitoyl-2-palmitoyl-GPC (16:0/16:1)*	Lipid	Phosphatidylcholine (PC)	2200	733	0.95	-0.08	0.6139	0.7324
M4544	methyl-4-hydroxybenzoate sulfate	Xenobiotics	Benzene Metabolism	2873	231	0.81	-0.31	0.6147	0.7324
M3103	palmitoyl sphingomyelin (d18:1/16:0)	Lipid	Sphingomyelins	2168	704	0.99	-0.02	0.6147	0.7324
M1445	alpha-ketoglutarate	Energy	TCA Cycle	2700	145	1.05	0.06	0.6205	0.7382
M3363	androstenediol (3beta,17beta) disulfate (1)	Lipid	Androgenic Steroids	3740	224	0.92	-0.12	0.6221	0.7387
M3105	stearyl sphingomyelin (d18:1/18:0)	Lipid	Sphingomyelins	2450	732	0.98	-0.04	0.6225	0.7387
M6447	bilirubin degradation product, C17H18N2O4 (3)	PCM	PCM	4906	313	0.93	-0.10	0.6235	0.7387
M3484	deoxycholic acid glucuronide	Lipid	Secondary Bile Acid Metabolism	4800	567	1.09	0.13	0.6241	0.7387
M4223	2'-O-methyluridine	Nucleotide	Pyrimidine Metabolism, Uracil containing	1831	257	0.94	-0.09	0.6252	0.7391
M6444	bilirubin degradation product, C16H18N2O5 (2)	PCM	PCM	3204	317	1.10	0.13	0.6282	0.7416
M1924	3-hydroxyoctanoic carnitine (1)	Lipid	Fatty Acid Metabolism (Acyl Carnitine, Hydroxy)	3445	304	1.06	0.08	0.6330	0.7453
M3353	etiocholanolone glucuronide	Lipid	Androgenic Steroids	4915	465	0.93	-0.11	0.6322	0.7453
M2582	1-palmitoyl-GPA (16:0)	Lipid	Lysophospholipid	5600	409	0.94	-0.09	0.6392	0.7517
M2277	N-formylphenylalanine	Amino Acid	Tyrosine Metabolism	2360	192	1.16	0.22	0.6454	0.7580
M3122	sphingomyelin (d18:1/20:1, d18:2/20:0)*	Lipid	Sphingomyelins	2450	758	0.98	-0.03	0.6468	0.7587
M1857	nonanoylcarnitine (C9)	Lipid	Fatty Acid Metabolism (Acyl Carnitine, Medium Chain)	1010	302	0.94	-0.09	0.6478	0.7588
M1985	3-hydroxylaurate	Lipid	Fatty Acid, Monohydroxy	5175	215	1.06	0.08	0.6548	0.7661
M4476	benzoate	Xenobiotics	Benzene Metabolism	1750	121	1.11	0.15	0.6587	0.7688
M4595	theobromine	Xenobiotics	Xanthine Metabolism	1600	181	0.91	-0.14	0.6589	0.7688
M1642	(14 or 15)-methylpalmitate (17:0 or 17:0)	Lipid	Fatty Acid, Branched	5695	269	1.05	0.07	0.6701	0.7738
M4448	2,3-dihydroxy-5-methylthio-4-pentoate (DMTPA)*	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	1156	177	1.03	0.05	0.6676	0.7738
M3367	3-methylglutamate	Amino Acid	Leucine, Isoleucine and Valine Metabolism	2700	99	0.96	-0.06	0.6661	0.7738
M3343	4-methyl-2-oxopentanoate	Amino Acid	Leucine, Isoleucine and Valine Metabolism	2170	129	1.03	0.04	0.6649	0.7738
M528	creatinine	Amino Acid	Creatine Metabolism	1947	132	0.93	-0.11	0.6688	0.7738
M4648	cysteine sulfonic acid	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	597	154	1.05	0.07	0.6676	0.7738
M4364	delta-tocopherol	Cofactors and Vitamins	Tocopherol Metabolism	2259	402	1.08	0.12	0.6711	0.7738
M4192	N2,N2-dimethylguanosine	Nucleotide	Purine Metabolism, Guanine containing	2210	312	1.05	0.07	0.6702	0.7738
M1114	N6-methyllysine	Amino Acid	Lysine Metabolism	2831	161	0.92	-0.12	0.6708	0.7738
M3126	sphingomyelin (d18:1/22:0, d18:2/22:0; d16:1/24:1)*	Lipid	Sphingomyelins	2775	786	0.98	-0.03	0.6716	0.7738
M2942	linoleoyl-arachidonylglycerol (18:2/20:4) [2]*	Lipid	Diacylglycerol	2650	659	0.96	-0.06	0.6745	0.7751
M1885	palmitoleoylcarnitine (C16:1)*	Lipid	Fatty Acid Metabolism (Acyl Carnitine, Monounsaturated)	1357	398	0.96	-0.06	0.6739	0.7751
M579	5-oxoproline	Amino Acid	Glutathione Metabolism	738.5	128	1.06	0.08	0.6803	0.7808
M1509	pentadecanolate (15:0)	Lipid	Long Chain Saturated Fatty Acid	5521	241	1.04	0.06	0.6824	0.7822
M3052	ceramide (d18:2/24:1, d18:1/24:2)*	Lipid	Ceramides	3858	647	1.03	0.04	0.6840	0.7831
M62	S-1-pyrroline-5-carboxylate	Amino Acid	Glutamate Metabolism	1528	114	0.97	-0.05	0.6864	0.7848
M1119	5-hydroxylysine	Amino Acid	Lysine Metabolism	2790	163	0.97	-0.05	0.6882	0.7859
M2906	palmitoyl-linoleoyl-glycerol (16:0/18:2) [1]*	Lipid	Diacylglycerol	3080	611	0.95	-0.07	0.6947	0.7923
M3514	glycurosoodeoxycholate	Lipid	Secondary Bile Acid Metabolism	5033	448	0.82	-0.29	0.6973	0.7942
M3116	sphingomyelin (d17:2/16:0, d18:2/15:0)*	Lipid	Sphingomyelins	1875	688	0.96	-0.06	0.6993	0.7956
M1929	3-hydroxyoleoylcarnitine	Lipid	Fatty Acid Metabolism (Acyl Carnitine, Hydroxy)	1406	442	0.94	-0.09	0.7013	0.7959
M1507	myristate (14:0)	Lipid	Long Chain Saturated Fatty Acid	5440	227	0.96	-0.06	0.7012	

M3504	ursodeoxycholate	Lipid	Secondary Bile Acid Metabolism	5055	391	0.81	-0.31	0.7414	0.8259
M1504	5-dodecanoate (12:1n7)	Lipid	Medium Chain Fatty Acid	5224	197	1.04	0.06	0.7454	0.8273
M1449	fumarate	Energy	TCA Cycle	3084	115	0.97	-0.05	0.7445	0.8273
M73	N-acetylhistidine	Amino Acid	Histidine Metabolism	2065	198	0.92	-0.11	0.7449	0.8273
M6252	5-hydroxy-2-methylpyridine sulfate	Xenobiotics	Chemical	2074	188	0.76	-0.39	0.7474	0.8285
M1705	3-carboxy-4-methyl-5-propyl-2-furanpropanoate (CMPPF)	Lipid	Fatty Acid, Dicarboxylate	2800	239	0.95	-0.07	0.7593	0.8390
M1927	3-hydroxydecanoylcarnitine	Lipid	Fatty Acid Metabolism (Acyl Carnitine, Hydroxy)	961	332	1.04	0.05	0.7589	0.8390
M287	serotonin	Amino Acid	Tryptophan Metabolism	2550	177	1.08	0.11	0.7596	0.8390
M476	succinyltaurine	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	2572	224	1.07	0.09	0.7605	0.8390
M1995	5-hydroxyhexanoate	Lipid	Fatty Acid, Monohydroxy	1267	131	1.05	0.08	0.7631	0.8408
M1239	pyruvate	Carbohydrate	Glycolysis, Gluconeogenesis, and Pyruvate Metabolism	1083	87	0.97	-0.04	0.7671	0.8441
M5328	N-methylpipecolate	Xenobiotics	Bacteria/Fungal	1932	144	0.91	-0.14	0.7684	0.8446
M2723	1-oleoyl-GPI (18:1)	Lipid	Lysophospholipid	5599	597	1.03	0.04	0.7711	0.8465
M36	aspartate	Amino Acid	Alanine and Aspartate Metabolism	1165	134	1.03	0.05	0.7727	0.8473
M1498	(2 or 3)-decanoate (10:1n7 or n8)	Lipid	Medium Chain Fatty Acid	4990	169	0.97	-0.05	0.7742	0.8479
M1136	glu-gly-asn-val	Peptide	Polypeptide	2675	418	1.07	0.10	0.7791	0.8512
M466	lanthionine	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	1730	209	1.02	0.03	0.7786	0.8512
M4408	bilirubin	Cofactors and Vitamins	Hemoglobin and Porphyrin Metabolism	1840	585	0.97	-0.04	0.7805	0.8517
M1982	3-hydroxydecanoate	Lipid	Fatty Acid, Monohydroxy	4634.7	187	1.03	0.05	0.7843	0.8528
M1573	arachidonate (20:4n6)	Lipid	Long Chain Polyunsaturated Fatty Acid (n3 and n6)	5535	303	1.03	0.04	0.7833	0.8528
M1768	butyrylcarnitine (C4)	Lipid	Fatty Acid Metabolism (also BCAA Metabolism)	2860	232	0.95	-0.08	0.7839	0.8528
M4407	heme	Cofactors and Vitamins	Hemoglobin and Porphyrin Metabolism	1124	616	1.14	0.20	0.7862	0.8539
M1840	acetylcarnitine (C2)	Lipid	Fatty Acid Metabolism (Acyl Carnitine, Short Chain)	2282	204	0.97	-0.04	0.7872	0.8539
M2841	glycerol	Lipid	Glycerolipid Metabolism	758	91	0.97	-0.04	0.7917	0.8578
M2325	1-stearoyl-2-linoleoyl-GPC (18:0/18:2)*	Lipid	Phosphatidylcholine (PC)	2450	787	0.99	-0.01	0.7956	0.8609
M1891	linoleoylcarnitine (C18:2)*	Lipid	Fatty Acid Metabolism (Acyl Carnitine, Polyunsaturated)	1430	424	0.98	-0.03	0.7997	0.8633
M2926	oleoyl-linoleoyl-glycerol (18:1/18:2) [1]	Lipid	Diacylglycerol	3115	637	1.03	0.04	0.7994	0.8633
M3380	5alpha-androstan-3alpha,17beta-diol disulfate	Lipid	Androgenic Steroids	4275	225	0.91	-0.13	0.8071	0.8703
M3106	behenoyl sphingomyelin (d18:1/22:0)*	Lipid	Sphingomyelins	3250	788	1.01	0.02	0.8097	0.8720
M4498	cathochol sulfate	Xenobiotics	Benzene Metabolism	1906	189	0.87	-0.20	0.8129	0.8744
M3047	ceramide (d18:1/14:0, d16:1/6:0)*	Lipid	Ceramides	2477	510	0.98	-0.03	0.8176	0.8784
M2333	1-stearoyl-2-arachidonoyl-GPC (18:0/20:4)	Lipid	Phosphatidylcholine (PC)	2400	811	1.01	0.01	0.8219	0.8821
M51	4-hydroxyglutamate	Amino Acid	Glutamate Metabolism	1141	164	1.02	0.03	0.8230	0.8822
M3500	glycocholic acid sulfate*	Lipid	Secondary Bile Acid Metabolism	5011	256	1.06	0.08	0.8258	0.8841
M33	N,N-dimethylalanine	Amino Acid	Alanine and Aspartate Metabolism	1370	118	0.94	-0.09	0.8289	0.8865
M4126	N1-methylnosine	Nucleotide	Purine Metabolism, (Hypo)Xanthine/Inosine containing	1430	283	0.97	-0.04	0.8330	0.8898
M449	2-hydroxy-4-(methylthio)butanoic acid	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	1065	149	0.98	-0.03	0.8345	0.8903
M1674	heptenedioate (C7:1-DC)*	Lipid	Fatty Acid, Dicarboxylate	2816	157	0.97	-0.04	0.8387	0.8938
M1439	citrate	Energy	TCA Cycle	582	191	0.98	-0.02	0.8451	0.8995
M2536	1-palmitoyl-2-linoleoyl-GPI (16:0/18:2)	Lipid	Phosphatidylinositol (PI)	2730	853	1.02	0.02	0.8528	0.9008
M556	5-methylthioadenosine (MTA)	Amino Acid	Polyamine Metabolism	2752	298	0.98	-0.03	0.8543	0.9008
M3193	cholesterol sulfate	Lipid	Sterol	681	465	0.98	-0.03	0.8505	0.9008
M1563	docosahexaenoate (DHA; 22:6n3)	Lipid	Long Chain Polyunsaturated Fatty Acid (n3 and n6)	5525	327	1.01	0.02	0.8516	0.9008
M3134	palmityl-sphingosine-phosphate/ethanolamine (d18:1/16:0)	Lipid	Ceramide PEs	2207	662	1.01	0.01	0.8538	0.9008
M3115	spingomyelin (d17:1/16:0, d18:1/15:0, d16:1/17:0)*	Lipid	Sphingomyelins	2082	690	0.99	-0.02	0.8473	0.9008
M3119	spingomyelin (d18:1/18:1, d18:2/18:0)	Lipid	Sphingomyelins	2167	730	1.01	0.02	0.8499	0.9008
M6205	trizma acetate	Xenobiotics	Chemical	1884	122	1.15	0.20	0.8509	0.9008
M4186	7-methylguanine	Nucleotide	Purine Metabolism, Guanine containing	2175	166	1.02	0.03	0.8658	0.9119
M4239	beta-alanine	Nucleotide	Pyrimidine Metabolism, Uracil containing	1905	90	0.99	-0.01	0.8687	0.9129
M3110	spingomyelin (d18:2/23:1)*	Lipid	Sphingomyelins	2500	798	1.01	0.02	0.8681	0.9129
M1562	docosapentaenoate (DPA; 22:5n3)	Lipid	Long Chain Polyunsaturated Fatty Acid (n3 and n6)	5571	329	1.02	0.02	0.8714	0.9146
M1929	3-hydroxyoctanoylcarnitine (2)	Lipid	Fatty Acid Metabolism (Acyl Carnitine, Hydroxy)	3497	304	0.98	-0.03	0.8741	0.9162
M3525	hyocholate	Lipid	Secondary Bile Acid Metabolism	5046	407	1.03	0.04	0.8749	0.9162
M4360	alpha-tocopherol	Cofactors and Vitamins	Tocopherol Metabolism	2522	430	0.99	-0.01	0.8760	0.9163
M4504	4-ethylacetohol sulfate	Xenobiotics	Benzene Metabolism	3379	217	0.90	-0.15	0.8799	0.9194
M1919	(R)-3-hydroxybutyrylcarnitine	Lipid	Fatty Acid Metabolism (Acyl Carnitine, Hydroxy)	2400	248	1.05	0.07	0.8829	0.9203
M647	gamma-glutamylvaline	Peptide	Gamma-glutamyl Amino Acid	2700	247	0.99	-0.02	0.8822	0.9203
M3280	5alpha-pregn-3beta,20alpha-diol disulfate	Lipid	Progesterin Steroids	3962	239	1.02	0.03	0.8911	0.9278
M133	6-oxopiperidine-2-carboxylate	Amino Acid	Lysine Metabolism	965	142	0.96	-0.06	0.8931	0.9289
M4450	pyridoxal	Cofactors and Vitamins	Vitamin B6 Metabolism	2343	168	1.00	-0.01	0.9015	0.9365
M3368	androstenediol (3alpha, 17alpha)-monosulfate (3)	Lipid	Androgenic Steroids	5180	369	1.02	0.03	0.9047	0.9388
M407	ethylmalonate	Amino Acid	Leucine, Isoleucine and Valine Metabolism	2785	131	1.03	0.04	0.9063	0.9394
M1668	3-hydroxyadipate	Lipid	Fatty Acid, Dicarboxylate	3131	161	1.02	0.03	0.9100	0.9422
M56	beta-ctrylglyutamate	Amino Acid	Glutamate Metabolism	900	322	0.98	-0.04	0.9148	0.9446
M2198	N-oleoylserrine	Lipid	Endocannabinoid	5600	368	0.99	-0.01	0.9155	0.9446
M5116	4-vinyloguaicol sulfate	Xenobiotics	Food Component/Plant	3354	229	1.10	0.13	0.9140	0.9446
M1663	2-hydroxyglutarate	Lipid	Fatty Acid, Dicarboxylate	958	166	1.04	0.06	0.9238	0.9495
M577	cysteinylglycine disulfide*	Amino Acid	Glutathione Metabolism	2547	298	1.01	0.01	0.9223	0.9495
M544	N-acetyl-isoptreanine	Amino Acid	Polyamine Metabolism	2305	203	0.96	-0.06	0.9244	0.9495
M1681	sebacate (C10:0C)	Lipid	Fatty Acid, Dicarboxylate	1788	201	1.02	0.03	0.9229	0.9495
M110	N2-acetyl,N6,N6-dimethyllysine	Amino Acid	Lysine Metabolism	2172	217	1.05	0.07	0.9294	0.9524
M1184	phenylacetylcarnitine	Peptide	Acetylated Peptides	3092	280	1.02	0.03	0.9290	0.9524
M2452	1,2-dilinoleoyl-GPE (18:2/18:2)*	Lipid	Phosphatidylethanolamine (PE)	2150	741	1.02	0.02	0.9316	0.9537
M1879	3-decanoylcarnitine	Lipid	Fatty Acid Metabolism (Acyl Carnitine, Monounsaturated)	1045	314	1.01	0.01	0.9373	0.9562
M1980	3-hydroxyocteate	Lipid	Fatty Acid, Monohydroxy	5674	299	1.02	0.02	0.9367	0.9562
M1862	myristoylcarnitine (C14)	Lipid	Fatty Acid Metabolism (Acyl Carnitine, Long Chain Saturated)	1350	372	0.99	-0.01	0.9367	0.9562
M1564	docosatrienoate (22:3n3)	Lipid	Long Chain Polyunsaturated Fatty Acid (n3 and n6)	5823	333	0.99	-0.01	0.9431	0.9610
M1920	(S)-3-hydroxybutyrylcarnitine	Lipid	Fatty Acid Metabolism (Acyl Carnitine, Hydroxy)	2340	248	1.01	0.02	0.9466	0.9626
M264	tryptophan betaine	Amino Acid	Tryptophan Metabolism	2673	247	0.98	-0.03	0.9467	0.9626
M2033	2S,3R-dihydroxybutyrate	Lipid	Fatty Acid, Dihydroxy	1660	119	0.99	-0.01	0.9527	0.9676
M428	3-hydroxyisobutyrate	Amino Acid	Leucine, Isoleucine and Valine Metabolism	1619	103	0.99	-0.01	0.9555	0.9694
M6254	3-hydroxy-2-methylpyridine sulfate	Xenobiotics	Chemical	1849	188	0.96	-0.06	0.9607	0.9736
M3461	glycochenodeoxycholate	Lipid	Primary Bile Acid Metabolism	5236.1	448	0.99	-0.01	0.9659	0.9777
M1852	octanoylcarnitine (C8)	Lipid	Fatty Acid Metabolism (Acyl Carnitine, Medium Chain)	950	288	1.00	0.01	0.9701	0.9809
M3219	4-cholesten-3-one	Lipid	Sterol	2520	385	1.00	0.00	0.9811	0.9865
M4251	cytidine	Nucleotide	Pyrimidine Metabolism, Cytidine containing	2124	244	1.00	0.01	0.9805	0.9865
M1346	fructose	Carbohydrate	Fructose, Mannose and Galactose Metabolism	2065	225	1.00	0.00	0.9808	0.9865
M267	kynurenine	Amino Acid	Tryptophan Metabolism	2739	209	1.00	0.00	0.9784	0.9865
M2927	oleoyl-linoleoyl-glycerol (18:1/18:2) [2]	Lipid	Diacylglycerol	3223	637	1.00	0.00	0.9777	0.9865
M3118	spingomyelin (d18:1/17:0, d17:3/18:0, d19:1/16:0)	Lipid	Sphingomyelins	2350	718	1.00	0.00	0.9824	0.9867
M1902	docosahexaenoylcarnitine (C22:6)*	Lipid	Fatty Acid Metabolism (Acyl Carnitine, Polyunsaturated)	1349	472	1.00	0.00	0.9843	0.9876
M1696	hexadecenedioate (C16:1-DC)*	Lipid	Fatty Acid, Dicarboxylate	4380	283	1.00	0.00	0.9874	0.9896
M4967	N-(2-furyl)glycine	Xenobiotics	Food Component/Plant	1525	168	1.01	0.02	0.9889	0.9900
M1682	decadienedioic acid (C10:2-DC)	Lipid	Fatty Acid, Dicarboxylate	2329.7	197	1.00	0.00	0.9940	0.9940

Supplementary data 2: UPLC-MS/MS metabolites in serum samples collected before the first NF

Compounds in column B for which no authentic standards were available for confirmation are marked with * after the compound name to designate these as Metabolomics Standards Initiative level 2/3

Fold change and log2 (fold change) were based on samples preceding vs. not preceding NF within 24 hours

p values are from Welch's two-sample t-test. q values are derived from p values after FDR correction for multiple testing

Color coding is column E was applied along the fold change gradient, with blue and red representing decreased and increased levels in NF vs. non-NF samples, respectively

Color coding in column H was applied along the q value gradient, with darker colors indicating more significant values

metabolite_code	metabolite	pathway	sub_pathway	foldchange	log2_foldchange	p	q
M397	2-methylbutyrylcarnitine (C5)	Amino Acid	Leucine, Isoleucine and Valine Metabolism	0.370871372	-1.431009186	1.20E-08	1.09E-05
M4120	hypoxanthine	Nucleotide	Purine Metabolism, (Hypo)Xanthine/Inosine containing	0.243273154	-2.039350971	2.58E-07	7.82E-05
M5	sarcosine	Amino Acid	Glycine, Serine and Threonine Metabolism	0.406750167	-1.297785157	1.78E-07	7.82E-05
M116	N6,N6,N6-trimethyllysine	Amino Acid	Lysine Metabolism	0.557239231	-0.856234883	5.34E-07	0.000121337
M4280	5,6-dihydrothymine	Nucleotide	Pyrimidine Metabolism, Thymine containing	0.053961552	-4.266411671	1.70E-06	0.000308421
M5410	celecoxib	Xenobiotics	Drug - Analgesics, Anesthetics	0.999999843	-2.27E-07	3.74E-06	0.00056603
M1857	nonanoylcarnitine (C9)	Lipid	Fatty Acid Metabolism (Acyl Carnitine, Medium Chain)	0.290098206	-1.78538672	4.76E-06	0.000617529
M3058	glycosy-N-stearoyl-sphingosine (d18:1/18:0)	Lipid	Hexosylceramides (HCKER)	0.449458773	-1.153739307	6.06E-06	0.000688198
M3082	glycosy1 ceramide (d18:2/24:1, d18:1/24:2)*	Lipid	Hexosylceramides (HCKER)	0.291841408	-1.7767435	7.82E-06	0.000790069
M2905	palmitoyl-oleoylglycerol (16:0/18:1) [2]*	Lipid	Diacylglycerol	0.49678811	-1.009297449	9.01E-06	0.000818917
M544	N-acetyl-isoproporeanine	Amino Acid	Pyrimidine Metabolism	0.3185180564	-0.1650496283	1.38E-05	0.001042433
M4231	5,6-dihydrouracil	Nucleotide	Pyrimidine Metabolism, Uracil containing	0.164954834	-2.599769578	1.33E-05	0.001042433
M354	isovalerylcarnitine (C5)	Amino Acid	Leucine, Isoleucine and Valine Metabolism	0.532672993	-0.908677957	1.57E-05	0.001097038
M434	methionine	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	0.474711687	-1.074860775	1.82E-05	0.001178733
M4316	1-methylnicotinamide	Cofactors and Vitamins	Nicotinate and Nicotinamide Metabolism	0.429048209	-1.220788331	2.64E-05	0.001197985
M527	guanidinoacetate	Amino Acid	Creatine Metabolism	0.300220855	-1.735855843	2.04E-05	0.001197985
M493	homogarginine	Amino Acid	Urea cycle; Arginine and Proline Metabolism	0.243663811	-2.037036097	2.25E-05	0.001197985
M546	N'(1)-acetylspiperidine	Amino Acid	Polyamine Metabolism	0.141234672	-2.823833791	2.45E-05	0.001197985
M1890	ximenylcarnitine (C26:1)*	Lipid	Fatty Acid Metabolism (Acyl Carnitine, Monounsaturated)	0.073505094	-3.766011962	2.60E-05	0.001197985
M3081	glycosy1 ceramide (d18:1/23:1, d17:1/24:1)*	Lipid	Hexosylceramides (HCKER)	0.147073723	-2.765388589	2.32E-05	0.001197985
M449	N-acetylarginine	Amino Acid	Urea cycle; Arginine and Proline Metabolism	0.439374309	-1.186477578	3.16E-05	0.001369683
M3161	sphingosine 1-phosphate	Lipid	Sphingosine	0.607479757	-0.719091759	6.41E-05	0.002648356
M4121	xanthine	Nucleotide	Purine Metabolism, (Hypo)Xanthine/Inosine containing	0.065320593	-3.936318307	9.77E-05	0.003861874
M107	N6-acetyllysine	Amino Acid	Lysine Metabolism	0.444630609	-1.08586399	0.000130292	0.003898219
M2662	1-palmitoyl-GPE (16:0)	Lipid	Lysophospholipid	0.463748204	-1.108586399	0.000130292	0.00473125
M7	betaine	Amino Acid	Glycine, Serine and Threonine Metabolism	0.594468915	-0.750326723	0.000138314	0.004835654
M1160	Fibrinopeptide A (4:15)	Peptide	Fibrinogen Cleavage Peptide	0.467298872	-1.295840276	0.000149499	0.004855905
M2904	palmitoyl-oleoylglycerol (16:0/18:1) [1]*	Lipid	Diacylglycerol	0.516937017	-0.951939579	0.000151113	0.004855905
M131	pipecolate	Amino Acid	Lysine Metabolism	0.3302405	-0.1598411036	0.000151949	0.004855905
M3063	glycosy1-N-ervenoyl-sphingosine (d18:1/24:1)*	Lipid	Hexosylceramides (HCKER)	0.235330612	-2.087239096	0.000163804	0.00496327
M545	spermidine	Amino Acid	Polyamine Metabolism	0.175998146	-2.056367864	0.000201647	0.005192801
M4931	histidine betaine (hercynine)*	Xenobiotics	Food Component/Plant	0.200469139	-2.318547935	0.000226913	0.006454744
M3363	androstenediol (3beta,17beta) disulfate (1)	Lipid	Androgenic Steroids	0.628207284	-0.644442997	0.000378215	0.007885694
M4219	uridine	Nucleotide	Pyrimidine Metabolism, Uracil containing	0.492416133	-1.022050064	0.000305253	0.008161023
M4235	2'-deoxyuridine	Nucleotide	Pyrimidine Metabolism, Uracil containing	0.241595201	-0.204936296	0.000317644	0.008249569
M3192	cholesterol	Lipid	Sterol	0.78385753	-0.351139946	0.000343576	0.008642931
M4182	guanosine	Nucleotide	Purine Metabolism, Guanine containing	0.073260153	-3.77082747	0.000361311	0.008642931
M554	N1,N12-diacetylsperrmine	Amino Acid	Polyamine Metabolism	0.062085261	-4.009605375	0.000361265	0.008642931
M1976	2-hydroxyneurovnotone*	Lipid	Fatty Acid, Monohydroxy	0.639739737	-0.644442997	0.000378215	0.008815328
M5206	tartromate (hydroxymalonate)	Xenobiotics	Food Component/Plant	0.374619206	-0.14650329	0.000390763	0.008809996
M1445	alpha-ketoglutarate	Energy	TCA Cycle	0.778896864	-0.360495786	0.00042781	0.009848592
M440	methionine sulfoxide	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	0.485897395	-0.041276396	0.000449938	0.009511484
M31	N-acetylananine	Amino Acid	Alanine and Aspartate Metabolism	0.663600919	-0.59161221	0.000441157	0.009511484
M2670	2-stearoyl-GPE (18:0)*	Lipid	Lysophospholipid	0.422828203	-1.241857099	0.000488892	0.009719152
M3386	Salpaha-androstan-3beta,17beta-diol disulfate	Lipid	Androgenic Steroids	0.457846173	-1.127065131	0.000476683	0.009719152
M512	N-methylhydroxyproline	Amino Acid	Urea cycle; Arginine and Proline Metabolism	0.164064994	-0.207660646	0.000491838	0.009719152
M3134	palmitoyl-sphingosine-phosphoethanolamine (d18:1/16:0)	Lipid	Ceramide PEs	0.851136164	-0.232538143	0.000504643	0.011419799
M6177	2,4-di-tert-butylphenol	Xenobiotics	Chemical	0.776167736	-0.365559631	0.00061697	0.01566968
M498	dimethylarginine (ADMA + SDMA)	Amino Acid	Urea cycle; Arginine and Proline Metabolism	0.466746032	-1.092903038	0.0006113	0.0156698
M650	gamma-glutamyl-2-aminobutyrate	Peptide	Gamma-glutamyl Amino Acid	0.417709344	-1.259428679	0.00061212	0.0156698
M2907	palmitoyl-linoleoylglycerol (16:0/18:2) [2]*	Lipid	Diacylglycerol	0.595846182	-0.746988149	0.000634908	0.0156698
M137	N,N-dimethyl-5-aminovalerate	Amino Acid	Lysine Metabolism	0.193554918	-2.369185129	0.000655451	0.0156698
M2833	1-(1-enyl-palmitoyl)-GPC (P-16:0)*	Lipid	Lysoplasmapagen	0.324808608	-1.622382828	0.000714702	0.012010202
M2233	phosphocholine	Lipid	Phospholipid Metabolism	0.652750391	-0.615396679	0.000704992	0.012010202
M3361	androstenediol (3beta,17beta) monosulfate (2)	Lipid	Androgenic Steroids	0.400617142	-1.319508475	0.00076313	0.012612464
M227	N-formylphenylalanine	Amino Acid	Tyrosine Metabolism	0.152121108	-2.716707746	0.000782786	0.012706288
M1889	nervonylcarnitine (C24:1)*	Lipid	Fatty Acid Metabolism (Acyl Carnitine, Monounsaturated)	0.400879055	-0.318761052	0.000857621	0.0137658
M2241	glycerophosphoserine*	Lipid	Phospholipid Metabolism	0.406959239	-1.297043794	0.000902462	0.01413762
M3103	palmitoyl sphingomyelin (d18:1/16:0)	Lipid	Sphingomyelins	0.861623165	-0.214871057	0.00093238	0.014364975
M2669	1-stearoyl-GPE (18:0)	Lipid	Lysophospholipid	0.509841667	-0.971878811	0.000955362	0.014464293
M2141	12-HETE	Lipid	Eicosanoid	0.053050387	-4.236492924	0.00097658	0.014464393
M4360	alpha-tocopherol	Cofactors and Vitamins	Tocopherol Metabolism	0.784936571	-0.349352016	0.001026988	0.015056962
M5063	stachydrine	Xenobiotics	Food Component/Plant	0.283894395	-1.816573727	0.00110546	0.015950203
M580	2-aminobutyrate	Amino Acid	Glutathione Metabolism	0.444515817	-1.318761052	0.000857621	0.0137658
M1869	lignocyercarnitine (C24)*	Lipid	Fatty Acid Metabolism (AcyL Carnitine, Long Chain Saturated)	0.43864793	-1.188846436	0.001283477	0.017948936
M11	N-acetylsarcosine	Amino Acid	Glycine, Serine and Threonine Metabolism	0.432929991	-1.20779435	0.001370637	0.018877414
M518	N-methylproline	Amino Acid	Urea cycle; Arginine and Proline Metabolism	0.123866683	-3.013137803	0.001417823	0.019253833
M2842	glycerol 3-phosphate	Lipid	Glycerolipid Metabolism	0.478198326	-1.064319016	0.002456907	0.019475419
M6422	metabolic lactone sulfate	Partially Characterized Molecules	Partially Characterized Molecules	0.511546413	-0.967062951	0.001516167	0.020310044
M2866	1-docosahexaenoyleglycerol (22:6)	Lipid	Monogacylglycerol	0.395369601	-1.338726144	0.001608625	0.02060928
M556	5-methylthioadenosine (MTA)	Amino Acid	Polyamine Metabolism	0.588662902	-0.764486385	0.001609746	0.02060928
M387	N-acetylisoleucine	Amino Acid	Leucine, Isoleucine and Valine Metabolism	0.583760141	-0.776552387	0.00169578	0.021409228
M40	asparagine	Amino Acid	Alanine and Aspartate Metabolism	0.530752898	-0.913887751	0.001831312	0.022475749
M642	gamma-glutamylmethionine	Peptide	Gamma-glutamyl Amino Acid	0.376265038	-1.410178852	0.001895803	0.022475749
M3091	lactosy1-N-ervenoyl-sphingosine (d18:1/24:1)*	Lipid	Lactosylceramides (LCER)	0.38574133	-1.374294364	0.001829684	0.022475749
M4241	N-acetyl-beta-alanine	Nucleotide	Pyrimidine Metabolism, Uracil containing	0.458407184	-1.125298442	0.001875981	0.022475749
M6241	perfluorooctanoate (PFOA)	Xenobiotics	Chemical	0.653182187	-0.614442646	0.001869875	0.022475749
M1865	margaroylcarnitine (C17)*	Lipid	Fatty Acid Metabolism (Acyl Carnitine, Long Chain Saturated)	0.3656513013	-1.451610675	0.002234522	0.025498916
M109	N2-acetyl,N6-methyllysine	Amino Acid	Lysine Metabolism	0.379975215	-1.396022778	0.002244129	0.025498916
M4353	threonate	Cofactors and Vitamins	Ascorbate and Aldarate Metabolism	0.609833285	-0.7135132	0.002201888	0.025498916
M2240	glycerophosphoethanolamine	Lipid	Phospholipid Metabolism	0.494135866	-1.017020319	0.00230001	0.025690348
M272	kynurene	Amino Acid	Tryptophan Metabolism	0.675868804	-0.565184869	0.002317501	0.025690348
M1971	2-hydroxystearate	Lipid	Fatty Acid, Monohydroxy	0.82380973	-0.279616928	0.002510325	0.027165299
M44	glutamate	Amino Acid	Glutamate Metabolism	0.773928641	-0.369727444	0.002508866	0.027165299
M2852	1-palmitoleoylglycerol (16:1)*	Lipid	Monogacylglycerol	0.285474159	-1.808567937	0.002626444	0.02770862
M16	2-methylserine	Amino Acid	Glycine, Serine and Threonine Metabolism	0.507030458	-0.979885668	0.002598152	0.02770862
M2914	palmitoyl-arachidonoylglycerol (16:0/20:4) [2]*	Lipid	Diacylglycerol	0.473564389	-1.078367496	0.002767275	0.028913254
M5044	S-allylcysteine	Xenobiotics	Food Component/Plant	0.189956907	-3.269255921	0.002913093	0.030152323
M56	beta-citrulline	Amino Acid	Glutamate Metabolism	0.420678194	-1.249180191	0.003039005	0.031038831
M2711	1-stearoyl-GPG (18:0)	Lipid	Lysophospholipid	0.143090672	-2.049984666	0.003207656	0.032397327
M438	S-methylmethionine	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	0.22844886	-2.130056852	0.003290103	0.032864878
M4119	inosine	Nucleotide	Purine Metabolism, (Hypo)Xanthine/Inosine containing	0.14300875	-2.805824674	0.003424483	0.032839337
M4601	3-methylkanthine	Xenobiotics	Xanthine Metabolism	0.44156055	-1.179316811	0.003508929	0.032496949
M2906	palmitoyl-linoleoylglycerol (16:0/18:2) [1]*	Lipid	Diacylglycerol	0.547143262	-0.870099462	0.003672438	0.033513254
M2941	linoleoyl-arachidonoylglycerol (18:2/20:4) [1]*	Lipid	Diacylglycerol	0.566658426	-0.819448736	0.003759707	0.035974466
M18	N-acetylthreonine	Amino Acid	Glycine, Serine and Threonine Metabolism	0.558770709	-0.839671698	0.003871564	0.036658867
M483	arginine	Amino Acid	Urea cycle; Arginine and Proline Metabolism	0.640177104</			

M4256	N4-acetylcytidine	Nucleotide	Pyrimidine Metabolism, Cytidine containing	0.623093705	-0.682478953	0.005747415	0.047066659
M3209	3beta-hydroxy-5-cholestenoate	Lipid	Sterol	0.46930891	-0.091390245	0.006281616	0.050087621
M4816	allin	Xenobiotics	Food Component/Plant	0.266599102	-1.907256172	0.006202521	0.050087621
M504	N-acetylcitrulline	Amino Acid	Urea cycle; Arginine and Proline Metabolism	0.263723738	-1.922900567	0.006228045	0.050087621
M1219	N,N-dimethyl-pro-pro	Peptide	Modified Peptides	0.533525947	-0.90636966	0.00689195	0.05476723
M2802	1-(1-enyl-palmitoyl)-2-palmitoyl-GPC (P:16:0/16:0)*	Lipid	Plasmalogens	0.46070206	-1.12006825	0.007878593	0.060181855
M2454	1-linoleoyl-2-arachidonoyl-GPE (18:2/20:4)*	Lipid	Phosphatidylethanolamine (PE)	0.672955721	-0.571416514	0.00780109	0.060181855
M48	N-acetylglutamine	Amino Acid	Glutamate Metabolism	0.506911138	-0.980194544	0.007820061	0.060181855
M17	threonine	Amino Acid	Glycine, Serine and Threonine Metabolism	0.406605015	-1.298300084	0.00768682	0.060181855
M3000	sphinganine	Lipid	Sphingolipid Synthesis	0.056015066	-4.158041272	0.008282898	0.062264098
M2999	3-ketosphinganine	Lipid	Sphingolipid Synthesis	0.656088433	-0.605288746	0.008562209	0.063768111
M641	gamma-glutamyl-epsilon-lysine	Peptide	Gamma-glutamyl Amino Acid	0.660369248	-0.598655156	0.008496629	0.063768111
M2913	palmitoyl-arachidonoyl-glycerol (16:0/20:4) [1]*	Lipid	Diacetylcerol	0.649365847	-0.622896586	0.00882295	0.063651105
M2861	1-dihomo-linolenoylglycerol (20:3)	Lipid	Monoaerylcerol	0.38864791	-1.363464338	0.008783923	0.063651105
M640	gamma-glutamyl-alpha-lysine	Peptide	Gamma-glutamyl Amino Acid	0.465284887	-1.103813767	0.008703074	0.063651105
M636	gamma-glutamylglycine	Peptide	Gamma-glutamyl Amino Acid	0.861424449	-0.215173679	0.009026231	0.063714105
M647	gamma-glutamylvaline	Peptide	Gamma-glutamyl Amino Acid	0.557686835	-0.84247288	0.009041936	0.063714105
M55	N-acetyl-aspartyl-glutamate (NAAG)	Amino Acid	Glutamate Metabolism	0.6328544	-0.660054477	0.008978666	0.063714105
M2196	N-oleoyserine	Lipid	Endocannabinoid	0.520595654	-0.941864594	0.009220539	0.064748488
M2862	1-arachidonylglycerol (20:4)	Lipid	Monoaerylcerol	0.695727554	-0.523405635	0.00937358	0.065042337
M4164	N6-carbamoylthreosine	Nucleotide	Purine Metabolism, Adenine containing	0.34249804	-1.545832364	0.009474357	0.065423867
M3087	lactosyl-N-palmitoyl-sphingosine (d18:1/16:0)	Lipid	Lactosylceramides (LCER)	0.514689337	-0.958226202	0.009801874	0.0656991755
M1831	3-hydroxybutyrylglycine	Lipid	Fatty Acid Metabolism (Acyl Glycine)	0.605667352	-0.72340449	0.010013999	0.067930787
M2232	choline	Lipid	Phospholipid Metabolism	0.359007677	-1.477913399	0.010142737	0.068294248
M5005	piperine	Xenobiotics	Food Component/Plant	0.715347974	-0.483282897	0.010320479	0.068859899
M1771	propionylcarnitine (C3)	Lipid	Fatty Acid Metabolism (also BCAA Metabolism)	0.653395002	-0.613972675	0.010669119	0.070789991
M1648	(16 or 17)-methylsteareate (a19:0 or i19:0)	Lipid	Fatty Acid, Branched	0.407064559	-1.296670476	0.010942176	0.072075677
M4602	7-methylxanthine	Xenobiotics	Xanthine Metabolism	0.530742514	-0.913915978	0.011172073	0.073060537
M6	dimethylglycine	Amino Acid	Glycine, Serine and Threonine Metabolism	0.572523223	-0.804593882	0.011302944	0.073883398
M105	lysine	Amino Acid	Lysine Metabolism	0.532710013	-0.908577697	0.011563379	0.074564889
M2836	1-(1-enyl-oleoyl)-GPE (P:18:1)*	Lipid	Cofactors and Vitamins	0.5551255719	-0.849035596	0.012827418	0.082113542
M4356	oxalate (ethanedioate)	Lipid	Ascorbate and Aldarate Metabolism	0.265553006	-1.912928232	0.013544023	0.086094525
M4206	dihydroorotate	Nucleotide	Pyrimidine Metabolism, Orotate containing	0.719172003	-0.475591236	0.013974421	0.087065156
M437	N-formylmethionine	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	0.745316458	-0.424074977	0.013949822	0.087605156
M3001	sphinganine-1-phosphate	Lipid	Sphingolipid Synthesis	0.637057348	-0.650504846	0.01412776	0.087959823
M2942	linoleoyl-arachidonoyl-glycerol (18:2/20:4) [2]*	Lipid	Diacetylcerol	0.548577293	-0.866233189	0.014266562	0.088219763
M638	gamma-glutamylisoleucine*	Peptide	Gamma-glutamyl Amino Acid	0.083652199	-3.579452724	0.014878955	0.09020394
M4283	3-aminoisobutyrate	Nucleotide	Pyrimidine Metabolism, Thymine containing	0.724533266	-0.464876164	0.014885139	0.09020394
M1840	acetyl carnitine (C2)	Lipid	Fatty Acid Metabolism (Acyl Carnitine, Short Chain)	0.445602448	-1.161670937	0.014752015	0.09020394
M519	N,N-trimethyl-alanylproline betaine (TMAP)	Amino Acid	Urea cycle; Arginine and Proline Metabolism	0.767162026	-0.382396785	0.016313414	0.098204594
M4221	pseudouridine	Nucleotide	Pyrimidine Metabolism, Uracil containing	0.485722802	-1.04179488	0.016674527	0.099347162
M3068	glycosyl-N-benzenoyl-sphingadiene (d18:2/22:0)*	Lipid	Hexosylceramides (HCKER)	0.346876153	-0.173801912	0.018806957	0.106944741
M4220	uracil	Nucleotide	Pyrimidine Metabolism, Uracil containing	0.389268622	-0.650720891	0.019934762	0.106944741
M1866	stearylcaritnine (C18)	Lipid	Fatty Acid Metabolism (Acyl Carnitine, Long Chain Saturated)	0.519915386	-1.361162038	0.016931315	0.099387376
M4893	ergothioneine	Xenobiotics	Food Component/Plant	0.548360693	-0.866802934	0.017113865	0.106058448
M471	taurine	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	0.397600867	-1.330607193	0.018371355	0.106058448
M4223	2'-O-methyluridine	Nucleotide	Pyrimidine Metabolism, Uracil containing	0.214195027	-0.223003111	0.018434802	0.106058448
M829	glycylvaline	Peptide	Dipeptide	0.609711257	-0.713801912	0.018806957	0.106944741
M123	2-aminoadipate	Amino Acid	Lysine Metabolism	0.774421169	-0.713801912	0.018806957	0.106944741
M457	5-methylcysteine	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	0.638947356	-0.646231025	0.018824151	0.106944741
M4264	2'-O-methylcytidine	Lipid	Pyrimidine Metabolism, Cytidine containing	0.382859155	-1.385114341	0.019233427	0.108591211
M93	1-methyl-5-imidazoleacetate	Nucleotide	Histidine Metabolism	1.533077004	-1.616430163	0.019405897	0.108903794
M1136	glu-gly-asn-val	Peptide	Polypeptide	0.252800551	-1.989328489	0.020640138	0.115103591
M1870	cerotylcarnitine (C26)*	Lipid	Fatty Acid Metabolism (Acyl Carnitine, Long Chain Saturated)	0.316684285	-0.165882817	0.022383784	0.12331343
M3167	hexadecaspinosine (d16:1)*	Lipid	Sphingosines	0.133975697	-2.899956773	0.02230275	0.12331343
M4126	N1-methylinosine	Nucleotide	Purine Metabolism, (Hypoxanthine/Inosine containing	0.74541357	-0.423887011	0.022656291	0.124063666
M4222	5,6-dihydrouridine	Nucleotide	Pyrimidine Metabolism, Uracil containing	0.796208886	-0.323781123	0.023842066	0.124321169
M551	acisog-e	Amino Acid	Polyamine Metabolism	0.398526961	-1.327250767	0.023727499	0.128382718
M1700	octadecadienoate (C18:2-DC)*	Lipid	Fatty Acid, Dicarboxylate	0.462770922	-1.111629878	0.026126679	0.139700892
M400	tiglyl carnitine (C5)	Amino Acid	Leucine, Isoleucine and Valine Metabolism	0.355867018	-1.49058966	0.026121392	0.139700892
M2871	2-oleoylglycerol (18:1)	Lipid	Monoaerylcerol	0.010124223	-6.626045283	0.029583095	0.152355353
M1951	docosahexaenoylcholine	Lipid	Fatty Acid Metabolism (Acyl Choline)	0.4304303476	-1.21579874	0.030167641	0.154058346
M3057	glycosyl-N-palmitoyl-sphingosine (d18:1/16:0)	Lipid	Hexosylceramides (HCKER)	0.492445191	-1.021964933	0.027629406	0.145172062
M2686	1-arachidonoyl-GPC (P:20:4n)*	Lipid	Lysophospholipid	0.544049083	-0.877234978	0.028496583	0.148870081
M1569	linolenate (18:3n or 3ng)	Lipid	Long Chain Polyunsaturated Fatty Acid (n3 and n6)	0.650752571	-0.619818988	0.028925111	0.152485282
M2034	2R,3R-dihydroxybutyrate	Lipid	Fatty Acid, Dihydroxy	0.377463393	-0.368413401	0.029666543	0.152355353
M6204	triethanolamine	Xenobiotics	Chemical	0.010124223	-6.626045283	0.029583095	0.152355353
M1867	arachidoylcarnitine (C20)*	Lipid	Fatty Acid Metabolism (Acyl Carnitine, Long Chain Saturated)	0.4304303476	-1.21579874	0.030167641	0.154058346
M453	cystathione	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	0.461247544	-1.116368665	0.030655899	0.154817949
M6452	glutamine_degradant*	Partially Characterized Molecules	Partially Characterized Molecules	0.559212388	-0.838531775	0.030650702	0.154817949
M1562	docosapentenoate (DPA; 22:5n3)	Lipid	Long Chain Polyunsaturated Fatty Acid (n3 and n6)	0.600838577	-0.734950651	0.031781533	0.158946067
M83	imidazole lactate	Amino Acid	Histidine Metabolism	0.772827171	-0.318227278	0.031822728	0.158946067
M1902	docosahexaenylcarnitine (C22:6)*	Lipid	Fatty Acid Metabolism (Acyl Carnitine, Polyunsaturated)	0.681166052	-0.55392156	0.033721486	0.166608776
M1	glycine	Amino Acid	Glycine, Serine and Threonine Metabolism	0.558721393	-0.837990934	0.033724989	0.166608776
M1932	camitine	Lipid	Carnitine Metabolism	0.691152093	-0.532924874	0.030530832	0.172144682
M2838	1-(1-enyl-stearoyl)-GPE (P:18:0)*	Lipid	Lysosomal amegogen	0.530113399	-0.915627089	0.035435652	0.173157289
M2173	N-stearyltaurine	Lipid	Endocannabinoid	0.596931096	-0.744363684	0.035622017	0.173157289
M4559	o-cresol sulfate	Xenobiotics	Benzooate Metabolism	0.403332467	-1.309958551	0.036401385	0.176004571
M121	fructosylsine	Amino Acid	Lysine Metabolism	0.613692958	-0.704411065	0.03707388	0.178307709
M2857	1-limonenoyleglycerol (18:3)	Lipid	Monoaerylcerol	0.532261578	-0.90972667	0.038528904	0.181465149
M4254	3-methylcytidine	Nucleotide	Pyrimidine Metabolism, Cytidine containing	0.756967796	-0.40169617	0.038455254	0.181465149
M1443	isocitrate	Energy	TCA Cycle	0.810020985	-0.303968811	0.038345682	0.181465149
M2937	stearyl-arachidonoyl-glycerol (18:0/20:4) [1]*	Lipid	Fatty Acid, Dicarboxylate	0.830620883	-0.215773951	0.037987497	0.181465149
M1698	cytosine	Nucleotide	Fatty Acid Metabolism, Cytidine containing	0.635555009	-0.653911095	0.039776801	0.183768665
M4252	cytosine	Lipid	Hexosylceramides (HCKER)	0.414041267	-0.764312911	0.041442576	0.191928754
M3078	glycosyl ceramide (d18:1/20:0, d16:1/22:0)*	Lipid	Lysine Metabolism	0.647011343	-0.628317079	0.041306594	0.191928754
M115	N6,N6-dimethyllysine	Amino Acid	Fatty Acid Metabolism (Acyl Choline)	0.358678096	-1.47923845	0.041519512	0.191928754
M1950	stearylcholine	Lipid	Long Chain Saturated Fatty Acid	0.413818161	-1.272933053	0.041834844	0.192059663
M573	cysteine-glutathione disulfide	Amino Acid	Glutathione Metabolism	0.648826384	-0.624095609	0.042565262	0.194312737
M1563	docosahexaenoate (DHA; 22:6n3)	Lipid	Long Chain Polyunsaturated Fatty Acid (n3 and n6)	0.355665727	-1.491406137	0.043439685	0.196451111
M1856	cis-3,4-methylenephentanoylcarnitine	Lipid	Fatty Acid Metabolism (Acyl Carnitine, Medium Chain)	0.720053191	-0.473824611	0.044605722	0.200740522
M2806	1-(1-enyl-palmitoyl)-2-oleoylglycerol (P:16:0/18:1)*	Lipid	Plasmalogens	0.638552145	-0.647123658	0.045317811	0.202259564
M644	gamma-glutamyltreonine	Peptide	Gamma-glutamyl Amino Acid	0.410836796	-0.872368269	0.046110729	0.204467172
M3032	N-stearyl-sphingadenine (d18:2/18:0)*	Lipid	Ceramides	0.828188084	-0.27196965	0.045931108	0.204467172
M1547	erucate (22:1n9)	Lipid	Long Chain Monounsaturated Fatty Acid	0.633226518	-0.661404398	0.047129393	0.205894389
M635	gamma-glutamylglutamine	Peptide	Gamma-glutamyl Amino Acid	0.594308992	-0.750714885	0.046792833	0.205894389
M385	isoleucine	Amino Acid	Leucine, Isoleucine and Valine Metabolism	0.655124336	-0.610159353	0.047339854	0.205894389
M1472	malonate	Lipid	Fatty Acid Synthesis	0.784905918	-0.349401741	0.047060192	0.205894389
M491	2-oxarginine*	Amino Acid	Urea cycle; Arginine and Proline Metabolism	0.398407554	-1.327683094	0.047643999</	

M4324	N1-Methyl-2-pyridone-5-carboxamide	Cofactors and Vitamins	Nicotinate and Nicotinamide Metabolism	0.582221207	-0.780360704	0.058884305	0.233737265
M1642	(14 or 15)-methylpalmitate (a17:0 or 17:0)	Lipid	Fatty Acid, Branched	0.680709312	-0.554889249	0.062875045	0.23435747
M2803	1-(1-enyl-palmitoyl)-2-palmitoleoyl-GPC (P-16:0/16:1)*	Lipid	Plasmalogen	0.501360234	-0.9966080525	0.060242232	0.234345747
M2444	1-oleoyl-2-linoleoyl-GPE (18:1/18:2)*	Lipid	Phosphatidylethanolamine (PE)	0.796653843	-0.327975106	0.062904689	0.234345747
M2281	1-palmitoyl-2-stearoyl-GPC (16:0/18:0)	Lipid	Phosphatidylcholine (PC)	0.729213853	-0.455586126	0.061540245	0.234345747
M4238	3-ureidopropionate	Nucleotide	Pyrimidine Metabolism, Uracil containing	0.459110527	-1.123086582	0.062604182	0.234345747
M3380	Salpaha-androstan-3-alpha,17beta-diol sulfate	Lipid	Androgenic Steroids	0.443359451	-1.173451266	0.061119922	0.234345747
M3315	cortisone	Lipid	Corticosteroids	1.770111911	0.823840574	0.062760397	0.234345747
M1887	ecicosoylcarnitine (C20:1)*	Lipid	Fatty Acid Metabolism (Acyl Carnitine, Monounsaturated)	0.429057062	-1.220758563	0.062198419	0.234345747
M445	glutamine	Amino Acid	Glutamate Metabolism	0.616167811	-0.698604777	0.061169506	0.234345747
M417	N-acetylyvaline	Amino Acid	Leucine, Isoleucine and Valine Metabolism	0.64449649	-0.633755593	0.061304001	0.234345747
M1864	palmitoylcarnitine (C16)	Lipid	Fatty Acid Metabolism (Acyl Carnitine, Long Chain Saturated)	0.553163737	-0.854221511	0.062797121	0.234345747
M3105	stearyl sphingomyelin (d18:1/18:0)	Lipid	Sphingomyelin	0.832927697	-0.263736828	0.059694148	0.234345747
M78	trans-urocanate	Amino Acid	Histidine Metabolism	0.490982038	-1.026257847	0.060009419	0.234345747
M4604	5-acetylaminoo-6-formylamino-3-methyluracil	Xenobiotics	Xanthine Metabolism	0.520042665	-0.943298107	0.060755444	0.234345747
M2888	dialeylglycerol (14:0/18:1, 16:0/16:1) [2]*	Lipid	Dialeylglycerol	0.403924208	-1.307843481	0.061330764	0.234345747
M140	phenylalanine	Amino Acid	Phenylalanine Metabolism	0.781037957	-0.356535432	0.063193489	0.240091879
M426	isobutyrylcarnitine (C4)	Amino Acid	Leucine, Isoleucine and Valine Metabolism	0.621856556	-0.685346262	0.062532948	0.240091879
M1516	nonadecanoate (19:0)	Lipid	Long Chain Saturated Fatty Acid	0.791544466	-0.37257696	0.065180947	0.240091879
M2813	1-(1-enyl-palmitoyl)-2-arachidonoyl-GPC (P-16:0/20:4)*	Lipid	Plasmalogen	0.583727208	-0.776521331	0.067225844	0.245735446
M224	dopamine 3-O-sulfate	Amino Acid	Tyrosine Metabolism	0.503062059	-0.991191709	0.06731367	0.245735446
M649	gamma-glutamylcitrulline*	Peptide	Gamma-glutamyl Amino Acid	0.592694243	-0.75464005	0.060963798	0.252119859
M254	tryptophan	Amino Acid	Tryptophan Metabolism	0.824854333	-0.27778873	0.069845663	0.259470444
M2814	1-(1-enyl-palmitoyl)-2-linoleoyl-GPC (P-16:0/18:2)*	Lipid	Plasmalogen	0.688280906	-0.538930607	0.071431826	0.253638789
M1643	cis-3,4-methylenephentanoate	Lipid	Fatty Acid, Branched	0.621604341	-0.685931515	0.070392843	0.253638789
M1240	lactate	Carbohydrate	Glycolysis, Gluconeogenesis, and Pyruvate Metabolism	0.799900873	-0.323716828	0.071224111	0.253638789
M3261	pregnenetriol sulfate*	Lipid	Pregnenolone Steroids	2.327317906	1.218701767	0.07097556	0.253638789
M3310	tetrahydrocyclic glucuronide	Lipid	Corticosteroids	3.66839087	1.875147367	0.071263836	0.253638789
M2938	stearyl-arachidonoyl-glycerol (18:0/20:4) [2]*	Lipid	Dialeylglycerol	0.493889109	-0.17171465	0.071838204	0.240589213
M127	glutarylcarnitine (C5:DC)	Amino Acid	Lysine Metabolism	0.716170782	-0.481624433	0.072172834	0.252823357
M3305	cortisol	Lipid	Corticosteroids	1.8955619	0.92265569	0.073302052	0.257264732
M2856	1-linoleoylglycerol (18:2)	Lipid	Monoaoylglycerol	0.508805869	-0.974812782	0.074566041	0.26094352
M4300	quinolinolate	Cofactors and Vitamins	Nicotinate and Nicotinamide Metabolism	0.493044204	-1.020211098	0.075074071	0.263590007
M2889	diacylglycerol (16:1/18:2) [2], 16:0/18:3 [1]*	Lipid	Dialeylglycerol	0.584161906	-0.775559813	0.076349077	0.263883312
M3090	lactosyl-N-behenoyl-phingosine (d16:1/22:0)*	Lipid	Lactosylceramides (LCER)	0.731832259	-0.450415085	0.076097805	0.263883312
M2834	1-(1-enyl-palmitoyl)-GPE (P-16:0)*	Lipid	Lysophospholipid	0.577600205	-0.791856841	0.077617056	0.264264832
M646	gamma-glutamyltyrosine	Peptide	Gamma-glutamyl Amino Acid	0.557423235	0.843154916	0.077617016	0.264264832
M1512	margarate (17:0)	Lipid	Long Chain Saturated Fatty Acid	0.717017275	-0.479919312	0.077507024	0.264264832
M282	picolinate	Amino Acid	Tryptophan Metabolism	0.646076195	-0.60223776	0.077018538	0.264264832
M10	serine	Amino Acid	Glycine, Serine and Threonine Metabolism	0.640765985	-0.642130531	0.078705956	0.266954919
M2841	glycerol	Lipid	Glycerolipid Metabolism	0.826605188	-0.274729677	0.0791678	0.266966865
M2924	oleoyl-oleoylglycerol (18:1/18:1) [2]*	Lipid	Dialeylglycerol	0.580040809	-0.785773369	0.079297089	0.266966865
M1447	succinylcarnitine (C4:DC)	Energy	TCA Cycle	0.559503159	-0.837791818	0.080780333	0.270956901
M2358	1-oleoyl-2-docosahexaenoyl-GPC (18:1/22:6)*	Lipid	Phosphatidylcholine (PC)	0.781662337	-0.35532569	0.081905311	0.270514901
M405	3-hydroxy-2-ethylpropionate	Amino Acid	Leucine, Isoleucine and Valine Metabolism	0.540397557	-0.887906941	0.082314948	0.271054901
M1921	3-hydroxyhexanoylcarnitine (1)	Lipid	Fatty Acid Metabolism (Acyl Carnitine, Hydroxy)	0.643511837	-0.635961408	0.082389431	0.271054901
M2002	9-hydroxystearate	Lipid	Fatty Acid, Monohydroxy	0.469607526	-1.094072564	0.081938074	0.271054901
M2934	linoleoyl-linoleoylglycerol (18:2/18:3) [2]*	Lipid	Dialeylglycerol	0.787160781	-0.345269753	0.081967229	0.271054901
M3031	N-palmitoyl-sphingadine (d18:2/16:0)*	Lipid	Ceramides	0.804842921	-0.313220851	0.082784493	0.271054901
M416	valine	Amino Acid	Leucine, Isoleucine and Valine Metabolism	0.819030272	-0.288011319	0.082896881	0.271054901
M274	N-formylanthranilic acid	Amino Acid	Tryptophan Metabolism	0.473015254	-1.080041387	0.084876793	0.276534066
M6260	3-bromo-5-chloro-2,6-dihydroxybenzoic acid*	Xenobiotics	Chemical	0.738836723	-0.43667252	0.087738069	0.284833574
M3064	glycosyl-(2-hydroxyervenoyl)-phingosine (d18:1/24:1(2OH))*	Lipid	Hexasylceramides (H6CR)	0.376813429	-1.408077715	0.088852881	0.287428004
M391	1-carboxybutyrylcarnitine	Amino Acid	Leucine, Isoleucine and Valine Metabolism	0.553658655	-0.852931304	0.089299671	0.287848938
M461	cysteine s-sulfate	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	0.831021712	-0.26701925	0.088966631	0.288009456
M1514	stearate (18:0)	Lipid	Long Chain Saturated Fatty Acid	0.817160387	-0.291308826	0.090040307	0.288201056
M492	citrulline	Amino Acid	Urea cycle: Arginine and Proline Metabolism	0.74955606	-0.415891713	0.09104433	0.290383824
M2731	1-arachidonoyl-GPI* (20:4)*	Lipid	Lysophospholipid	0.785631198	-0.348075874	0.091731069	0.290452107
M2851	1-palmitoylglycerol (16:0)	Lipid	Monoaoylglycerol	0.559889593	-0.836785731	0.091978429	0.290452107
M1886	oleoylcarnitine (C18:1)	Lipid	Fatty Acid Metabolism (Acyl Carnitine, Monounsaturated)	0.492035992	-1.023164242	0.092024243	0.290452107
M336	N-acetylleucine	Amino Acid	Leucine, Isoleucine and Valine Metabolism	0.616632883	-0.697516269	0.092752093	0.291701509
M5374	4-acetamidophenol	Xenobiotics	Drug - Analgesics, Anesthetics	1.616436328	-2.613199403	0.09415627	0.295132055
M92	1-methyl-5-imidazoleacetate	Amino Acid	Histidine Metabolism	1.445296321	-0.53136531	0.096504687	0.299395087
M399	2-methylbutyrylglycine (C5)	Amino Acid	Leucine, Isoleucine and Valine Metabolism	0.507109098	-0.979361937	0.096266631	0.299395087
M4544	methyl-4-hydroxybenzoate sulfate	Xenobiotics	Benzoate Metabolism	0.181580035	-0.46132251	0.096079308	0.299395087
M4239	beta-alanine	Nucleotide	Pyrimidine Metabolism, Uracil containing	0.788935367	-0.342020982	0.096945056	0.299736585
M1460	2-methylcitrate/homocitrate	Energy	TCA Cycle	0.847369213	-0.238937382	0.097808204	0.300363708
M2939	oleoyl-arachidonoylglycerol (18:1/20:4) [1]*	Lipid	Dialeylglycerol	0.626453171	-0.674721426	0.097734573	0.300363708
M3378	Salpaha-androstan-3-alpha,17beta-diol monosulfate (1)	Lipid	Androgenic Steroids	0.524696105	-0.930446015	0.099201993	0.302599657
M1507	myristate (14:0)	Lipid	Long Chain Saturated Fatty Acid	0.680591847	-0.55138262	0.099016785	0.302599657
M1894	arachidonoylcarnitine (C20:4)	Lipid	Fatty Acid Metabolism (Acyl Carnitine, Polyunsaturated)	0.39724872	-1.331972135	0.099574806	0.302727031
M2197	N-stearylserine*	Lipid	Endocannabinoid	0.451302947	-0.101219758	0.09104433	0.303867331
M458	5-methylcytathione sulfoxide	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	0.641980954	-0.639397599	0.101074732	0.305676943
M2671	1-oleoyl-GPE (18:1)	Lipid	Lysophospholipid	0.548404344	-0.866688097	0.102365425	0.306540564
M2601	2-palmitoyl-GPC* (16:0)*	Lipid	Lysophospholipid	0.549872937	-0.862829812	0.102340917	0.306540564
M162	tyrosine	Amino Acid	Tyrosine Metabolism	0.685698042	-0.544354693	0.102517416	0.306540564
M2923	oleoyl-oleoylglycerol (18:1/18:1) [1]*	Lipid	Dialeylglycerol	0.615813059	-0.617431039	0.103872011	0.308560974
M4131	urate	Nucleotide	Purine Metabolism, (Hypo)Xanthine/Inosine containing Food Component/Plant	0.683486574	-0.549015096	0.103603678	0.308560974
M5214	3-indolegycylic acid	Xenobiotics	Food Component/Plant	0.759155193	-0.397332351	0.107331494	0.31785332
M4304	nicotinamide	Cofactors and Vitamins	Nicotinate and Nicotinamide Metabolism	0.556078566	-0.846639366	0.107794591	0.318079778
M1944	oleoylcholine	Lipid	Fatty Acid Metabolism (Acyl Choline)	0.513438053	-0.961737872	0.108476793	0.318079778
M1468	phosphate	Energy	Oxidative Phosphorylation	0.681375389	-0.553478257	0.108293098	0.318079778
M4244	3-(3-amino-3-carboxypropyl)uridine*	Nucleotide	Pyrimidine Metabolism, Uracil containing	0.610687187	-0.711494534	0.109039723	0.31872664
M2713	1-oleoyl-GPE (18:1)*	Lipid	Lysophospholipid	0.371909358	-1.426977047	0.109397293	0.31872664
M505	N-acetylproline	Amino Acid	Urea cycle: Arginine and Proline Metabolism	0.685054046	-0.544762885	0.110626215	0.321275494
M264	tryptophan betaine	Amino Acid	Tryptophan Metabolism	0.500244931	-0.99923451	0.112241618	0.321983339
M1531	10-heptadecenoate (17:1n7)	Lipid	Long Chain Monounsaturated Fatty Acid	0.604388348	-0.764524248	0.112022952	0.322243238
M3502	tauroithocholate 3-sulfate	Lipid	Secondary Bile Acid Metabolism	0.330668214	-1.595643724	0.11173941	0.322243238
M1958	alpha-hydroxycaproate	Lipid	Fatty Acid, Monohydroxy	1.288100954	0.365245668	0.112948379	0.322861876
M70	histidine	Amino Acid	Sphingomyelin	0.691380808	0.532441278	0.112643823	0.322861876
M36	aspartate	Amino Acid	Alanine and Aspartate Metabolism	0.674942945	-0.567056784	0.116533686	0.330432334
M634	gamma-glutamylglutamate	Peptide	Gamma-glutamyl Amino Acid	0.655268536	-0.609864232	0.116687328	0.330432334
M37	N-acetylaspartate (NAA)	Amino Acid	Alanine and Aspartate Metabolism	0.700152025	-0.514259884	0.116087736	0.330432334
M5380	2-methoxyacetaminophen sulfate*	Xenobiotics	Drug - Analgesics, Anesthetics	0.306552148	-1.7057958	0.117889444	0.332801115
M1989	3-hydroxystearate	Lipid	Fatty Acid, Monohydroxy	0.565058784	-0.823527247	0.11946254	0.33474602
M3106	behenoyl sphingomyelin (d18:1/22:0)*	Lipid	Sphingomyelin	1.170333026	-0.22691917	0.119176188	0.33474602
M278	xanthurene	Amino Acid	Tryptophan Metabolism	0.519349743	-0.945221682	0.119515122	0.33474602
M3052	ceramide (d18:2/24:1, d18:1/21:2)*	Lipid	Ceramides	0.714522037</			

M5210	(S)-a-amino-omega-caprolactam	Xenobiotics	Fatty Acid Metabolism (Acyl Carnitine, Hydroxy)	0.816460862	-0.292544365	0.147089358	0.385314773
M1920	(S)-3-hydroxybutyrylcarnitine	Lipid	Purine Metabolism, Adenine containing	0.639802925	-0.644300506	0.148965323	0.389107698
M4153	1-methyladenosine	Nucleotide	Fatty Acid Metabolism (Acyl Carnitine, Medium Chain)	0.77898926	-0.360323424	0.149948659	0.390553956
M1844	hexanoylcarnitine (C6)	Lipid	TCA Cycle	0.732642945	-0.448817826	0.150840171	0.391177666
M1448	succinate	Energy	Fatty Acid Metabolism (Acyl Carnitine, Polyunsaturated)	0.680205582	-0.555957249	0.15104884	0.391177666
M1891	linoleoylcarnitine (C18:2)*	Lipid	Long Chain Polysaturated Fatty Acid (n3 and n6)	0.535824344	-0.90167967	0.153034228	0.39519305
M2613	1-oleoyl-GPC (18:1)	Lipid	Fatty Acid, Dicarboxylate	0.635273137	-0.65451081	0.15436199	0.39525366
M1576	docosapentenoate (n6 DPA; 22:5n6)	Lipid	Gamma-glutamyl Amino Acid	0.640641675	-0.642410443	0.15402042	0.39525366
M1674	heptenedioate (C7:1-DC)*	Lipid	Alanine and Aspartate Metabolism	0.570251729	-0.810329178	0.153522229	0.39525366
M643	gamma-glutamylphenylalanine	Peptide	Alanine, Isoleucine and Valine Metabolism	0.842888846	-0.246585703	0.155700457	0.396625109
M43	hydroxyasparagine	Amino Acid	Nicotinate and Nicotinamide Metabolism	1.186169063	0.24630965	0.155770257	0.396625109
M2611	1-stearoyl-GPC (18:0)	Lipid	Leucine, Isoleucine and Valine Metabolism	0.499124845	-1.00257377	0.159313615	0.402266878
M35	N-carbamoylalanine	Amino Acid	Phospholipid Metabolism	0.502632768	0.992423368	0.160235557	0.40384019
M4325	N1-Methyl-4-pyridone-3-carboxamide	Cofactors and Vitamins	Primary Bile Acid Metabolism	0.616636758	0.697507202	0.160814422	0.403813009
M429	2,3-dihydroxy-2-methylbutyrate	Amino Acid	Lysophospholipid	0.881289944	0.182311352	0.16199582	0.405657607
M2236	glycerophosphocholine (GPC)	Lipid	Phosphatidylethanolamine (PE)	0.585658058	-0.771869514	0.164701605	0.408095048
M3477	glycocholate sulfate	Lipid	Phosphatidylethanolamine (PE)	0.669606162	-0.57881529	0.164597641	0.408095048
M2673	1-linoleoyl-GPE (18:2)*	Lipid	Purine Metabolism, (Hypoxanthine/Inosine containing	0.681551612	-0.553105182	0.164764447	0.408095048
M2416	1-palmitoyl-2-arachidonoyl-GPE (16:0/20:4)*	Lipid	Drug - Antibiotic	1.000011955	1.722-05	0.164244682	0.408095048
M4133	allantoin	Nucleotide	Pyrimidine Metabolism, Uracil containing	0.799607661	-0.322635801	0.166200375	0.40532992
M5505	metronidazole	Xenobiotics	Lysophospholipid	0.685350179	-0.545086774	0.167000461	0.41391338
M4224	5-methyluridine (ribothymidine)	Nucleotide	Phosphatidylethanolamine (PE)	0.688663293	0.538129314	0.168802016	0.417054094
M2600	1-palmitoyl-GPC (16:0)	Lipid	Fatty Acid Metabolism (Acyl Glycine)	0.83996384	-0.251600873	0.16970371	0.415788781
M2447	1-oleoyl-2-arachidonoyl-GPE (18:1/20:4)*	Lipid	Ceramides	0.86489995	0.209394841	0.170946885	0.417116985
M1837	picolinoylglycine	Lipid	Phosphatidylcholine (PC)	0.861246388	-0.215502067	0.171475424	0.417885149
M3025	N-stearoyl-sphingosine (d18:1/18:0)*	Lipid	Plasmalogen	0.762025605	0.392088621	0.172264538	0.418301882
M2297	1-palmitoyl-2-arachidonoyl-GPC (16:0/20:4n6)	Lipid	Chemical	0.799607661	-0.415045411	0.173026961	0.418301882
M2818	1-(1-enyl-stearoyl)-2-arachidonoyl-GPE (P-18:0/20:4)*	Lipid	Long Chain Monounsaturated Fatty Acid	0.665035427	0.805507803	0.174613898	0.421018657
M6259	3,5-dichloro-2,6-dihydroxybenzoic acid	Xenobiotics	Fatty Acid, Dihydroxy	0.572106055	0.921340833	0.176368905	0.424152224
M6213	4-hydroxychlorothalanol	Xenobiotics	Monoaurylycerol	0.529851202	0.1002771108	0.178162058	0.427306887
M1529	palmitoleate (16:1n7)	Lipid	Fatty Acid Metabolism (Acyl Choline)	0.499040529	-0.885270588	0.181131015	0.433284454
M2033	25,3R-dihydroxybutyrate	Lipid	Fatty Acid, Dicarboxylate	1.407932317	0.493577932	0.181652771	0.43392044
M2868	2-palmitoylglycerol (16:0)	Lipid	Fatty Acid Metabolism (Acyl Glycine)	0.715204013	-0.483573263	0.182480246	0.434265554
M1952	arachidonoylcholine	Lipid	Food Component/Plant	0.178243333	-0.248807999	0.182986792	0.434295024
M1707	3-carboxy-4-methyl-5-pentyl-2-furanpropionate (3-CMPFP)	Lipid	Glutathione Metabolism	0.718204099	-0.4775326	0.184079821	0.43575145
M1823	N-palmitoylglycine	Lipid	Drug - Analgesics, Anesthetics	0.380502126	0.1393951036	0.185832566	0.43877929
M5077	thymol sulfate	Xenobiotics	Fatty Acid, Amino	0.753354155	-0.408599853	0.187302045	0.440187159
M579	5-oxoproline	Amino Acid	Long Chain Monounsaturated Fatty Acid	0.645765229	0.630918333	0.18942762	0.444923231
M5376	3-(N-acetyl-L-cystein-S-yl) acetaminophen	Xenobiotics	Medium Chain Fatty Acid	0.552908116	-0.854888346	0.190287069	0.450851406
M1750	2-aminoheptanoate	Lipid	Plasmalogen	0.851692843	0.231594869	0.192212773	0.448870252
M1540	10-nonadecenoate (19:1n9)	Lipid	Monoaurylycerol	0.557767837	-0.842263349	0.192584597	0.448707052
M1495	cis-4-decenote (10:1n6)*	Lipid	Monoacylglycerol	0.687457957	-0.540618815	0.193526146	0.449636335
M2801	1-(1-enyl-palmitoyl)-2-linoleoyl-GPE (P-16:0/18:2)*	Lipid	Gamma-glutamyl Amino Acid	0.597696537	-0.742514911	0.193902578	0.449636335
M2872	2-linoleoylglycerol (18:2)	Lipid	Long Chain Saturated Fatty Acid	0.498902054	-0.203952883	0.213579769	0.449657515
M2873	2-arachidonoylglycerol (20:4)	Lipid	Tryptophan Metabolism	0.868168581	-0.209601808	0.212714145	0.449657515
M632	gamma-glutamylalanine	Peptide	Long Chain Polysaturated Fatty Acid (n3 and n6)	0.707301973	0.792389198	0.212714145	0.449657515
M1346	fructose	Carbohydrate	Fibrinogen Cleavage Peptide	1.565920793	0.64701124	0.196201072	0.453805857
M3236	cortolone glucuronide (1)	Lipid	Endocannabinoid	2.210595783	0.147369084	0.196837098	0.454303899
M3206	7-HOCA	Lipid	Sterol	0.74988077	-0.415268687	0.198106687	0.454744894
M2926	oleoyl-linoleoyl-glycerol (18:1/18:2) [1]	Lipid	Diacylglycerol	0.676189565	0.564503042	0.197624347	0.454744894
M1918	octadecenoylcarnitine (C18:1-DC)*	Lipid	Fatty Acid Metabolism (Acyl Carnitine, Dicarboxylate)	0.597889871	-0.740248325	0.205206345	0.469855333
M1430	N-acetylglucosaminylasparagine	Carbohydrate	Aminosugar Metabolism	1.319474255	0.39963201	0.205730301	0.469877662
M1968	2-hydroxyalpimate	Lipid	Fatty Acid, Monohydroxy	0.830532503	-0.267891465	0.213422245	0.480695715
M1519	behenate (22:0)*	Lipid	Long Chain Saturated Fatty Acid	0.498902054	-0.1003171486	0.214442844	0.480695715
M261	C-glycosytryptophan	Amino Acid	Tryptophan Metabolism	0.868168581	-0.203952883	0.213579769	0.480695715
M1577	docosadienoate (22:2n6)	Lipid	Long Chain Polysaturated Fatty Acid (n3 and n6)	0.707301973	0.499601808	0.212714145	0.480695715
M1158	Fibrinopeptide A (1:25)	Peptide	Fibrinogen Cleavage Peptide	0.613601463	0.704626173	0.214700176	0.480695715
M6399	glutamine conjugate of C6H10O2 (1)*	Partially Characterized Molecules	Partially Characterized Molecules	0.567466471	-0.817392941	0.211221598	0.480695715
M4357	guanolate*	Cofactors and Vitamins	Ascorbate and Aldarate Metabolism	1.348706173	0.43157608	0.214239421	0.480695715
M3021	N-palmitoyl-sphingosine (d18:1/16:0)	Lipid	Ceramides	0.84162679	-0.248747467	0.213538494	0.480695715
M3033	N-behenoyl-sphingadine (d18:2/22:0)*	Lipid	Ceramides	0.868921945	-0.202701509	0.216701248	0.480695715
M2603	2-palmitoleoyl-GPC* (16:1)*	Lipid	Lysophospholipid	0.638200454	-0.64791846	0.218748265	0.486166682
M245	thyroxine	Amino Acid	Tyrosine Metabolism	0.818851057	-0.28827035	0.218449651	0.486166682
M2635	1-arachidonoyl-GPC* (20:4)*	Lipid	Lysophospholipid	0.609356941	-0.714640536	0.221972541	0.487374492
M2539	1-palmitoyl-2-arachidonoyl-GPI (16:0/20:4)*	Lipid	Phosphatidylinositol (PI)	0.883113673	-0.179328943	0.221651756	0.487374492
M332	leucine	Amino Acid	Fatty Acid Metabolism (Acyl Glycine)	0.811069928	-0.30210179	0.220804498	0.487374492
M4174	N6-succinyladenosine	Nucleotide	Purine Metabolism, Adenine containing	0.638040726	-0.64827958	0.221159536	0.487374492
M5017	sulfate of piperine metabolite C16H19NO3 (2)*	Xenobiotics	Food Component/Plant	0.700408914	0.513730649	0.22181364	0.487374492
M1449	fumarate	Energy	TCA Cycle	0.819418287	-0.287328005	0.224020406	0.48962967
M2159	oleoyl ethanolamide	Lipid	Endocannabinoid	0.690166049	0.534984589	0.22407076	0.48962967
M2616	1-linoleoyl-GPC (18:2)	Lipid	Lysophospholipid	0.621105823	-0.687089002	0.225449302	0.490271333
M3262	pregnenetriol distufate*	Lipid	Pregnenolone Steroids	2.409109811	0.126850155	0.225384277	0.490271333
M645	gamma-glutamyltryptophan	Peptide	Gamma-glutamyl Amino Acid	0.682149518	-0.551840102	0.2271739	0.491536993
M150	phenylpyruvate	Amino Acid	Phenylalanine Metabolism	0.810485777	0.303141239	0.226923231	0.491536993
M1504	5-dodecanoate (12:1n7)	Lipid	Medium Chain Fatty Acid	0.518222261	-0.948357106	0.220956962	0.492170699
M639	gamma-glutamylleucine	Peptide	Gamma-glutamyl Amino Acid	0.816822377	0.291905705	0.229216688	0.492170699
M73	N-acetylhistidine	Amino Acid	Histidine Metabolism	0.575120645	-0.798063467	0.228911254	0.492170699
M1943	palmitoylcholine	Lipid	Fatty Acid Metabolism (Acyl Choline)	0.577427131	0.792389198	0.228600117	0.492170699
M2725	1-linoleoyl-GPI* (18:2)*	Lipid	Lysophospholipid	0.860067359	-0.217478442	0.233424114	0.498081032
M2410	1-palmitoyl-2-linoleoyl-GPE (16:0/18:2)	Lipid	Phosphatidylethanolamine (PE)	0.735542057	-0.443120261	0.233192945	0.498081032
M263	oxindolylalanine	Amino Acid	Tryptophan Metabolism	1.607338887	0.247374492	0.232119536	0.498081032
M1500	10-decenoate (11:1n1)	Lipid	Medium Chain Fatty Acid	0.521734273	-0.938612888	0.232818378	0.503953762
M1699	octadecenoate (C18:1-DC)	Lipid	Fatty Acid, Dicarboxylate	0.68673061	0.542940316	0.239312044	0.507073771
M6401	glutamine conjugate of C7H12O2*	Partially Characterized Molecules	Partially Characterized Molecules	0.558405733	-0.840614341	0.240527039	0.508642973
M2602	1-palmitoleoyl-GPC* (16:1)*	Lipid	Lysophospholipid	0.655954496	-0.608354131	0.245268867	0.515150196
M223	dopamine 4-sulfate	Amino Acid	Tyrosine Metabolism	0.578707043	-0.789094892	0.248790909	0.515150196
M4895	erythritol	Xenobiotics	Food Component/Plant	1.252124302	-0.3243779	0.248402528	0.515150196
M1433	N-acetylglucosamine/N-acetylgalactosamine	Carbohydrate	Aminosugar Metabolism	0.897439342	-0.156113665	0.247807571	0.515150196
M1510	palmitate (16:0)	Lipid	Long Chain Saturated Fatty Acid	0.831907888	-0.265504125	0.247956758	0.515150196
M2162	palmitoyl ethanolamide	Lipid	Endocannabinoid	0.740651139	0.433133939	0.247138864	0.515150196
M3130	sphingomyelin (d18:2/24:1, d18:1/24:2)*	Lipid	Sphingomyelin	0.856554791	-0.223382562	0.247395577	0.515150196
M3541	taurochenodeoxycholic acid 3-sulfate	Lipid	Secondary Bile Acid Metabolism	1.62576847	0.701121814	0.244905313	0.515150196
M3311	tetrahydrocortisol sulfate (1)	Lipid	Corticosteroids	3.715443482	1.893534424	0.248761151	0.515150196
M3252	hydrocholate	Lipid	Secondary Bile Acid Metabolism	1.57411673	0.654537895	0.250045602	0.516571482
M1557	steardionate (18:4n3)	Lipid	Long Chain Polysaturated Fatty Acid (n3 and n6)	0.710589086	-0.49212564	0.252476825	0.520414124
M4147	adenine	Nucleotide	Purine Metabolism, Adenine containing	0.873244128	-0.155403509	0.256162572	0.526813977
M327	6-bromotryptophan	Amino Acid	Tryptophan Metabolism	0.56159495	-0.832398132	0.259554211	0.532584149
M1948	linoleoylcholine*	Lipid	Fatty Acid Metabolism (Acyl Choline)	0.619352784	0.627811646	0.260893112	0.532928105
M2343	pregnen						

M1885	palmitoleoylcarnitine (C16:1)*	Lipid	Fatty Acid Metabolism (Acyl Carnitine, Monounsaturated)	0.611181158	-0.710328028	0.29359108	0.573932308
M4451	pyridoxate	Cofactors and Vitamins	Vitamin B6 Metabolism	1.123926684	0.168547928	0.299763845	0.582490376
M5009	glucuronide of piperine metabolite C17H21NO3 (4)*	Xenobiotics	Food Component/Plant	0.646667272	-0.628904498	0.299198205	0.583480376
M4376	delta-CEHC	Cofactors and Vitamins	Tocopherol Metabolism	3.271377984	0.1709898462	0.301857038	0.585049142
M139	N-acetyl-2-amino adipate	Amino Acid	Lysine Metabolism	0.739106069	-0.436146675	0.301806888	0.585049142
M5381	2-methoxyacetaminophen glucuronide*	Xenobiotics	Drug - Analgesics, Anesthetics	0.451944551	-1.145782316	0.304737234	0.586877427
M1907	adipoylcarnitine (C6:DC)	Lipid	Fatty Acid Metabolism (Acyl Carnitine, Dicarboxylate)	0.613590457	-0.704652049	0.303468911	0.586877427
M117	hydroxy-N6,N6,N6-trimethyllysine*	Amino Acid	Lysine Metabolism	0.706350928	-0.501542975	0.304204636	0.586877427
M4476	benzoate	Xenobiotics	Benzoate Metabolism	0.618141571	-0.693990804	0.307855779	0.591628917
M4369	gamma-CEHC glucuronide*	Cofactors and Vitamins	Tocopherol Metabolism	2.234100553	1.15969412	0.3128315	0.599039038
M2911	palmitoleyl-linoleoyl-glycerol (16:1/18:2) [1]*	Lipid	Diacetyl/glycerol	0.626753824	-0.674029201	0.313029201	0.599039038
M2438	1-stearoyl-2-arachidonoyl-GPE (18:0/20:4)	Lipid	Glutamate Metabolism	0.80749752	-0.308470266	0.314422435	0.600206902
M60	2-pyridolinone	Amino Acid	Lysophospholipid	0.733537412	-0.447057546	0.318548358	0.601528071
M2715	1-linoleoyl-GPG (18:2)*	Lipid	Phosphatidylcholine (PC)	0.929532581	-0.105418472	0.319623872	0.601528071
M2286	1-palmitoyl-2-linoleoyl-GPC (16:0/18:2)	Lipid	Mevalonate Metabolism	0.884640283	-0.176837156	0.316416979	0.601528071
M3175	3-hydroxy-3-methylglutarate	Lipid	Aminosugar Metabolism	1.156747879	0.210074454	0.319288868	0.601528071
M1406	glucuronate	Carbohydrate	Sphingomyelin	0.944098347	-0.082990941	0.317331748	0.601528071
M3108	lignoceroyl sphingomyelin (d18:1/24:0)	Lipid	Sphingomyelin	0.863710427	-0.211380388	0.318632938	0.601528071
M3110	sphingomyelin (d18:2/23:1)*	Lipid	Partially Characterized Molecules	0.694409493	-0.526076087	0.322070556	0.603358168
M6431	branched-chain, straight-chain, or cyclopropyl 10:1 fatty acid (2)*	Xenobiotics	Secondary Bile Acid Metabolism	1.503334636	0.613847116	0.321508867	0.603358168
M3484	deoxycholic acid glucuronide	Lipid	Histidine Metabolism	2.039072736	1.027913239	0.322587536	0.603358168
M75	N-acetyl-3-methylhistidine*	Amino Acid	Guanidino and Acetamido Metabolism	2.323176234	1.2160986	0.323543244	0.603903098
M564	guanidinosuccinate	Amino Acid	Phosphatidylethanamine (PE)	0.671893393	-0.573695751	0.327246327	0.60749568
M2418	1-palmitoyl-2-docosahexaenoyl-GPE (16:0/22:6)*	Lipid	Phenylalanine Metabolism	0.581604862	-0.78188766	0.328615633	0.606749568
M156	2-hydroxyphenylacetate	Amino Acid	Leucine, Isoleucine and Valine Metabolism	0.813967995	-0.296956026	0.329071695	0.606749568
M364	beta-hydroxysovaleryl/carnitine	Amino Acid	Fibrinogen Cleavage Peptide	0.735081273	-0.444024327	0.327125421	0.606749568
M1179	Fibrinopeptide B (1-12)	Peptide	Histidine Metabolism	0.632791596	-0.600197655	0.327753325	0.606749568
M86	N-acetylcarnosine	Amino Acid	Vitamin B6 Metabolism	0.907807787	-0.139541231	0.327386622	0.606749568
M4450	pyridoxal	Cofactors and Vitamins	Fibrinogen Cleavage Peptide	0.673738385	-0.56964217	0.332327271	0.609588171
M1159	Fibrinopeptide A (3-15)	Peptide	Gamma-glutamyl Amino Acid	0.740494616	-0.433438849	0.333214268	0.609588171
M648	gamma-glutamylserine	Peptide	Sphingomyelins	0.858292604	-0.220458528	0.333295182	0.609588171
M3116	sphingomyelin (d17:2/16:0, d18:2/15:0)*	Lipid	Sphingomyelins	0.898283092	-0.154757916	0.333102438	0.609588171
M3117	sphingomyelin (d18:2/16:0, d18:1/16:1)*	Lipid	Lysine Metabolism	0.749627891	-0.415753463	0.337023976	0.613937463
M119	5-hydroxylysine	Amino Acid	Glycolysis, Gluconeogenesis, and Pyruvate Metabolism	0.829391783	-0.270048297	0.336909862	0.613937463
M1243	glycerate	Carbohydrate	Lysine Metabolism	0.719236921	-0.1046133764	0.341390818	0.614949572
M5378	4-acetamidophenylglucuronide	Xenobiotics	Drug - Analgesics, Anesthetics	0.484264192	-0.146377402	0.341390818	0.614949572
M3271	Salpha-pregnan-3beta,20beta-diol monosulfate (1)	Lipid	Progestin Steroids	1.886237659	0.900132722	0.342012075	0.619449572
M6400	glutamine conjugate of GH1002 (2)*	Xenobiotics	Partially Characterized Molecules	0.634338548	-0.656657508	0.342094263	0.619449572
M2534	1-palmitoyl-2-oleoyl-GPI (16:0/18:1)*	Lipid	Phosphatidylinositol (PI)	0.864775545	-0.209602369	0.345648298	0.624536444
M1451	malate	Energy	TCA Cycle	0.792130802	-0.336189418	0.346227763	0.624536444
M6423	pentose acid*	Xenobiotics	Partially Characterized Molecules	0.810243719	-0.303588189	0.347906849	0.626232327
M1862	myristoylcarnitine (C14)	Lipid	Fatty Acid Metabolism (Acyl Carnitine, Long Chain Saturated)	0.639355195	-0.64531045	0.348593937	0.626232338
M1333	6-oxopiperidine-2-carboxylate	Amino Acid	Lysine Metabolism	0.831781806	-0.265722967	0.351012675	0.626250267
M2365	1-linoleoyl-2-arachidonoyl-GPC (18:2/20:4n6)*	Lipid	Phosphatidylcholine (PC)	1.1650651046	0.723035161	0.351417333	0.627580267
M6261	dibutyl sulfosuccinate	Xenobiotics	Chemical	0.797499472	-0.326444531	0.354886982	0.630063021
M1439	citrate	Energy	TCA Cycle	0.784741119	-0.349760936	0.353705888	0.630063021
M1572	dihomolinolenate (20:3n or 3n6)	Lipid	Long Chain Polyunsaturated Fatty Acid (n3 and n6)	0.784741119	-0.437508057	0.354590507	0.630063021
M3514	glycoconsoeoxycholate	Lipid	Secondary Bile Acid Metabolism	0.596632715	-0.264523279	0.354609382	0.633483144
M1947	dihomo-limonenoyl-choline	Lipid	Fatty Acid Metabolism (Acyl Choline)	0.581871861	-0.781226616	0.357806568	0.633483144
M3260	pregnen-diol disulfate*	Lipid	Pregnanolone Steroids	1.563747711	-0.454561014	0.349446222	0.626251222
M2404	1,2-dipalmitoyl-GPC (16:0/16:0)*	Lipid	Phosphatidylethanamine (PE)	0.699291262	-0.156302759	0.359994427	0.635373907
M2810	1-(1-enyl-stearyl)-2-oleoyl-GPE (P-18:0/18:2)*	Lipid	Plasmalogens	0.882163726	-0.180816156	0.362072259	0.635373907
M3500	glycocholotholate sulfate*	Lipid	Secondary Bile Acid Metabolism	0.5410208233	-0.886605558	0.361679874	0.635373907
M1881	undecenoylcarnitine (C11:1)	Lipid	Fatty Acid Metabolism (Acyl Carnitine, Monounsaturated)	0.75058138	-0.413919593	0.360714442	0.642534052
M1768	butyrylcarnitine (C4)	Lipid	Fatty Acid Metabolism (also BCAA Metabolism)	0.803512249	-0.315608077	0.364750844	0.636388709
M4498	cetearyl sulfate	Xenobiotics	Benzoate Metabolism	1.747716666	0.805471319	0.364043119	0.636388709
M3398	Salpha-androstan-3beta,17alpha-diol disulfate	Lipid	Androgenic Steroids	0.643505272	-0.635976126	0.36417813	0.636388709
M2198	N-palmitoylserine	Lipid	Endocannabinoid	0.585983946	-0.771066956	0.3635842705	0.637070918
M529	creatinine	Amino Acid	Creatine Metabolism	0.897909562	-0.155357952	0.36849103	0.640455728
M6430	branched-chain, straight-chain, or cyclopropyl 10:1 fatty acid (1)*	Xenobiotics	Partially Characterized Molecules	0.638112858	-0.648164911	0.370146567	0.6421054
M2408	1-palmitoyl-2-oleoyl-GPE (16:0/18:1)*	Lipid	Phosphatidylethanamine (PE)	0.750497812	-0.405507111	0.372237139	0.642534052
M375	3-methylglutarylcarnitine (2)	Amino Acid	Fatty Acid, Dihydroxy	1.149547847	0.579735174	0.372512421	0.642534052
M4368	gamma-CEHC	Cofactors and Vitamins	Tocopherol Metabolism	2.104146235	0.173234973	0.372352420	0.642534052
M3128	sphingomyelin (d18:2/23:0, d18:1/23:1, d17:1/24:1)*	Lipid	Sphingomyelin	0.891396435	-0.156809004	0.373254625	0.64259177
M2333	1-stearoyl-2-arachidonoyl-GPC (18:0/20:4)	Lipid	Phosphatidylcholine (PC)	0.91093794	-0.134575252	0.377324954	0.643821344
M1164	Fibrinopeptide A (8-16)	Peptide	Fibrinogen Cleavage Peptide	0.842942626	-0.246494279	0.378863657	0.649786913
M2283	1-palmitoyl-2-oleoyl-GPC (16:0/18:1)	Lipid	Phosphatidylcholine (PC)	0.890259652	-0.167701923	0.381946845	0.6538241209
M1487	butyrate/isobutyrate (4:0)	Lipid	Short Chain Fatty Acid	2.171088632	1.118418624	0.386510246	0.660490424
M2031	9,10-DHOME	Lipid	Fatty Acid, Dihydroxy	0.561087643	-0.383701954	0.388202777	0.662056282
M3453	cholate	Lipid	Primary Bile Acid Metabolism	7.600061034	0.296010384	0.389648461	0.663279999
M2556	1-stearoyl-2-arachidonoyl-GPI (18:0/20:4)	Lipid	Phosphatidylinositol (PI)	0.821414001	-0.283818556	0.391114401	0.664528955
M3281	Salpha-pregnan-3beta,17alpha-diol disulfate	Lipid	Progesterin Steroids	2.154148633	1.10709518	0.392470437	0.665568857
M4959	mannone*	Xenobiotics	Food Component/Plant	1.506410809	0.591115257	0.395237043	0.669032537
M1262	ribitol	Carbohydrate	Pentose Metabolism	0.936033576	-0.053687814	0.396682556	0.670229943
M1974	2-hydroxybehenate	Lipid	Fatty Acid, Monohydroxy	0.773169512	-0.371143346	0.397754433	0.670734884
M1924	3-hydroxyoctanoylcarnitine (1)	Lipid	Fatty Acid Metabolism (Acyl Carnitine, Hydroxy)	0.650514512	-0.621146272	0.399142101	0.671889204
M1178	gamma-glutamylhistidine	Peptide	Fibrinogen Cleavage Peptide	0.802651381	-0.317154583	0.40474288	0.677344028
M637	gamma-glutamylhistidine	Peptide	Gamma-glutamyl Amino Acid	0.797782462	-0.325923687	0.405363202	0.677344028
M2182	linoleoyl ethanalamide	Lipid	Endocannabinoid	0.778782069	-0.360689903	0.404021906	0.677344028
M5117	pyrraline	Xenobiotics	Food Component/Plant	0.680591125	-0.555139545	0.404191212	0.677344028
M1567	linoleate (18:2n6)	Lipid	Long Chain Polyunsaturated Fatty Acid (n3 and n6)	0.774349416	-0.568885945	0.406982856	0.678802598
M2262	1-myristoyl-2-palmitoyl-GPC (14:0/16:0)	Lipid	Phosphatidylcholine (PC)	1.464372875	0.550282955	0.422235299	0.689501305
M2721	1-stearoyl-GPI (18:0/18:0)	Lipid	Lysophospholipid	0.881071915	0.182668315	0.424102488	0.689501305
M4448	2,3-dihydroxy-5-methylthio-4-pentenoate (DMTPA)*	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	0.913293445	-0.130849616	0.422171646	0.689501305
M1973	2-hydroxyarachidate*	Lipid	Fatty Acid, Monohydroxy	0.757478626	-0.40707574	0.426480114	0.689501305
M3253	21-hydroxyregnenolone disulfate	Lipid	Pregnenolone Steroids	1.33996659	0.42222933	0.422294676	0.689501305
M5386	3-(methylthio)acetaminophen sulfate*	Xenobiotics	Drug - Analgesics, Anesthetics	0.603057634	-0.129632208	0.425160418	0.689501305
M72	3-methylhistidine	Amino Acid	Histidine Metabolism	1.221816915	0.289028118	0.415785533	0.691498565
M446	alpha-ketoglutarate*	Amino Acid	Glutamate Metabolism	0.879239633	-0.185671676	0.423568765	0.693501305
M275	anthranilate	Amino Acid	Tryptophan Metabolism	0.834609487	-0.260826776	0.418187684	0.693501305
M3100	behenoyl dihydrospingomyelin (d18:0/22:0)*	Lipid	Dihydrospingomyelins	1.239095399	0.309282766	0.427432206	0.693501305
M6448	bilirubin degradation product, C17H20N2OS (1)	Lipid	Partially Characterized Molecules	0.664441294	-0.389786358	0.418572866	0.693501305
M1161	Fibrinopeptide A (3-16)	Peptide	Fibrinogen Cleavage Peptide	1.379675070	0.464330037	0.418984059	0.693501305
M1166	ADPGSEGDFAKAEGGGV*	Peptide	Fibrinogen Cleavage Peptide	1.256625933	-0.421160938	0.419916434	0.693501305
M2242	glycerophosphoinositol*	Lipid	Phospholipid Metabolism	0.752023816	-0.41160938	0.421152255	0.693501305
M3517	glycoconsoeoxycholic acid sulfate (1)	Lipid	Secondary Bile Acid Metabolism	1.541821386	0.943418402	0.422418589	0.693501305
M4501	guaiacol sulfate	Xenobiotics	Benzoate Metabolism	1.923079497	0.494301822	0.422418589	0.693501305
M47	N-acetylglutamate						

M1352	mannose	Carbohydrate	Fructose, Mannose and Galactose Metabolism	1.341040828	0.42335316	0.460468476	0.716722337
M487	ornithine	Amino Acid	Urea cycle; Arginine and Proline Metabolism	0.835581537	0.25914748	0.458640494	0.716722337
M4530	4-vinylcatechol sulfate	Xenobiotics	Benzoate Metabolism	7.996826657	2.999427616	0.462536141	0.718710004
M1498	(2 or 3)-deenoate (10:1n or n8)	Lipid	Medium Chain Fatty Acid	0.651796769	-0.617505894	0.463687492	0.719269505
M4967	N-(2-fuoyl)glycine	Xenobiotics	Food Component/Plant	8.704316118	3.121730952	0.467119519	0.723358847
M4410	bilirubin (E,Z or Z,E)*	Cofactors and Vitamins	Hemoglobin and Porphyrin Metabolism	0.850693708	-0.233288311	0.471820143	0.729395425
M3340	androsterone glucuronide	Lipid	Androgenic Steroids	0.715286498	-0.483406885	0.480313579	0.731331731
M1671	maleate	Lipid	Fatty Acid, Dicarboxylate	1.203364864	0.267074138	0.474464098	0.731331731
M2915	palmitoleoyl-archidonoyl-glycerol (16:1/20:4) [2]*	Lipid	Diaclylglycerol	0.829138102	-0.270315676	0.478110779	0.731331731
M62	5-1-pyrorline-5-carboxylate	Amino Acid	Glutamate Metabolism	0.654301733	-0.611972002	0.479110124	0.731331731
M3114	sphingomyelin (d18:2/14:0, d18:1/14:1)*	Lipid	Sphingomyelin	1.159844341	0.213931199	0.477482831	0.731331731
M5151	trans-3,4-methylenephantanoate	Xenobiotics	Food Component/Plant	0.682453157	-0.551198071	0.47678289	0.731331731
M6254	3-hydroxy-2-methylpyridine sulfate	Xenobiotics	Chemical	6.552480702	2.712261358	0.470692969	0.731331731
M3307	cortisol 21-sulfate	Lipid	Corticosteroids	1.331231435	0.412761407	0.479647059	0.731331731
M5404	salicylicuric glucuronide*	Xenobiotics	Drug - Analgesics, Anesthetics	6.063582225	2.600170357	0.476533189	0.731331731
M353	isovalerylglycine	Amino Acid	Leucine, Isoleucine and Valine Metabolism	0.642670318	-0.637849253	0.48425817	0.731331731
M5116	4-vinylguaiacol sulfate	Xenobiotics	Food Component/Plant	5.978191872	2.579709201	0.485932107	0.737854313
M2809	1-(1-enyl-stearoyl)-2-oleoyl-GPE (P-18:0/18:1)	Lipid	Phosphatidylcholine (PC)	0.706102811	-0.502049835	0.487357037	0.737854313
M2310	1-palmitoleoyl-2-linolenoyl-GPC (16:1/18:3)*	Lipid	Phosphatidylcholine (PC)	0.923592506	-0.114671628	0.491030196	0.740080038
M2278	1,2-dipalmitoyl-GPC (16:0/16:0)	Lipid	Phosphatidylinositol (PI)	0.833570933	-0.262632124	0.497499991	0.740080038
M2543	1-stearyl-2-linoleoyl-GPL (18:0/18:2)	Lipid	Chemical	4.427142686	2.146375872	0.494445841	0.740080038
M6221	3-hydroxypropanoate	Xenobiotics	Tyrosine Metabolism	0.789668634	-0.340680707	0.496850328	0.740080038
M204	3-methoxytyrosine	Amino Acid	Leucine, Isoleucine and Valine Metabolism	0.860419186	-0.21688399	0.495268979	0.740080038
M347	alpha-hydroxyisocaproate	Amino Acid	Partially Characterized Molecules	1.645356699	0.718403082	0.492743776	0.740080038
M6435	GlcNAc sulfate conjugate of C21H34O2 steroid	Partially Characterized Molecules	Medium Chain Fatty Acid	0.851988292	-0.2310949	0.495062606	0.740080038
M1490	heptanoate (7:0)	Lipid	Progestin Steroids	1.31511022	0.395183718	0.498217484	0.740080038
M3283	pregnanediol-3-glucuronide	Lipid	Sphingomyelin	0.913119351	-0.31124651	0.498271706	0.740080038
M3119	sphingomyelin (d18:1/18:1, d18:2/18:0)	Lipid	Chemical	5.441090336	2.443895781	0.494497147	0.740080038
M6252	5-hydroxy-2-methylpyridine sulfate	Xenobiotics	Tyrosine Metabolism	1.626953061	0.702172628	0.497886102	0.740080038
M219	gentisate	Amino Acid	Urea cycle; Arginine and Proline Metabolism	1.650696477	0.723074868	0.500180499	0.741703219
M515	polyhydroxyproline	Amino Acid	Benzoate Metabolism	4.046142133	1.239516034	0.513373371	0.751459573
M4466	2-hydroxyhippurate (salicylate)	Xenobiotics	Tyrosine Metabolism	0.836135693	-0.258919004	0.5084945	0.751459573
M181	3-(4-hydroxyphenyl)lactate (HPLA)	Amino Acid	Fatty Acid Metabolism (Acyl Glutamine)	0.82297469	-0.281080033	0.511093891	0.751459573
M1781	hexanoylglutamine	Lipid	Fatty Acid, Amino	0.806192125	0.310804386	0.511043099	0.751459573
M1756	N-acetyl-2-aminooctanoate*	Lipid	Glycogen, Gluconeogenesis, and Pyruvate Metabolism	0.702576376	0.472776741	0.518844496	0.750455967
M419	N-carbamoylvaline	Amino Acid	Lysophospholipid	0.633926904	-0.657615196	0.517351979	0.753642547
M3325	sucrose	Carbohydrate	Sphingomyelin	1.290573839	0.368012686	0.508567967	0.751459573
M3536	taurocholenate sulfate*	Lipid	Disaccharides and Oligosaccharides	0.562323068	-0.830528664	0.51318268	0.751459573
M228	vanillic alcohol sulfate	Amino Acid	Secondary Bile Acid Metabolism	0.760268627	-0.395418837	0.511234331	0.751459573
M1995	5-hydroxyhexanoate	Lipid	Tyrosine Metabolism	0.614627135	0.702216633	0.511941716	0.751459573
M5959	salicylate	Xenobiotics	Fatty Acid, Monohydroxy	0.704028304	-0.506294663	0.516401914	0.753466034
M1220	1,5-hydroxyglucitol (1,5-AG)	Carbohydrate	Drug - Topical Agents	3.902796217	0.75998096	0.515599008	0.753466034
M2649	1-lignoceroyl-GPC (24:0)	Lipid	Glycology, Gluconeogenesis, and Pyruvate Metabolism	0.633926904	-0.657615196	0.517351979	0.753642547
M3129	sphingomyelin (d18:1/24:1, d18:2/24:0)*	Lipid	Lysophospholipid	0.702576376	0.472776741	0.518844496	0.750455967
M1925	3-hydroxyoctanoyl carnitine (2)	Lipid	Sphingomyelin	0.902526868	-0.147958213	0.516960166	0.756429997
M1929	3-hydroxyoleoylcarnitine	Lipid	Fatty Acid Metabolism (Acyl Carnitine, Hydroxy)	0.699151625	-0.516322729	0.523414134	0.755980906
M3051	ceramide (d16:2/24:1, d18:1/22:1)*	Lipid	Fatty Acid Metabolism (Acyl Carnitine, Hydroxy)	0.656543509	0.607037473	0.524648992	0.755980906
M4429	retinol (Vitamin A)	Cofactors and Vitamins	Ceramides	0.920943671	-0.118815177	0.524778862	0.755980906
M513	hydroxyproline	Amino Acid	Vitamin A Metabolism	0.912506507	-0.132093249	0.523880608	0.755980906
M2425	1-stearyl-2-oleoyl-GPE (18:0/18:1)	Lipid	Urea cycle; Arginine and Proline Metabolism	0.824569541	-0.278129695	0.52211889	0.755980906
M3337	dehydoroepiandrosterone sulfate (DHEA-S)	Lipid	Phosphatidylethanolamine (PE)	0.867805359	-0.204565458	0.526062371	0.756754761
M226	tyramine O-sulfate	Lipid	Androgenic Steroids	1.289856914	0.367211034	0.527688007	0.756754761
M4603	5-acetylamino-6-amino-3-methyluracil	Amino Acid	Tyrosine Metabolism	3.886669964	0.562329323	0.527688007	0.756754761
M6450	bilirubin degradation product, C16H18N20S (3)	Partially Characterized Molecules	Xanthine Metabolism	0.790514531	-0.339136112	0.533938805	0.765433297
M1689	dodecanoate (12:2)*	Lipid	Partially Characterized Molecules	1.050962932	0.59068626	0.537341427	0.7655852
M4506	4-allylcetohol sulfate	Xenobiotics	Fatty Acid, Dicarboxylate	2.596464032	0.732326293	0.535973196	0.7655852
M6443	bilirubin degradation product, C16H18N20S (1)	Partially Characterized Molecules	Benzoate Metabolism	0.550031668	0.632397691	0.542677742	0.771978197
M1659	glutarate (5-DC)	Lipid	Partially Characterized Molecules	0.789234442	-0.341474179	0.543691325	0.772211585
M6433	branched-chain, straight-chain, or cyclopropyl 12:1 fatty acid*	Partially Characterized Molecules	Xanthine Metabolism	0.742892323	-0.428774798	0.544959517	0.772805306
M4590	caffeine	Xenobiotics	Monooacylglycerol	2.040075303	1.02622406	0.545916255	0.772956193
M2850	1-pentadecanoylglycerol (15:0)	Lipid	Histidine Metabolism	0.642889256	0.637357855	0.552234743	0.774803847
M96	1-ribosyl-imidazoleacetate*	Amino Acid	Phosphatidylethanolamine (PE)	0.895290073	-0.159572906	0.554688792	0.774803847
M2339	1-stearyl-2-docosahexaenyl-GPC (18:0/22:6)	Lipid	Food Component/Plant	1.28498053	0.361746499	0.554824973	0.774803847
M4772	2,3-dihydroxyisovalerate	Xenobiotics	Leucine, Isoleucine and Valine Metabolism	0.813926184	-0.297030134	0.550937372	0.774803847
M428	3-hydroxyisobutyrate	Amino Acid	Chemical	0.813926184	-0.164819835	0.554547329	0.774803847
M6235	6-hydroxyindole sulfate	Xenobiotics	Hemoglobin and Porphyrin Metabolism	0.892039911	-0.164819835	0.554547329	0.774803847
M4411	biliverdin	Cofactors and Vitamins	Xanthine Metabolism	1.764384586	0.819165062	0.552412157	0.774803847
M255	N-acetyltryptophan	Amino Acid	Tryptophan Metabolism	1.163438312	0.218394717	0.551051933	0.774803847
M3102	sphingomyelin (d18:0/20:0, d16:0/22:0)*	Lipid	Dihydroxygomyelins	0.329093305	0.410442388	0.5513669	0.774803847
M3111	sphingomyelin (d18:2/24:2)*	Lipid	Sphingomyelin	0.914678345	-0.128663599	0.556697263	0.774803847
M202	vanillylmandelate (VMA)	Amino Acid	Tyrosine Metabolism	1.261214742	0.334710959	0.555218628	0.774803847
M2708	1-palmityl-GPG (16:0)*	Lipid	Long Chain Fatty Acid	0.798066345	-0.325419048	0.5589281	0.776859212
M1686	dodecanoate (C12)	Lipid	Fatty Acid, Dicarboxylate	1.804782272	0.851284802	0.565402066	0.784572128
M4594	1-methylurate	Xenobiotics	Xanthine Metabolism	1.271720072	0.467811143	0.566975506	0.785641364
M1431	erythronate*	Carbohydrate	Aminosugar Metabolism	1.082123858	0.113856537	0.571101421	0.791504221
M5936	diphenylhydramine	Xenobiotics	Drug - Respiratory	2.530016651	1.33914688	0.57299944	0.791575214
M3098	myristoyl dihydroxygomyelin (d18:0/14:0)*	Lipid	Dihydroxygomyelins	1.429327552	0.51335657	0.574036766	0.791804887
M340	1-carboxyethylleucine	Amino Acid	Leucine, Isoleucine and Valine Metabolism	0.912062817	-0.132794903	0.586415994	0.793550684
M4600	1-methoxykantchine	Xenobiotics	Xanthine Metabolism	0.713007682	0.488010475	0.5822367	0.793550684
M1966	2-hydroxylaurate	Lipid	Fatty Acid, Monohydroxy	1.20730815	0.271821036	0.586292241	0.793550684
M5129	2-keto-3-deoxy-gluconate	Xenobiotics	Food Component/Plant	1.230125916	0.298805958	0.580225833	0.793550684
M4502	3-methyl catechol sulfate (1)	Xenobiotics	Benzene Metabolism	2.261349541	1.177184009	0.577394317	0.793550684
M1277	arachidate (20:0)	Carbohydrate	Pentose Metabolism	1.0722765482	0.107373832	0.582554472	0.793550684
M6447	bilirubin degradation product, C17H18N20A (3)	Partially Characterized Molecules	Partially Characterized Molecules	0.745057565	-0.424498747	0.586561331	0.793550684
M1491	caprylate (8:0)	Lipid	Medium Chain Fatty Acid	0.961904391	0.306540591	0.586381325	0.793550684
M3050	ceramide (d18:1/20:0, d16:1/22:0, d20:1/18:0)*	Lipid	Ceramides	0.723058132	0.312182532	0.582952816	0.79881778
M1564	docosatrienoate (22:3n)	Lipid	Long Chain Polyunsaturated Fatty Acid (n3 and n6)	0.798055823	-0.325438431	0.578236375	0.793550684
M407	glycine conjugate of C10H12O2*	Amino Acid	Leucine, Isoleucine and Valine Metabolism	1.142707654	0.19246357	0.578251533	0.793550684
M6239	thioproline	Xenobiotics	Partially Characterized Molecules	0.904157319	-0.145325588	0.583740051	0.793550684
M1184	phenylacetylcarnitine	Peptide	Chemical	1.151468073	0.203474409	0.585641589	0.793550684
M2452	1,2-dilinoleoyl-GPE (18:2/18:2)*	Lipid	Acetylated Peptides	1.557308262	0.639075484	0.585834789	0.79466212
M1860	decanylcarnitine (C10)	Lipid	Phosphatidylethanolamine (PE)	0.810077601	-0.303867979	0.593182262	0.798817878
M1982	3-hydroxydecanoate	Lipid	Fatty Acid Metabolism (Acyl Carnitine, Medium Chain)	0.820282856	-0.285806119	0.597111181	0.800551716
M3360	androstenediol (3beta,17beta) monosulfate (1)	Lipid	Acetylated Peptides	0.873283605	-0.19547784	0.5965837	0.800551716
M3121	sphingomyelin (d18:1/20:0, d16:1/22:0)*	Lipid	Sphingomyelin	1.052218722	0.073424626	0.595412081	0.800551716
M367	3-methylglutamate	Amino Acid	Leucine, Isoleucine and Valine Metabolism	1.329059401	0.41044664	0.598228348	0.800551727
M5157	arachidate (20:0)	Lipid	Long Chain Saturated Fatty Acid	0.813159841	0.298389127	0.602396864	0.800551727
M1462	citrate/acetoglutarate	Energy	TCA Cycle	1.775881704	0.		

M4322	trigonelline (N'-methylnicotinate)	Cofactors and Vitamins	Nicotinate and Nicotinamide Metabolism	1.230856187	0.299662207	0.632324053	0.820773844
M279	8-methoxykynurename	Amino Acid	Tryptophan Metabolism	0.744701411	-0.425266004	0.632864949	0.820773844
M420	1-carboxyethylvaline	Amino Acid	Leucine, Isoleucine and Valine Metabolism	0.914502206	-0.128941444	0.641750899	0.822468444
M5961	2,6-dihydroxybenzoic acid	Xenobiotics	Drug - Topical Agents	1.244031695	0.315023243	0.644945652	0.822468444
M1755	2-aminooctanoate	Lipid	Fatty Acid, Amino	0.806856899	-0.30961527	0.647840931	0.822468444
M1927	3-hydroxydecanoylcarnitine	Lipid	Fatty Acid Metabolism (Acyl Carnitine, Hydroxy)	0.763093569	-0.390068127	0.646790957	0.822468444
M447	5-methylthioribose	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	1.088762466	0.122689237	0.646384234	0.822468444
M4139	AMP	Nucleotide	Purine Metabolism, Adenine containing	0.932177703	-0.101323089	0.643986702	0.822468444
M3368	androstenediol (3alpha, 17alpha) monosulfate (3)	Lipid	Androgenic Steroids	0.840803839	-0.250158839	0.63710967	0.822468444
M4432	carotene diol (2)	Cofactors and Vitamins	Vitamin A Metabolism	1.185608389	0.245627561	0.642872403	0.822468444
M462	cystine	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	0.930677114	-0.103647364	0.640066358	0.822468444
M1543	eicosanoate (20:1n9 or 1n11)	Lipid	Long Chain Monounsaturated Fatty Acid	0.807285664	-0.308848824	0.646856921	0.822468444
M77	hydantoin-5-propionate	Amino Acid	Histidine Metabolism	1.194515656	0.256425763	0.647123426	0.822468444
M1533	oleate/vaccenate (18:1)	Lipid	Long Chain Monounsaturated Fatty Acid	0.858065267	-0.220840706	0.643071564	0.822468444
M4591	paraxanthine	Xenobiotics	Xanthine Metabolism	1.373317358	0.457665055	0.636692214	0.822468444
M4592	theobromine	Xenobiotics	Xanthine Metabolism	0.768182704	-0.380478613	0.647524717	0.822468444
M3401	11beta-hydroxyandrosterone glucuronide	Lipid	Androgenic Steroids	1.349476159	0.432399489	0.652986029	0.822685588
M3461	glycochenodeoxycholate	Lipid	Primary Bile Acid Metabolism	1.615490983	0.691972609	0.652835528	0.822685588
M1502	laurate (12:0)	Lipid	Medium Chain Fatty Acid	1.52061766	0.604657451	0.653442238	0.822685588
M4905	quinate	Xenobiotics	Food Component/Plant	1.514856446	0.599181085	0.651079894	0.822685588
M3124	sphingomyelin (d18:1:21:0, d17:1:22:0, d16:1:23:0)*	Lipid	Sphingomyelin	1.048340939	0.681079883	0.651442537	0.822685588
M2243	trimethylamine N-oxide	Lipid	Phospholipid Metabolism	1.595505232	0.674013339	0.651231001	0.822685588
M3519	taurosoodeoxycholic acid sulfate (1)	Lipid	Secondary Bile Acid Metabolism	1.215090366	0.28106361	0.661728863	0.83017039
M1550	tetradecadienoate (14:2)*	Lipid	Long Chain Polyunsaturated Fatty Acid (n3 and n6)	0.799645791	-0.322567006	0.661627202	0.83017039
M576	cysteinylglycine	Amino Acid	Glutathione Metabolism	1.226381228	0.29440752	0.663531716	0.83193831
M58	carboxyethyl-GABA	Amino Acid	Glutamate Metabolism	1.328091018	0.409354023	0.665790758	0.833614048
M2030	12,13-DHOME	Lipid	Fatty Acid, Dihydroxy	0.684552543	-0.546766815	0.666864994	0.835703325
M80	imidazole propionate	Amino Acid	Histidine Metabolism	1.319148669	0.399607167	0.669298152	0.835703325
M51	4-hydroxyglutamate	Amino Acid	Glutamate Metabolism	1.12720312	0.172747511	0.67331503	0.839556564
M2266	1-myristoyl-2-arachidonoyl-GPC (14:0/20:4)*	Lipid	Phosphatidylcholine (PC)	1.154917361	0.207789624	0.678327174	0.841197929
M3339	16a-hydroxy DHEA 3-sulfate	Lipid	Androgenic Steroids	1.518368355	0.60252183	0.677794836	0.841197929
M3535	ethocholanolone glucuronide	Lipid	Androgenic Steroids	1.230141831	0.298824663	0.678077588	0.841197929
M5736	ondansetron	Xenobiotics	Drug - Gastrointestinal	0.667146331	-0.583924859	0.677703609	0.841197929
M1165	DSEGEDF1XAEGGVR*	Peptide	Fibrinogen Cleavage Peptide	1.123533429	0.168043051	0.682391062	0.845084678
M2279	1-palmitoyl-2-palmitoleoyl-GPC (16:0/16:1)*	Lipid	Phosphatidylcholine (PC)	1.195626585	0.257766881	0.685489525	0.847786787
M3122	sphingomyelin (d18:1:20:1, d18:2:20:0)*	Lipid	Sphingomyelins	0.961470326	-0.056685763	0.687658937	0.849261559
M3112	sphingomyelin (d17:1:14:0, d16:1:15:0)*	Lipid	Sphingomyelins	1.174699446	0.232291682	0.689992981	0.850494636
M578	cys-gly, oxidized	Amino Acid	Glutathione Metabolism	1.253379278	0.325823047	0.695933094	0.853715496
M2123	glucose	Carbohydrate	Glycolysis, Glconeogenesis, and Pyruvate Metabolism	1.091767919	0.126666221	0.693409178	0.853715496
M1706	hydroxy-CMP*	Lipid	Fatty Acid, Dicarboxylate	1.220669853	0.287673056	0.695641028	0.853715496
M138	N,N,N-trimethyl-5-monovalerate	Amino Acid	Lysine Metabolism	0.913158509	-0.311062785	0.695591548	0.853715496
M141	N-acetylphenylalanine	Amino Acid	Phenylalanine Metabolism	0.885339385	-0.175608685	0.697103783	0.853991009
M1688	dodecenodioate (C12:2-D)*	Lipid	Fatty Acid, Dicarboxylate	0.883401195	-0.178859311	0.703872055	0.861310146
M1570	dihomolinoleate (20:6)	Lipid	Long Chain Polyunsaturated Fatty Acid (n3 and n6)	0.83736318	-0.256074613	0.706085569	0.862767126
M6451	bilirubin degradation product, C16H18N2O5 (4)	Partially Characterized Molecules	Pantothenate and CoA Metabolism	0.869657037	0.20481531	0.721083503	0.870470769
M455	cysteine	Amino Acid	Pantothenate, Cysteine, SAM and Taurine Metabolism	1.284275737	0.358931532	0.711761422	0.864961408
M5514	fluconazole	Xenobiotics	Methionine, Cysteine, SAM and Taurine Metabolism	1.15811939	0.211789375	0.71093677	0.864961408
M1690	tridecenodioate (C13:1-DC)*	Lipid	Fatty Acid, Dicarboxylate	1.277754002	0.35361011	0.710951632	0.864961408
M485	urea	Amino Acid	Urea cycle; Arginine and Proline Metabolism	0.919967905	-0.12034565	0.713540428	0.86556562
M1960	2-hydroxyoctanoate	Lipid	Fatty Acid, Monohydroxy	0.841178562	0.249516013	0.717760306	0.868767135
M1668	3-hydroxyadipate	Lipid	Fatty Acid, Dicarboxylate	0.853722076	-0.228161609	0.716900716	0.868767135
M4436	pantothenate (Vitamin B5)	Cofactors and Vitamins	Pantothenate, Cysteine, SAM and Taurine Metabolism	0.869657037	0.20481531	0.721083503	0.870470769
M1681	sebacate (C10:DC)	Lipid	Fatty Acid, Dicarboxylate	1.321438289	0.402109053	0.720875567	0.870470769
M3012	N-stearyl-3-sphinganine (d18:0/18:0)*	Lipid	Dihydroceramides	1.169020853	0.22530665	0.722707521	0.871265721
M2582	1-palmitoyl-GPA (16:0)	Lipid	Lysophospholipid	0.867404184	-0.20523693	0.727298449	0.871406138
M159	4-hydroxyphenylacetate	Amino Acid	Phenylalanine Metabolism	1.414356365	0.500145671	0.727347279	0.871406138
M1704	docosidioate (C22:DC)	Lipid	Fatty Acid, Dicarboxylate	1.333515233	0.415234305	0.727609746	0.871406138
M3099	palmitoyl dihydroosphingomyelin (d18:0/16:0)*	Lipid	Dihydroosphingomyelins	0.981179919	-0.027410387	0.727204142	0.871406138
M476	succinoyltaurine	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	1.30442825	0.383417591	0.726963148	0.871406138
M3113	sphingomyelin (d18:1/14:0, d16:1/16:0)*	Lipid	Sphingomyelins	1.046661544	0.06579498	0.729777883	0.872852638
M2325	1-stearoyl-2-linoleoyl-GPC (18:0/18:2)*	Lipid	Phosphatidylcholine (PC)	0.962634311	-0.05494025	0.732442725	0.87340731
M299	indoleacetate	Amino Acid	Tryptophan Metabolism	1.306561774	0.385757537	0.731701027	0.87340731
M348	2-ketocaprylate	Amino Acid	Leucine, Isoleucine and Valine Metabolism	0.886767738	-0.204768781	0.737177738	0.877087622
M4817	N-acetyllallin	Xenobiotics	Food Component/Plant	0.858177766	-0.220617949	0.736999422	0.877087622
M3439	ascorbic acid 3-sulfate*	Cofactors and Vitamins	Ascorbate and Aldarate Metabolism	1.251055046	0.323145269	0.738853366	0.877931639
M1962	2-hydroxydecanoate	Lipid	Fatty Acid, Monohydroxy	1.349130953	0.432001517	0.751249261	0.890318906
M6444	bilirubin degradation product, C16H18N2O5 (2)	Partially Characterized Molecules	Pantothenate and CoA Metabolism	1.208420961	0.273123114	0.752216633	0.890318906
M439	methionine sulfone	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	1.211533277	0.276834032	0.751854752	0.890318906
M449	2-hydroxy-4-(methylthio)butanoic acid	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	1.196092699	0.258329204	0.755454878	0.890700475
M4435	beta-cryptoxanthin	Cofactors and Vitamins	Vitamin A Metabolism	0.863109537	-0.212384432	0.755116897	0.890700475
M363	beta-hydroxyisovalerate	Amino Acid	Leucine, Isoleucine and Valine Metabolism	0.925854092	-0.111143242	0.758418226	0.890700475
M6446	bilirubin degradation product, C17H18N2O4 (2)	Partially Characterized Molecules	Pantothenate and CoA Metabolism	0.839295179	-0.2527498	0.755705622	0.890700475
M4938	indolin-2-one	Xenobiotics	Food Component/Plant	0.919666759	-0.120816899	0.751717921	0.890700475
M867	leucylalanine	Peptide	Dipeptidase	1.257074731	0.330070418	0.757765602	0.890700475
M1162	Fibrinopeptide A (5-6)*	Peptide	Fibrinogen Cleavage Peptide	0.962410027	-0.055276421	0.761052084	0.892633333
M4433	carotene diol (3)	Cofactors and Vitamins	Vitamin A Metabolism	1.120232983	0.163798812	0.7630972485	0.893072707
M6418	glycine conjugate of C10H14O2 (1)*	Partially Characterized Molecules	Pantothenate and CoA Metabolism	0.955615032	0.065498547	0.764371911	0.893072707
M2120	homovanillate (HVA)	Amino Acid	Tyrosine Metabolism	1.054551242	0.0766292	0.763535534	0.893072707
M4636	2-piperidone	Xenobiotics	Food Component/Plant	1.229085133	0.297584848	0.771393581	0.893483633
M1936	acetocetate	Lipid	Ketone Bodies	0.879439563	-0.185255076	0.768627017	0.893483633
M3364	androstenediol 3(beta,17beta) disulfate (2)	Lipid	Androgenic Steroids	1.211779241	0.20481531	0.771260997	0.894383633
M6445	p-cresol sulfate	Xenobiotics	Benzene Metabolism	0.849936489	-0.23473054	0.771141515	0.894383633
M3462	taurochenodeoxycholate	Lipid	Primary Bile Acid Metabolism	1.301246236	0.279883991	0.769077662	0.894383633
M3526	glycochoyolate	Lipid	Secondary Bile Acid Metabolism	0.853912271	-0.227840237	0.775544969	0.897941116
M466	lanthionine	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	1.081018189	0.112391638	0.776934455	0.898515801
M2587	1-linoleoyl-GPA (18:2)*	Lipid	Lysophospholipid	0.881038493	-0.182723042	0.778927681	0.898876591
M4999	phytanate	Xenobiotics	Food Component/Plant	0.839525165	-0.252334524	0.779224152	0.898876591
M97	4-imidazoleacetaete	Amino Acid	Histidine Metabolism	0.844555056	-0.243736621	0.781426462	0.900274593
M6190	perfluoroctanesulfonate (PFOS)	Xenobiotics	Chemical	0.932659634	0.100577417	0.783165	0.901214069
M1705	3-carboxy-4-methyl-5-propyl-2-furanpropanoate (CMFP)	Lipid	Fatty Acid, Dicarboxylate	1.187016728	0.247340267	0.785216689	0.901214069
M1180	Fibrinopeptide B (1-13)	Peptide	Fibrinogen Cleavage Peptide	0.946226689	0.09742241	0.785189044	0.901214069
M1959	2-hydroxyheptanoate*	Lipid	Fatty Acid, Monohydroxy	1.076807474	0.106760328	0.789269054	0.902442758
M2037	3,4-dihydroxybutyrate	Lipid	Fatty Acid, Dihydroxy	1.032213035	0.054704554	0.788723124	0.902442758
M3131	sphingomyelin (d18:1/25, 0, d19:0/24:1, d20:1/23:0, d19:1/24:0)*	Lipid	Sphingomyelins	0.105838046	0.11880894	0.788910133	0.902442758
M427	isobutyrylglycine (C4)	Amino Acid	Leucine, Isoleucine and Valine Metabolism	0.854558465	-0.226788987	0.79138596	0.903703952
M1494	caproate (10:0)	Lipid	Medium Chain Fatty Acid	1.240244221	0.310624235	0.794969008	0.906835999
M3531	mannitol/sorbitol	Carbohydrate	Fructose, Mannose and Galactose Metabolism	1.108691049	0.148857396	0.799116682	0.91027201
M4597	1,7-dimethylurate	Xenobiotics	Xanthine Metabolism	1.152247232	0.204450412	0.802124046	0.910242225
M2618	1-linolenoyl-GPC (18:3)*	Lipid	Lysophospholip				

M76	N-acetyl-1-methylhistidine*	Amino Acid	Histidine Metabolism	0.913638914	-0.130303995	0.847372275	0.941035295
M1441	aconitate [cis or trans]	Energy	TCA Cycle	0.97162354	-0.041530652	0.849390279	0.941576016
M3047	ceramide (d18:1/14:0, d16:1/16:0)*	Lipid	Ceramides	1.054047148	0.075939401	0.850422343	0.941576016
M1985	3-hydroxyflaureate	Lipid	Fatty Acid, Monohydroxy	0.912259338	-0.132484081	0.853593073	0.942130933
M163	N-acetyltyrosine	Amino Acid	Tyrosine Metabolism	0.925941062	-0.11007729	0.850449297	0.942130933
M3120	sphingomyelin (d18:1/19:0, d19:1/18:0)*	Lipid	Sphingomyelins	0.969441112	-0.044774883	0.855069328	0.942130933
M3455	taurocholate	Lipid	Primary Bile Acid Metabolism	1.240920422	0.311410601	0.85492021	0.942130933
M2322	1-stearoyl-2-oleoyl-GPC (18:0/1:8:1)	Lipid	Phosphatidylcholine (PC)	1.03312787	0.047018827	0.86340111	0.950159333
M3101	sphingomyelin (d18:0/18:0, d19:0/17:0)*	Lipid	Dihydro sphingomyelins	0.942626949	-0.085241167	0.866336544	0.952236903
M582	2-hydroxybutyrate/2-hydroxyisobutyrate	Amino Acid	Glutathione Metabolism	0.933286	-0.099608841	0.870161861	0.955090904
M1880	cis-4-decenoylcarnitine (C10:1)	Lipid	Fatty Acid Metabolism (Acyl Carnitine, Monounsaturated)	0.93846862	-0.091619589	0.871041968	0.955090904
M79	cis-urocanate	Amino Acid	Histidine Metabolism	0.902432344	-0.148109318	0.873393597	0.955372779
M1703	eicosenedioate (C20:1-DC)*	Lipid	Fatty Acid, Dicarboxylate	1.024320414	0.048683176	0.87252507	0.955372779
M2536	1-palmitoyl-2-linoleoyl-GPI (16:0/18:2)	Lipid	Phosphatidylinositol (PI)	0.985681356	-0.020806757	0.879717199	0.955486335
M4470	4-hydroxyhippurate	Xenobiotics	Benzoate Metabolism	0.973794275	-0.038311076	0.87614768	0.955486335
M4431	carcotoe diol (1)	Cofactors and Vitamins	Vitamin A Metabolism	0.955286129	-0.065995178	0.87955566	0.955486335
M3043	N-palmitoyl-heptadecasparginosine (d17:1/16:0)*	Lipid	Ceramides	0.971112301	-0.042289954	0.879697491	0.955486335
M402	tglo/glycine	Amino Acid	Leucine, Isoleucine and Valine Metabolism	0.9604644	-0.051895955	0.878084249	0.955486335
M5249	2-acetamidophenol sulfate	Xenobiotics	Food Component/Plant	0.921433542	-0.118079293	0.877325014	0.955486335
M1986	3-hydroxymyristate	Lipid	Fatty Acid, Monohydroxy	0.933639089	-0.099606313	0.884110156	0.955741101
M1489	caproate (6:0)	Lipid	Medium Chain Fatty Acid	1.057190107	0.080234829	0.883629657	0.955741101
M528	creatine	Amino Acid	Creatine Metabolism	0.926638524	-0.109921433	0.882987705	0.955741101
M3104	hydroxylpalmitoyl sphingomyelin (d18:1/16:0(OH))	Lipid	Sphingomyelins	0.977033754	-0.03351969	0.884244517	0.955741101
M4933	homostachydine	Xenobiotics	Food Component/Plant	0.92032635	-0.119819736	0.88608808	0.956510697
M343	4-methyl-2-oxopentanoate	Amino Acid	Leucine, Isoleucine and Valine Metabolism	1.03330431	0.047265192	0.888284795	0.956695354
M4348	ascorbic acid 2-sulfate	Cofactors and Vitamins	Ascorbate and Aldarate Metabolism	1.025412379	0.036204222	0.88800776	0.956695354
M5328	N-methylpipecolate	Xenobiotics	Bacterial/Fungal	0.929684674	-0.105186622	0.889426893	0.95679177
M23	O-acetylhomoserine	Amino Acid	Glycine, Serine and Threonine Metabolism	1.132209852	0.179141383	0.890544456	0.956861596
M3342	epiandrosterone sulfate	Lipid	Androgenic Steroids	0.921885988	-0.117339755	0.892801091	0.95815709
M4408	bilirubin	Cofactors and Vitamins	Hemoglobin and Porphyrin Metabolism	1.048739419	0.068656255	0.894319533	0.958650816
M395	2-hydroxy-3-methylvalerate	Amino Acid	Leucine, Isoleucine and Valine Metabolism	1.059224449	0.12858963	0.898874417	0.960243902
M3472	glycochenodeoxycholate glucuronide (1)	Lipid	Primary Bile Acid Metabolism	0.946628456	-0.07192904	0.898726087	0.960243902
M1694	tetradeциnedioate (C14:2-DC)*	Lipid	Fatty Acid, Dicarboxylate	1.070876378	0.089781945	0.898974214	0.960243902
M1702	eicosenedioate (C20-DC)	Lipid	Fatty Acid, Dicarboxylate	1.08073108	0.112007579	0.91116578	0.972124054
M350	androsterone sulfate	Lipid	Androgenic Steroids	1.066779846	0.093262475	0.915276712	0.972135136
M4963	methyl indole-3-acetate	Xenobiotics	Food Component/Plant	1.100918199	0.138707277	0.913418128	0.972135136
M1884	myristoleylcarnitine (C14:1)*	Lipid	Fatty Acid Metabolism (Acyl Carnitine, Monounsaturated)	0.944371846	0.082573063	0.91545399	0.972135136
M3123	sphingomyelin (d18:1/20:2, d18:2/20:1, d16:1/22:2)*	Lipid	Sphingomyelins	0.959991998	-0.058905741	0.913192577	0.972135136
M538	N-acetylputrescine	Amino Acid	Polyamine Metabolism	0.970724841	0.042865684	0.918932253	0.974690103
M5088	4-allylphenol sulfate	Xenobiotics	Food Component/Plant	0.917947493	-0.123516462	0.922479327	0.976357776
M4462	hippurate	Xenobiotics	Benzoate Metabolism	1.074890464	0.104189651	0.922652713	0.976357776
M3297	corticosterone	Lipid	Corticosteroids	1.041305434	0.05839333	0.924754091	0.977443568
M4780	2-isopropylmalate	Xenobiotics	Food Component/Plant	0.936299201	-0.094958469	0.92873579	0.977795189
M1938	3-hydroxybutyrate (BHBA)	Lipid	Ketone Bodies	0.938322328	-0.081844499	0.929022294	0.977795189
M3048	ceramide (d18:1/17:0, d17:1/18:0)*	Lipid	Ceramides	1.011506668	0.016505883	0.930701027	0.977795189
M1696	hexadecenedioate (C16:1-DC)*	Lipid	Fatty Acid, Dicarboxylate	0.963879345	-0.053075529	0.930562976	0.977795189
M307	indoleacetylglutamine	Amino Acid	Tryptophan Metabolism	0.926276439	-0.110485278	0.928071896	0.977795189
M1772	propionylglycine (C3)	Lipid	Fatty Acid Metabolism (also BCAA Metabolism)	0.933481383	-0.099306845	0.932616533	0.977795189
M201	vanillate	Amino Acid	Tyrosine Metabolism	1.022216814	0.031701227	0.932067717	0.977795189
M1679	azelate (C9-DC)	Lipid	Fatty Acid, Dicarboxylate	1.048304826	0.068058285	0.933697214	0.977804243
M1861	laurylcarnitine (C12)	Lipid	Fatty Acid Metabolism (Acyl Carnitine, Medium Chain)	0.973126873	-0.039246814	0.935893646	0.977847499
M6086	sulfate*	Cofactors and Vitamins	Chemical	0.982423931	-0.025582391	0.935348577	0.977847499
M1882	5-dodecenoylcarnitine (C12:1)	Lipid	Fatty Acid Metabolism (Acyl Carnitine, Monounsaturated)	0.96330263	-0.053938991	0.941463364	0.980700059
M4409	bilirubin (E,E)*	Cofactors and Vitamins	Hemoglobin and Porphyrin Metabolism	0.966662612	-0.048915652	0.941860452	0.980700059
M2931	linoleoyl-linoleoyl-glycerol (18:2/18:2) [1]*	Lipid	Diacylglycerol	0.977709947	-0.032521564	0.940889986	0.980700059
M81	formiminoglutamate	Amino Acid	Histidine Metabolism	1.016093101	0.023032597	0.94478668	0.982621386
M1939	cholesterol sulfate	Lipid	Sterol	0.11156186	0.016584547	0.947502087	0.9836174
M267	kynurene	Amino Acid	Tryptophan Metabolism	0.970766332	-0.042804021	0.947908517	0.9836174
M1814	cis-3,4-methylenehexanoylethanol/glycine	Lipid	Fatty Acid Metabolism (Acyl Glycine)	1.018557502	0.026527429	0.955155276	0.987754433
M3009	N-palmitoyl-sphinganine (d18:0/16:0)	Lipid	Dihydroceramides	0.977872258	-0.03228208	0.954406016	0.987754433
M3127	sphingomyelin (d18:1/22:2, d18:2/22:1, d16:1/24:2)*	Lipid	Sphingomyelins	0.99165215	-0.012093952	0.953648601	0.987754433
M3115	sphingomyelin (d17:1/16:0, d18:1/15:0, d16:1/17:0)*	Lipid	Sphingomyelins	1.007106928	0.010216867	0.958346679	0.989928558
M2800	1-(1-enyl-palmitoyl)-2-oleoyl-GPE (P-16:0/18:1)*	Lipid	Plasmalogens	1.008608687	0.012366556	0.962028872	0.992028147
M2848	1-myristoylglycerol (14:0)	Lipid	Monoglyclycerol	0.964713131	-0.051820891	0.969110005	0.992028147
M1979	3-hydroxyhexanoate	Lipid	Fatty Acid, Monohydroxy	0.984393334	-0.022693207	0.967004561	0.992028147
M577	cysteinylglycine disulfide*	Amino Acid	Glutathione Metabolism	0.989731429	-0.014891003	0.965285777	0.992028147
M4437	retinal	Cofactors and Vitamins	Vitamin A Metabolism	1.02905606	0.041321578	0.965784369	0.992028147
M1691	tetradecanedioate (C14)	Lipid	Fatty Acid, Dicarboxylate	0.986974171	-0.018915764	0.962743749	0.992028147
M5738	diphenoxylate	Xenobiotics	Drug - Gastrointestinal	1.0000001	-1.44E-07	0.968305865	0.992028147
M5218	vanillic acid glycine	Xenobiotics	Food Component/Plant	0.962131327	-0.055694265	0.968315326	0.992028147
M2010	16-hydroxypalmitate	Lipid	Fatty Acid, Monohydroxy	1.015424825	0.022083436	0.972359781	0.993118024
M322	3-indoxyl sulfate	Amino Acid	Tryptophan Metabolism	0.993907188	0.008816957	0.971918595	0.993118024
M3372	galactonate	Carbohydrate	Fructose, Mannose and Galactose Metabolism	1.027781658	0.032498194	0.975877471	0.995502994
M180	4-hydroxyphenylacetoxycarnitine	Amino Acid	Tyrosine Metabolism	1.017744441	0.025573542	0.978194831	0.995682851
M3280	Salp α -pregnan-3 β eta,20 α lpha-diol disulfate	Lipid	Progesterin Steroids	0.984364033	-0.02273615	0.979252441	0.995682851
M2	N-acetyl-glycine	Amino Acid	Glycine, Serine and Threonine Metabolism	0.988710608	-0.016379784	0.977131609	0.995682851
M151	phenylalactate (PLA)	Amino Acid	Phenylalanine Metabolism	0.99047638	-0.013805524	0.981083956	0.99643052
M1682	decadienedioic acid (C10:2-DC)	Lipid	Fatty Acid, Dicarboxylate	1.008288648	0.011908706	0.983374859	0.997642574
M1709	2-hydroxysebacate	Lipid	Fatty Acid, Dicarboxylate	1.01047171	0.014993895	0.985598609	0.998697003
M5073	tartarate	Xenobiotics	Food Component/Plant	0.981567617	-0.026840441	0.986611561	0.998697003
M2360	1-linoleoyl-2-linolenoyl-GPC (18:2/18:3)*	Lipid	Phosphatidylcholine (PC)	0.99716406	-0.004097208	0.994190077	0.999110486
M6175	2-naphthol sulfate	Xenobiotics	Chemical	1.001293242	0.001864548	0.99758319	0.999110486
M4382	gamma-tocopherol/beta-tocopherol	Cofactors and Vitamins	Tocopherol Metabolism	0.998575532	-0.002056537	0.99727119	0.999110486
M3540	glycodeoxycholate 3-sulfate	Lipid	Secondary Bile Acid Metabolism	0.997974705	-0.002924845	0.99801354	0.999110486
M351	isovalerate (C5)	Amino Acid	Leucine, Isoleucine and Valine Metabolism	0.998867107	-0.001635346	0.996624777	0.999110486
M410	methylsuccinate	Amino Acid	Leucine, Isoleucine and Valine Metabolism	1.00696369	0.010011662	0.990463652	0.999110486
M110	N2-acetyl,N6,N6-dimethyllysine	Amino Acid	Lysine Metabolism	0.996316144	-0.00525861	0.993955286	0.999110486
M4209	ortotidine	Nucleotide	Pyrimidine Metabolism, Orotate containing	0.99134111	-0.012546536	0.989754736	0.999110486
M1239	pyruvate	Carbohydrate	Glycolysis, Gluconeogenesis, and Pyruvate Metabolism	1.002149566	0.003097839	0.991332105	0.999110486
M3504	ursodeoxycholate	Lipid	Secondary Bile Acid Metabolism	0.995348987	-0.006725646	0.993737204	0.999110486
M510	N ₂ ,N ₅ -diacetylornithine	Amino Acid	Urea cycle; Arginine and Proline Metabolism	0.99996451	-5.12E-05	0.999737557	0.999737557

Supplementary data 3: UPLC-MS/MS metabolites in serum samples collected after the first NF

Compounds in column B for which no authentic standards were available for confirmation are marked with * after the compound name to designate these as Metabolomics Standards Initiative level 2/3

Fold change and log2 (fold change) were based on samples preceding vs. not preceding NF within 24 hours

p values are from Welch's two-sample t-test. q values are derived from p values after FDR correction for multiple testing

Color coding is column E was applied along the fold change gradient, with blue and red representing decreased and increased levels in NF vs. non-NF samples, respectively

Color coding in column H was applied along the q value gradient, with darker colors indicating more significant values

metabolite_code	metabolite	pathway	sub_pathway	foldchange	log2_foldchange	p	q
M2834	1-(1-enyl-palmitoyl)-GPE (P-16:0)*	Lipid	Lysoplasmalogen	0.674570614	-0.567958623	2.80E-06	0.000926257
M105	lysine	Amino Acid	Lysine Metabolism	0.739030421	-0.436294343	3.30E-06	0.000926257
M17	threonine	Amino Acid	Glycine, Serine and Threonine Metabolism	0.647591826	-0.626843319	3.30E-06	0.000926257
M4219	uridine	Nucleotide	Pyrimidine Metabolism, Uracil containing	0.553579757	-0.853136906	4.08E-06	0.000926257
M2838	1-(1-enyl-stearoyl)-GPE (P-18:0)*	Lipid	Lysoplasmalogen	0.664253797	-0.590193526	6.35E-06	0.000964415
M2602	1-palmityleoyl-GPC* (16:1)*	Lipid	Lyso phospholipid	0.559967027	-0.836586217	8.47E-06	0.000964415
M2708	1-palmityl-GPG (16:0)*	Lipid	Lyso phospholipid	0.665299869	-0.587923344	7.29E-06	0.000964415
M2601	2-palmityl-GPC* (16:0)*	Lipid	Lyso phospholipid	0.771489373	-0.37428181	8.99E-06	0.000964415
M40	asparagine	Amino Acid	Alanine and Aspartate Metabolism	0.56408009	-0.826028078	1.55E-05	0.00137539
M2673	1-linoleoyl-GPE (18:2)*	Lipid	Lyso phospholipid	1.6386170852	-0.7125261	1.66E-05	0.00137539
M2182	linoleoyl ethanalamide	Lipid	Endocannabinoid	0.574778096	-0.798923011	2.32E-05	0.00175645
M2833	1-(1-enyl-palmitoyl)-GPC (P-16:0)*	Lipid	Lysoplasmalogen	0.537594731	-0.895409098	3.37E-05	0.00203594
M121	fructosyllamine	Amino Acid	Lysine Metabolism	0.389657786	-1.359720451	3.39E-05	0.00203594
M527	guanidinoacetate	Amino Acid	Creatine Metabolism	0.678062534	-0.560509762	4.74E-05	0.002559294
M2616	1-linoleoyl-GPC (18:2)	Lipid	Lyso phospholipid	0.73458052	-0.445007457	5.02E-05	0.002559294
M2600	1-palmityl-GPC (16:0)	Lipid	Lyso phospholipid	0.550595589	-0.860935043	5.14E-05	0.002559294
M2603	2-palmityl-GPC* (16:1)*	Lipid	Lyso phospholipid	1.426473135	-0.51245277	5.02E-05	0.002559294
M3315	cortisone	Lipid	Corticosteroids	0.652597953	-0.615733633	5.75E-05	0.00272093
M644	gamma-glutamyltheanine	Peptide	Gamma-glutamyl Amino Acid	0.734039008	-0.446071362	6.06E-05	0.00272093
M2613	1-oleyl-GPC (18:1)	Lipid	Lyso phospholipid	0.637096532	-0.834308846	6.52E-05	0.00280838
M2618	1-linolenoyl-GPC (18:3)*	Lipid	Lyso phospholipid	0.571620647	-0.411957946	6.94E-05	0.00280838
M2236	glycerophosphorycholine (GPC)	Lipid	Phospholipid Metabolism	0.693454813	-0.528126218	7.59E-05	0.002976928
M2365	1-linoleyl-2-arachidonoyl-GPC (18:2/20:4n6)*	Lipid	Phosphatidylcholine (PC)	4.086393608	2.030828174	7.86E-05	0.002976928
M5382	3-(cystein-S-yl)acetaminophen*	Xenobiotics	Drug - Analgesics, Anesthetics	0.642814627	-0.637525337	9.18E-05	0.003254768
M640	gamma-glutamyl-alpha-lysine	Peptide	Gamma-glutamyl Amino Acid	0.773138269	-0.371201644	9.31E-05	0.003254768
M2240	glycerophosphocholanamine	Lipid	Phospholipid Metabolism	0.575940624	-0.796080008	0.000109415	0.003683629
M649	gamma-glutamylcitrulline*	Peptide	Gamma-glutamyl Amino Acid	0.490870428	-1.026585839	0.000119549	0.003881086
M2649	1-lignoceroyl-GPC (24:0)	Lipid	Plasmalogens	0.630618033	-0.66516167	0.000153738	0.004619947
M2801	1-(1-enyl-palmitoyl)-2-linoleoyl-GPE (P-16:0/18:2)*	Lipid	Cofactors and Vitamins	0.389183072	-1.361479136	0.000157556	0.004619947
M4429	retinol (Vitamin A)	Vitamin A	Vitamin A Metabolism	0.690110004	-0.535101748	0.000170644	0.00487357
M5117	pyraline	Xenobiotics	Food Component/Plant	0.723317555	-0.467289828	0.000191734	0.005163072
M2359	1,2-dilinoleoyl-GPC (18:2/18:2)	Lipid	Phosphatidylcholine (PC)	0.707084124	-0.500046228	0.000193118	0.005163072
M2686	1-arachidonoyl-GPE (20:4n6)*	Lipid	Lyso phospholipid	0.733919114	-0.446307024	0.000569949	0.012520761
M492	citrulline	Amino Acid	Urea cycle; Arginine and Proline Metabolism	0.730501297	-0.453041216	0.000223368	0.005081179
M2611	1-stearoyl-GPC (18:0)	Lipid	Lyso phospholipid	0.537351351	-0.466433958	0.000233443	0.005894437
M2635	1-arachidonoyl-GPC* (20:4)*	Lipid	Lyso phospholipid	0.534600534	-0.903466815	0.002992942	0.007351657
M48	N-acetylglutamine	Amino Acid	Glutamate Metabolism	1.348511635	-0.43126797	0.00361539	0.00864801
M1352	mannose	Carbohydrate	Fructose, Mannose and Galactose Metabolism	0.793005933	-0.334596435	0.009031774	0.009188699
M29	alanine	Amino Acid	Alanine and Aspartate Metabolism	0.816474119	-0.29252094	0.000404433	0.009188699
M445	glutamine	Amino Acid	Glutamate Metabolism	0.733919114	-0.446307024	0.000569949	0.012520761
M2804	1-(1-enyl-palmitoyl)-2-arachidonoyl-GPE (P-16:0/20:4)*	Lipid	Plasmalogens	0.318497052	-0.450648074	0.000578517	0.012520761
M2621	dibutyl sulfosuccinate	Xenobiotics	Chemical	0.708944032	-0.496256358	0.00059414	0.012559852
M2836	1-(1-enyl-oleoyl)-GPE (P-18:1)*	Lipid	Lyso plasmalogen	0.696596576	-0.521604713	0.000673343	0.013305852
M2810	1-(1-enyl-stearoyl)-2-linoleoyl-GPE (P-18:0/18:2)*	Lipid	Plasmalogens	0.574326438	-0.800057121	0.000651914	0.013305852
M1890	ximenoxy carnitine (C26:1)*	Lipid	Fatty Acid Metabolism (Acyl Carnitine, Monounsaturated)	0.267384258	-1.903013562	0.00066819	0.013305852
M429	2,3-dihydroxy-2-methylbutyrate	Amino Acid	Leucine, Isoleucine and Valine Metabolism	0.170517087	-2.552017779	0.000714097	0.013809933
M438	S-methylmethionine	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	0.603863572	-0.7770545	0.000836318	0.016364238
M2198	N-palmitoylserine	Lipid	Endocannabinoid	0.564771093	-0.824262	0.000901773	0.016394228
M493	homarginine	Amino Acid	Urea cycle; Arginine and Proline Metabolism	0.737056005	-0.440115389	0.000885655	0.016394228
M2197	N-stearylserine*	Lipid	Endocannabinoid	0.715371134	-0.483236189	0.000951391	0.016738645
M2671	1-oleoyl-GPE (18:1)	Lipid	Lyso phospholipid	0.835634489	-0.291157764	0.001295922	0.019965987
M5376	3-(N-acetyl-L-cystein-S-yl) acetaminophen	Xenobiotics	Drug - Analgesics, Anesthetics	2.903140527	1.537614408	0.000975961	0.016738645
M70	histidine	Amino Acid	Histidine Metabolism	0.755208032	-0.450503397	0.000954988	0.017729986
M635	gamma-glutamylglutamine	Peptide	Gamma-glutamyl Amino Acid	0.781114552	-0.356393958	0.001054506	0.017705844
M5379	2-hydroxyacetaminophen sulfate*	Xenobiotics	Drug - Analgesics, Anesthetics	2.334978885	1.223405904	0.001145559	0.018273135
M224	dopamine 3-O-sulfate	Amino Acid	Tyrosine Metabolism	0.559758242	-0.837124229	0.001115389	0.018273135
M2159	oleoyl ethanalamide	Lipid	Endocannabinoid	1.430964098	-0.516987477	0.001165943	0.018273135
M6086	sulfate*	Xenobiotics	Chemical	0.835634489	-0.295060506	0.001148791	0.018273135
M307	indoleacetylglutamine	Amino Acid	Tryptophan Metabolism	0.531758184	-0.491157764	0.001295922	0.019965987
M92	1-methyl-5-imidazoleacetate	Amino Acid	Histidine Metabolism	0.470772471	-1.086881324	0.001832313	0.02277986
M5380	2-methoxyacetaminophen sulfate*	Xenobiotics	Drug - Analgesics, Anesthetics	4.174724077	2.061680848	0.00186068	0.02277986
M279	8-methoxykyurenate	Amino Acid	Tryptophan Metabolism	0.467072991	-0.109841433	0.001891915	0.02277986
M2809	1-(1-enyl-stearoyl)-2-oleoyl-GPE (P-18:0/20:1)	Lipid	Plasmalogens	0.776873971	-0.36424752	0.002020023	0.00886255
M3078	glycosyl ceramide (d18:1/20:0, d16:1/22:0)*	Lipid	Hexosylceramides (HCR)	0.710870667	-0.492340909	0.002032127	0.00886255
M632	gamma-glutamylalanine	Peptide	Gamma-glutamyl Amino Acid	0.667243227	-0.583715338	0.002127171	0.02297454
M2818	1-(1-enyl-stearoyl)-2-arachidonoyl-GPE (P-18:0/20:4)*	Lipid	Plasmalogens	0.729770736	-0.454445258	0.002240155	0.030392549
M3108	lignoceroyl sphingomyelin (d18:1/24:0)	Lipid	Sphingomyelin	0.830073968	-0.2668868194	0.002235575	0.030392549
M223	dopamine 4-sulfate	Amino Acid	Tyrosine Metabolism	0.422763562	-1.242077058	0.002607033	0.0348499
M2034	2R,3R-dihydroxybutyrate	Lipid	Fatty Acid, Dihydroxy	0.726729879	-0.460508872	0.002823859	0.037201274
M495	proline	Amino Acid	Urea cycle; Arginine and Proline Metabolism	0.795923615	-0.322988114	0.002930661	0.038056725
M1894	arachidonoylcarnitine (C20:4)	Lipid	Fatty Acid Metabolism (Acyl Carnitine, Polyunsaturated)	0.697114327	-0.520328217	0.003077328	0.03885127
M3261	pregnenetriol sulfate*	Lipid	Pregnenolone Steroids	1.718784438	-0.78138862	0.003067143	0.03885127
M1870	cerotoly carnitine (C26)*	Lipid	Fatty Acid Metabolism (Acyl Carnitine, Long Chain Saturated)	0.662192481	-0.594674766	0.003142247	0.039127426
M4420	uracil	Nucleotide	Pyrimidine Metabolism, Uracil containing	0.474032012	-1.076943606	0.003274585	0.040224295
M454	alpha-ketobutyrate	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	1.538325348	-0.621360568	0.003327988	0.040335334
M2010	16-hydroxypalmitate	Lipid	Fatty Acid, Monohydroxy	0.784402371	-0.350334199	0.003688279	0.043504847
M5585	dexamethasone	Xenobiotics	Fatty Acid, Antiinflammatory, Immunosuppressant	0.106814657	-2.262818741	0.00368795	0.043504847
M5374	4-acetamidophenol	Xenobiotics	Drug - Analgesics, Anesthetics	2.999036562	1.584499111	0.004057933	0.047295023
M5386	3-(methylthio)acetaminophen sulfate*	Xenobiotics	Drug - Analgesics, Anesthetics	2.245499911	-0.945676665	0.004193348	0.048250309
M93	1-methyl-5-imidazoleacetate	Amino Acid	Histidine Metabolism	0.516401831	-0.953433978	0.004465079	0.050364742
M646	gamma-glutamyltyrosine	Peptide	Gamma-glutamyl Amino Acid	0.744412665	-0.425825494	0.004487945	0.050364742
M391	1-carboxyethylsucrose	Amino Acid	Leucine, Isoleucine and Valine Metabolism	0.597419767	-0.743183122	0.004680587	0.051087682
M504	N-acetyltrulline	Amino Acid	Urea cycle; Arginine and Proline Metabolism	0.356789923	-1.486853227	0.004684619	0.051305043
M2888	diacylglycerol (14:0/18:1, 16:0/16:1) [2]*	Lipid	Diacylglycerol	0.464335725	-1.06795221	0.004770762	0.051625491
M175	4-hydroxyphenylpyruvate	Amino Acid	Tyrosine Metabolism	0.676502254	-0.563833354	0.004847149	0.05175958
M3472	glycochenodeoxycholic glucuronide (1)	Lipid	Primary Bile Acid Metabolism	1.796667975	-0.485322875	0.004896225	0.05175958
M2556	1-stearoyl-2-arachidonoyl-GPI (18:0/20:4)	Lipid	Phosphatidylinositol (PI)	0.811106928	-0.302035978	0.004993938	0.052234466
M423	3-methyl-2-oxobutyrate	Amino Acid	Leucine, Isoleucine and Valine Metabolism	1.150114968	-0.301701014	0.0049932761	0.052277236
M1659	glutarate (C5-C6)	Lipid	Fatty Acid, Dicarboxylate	0.614964967	-0.701423869	0.005118453	0.052277236
M4322	triglycerol (N'-methylnicotinate)	Cofactors and Vitamins	Nicotinate and Nicotinamide Metabolism	0.444594591	-1.168268949	0.005272328	0.032520512
M5377	4-acetaminophen sulfate	Xenobiotics	Drug - Analgesics, Anesthetics	2.415269823	1.272184369	0.005402865	0.039699282
M4502	3-methyl catechol sulfate (1)	Xenobiotics	Benzoate Metabolism	0.188882959	-2.40436199	0.005571615	0.050502611
M4356	oxalate (ethanedioate)	Cofactors and Vitamins	Ascorbate and Aldarate Metabolism	0.707839942	-0.498504923	0.005540191	0.054502611
M3519	taurosoodeoxycholic acid sulfate (1)	Lipid	Secondary Bile Acid Metabolism	2.785001279	-1.47767799	0.005867386	0.056738873
M3161	sphingosine 1-phosphate	Lipid	Sphingosine	0.807101014	-0.309178848	0.005932761	0.056767156
M4772	2,3-dihydroxyvalerate	Xenobiotics	Food Component/Plant	0.397803107	-1.329873552	0.006196353	0.058673392
M1976	2-hydroxyneuro						

M5151	trans-3,4-methyleneheptanoate	Xenobiotics	Food Component/Plant	1.339605537	0.42180244	0.00867655	0.071736956
M75	N-acetyl-3-methylhistidine*	Amino Acid	Histidine Metabolism	0.365655193	-1.45144425	0.00873938	0.071736956
M5378	4-acetamidophenylglucuronide	Xenobiotics	Drug - Analgesics, Anesthetics	1.968171563	0.976855984	0.009074319	0.072996067
M4602	7-methoxykantchine	Xenobiotics	Xanthine Metabolism	0.463953655	-1.07947395	0.009357168	0.073324706
M3102	sphingomyelin (d18:0/20:0, d16:0/22:0)*	Lipid	Dihydro sphingomyelins	0.751472265	-0.412208236	0.009244379	0.073324706
M3107	tricosanoyl sphingomyelin (d18:1/23:0)*	Lipid	Sphingomyelin	0.806255887	-0.310690305	0.009331481	0.073324706
M2814	1-(1-enyl-palmitoyl)-2-linoleoyl-GPC (P-16:0/18:2)*	Lipid	Plasmalogen	0.842460639	-0.247318811	0.009982288	0.076897459
M4324	N1-Methyl-2-pyridone-5-carboxamide	Cofactors and Vitamins	Nicotinate and Nicotinamide Metabolism	0.651257571	-0.618699856	0.009914035	0.076897459
M4231	5,6-dihydrouracil	Nucleotide	Pyrimidine Metabolism, Uracil containing	0.481243974	-1.05515962	0.010170155	0.077686311
M2266	1-myristoyl-2-arachidonoyl-GPC (14:0/20:4)*	Lipid	Phosphatidylcholine (PC)	0.670136712	-0.577472651	0.010563159	0.077923972
M4603	5-acetylaminio-6-amino-3-methyluracil	Xenobiotics	Xanthine Metabolism	0.402081553	-1.314439952	0.010473618	0.077923972
M461	cysteine s-sulfate	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	0.880305084	-0.183924496	0.010409393	0.077923972
M6154	ectoine	Xenobiotics	Chemical	0.604223423	-0.726845982	0.010629893	0.077923972
M1683	undecanedioate (C11-DC)	Lipid	Fatty Acid, Dicarboxylate	0.677099237	-0.562560801	0.01038174	0.077923972
M2141	12-HETE	Lipid	Eicosanoid	0.151808025	-2.719679782	0.01118265	0.076375001
M2173	N-stearoyltaurine	Lipid	Endocannabinoid	0.707709985	-0.49876982	0.011214082	0.076375001
M510	N2,N5-diacytelylornithine	Amino Acid	Urea cycle; Arginine and Proline Metabolism	0.660635878	-0.598072772	0.011163911	0.076375001
M4353	threonate	Cofactors and Vitamins	Ascorbate and Aldarate Metabolism	0.729437237	-0.455144245	0.010974562	0.076375001
M641	gamma-glutamyl-epsilon-lysine	Peptide	Gamma-glutamyl Amino Acid	0.677111881	-0.562533886	0.011359525	0.070707612
M3474	glycochenodeoxycholate 3-sulfate	Lipid	Primary Bile Acid Metabolism	0.203471508	1.016832535	0.011574703	0.070707612
M3058	glycosy-N-stearoyl-sphingosine (d18:1/18:0)	Lipid	Hexosylceramides (HCR)	0.748986015	-0.416989313	0.011504902	0.070707612
M131	pipecolate	Amino Acid	Lysine Metabolism	0.61162252	-0.709286566	0.01148145	0.070707612
M263	oxindolylalanine	Amino Acid	Tryptophan Metabolism	0.730511179	-0.453021745	0.01212769	0.083195302
M2715	1-linoleoyl-GPG (18:2)*	Lipid	Lyso phospholipid	0.820121631	-0.286090205	0.012399502	0.084113042
M228	vanillic alcohol sulfate	Amino Acid	Tyrosine Metabolism	0.172888449	-2.532086616	0.012981422	0.087404245
M4594	1-methylurate	Xenobiotics	Xanthine Metabolism	0.493191116	-1.019781282	0.013440272	0.088911378
M58	carboxyethyl-GABA	Amino Acid	Glutamate Metabolism	0.781943279	-0.354846134	0.013498097	0.088911378
M505	N-acetylproline	Amino Acid	Urea cycle; Arginine and Proline Metabolism	0.70816973	-0.47832917	0.01339677	0.088911378
M637	gamma-glutamylhistidine	Peptide	Gamma-glutamyl Amino Acid	0.749491627	-0.416015735	0.013907975	0.088949881
M3068	glycosy-N-behenoyl-sphingadienine (d18:2/22:0)*	Lipid	Hexosylceramides (HCR)	0.7510464615	-0.413025641	0.013937629	0.088949881
M4499	N-acetylarginine	Amino Acid	Urea cycle; Arginine and Proline Metabolism	0.680719305	-0.55486807	0.014035955	0.088949881
M442	N-acetylasparagine	Amino Acid	Alanine and Aspartate Metabolism	0.725543016	-0.462866943	0.013754922	0.088949881
M72	3-methylhistidine	Amino Acid	Histidine Metabolism	0.554988951	-0.849469046	0.014468214	0.091962979
M447	5-methylthioribose	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	1.16179982	0.216361511	0.014605157	0.092195052
M1165	DSEEDFDAEGGGVR*	Peptide	Fibrinogen Cleavage Peptide	1.34284999	0.425298151	0.01475623	0.092506439
M4133	allantoin	Nucleotide	Purine Metabolism, (Hypo)Xanthine/Inosine containing	0.564206101	-0.825705829	0.014992926	0.09291996
M4817	N-acetylallilin	Xenobiotics	Food Component/Plant	0.273509775	-2.087127313	0.01502699	0.09291996
M6435	GlcNAc sulfate conjugate of C21H34O2 steroid	Partially Characterized Molecules	Partially Characterized Molecules	0.624605277	1.061518607	0.015144827	0.09301789
M2360	1-linoleoyl-2-linolenoyl-GPC (18:2/18:3)*	Lipid	Phosphatidylcholine (PC)	0.704254544	-0.505831127	0.015683311	0.094541631
M4816	allin	Xenobiotics	Food Component/Plant	0.31806666	-1.652589842	0.015704935	0.094541631
M576	cysteinylglycine	Amino Acid	Glutathione Metabolism	1.503328124	0.588159933	0.015599457	0.094541631
M1240	lactate	Carbohydrate	Glycosylation, Gluconeogenesis, and Pyruvate Metabolism	0.851025967	-0.232724941	0.016215065	0.096973558
M4601	3-methylkantchine	Xenobiotics	Xanthine Metabolism	0.436791777	-0.194982397	0.016941284	0.095516069
M1494	caprate (10:0)	Lipid	Medium Chain Fatty Acid	1.730198512	-0.453639366	0.016961691	0.095516069
M1880	cis-4-decenoylearnitine (C10:1)	Lipid	Fatty Acid Metabolism (Acyl Carnitine, Monounsaturated)	1.569841486	0.650618891	0.016798122	0.095516069
M1462	citraconate/glutonate	Energy	TCA Cycle	0.626495277	-0.674624462	0.017251696	0.100524307
M420	1-carboxyethylvaline	Amino Acid	Leucine, Isoleucine and Valine Metabolism	0.745288479	-0.424129137	0.017496697	0.101302552
M4252	cytosine	Nucleotide	Pyrimidine Metabolism, Cytidine containing	0.347510778	-0.124870369	0.018817825	0.108262046
M2662	1-palmitoyl-GPE (16:0)	Lipid	Lyso phospholipid	0.800135858	-0.321683114	0.018942505	0.108293946
M1974	2-hydroxybehenate	Lipid	Fatty Acid, Monohydroxy	1.166794006	0.22254988	0.019071931	0.108352409
M1702	eicosanedioate (C20-DC)	Lipid	Fatty Acid, Dicarboxylate	0.787682368	-0.344314113	0.019883182	0.115567642
M3124	spingomyelin (d18:1/21:0, d17:1/22:0, d16:1/23:0)*	Lipid	Sphingomyelin	0.7968401433	-0.327702954	0.019879206	0.115567642
M5353	glycocholate sulfate*	Lipid	Secondary Bile Acid Metabolism	2.246077243	1.167407543	0.020065547	0.115897279
M1950	stearylcholine*	Lipid	Fatty Acid Metabolism (Acyl Choline)	0.646121716	-0.630142225	0.022231822	0.1232394
M6431	branched-chain, straight-chain, or cyclopropyl 10:1 fatty acid (2)*	Partially Characterized Molecules	Partially Characterized Molecules	1.401726494	0.487204877	0.022672415	0.124120277
M2323	choline	Lipid	Phospholipid Metabolism	0.834825459	-0.260354841	0.022956355	0.124120277
M3541	taurochendoxycyclic acid 3-sulfate	Lipid	Secondary Bile Acid Metabolism	2.72644608	1.447021624	0.023924191	0.124120277
M1881	undecenoyl carnitine (C11:1)	Lipid	Fatty Acid Metabolism (Acyl Carnitine, Monounsaturated)	1.465982052	0.551867441	0.022714714	0.124120277
M3536	taurocholate sulfate*	Lipid	Secondary Bile Acid Metabolism	2.733150296	1.450564796	0.023278527	0.125208169
M460	S-carboxymethylcysteine	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	0.655661445	-0.608977033	0.023596428	0.126171489
M2905	palmitoyl-oleyl-glycerol (16:0/18:1) [2]*	Lipid	Diacylglycerol	0.755022568	-0.405408327	0.023795893	0.126493671
M3209	3beta-hydroxy-5-cholenenonate	Lipid	Sterol	0.729946463	-0.450402218	0.028234466	0.130380099
M3389	5alpha-androstan-3beta,17alpha-diol disulfate	Lipid	Androgenic Steroids	0.474134158	-1.076632762	0.024711562	0.140390438
M278	xanthurene	Amino Acid	Tryptophan Metabolism	0.67666194	-0.563492851	0.026927159	0.140671194
M261	C-glycosytryptophan	Amino Acid	Tryptophan Metabolism	0.838328357	-0.2254567188	0.027336943	0.141521486
M1166	ADpSSEGDFKAEGGGV*	Peptide	Fibrinogen Cleavage Peptide	1.406635639	0.492248675	0.027556989	0.141521486
M1866	stearoylcarnitine (C18)	Lipid	Fatty Acid Metabolism (Acyl Carnitine, Long Chain Saturated)	0.763652977	-0.389010904	0.027502639	0.141521486
M5206	tartarone (hydroxymalonate)	Xenobiotics	Food Component/Plant	0.70423184	-0.505877639	0.027952184	0.142744582
M3091	lactosyl-N-nervonyl-sphingosine (d18:1/24:1)*	Lipid	Lactosylceramides (LCER)	0.729946463	-0.454042218	0.028234466	0.143380613
M5961	2,6-dihydroxybenzoic acid	Xenobiotics	Drug - Topical Agents	0.464488028	-1.062686684	0.028497116	0.143910438
M6252	5-hydroxy-2-methylpyridine sulfate	Xenobiotics	Chemical	0.17479532	-2.514776648	0.028813983	0.144706686
M4120	hypoxanthine	Nucleotide	Purine Metabolism, (Hypo)Xanthine/Inosine containing	0.689201368	-0.537002529	0.029533908	0.147507264
M3386	5alpha-androstan-3beta,17beta-diol disulfate	Lipid	Androgenic Steroids	0.630803816	-0.664736708	0.030380819	0.150087852
M1517	arachidate (20:0)	Lipid	Long Chain Saturated Fatty Acid	1.235695649	0.305323452	0.030354701	0.150087852
M4504	4-ethylcatechol sulfate	Xenobiotics	Benzoate Metabolism	0.335282807	-1.576549588	0.031389746	0.150969732
M4523	4-ethylphenyl sulfate	Xenobiotics	Benzoate Metabolism	0.375897178	-1.4115901	0.031107127	0.150969732
M1489	caproate (6:0)	Lipid	Medium Chain Fatty Acid	0.884960132	-0.176315632	0.031178713	0.150969732
M35	N-carbamoylalanine	Amino Acid	Alanine and Aspartate Metabolism	0.579581166	-0.78691782	0.031295931	0.150969732
M3477	glycocholate sulfate	Lipid	Primary Bile Acid Metabolism	2.882891728	1.527516655	0.03118303	0.150969732
M1	glycine	Amino Acid	Glycine, Serine and Threonine Metabolism	0.834990903	-0.260135573	0.031261975	0.153090702
M1936	acetooacetate	Lipid	Ketone Bodies	1.744429121	0.302714921	0.032996061	0.156215727
M1491	caprylate (8:0)	Lipid	Medium Chain Fatty Acid	0.718816554	-0.476304462	0.032945453	0.156215727
M1543	ecosanoate (20:1n9 or 1n11)	Lipid	Long Chain Monounsaturated Fatty Acid	1.297681219	0.357937034	0.033728655	0.158824954
M4591	paraxanthine	Xenobiotics	Diacylglycerol	0.583566652	-0.777030651	0.034152808	0.160025629
M2889	diacylglycerol (16:18:2 [2], 16:0/18:3 [1])*	Lipid	Medium Chain Fatty Acid	0.752801999	-0.409643837	0.035377815	0.164917076
M1567	linoleate (18:2n6)	Lipid	Long Chain Polyunsaturated Fatty Acid (n3 and n6)	1.193208208	0.254839278	0.036273192	0.16737224
M202	vanillylmandelate (VMA)	Amino Acid	Tyrosine Metabolism	1.331186353	-0.292194272	0.036104441	0.16737224
M3098	myristoyl dihydro sphingomyelin (d18:0/14:0)*	Lipid	Dihydro sphingomyelins	0.816658597	-0.292194372	0.037078406	0.170223599
M4600	1-methylkantchine	Xenobiotics	Xanthine Metabolism	0.447007472	-1.161629149	0.037598033	0.170964133
M6221	3-hydroxyxypidine sulfate	Xenobiotics	Chemical	1.508019197	-2.729108019	0.037615871	0.170964133
M1690	tridecanoate (C13:1-DC)*	Lipid	Glutathione Metabolism	1.197794895	-0.462396457	0.047436219	0.170863897
M2587	1-linoleoyl-GPA (18:2)*	Lipid	Fatty Acid, Dicarboxylate	1.368256489	0.452338699	0.037963498	0.170863897
M1277	arabitol/syntol	Carbohydrate	Lysophospholipid	0.723208065	-0.467517329	0.038667196	0.170402338
M446	alpha-ketoglutarate*	Amino Acid	Pentose Metabolism	0.838048734	-0.25489353	0.041522711	0.185020314
M457	5-methylcytosine	Amino Acid	Glutamate Metabolism	0.774304948	-0.368668644	0.043510569	0.192932633
M1570	dihomolinoleate (20:2n6)	Lipid	Methionine, Cysteine, SAM and Taurine Metabolism	1.21949398	-0.286282637	0.043729848	0.192932632
M6418	glycine conjugate of C10H14O2 (1*)	Partially Characterized Molecules	Partially Characterized Molecules	1.049413781	0.495059526	0.044439163	0.195145899
M582	2-hydroxybutyrate/2-hydroxyisobutyrate	Amino Acid	Glutathione Metabolism	1.197794895	-0.260382525	0.044671703	0.195223933
M3361	androstenediol (3beta,17beta) monosulfate (2)	Lipid	Androgenic Steroids	0.587944251	-0.76624873	0.045389947	

M3259	pregnenediol sulfate (C21H34O5S)*	Lipid	Pregnenolone Steroids	1.562548139	0.643900637	0.051782991	0.203762362
M3101	sphingomyelin (d18:0/18:0, d19:0/17:0)*	Lipid	Dihydroxyphosphoglycerins	0.789720709	-0.340585572	0.052005355	0.203762362
M4485	urea	Amino Acid	Urea cycle; Arginine and Proline Metabolism	0.817828961	-0.290128943	0.050302989	0.203762362
M4604	5-acetylamino-6-formylamino-3-methyluracil	Xenobiotics	Xanthine Metabolism	0.648092093	-0.625772962	0.050864226	0.203762362
M3262	pregnenetriol distulfate*	Lipid	Pregnenolone Steroids	1.437305114	0.523366353	0.052916841	0.206059638
M137	N,N-dimethyl-5-aminovalerate	Amino Acid	Lysine Metabolism	0.423607775	-1.23919911	0.053045055	0.206059638
M1867	arachidoylcarnitine (C20)*	Lipid	Fatty Acid Metabolism (Acyl Carnitine, Long Chain Saturated)	0.702131208	-0.510187441	0.053756041	0.206178235
M80	imidazole propionate	Amino Acid	Histidine Metabolism	2.357049557	1.236982091	0.053641089	0.206178235
M2904	palmitoyl-oleoylglycerol (16:0/18:1) [1]*	Lipid	Diacylglycerol	0.776447048	-0.365040555	0.053743871	0.206178235
M1971	2-hydroxystearate	Lipid	Fatty Acid, Monohydroxy	1.14171197	0.191198735	0.054479908	0.206987394
M1947	dihydro-limonenyl-choline	Lipid	Fatty Acid Metabolism (Acyl Choline)	0.655603003	-0.609105632	0.054650137	0.206987394
M4121	xanthine	Nucleotide	Purine Metabolism, (Hypo)Xanthine/Inosine containing	0.474645525	-1.075077614	0.054471765	0.206987394
M3100	behenoyl dihydrophosphogomyelin (d18:0/22:0)*	Lipid	Dihydrophosphoglycerins	0.811857443	-0.300701674	0.055082318	0.207762015
M2924	oleoyl-oleoylglycerol (18:1/18:1) [2]*	Lipid	Diacylglycerol	0.791029112	-0.338197304	0.055618809	0.208915278
M4182	guanosine	Nucleotide	Purine Metabolism, Guanine containing	0.559035348	-0.838985888	0.055960201	0.209332603
M1495	cis-4-deceneoate (10:1n:6)*	Lipid	Medium Chain Fatty Acid	1.270379572	0.345259619	0.057464063	0.213203399
M3064	glycosy-N-(2-hydroxynervonoyl)-sphingosine (d18:1/24:1(20H))*	Lipid	Hexosylceramides (HCER)	0.75527361	-0.404928717	0.057361177	0.213203399
M2670	2-stearoyl-GPE (18:0)*	Lipid	Lyso phospholipid	0.802424552	-0.317562345	0.057721557	0.213288193
M2293	1-palmitoyl-2-dihydro-limonenoyl-GPC (16:0/20:3n 6)*	Lipid	Phosphatidylcholine (PC)	0.915773884	-0.126936672	0.059039295	0.215075732
M2442	1-stearoyl-2-docosahexanoyl-GPE (18:0/22:6)*	Lipid	Phosphatidylethanolamine (PE)	1.21527253	0.281279881	0.050989441	0.215075732
M636	gamma-glutamylglycine	Peptide	Gamma-glutamyl Amino Acid	0.807593504	-0.308298788	0.058693506	0.215075732
M2172	N-oleyloyltaurine	Lipid	Endocannabinoid	0.689822406	-0.535703106	0.059325009	0.215075732
M2418	1-palmitoyl-2-docosahexaenoyl-GPE (16:0/22:6)*	Lipid	Phosphatidylethanolamine (PE)	1.199493886	0.262425804	0.060408555	0.217041014
M3128	sphingomyelin (d18:2/23:0, d18:1/23:1, d17:1/24:1)*	Lipid	Sphingomyelins	0.866500234	-0.205727956	0.060185731	0.217041014
M219	gentisate	Amino Acid	Tyrosine Metabolism	0.471296798	-1.085292215	0.060057125	0.217041014
M3104	hydroxypalmitoyl sphingomyelin (d18:1/16:0(OH))	Lipid	Sphingomyelins	1.118559349	0.161641806	0.06153418	0.22021484
M458	5-methylcysteine sulfoxide	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	0.743375422	-0.427837104	0.061899662	0.22059456
M471	taurine	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	0.832720525	-0.264095711	0.062118571	0.22059456
M2408	1-palmitoyl-2-oleoyl-GPE (16:0/18:1)	Lipid	Phosphatidylethanolamine (PE)	1.223321895	0.290804072	0.063749538	0.221396414
M1707	3-carboxy-4-methyl-5-pentyl-2-furanpropionate (3-CMPFP)	Lipid	Fatty Acid, Dicarboxylate	0.766829953	-0.379263552	0.063598798	0.221396414
M3337	dehydroepiandrosterone sulfate (DHEA-S)	Lipid	Androgenic Steroids	1.439402588	0.525470158	0.062950468	0.221396414
M2842	glycerol-3-phosphate	Lipid	Glycerolipid Metabolism	0.792544559	-0.335436045	0.063812828	0.221396414
M4552	p-cresol sulfate	Xenobiotics	Benzene Metabolism	0.507582432	-0.978285958	0.062936454	0.221396414
M1889	nervonyoylcarnitine (C24:1)*	Lipid	Fatty Acid Metabolism (Acyl Carnitine, Monounsaturated)	0.698868724	-0.51690661	0.063182267	0.221396414
M505	metronidazole	Xenobiotics	Drug - Antibiotic	2.340956415	1.227080704	0.064804988	0.223987779
M1865	margaroylcarnitine (C17)*	Lipid	Fatty Acid Metabolism (Acyl Carnitine, Long Chain Saturated)	0.771228173	-0.374660054	0.062552036	0.224681335
M5116	nonadecanoate (19:0)	Lipid	Long Chain Saturated Fatty Acid	1.169162691	0.225475698	0.065990255	0.226359026
M4222	5,6-dihydroxyuridine	Nucleotide	Pyrimidine Metabolism, Uracil containing	0.762420459	-0.391341262	0.066782413	0.22815088
M3208	3beta,7alpha-dihydroxy-5-cholestenoate	Lipid	Sterol	1.137951947	0.186463968	0.067670644	0.230384327
M3360	androstanediol (3beta,17beta) monosulfate (1)	Lipid	Androgenic Steroids	1.465650088	0.551540713	0.06810856	0.230759553
M1704	docosadiolate (C22:DC)	Lipid	Fatty Acid, Dicarboxylate	0.851269331	-0.232312439	0.068312353	0.230759553
M2923	oleoyl-oleoylglycerol (18:1/18:1) [1]*	Lipid	Diacylglycerol	0.827257021	-0.273592464	0.068552986	0.230759553
M4264	2'-O-methylcytidine	Nucleotide	Pyrimidine Metabolism, Cytidine containing	1.318805251	0.398443639	0.069029607	0.231542115
M3253	21-hydroxy pregnenolone sulfate	Lipid	Pregnenolone Steroids	1.296073071	0.37147058	0.070539353	0.232319816
M1882	5-dodecenoylcarnitine (C12:1)	Lipid	Fatty Acid Metabolism (Acyl Carnitine, Monounsaturated)	1.223702275	0.291252595	0.070248139	0.232319816
M1948	linoleoylcarnitine*	Lipid	Fatty Acid Metabolism (Acyl Choline)	0.782891772	-0.353115215	0.070391564	0.232319816
M336	N-acetylleucine	Amino Acid	Leucine, Isoleucine and Valine Metabolism	0.788879631	-0.342122907	0.069563221	0.232319816
M1404	phenylalanine	Amino Acid	Phenylalanine Metabolism	1.109727775	0.150205784	0.069844429	0.232319816
M5410	celecoxib	Xenobiotics	Drug - Analgesics, Anesthetics	1.185099967	0.245008761	0.070859796	0.232532688
M5095	salicylate	Xenobiotics	Drug - Topical Agents	0.086928145	-0.524032827	0.071275147	0.233054348
M2438	1-stearyl-2- arachidonoyl-GPE (18:0/20:4)	Lipid	Phosphatidylethanolamine (PE)	1.159607445	0.213636501	0.071665593	0.233492253
M4931	histidine betaine (hercynine)*	Xenobiotics	Food Component/Plant	1.500876051	0.585804838	0.072637975	0.235813996
M3112	sphingomyelin (d17:1/14:0, d16:1/15:0)*	Lipid	Sphingomyelins	0.798797522	-0.324098237	0.074747037	0.241797353
M4147	adenine	Nucleotide	Purine Metabolism, Adenine containing	1.197175557	0.259634728	0.075390669	0.24310467
M97	4-imidazolacetate	Amino Acid	Histidine Metabolism	0.686901844	-0.554481254	0.076026512	0.244198232
M3048	ceramide (d18:1/17:0, d17:1/18:0)*	Lipid	Ceramides	1.225781706	0.293708435	0.076804324	0.245827926
M639	gamma glutamylleucine	Peptide	Gamma-glutamyl Amino Acid	0.864959418	-0.209235605	0.078213154	0.249457976
M513	hydroxyprolin	Amino Acid	Urea cycle; Arginine and Proline Metabolism	0.851760131	-0.231480892	0.079434040	0.254669333
M3260	pregnen-diol sulfate*	Lipid	Pregnenolone Steroids	1.319713329	0.400224579	0.080641161	0.259410506
M4505	4-methylcatechol sulfate	Xenobiotics	Benzene Metabolism	0.522753434	-0.93579746	0.083142098	0.259719113
M1441	aconitate [cis or trans]	Energy	TCA Cycle	1.161895705	0.216480574	0.082840538	0.259719113
M5152	margarate (17:0)	Lipid	Long Chain Saturated Fatty Acid	1.185566287	0.245576328	0.083136477	0.259719113
M4131	urate	Nucleotide	Purine Metabolism, (Hypo)Xanthine/Inosine containing	0.805567561	-0.319225056	0.082728267	0.259719113
M4466	2-hydroxyhippurate (salicylurate)	Xenobiotics	Benzene Metabolism	0.055158459	-4.180274036	0.083826261	0.260061512
M298	indoleacetate	Amino Acid	Tryptophan Metabolism	0.814971423	-0.295274219	0.083810107	0.260061512
M3009	N-palmitoyl-sphinganine (d18:0/16:0)	Lipid	Dihydroxyacetones	1.173979391	0.231407083	0.084379098	0.260863996
M4597	1,7-dimethylurate	Xenobiotics	Xanthine Metabolism	0.579926872	-0.786057105	0.084765575	0.261192906
M3113	sphingomyelin (d18:1/14:0, d16:1/16:0)*	Lipid	Sphingomyelins	0.885461759	-0.175498093	0.085497632	0.262558605
M6254	3-hydroxy-2-methylpyridine sulfate	Xenobiotics	Chemical	0.240398305	-0.205601372	0.087797432	0.268713353
M78	trans-urocanate	Amino Acid	Histidine Metabolism	3.902649905	0.196445045	0.089180666	0.270229127
M1180	Fibroinopeptide B (1-13)	Peptide	Fibrinogen Cleavage Peptide	1.202696461	0.266272578	0.090283169	0.27881003
M1695	hexadecanedioate (C16)	Lipid	Fatty Acid, Dicarboxylate	1.296100802	0.374177925	0.090359936	0.27881003
M1943	palmitoyl-choline	Lipid	Fatty Acid Metabolism (Acyl Choline)	1.159607445	0.213636501	0.071665593	0.27881003
M1915	suberylcarnitine (C8-DC)	Lipid	Fatty Acid Metabolism (Acyl Carnitine, Dicarboxylate)	1.675739082	-0.744797534	0.091438702	0.275713261
M5203	caffeoic acid sulfate	Xenobiotics	Food Component/Plant	0.298494658	-1.74422981	0.091724242	0.275713261
M3401	11beta-hydroxyandrosterone glucuronide	Lipid	Androgenic Steroids	1.415950125	0.50177045	0.092101677	0.275391634
M5404	salicylicuronicid*	Xenobiotics	Drug - Analgesics, Anesthetics	0.162044455	-2.625338441	0.092410497	0.275413581
M1443	isocitrate	Energy	TCA Cycle	1.180564663	0.239477065	0.093254525	0.277020795
M494	homocitrulline	Amino Acid	Urea cycle; Arginine and Proline Metabolism	0.737152935	-0.439964133	0.095605644	0.283082569
M1406	glucuronate	Carbohydrate	Aminosugar Metabolism	1.503768904	0.585852874	0.096927047	0.286060668
M1533	oleate/vaccenate (18:1)	Lipid	Long Chain Monounsaturated Fatty Acid	1.162490385	0.585852874	0.096927047	0.286060668
M117	hydroxy-N6,N6-trimethyllysine*	Amino Acid	Lysine Metabolism	0.777245294	-0.363558118	0.097764032	0.286669337
M4207	orotate	Nucleotide	Pyrimidine Metabolism, Orotate containing	0.364905708	0.287795775	0.099064674	0.287690005
M4780	2-isopropylmalate	Xenobiotics	Food Component/Plant	0.563083985	-0.82587975	0.099064674	0.287690005
M1864	palmitoylcarnitine (C16)	Lipid	Fatty Acid Metabolism (Acyl Carnitine, Long Chain Saturated)	0.856516264	-0.223453568	0.098897228	0.287690005
M4254	3-methylcytidine	Nucleotide	Pyrimidine Metabolism, Cytidine containing	1.234587122	0.304028648	0.099750726	0.288433739
M5514	fluconazole	Xenobiotics	Drug - Antibiotic	0.525099335	-0.92711399	0.099952286	0.288433739
M1884	myristoylcarnitine (C14:1)*	Lipid	Fatty Acid Metabolism (Acyl Carnitine, Monounsaturated)	1.236759239	0.306564677	0.101398001	0.291769692
M1418	N-acetylneuraminate	Carbohydrate	Aminosugar Metabolism	0.891836923	-0.165148164	0.101869027	0.292110329
M3526	glycochocholate	Lipid	Secondary Bile Acid Metabolism	1.762284246	0.817936287	0.102197839	0.292131559
M3281	Salpaha-pregnan-diol disulfate	Lipid	Progesterin Steroids	1.70656834	0.771098188	0.102736069	0.292739489
M3081	glycosyl ceramide (d18:1/23:1, d17:1/24:1)*	Lipid	Hexosylceramides (HCER)	0.582689253	-0.779201933	0.103756575	0.29473352
M340	1-carboxybutylicleucine	Amino Acid	Leucine, Isoleucine and Valine Metabolism	0.763588846	-0.389132065	0.105655739	0.297706224
M2848	1-myristoylglycerol (14:0)	Lipid	Monooacylglycerol	0.567887208	0.105875865	0.105875865	0.297076324
M5214	3-indolegycylic acid	Xenobiotics	Food Component/Plant	0.824672705	-0.278106437	0.105885191	0.297076324
M4493	ergothioneine	Xenobiotics	Food Component/Plant	1.606517402	-0.283310782	0.106959954	0.297076324
M2669	1-stearyl-GPE (18:0)	Lipid	Lyso phospholipid	0.853633807	-0.228310782	0.106959954	0.298326556
M3120	sphingomyelin (d18:1/19:0, d19:1/18:0						

M4431	carotene diol (1)	Cofactors and Vitamins	Vitamin A Metabolism	0.810434956	-0.303231693	0.117897651	0.308844279
M1448	succinate	Energy	TCA Cycle	0.876399638	-0.190339206	0.11852499	0.309595448
M1161	Fibrinopeptide A (3:16)	Peptide	Fibringen Cleavage Peptide	1.229936397	0.298583712	0.119594145	0.310603079
M2162	palmitoyl ethanolamide	Lipid	Endocannabinoid	1.106876791	0.146494641	0.119526284	0.310603079
M3454	glycocholate	Lipid	Primary Bile Acid Metabolism	1.496746193	0.581829601	0.1199814	0.31271061
M3082	glycosyl ceramide (d18:2/24:1, d18:1/24:2)*	Lipid	Hexosylceramides (HCKER)	0.759300479	-0.397257177	0.122173609	0.313792076
M3025	N-stearoyl-sphingosine (d18:1/18:0)*	Lipid	Ceramides	1.176815033	0.234887582	0.122202855	0.313792076
M3121	sphingomyelin (d18:1/20:0, d16:1/22:0)*	Lipid	Sphingomyelin	0.918296295	-0.12296837	0.121662249	0.313792076
M1487	butyrate/isobutyrate (4:0)	Lipid	Short Chain Fatty Acid	0.789374625	-0.341217951	0.125010673	0.319198599
M1689	dodecadienoate (12:2)*	Lipid	Fatty Acid, Dicarboxylate	1.158720002	0.12553199	0.124688776	0.319198599
M2002	9-hydroxystearate	Lipid	Fatty Acid, Monohydroxy	0.796329649	-0.328562323	0.126524988	0.321260374
M1262	ribitol	Carbohydrate	Pentose Metabolism	0.897545876	-0.155942414	0.12646229	0.321260374
M123	2-aminoisopropate	Amino Acid	Lysine Metabolism	0.859120379	0.219066792	0.127616615	0.323129534
M2937	stearyl-arachidonoyl-glycerol (18:0/20:4) [1]*	Lipid	Diacetyl/glycerol	0.854183852	-0.227381471	0.128649812	0.324386276
M375	3-methylglutaryl carnitine (2)	Amino Acid	Leucine, Isoleucine and Valine Metabolism	0.773355535	0.370796278	0.130318906	0.327273752
M2031	9,10-DHOME	Lipid	Fatty Acid, Dihydroxy	1.635777082	0.709976157	0.130182019	0.327273752
M274	N-formylanthranilic acid	Amino Acid	Tryptophan Metabolism	1.474808281	0.560597852	0.131636662	0.329635609
M1706	hydroxy-CMP*	Lipid	Fatty Acid, Dicarboxylate	0.801155046	-0.319846623	0.132709059	0.331408062
M4316	1-methylnicotinamide	Cofactors and Vitamins	Nicotinate and Nicotinamide Metabolism	0.736156015	-0.441916544	0.133367165	0.33213905
M3490	taurodoxocholic acid 3-sulfate	Lipid	Secondary Bile Acid Metabolism	1.704567398	0.769405644	0.135420125	0.33633031
M1979	3-hydroxyhexanoate	Lipid	Fatty Acid, Monohydroxy	1.207565506	0.272090699	0.136942384	0.338263685
M462	cysteine	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	0.920618334	-0.11932492	0.136596051	0.338263685
M1643	cis-3,4-methyleneheptanoate	Lipid	Fatty Acid, Branched	1.167895449	0.223911128	0.138425537	0.340994949
M4636	2-piperidinone	Xenobiotics	Food Component/Plant	0.478752105	0.162649264	0.139067641	0.341240557
M1468	phosphate	Energy	Oxidative Phosphorylation	0.845102545	-0.242801685	0.139274199	0.341240557
M3224	campesterol	Lipid	Sterol	1.394513934	0.47976235	0.141945254	0.344075295
M4357	gulonate*	Cofactors and Vitamins	Ascorbate and Aldarate Metabolism	0.681964043	-0.552232448	0.141114695	0.344075295
M2931	linoleoyl-linoleoyl-glycerol (18:2/18:2) [1]*	Lipid	Diacetyl/glycerol	1.532529864	0.165191588	0.141942737	0.344075295
M3021	N-palmitoyl-sphingosine (d18:1/16:0)	Lipid	Ceramides	1.135697717	0.183578891	0.141338984	0.344075295
M1460	2-methylcitrate/homocitrate	Energy	TCA Cycle	1.125201397	0.170183249	0.143641189	0.346339101
M1157	ADSGEDGFXAEGGVR*	Peptide	Fibringen Cleavage Peptide	1.315902883	0.396053019	0.143852415	0.346339101
M468	cysteine sulfenic acid	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	1.203425805	0.267147198	0.145527534	0.34995907
M55	N-acetyl-aspartyl-glutamate (NAAG)	Amino Acid	Glutamate Metabolism	1.211246003	0.276491905	0.146754159	0.351977654
M1869	lignoceroylcarnitine (24:4)*	Lipid	Fatty Acid Metabolism (Acyl Carnitine, Long Chain Saturated)	0.872656464	-0.196514271	0.148489643	0.352705655
M47	N-acetylglutamate	Amino Acid	Glutamate Metabolism	0.878169058	-0.187423932	0.148462276	0.352705655
M4280	5,6-dihydrothymine	Nucleotide	Pyrimidine Metabolism, Thymine containing	0.520227798	-0.942645448	0.14915462	0.354925998
M1514	stearate (18:0)	Lipid	Long Chain Saturated Fatty Acid	1.10906946	0.149384844	0.150155341	0.356373903
M6430	branched-chain, straight-chain, or cyclopropyl 10:1 fatty acid (1)*	Partially Characterized Molecules	Partially Characterized Molecules	1.325420832	0.4064505	0.150924702	0.357267067
M4476	benzoate	Xenobiotics	Benzoate Metabolism	1.343030612	0.425492188	0.151937628	0.358730666
M2725	1-linoleoyl-GPI* (18:2)*	Lipid	Lysophospholipid	1.112806854	0.154203211	0.154920591	0.363883249
M1814	cis-3,4-methylenehentanoyl/glycine	Lipid	Fatty Acid Metabolism (Acyl Glycine)	1.298905279	0.377296228	0.154550617	0.363883249
M491	2-oxoarginine*	Amino Acid	Urea cycle; Arginine and Proline Metabolism	0.798451337	-0.324723612	0.156194173	0.365048955
M3531	mannitol/sorbitol	Carbohydrate	Fructose, Mannose and Galactose Metabolism	0.458328695	-0.125545483	0.156252079	0.365048955
M736	ondansetron	Xenobiotics	Drug - Gastrointestinal	1.678313619	0.747012331	0.156621664	0.365048955
M1162	Fibrinopeptide A (5:16)*	Peptide	Fibringen Cleavage Peptide	1.145261058	0.195676493	0.158751536	0.368982045
M2242	glycerophosphoinositol*	Lipid	Phospholipid Metabolism	1.132228181	0.179164738	0.15912097	0.368982045
M5116	4-vinylguaiacol sulfate	Xenobiotics	Food Component/Plant	0.479267972	-1.061095563	0.161156193	0.372750583
M1952	arachidonylcholine	Lipid	Fatty Acid Metabolism (Acyl Choline)	0.822528653	0.281862158	0.161902894	0.373527234
M2404	1,2-dipalmitoyl-GPC (16:0/16:0)*	Lipid	Phosphatidylethanolamine (PE)	1.268935628	0.343618885	0.163523807	0.376311748
M254	tryptophan	Amino Acid	Tryptophan Metabolism	0.910041319	-0.135984803	0.164497749	0.377597106
M489	3-amino-2-piperidone	Amino Acid	Urea cycle; Arginine and Proline Metabolism	0.863887568	-0.211084532	0.166025194	0.379181935
M3114	spingomyelin (d18:2/14:0, d18:1/14:1)*	Lipid	Sphingomyelin	0.860279471	0.235931904	0.165912074	0.379181935
M79	cis-urocanate	Amino Acid	Histidine Metabolism	1.194062533	0.956400578	0.168944514	0.384567024
M1951	docosahexaenoylcholine	Lipid	Fatty Acid Metabolism (Acyl Choline)	0.805485524	-0.312069433	0.169649479	0.384567024
M1164	Fibrinopeptide A (8:16)	Peptide	Fibringen Cleavage Peptide	0.848955974	-0.236850658	0.160933739	0.384567024
M5249	2-acetamidophenyl sulfate	Xenobiotics	Food Component/Plant	0.657735919	-0.6052462	0.170196964	0.384884358
M1959	2-hydroxyheptanoate*	Lipid	Fatty Acid, Monohydroxy	1.206477618	0.270801152	0.170891505	0.385499595
M453	cystathione	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	1.762219556	0.817393682	0.17369987	0.390284707
M3090	lactosyl-N-benzenoyl-sphingosine (d18:1/22:0)*	Lipid	Lactosylceramides (LCER)	0.860279471	0.217122684	0.174457649	0.391560501
M138	N,N,N-trimethyl-5-aminovaleate	Amino Acid	Lysine Metabolism	0.858669642	-0.219284909	0.175976741	0.399391785
M1648	(16 or 17)-methylstearte (19:0 or 19:0)	Lipid	Fatty Acid, Branched	1.147355387	0.956400578	0.168944514	0.384567024
M2850	1-pentadecanoylglycerol (15:0)	Lipid	Monoaerylglycerol	0.670758171	0.576135572	0.179104708	0.390591119
M2711	1-stearoyl-GPG (18:0)	Lipid	Lysophospholipid	0.400856894	-0.1884081	0.178843184	0.390591119
M2281	1-palmitoyl-2-stearoyl-GPC (16:0/18:0)	Lipid	Fatty Acid, Monohydroxy	0.538418387	-0.893200415	0.182136332	0.403809574
M2717	1-palmitoyl-GPI* (16:0)	Lipid	Lysophospholipid	0.881464829	-0.182025089	0.182948143	0.403969624
M5250	2-aminophenol sulfate	Xenobiotics	Food Component/Plant	0.5627431	-0.829451632	0.184364938	0.403969624
M363	beta-hydroxyisovalerate	Amino Acid	Leucine, Isoleucine and Valine Metabolism	1.187329102	0.247719875	0.184334189	0.403969624
M3063	glycosyl-N-nercynoyl-sphingosine (d18:1/24:1)*	Lipid	Hexosylceramides (HCKER)	0.7158216	0.482328016	0.184271233	0.403969624
M83	imidazole lactate	Amino Acid	Creatine Metabolism	0.893448558	-0.162483636	0.184430577	0.403969624
M2871	2-oleoylglycerol (18:1)	Lipid	Hemoglobin and Porphyrin Metabolism	0.691589887	-0.5320132	0.186455165	0.406759262
M4241	N-acetyl-beta-alanine	Nucleotide	Ceramides	0.79978218	-0.32320958	0.186598062	0.406759262
M2938	stearyl-arachidonoyl-glycerol (18:0/20:4) [2]*	Lipid	Diacetyl/glycerol	0.839237718	-0.252848577	0.187291179	0.407299966
M2800	1-(1-enyl-palmitoyl)-2-palmitoyl-GPC (P-16:0/18:1)*	Lipid	Plasmalogens	0.650240116	-0.615967368	0.194614158	0.41496941
M2534	1-palmitoyl-2-oleoyl-GPI (16:0/18:1)*	Lipid	Phosphatidylinositol (PI)	0.888016201	-0.171342098	0.192725991	0.41455854
M4409	bilirubin (E,E)*	Cofactors and Vitamins	Ceramides	0.847501056	-0.238712929	0.192101664	0.41455854
M3033	N-behenoyl-sphingadenine (d18:2/22:0)*	Lipid	Hemoglobin and Porphyrin Metabolism	0.898632967	-0.154196106	0.19199228	0.41455854
M6204	triethanolamine	Xenobiotics	Chemical	0.070314552	-0.3830032892	0.192493987	0.41455854
M2806	1-(1-enyl-palmitoyl)-2-oleoyl-GPC (P-16:0/18:1)*	Lipid	Plasmalogens	0.907661619	-0.139775846	0.196220415	0.41496941
M2721	1-stearoyl-GPI (18:0)	Lipid	Lysophospholipid	0.920820383	-0.147521225	0.19776309	0.41496941
M322	3-indoxyl sulfate	Amino Acid	Tryptophan Metabolism	0.652040116	-0.615967368	0.194614158	0.41496941
M1995	5-hydroxyhexanoate	Lipid	Fatty Acid, Monohydroxy	1.300241846	0.378760396	0.196686215	0.41496941
M6235	6-hydroxyindole sulfate	Xenobiotics	Chemical	0.66999121	-0.57778526	0.19790063	0.41496941
M529	creatine	Amino Acid	Creatine Metabolism	1.070185275	0.197860583	0.197320372	0.41496941
M2932	linoleoyl-linoleoyl-glycerol (18:2/18:2) [2]*	Lipid	Diacetyl/glycerol	1.314150059	0.394130022	0.193457784	0.41496941
M1756	N-acetyl-2-monoisoctanoate*	Lipid	Fatty Acid, Amino	0.722001279	-0.469926702	0.197571284	0.41496941
M270	N-acetylkynurenine (2)	Amino Acid	Tryptophan Metabolism	0.743414726	-0.427760828	0.196249555	0.41496941
M5005	piperine	Xenobiotics	Food Component/Plant	0.6354451571	-0.654227651	0.197897885	0.41496941
M5077	thymol sulfate	Xenobiotics	Food Component/Plant	0.493867891	-0.107802921	0.195236482	0.41496941
M23	O-acetylhomoserine	Amino Acid	Glycine, Serine and Threonine Metabolism	0.1073373187	-0.581707844	0.200556871	0.414904702
M1569	linolenate (18:3n3 or 3n6)	Lipid	Long Chain Polyunsaturated Fatty Acid (n3 and n6)	1.142861577	0.192650676	0.2010991	0.41263949
M299	indoleacetate	Amino Acid	Tryptophan Metabolism	0.828280267	-0.271809076	0.20229232	0.41829508
M5936	diphenylhydramine	Xenobiotics	Drug - Respiratory	0.333052089	1.467776324	0.201844904	0.419825908
M180	4-hydroxyphenylacetoxycarnitine	Amino Acid	Tyrosine Metabolism	1.495815773	0.580932502	0.203449577	0.420254549
M4590	caffein	Xenobiotics	Xanthine Metabolism	0.71272538	0.488574727	0.204810523	0.420254549
M634	gamma-glutamylglutamate	Peptide	Gamma-glutamyl Amino Acid	0.793828343	-0.33101021	0.203951047	0.420254549
M44	glutamate	Amino Acid	Glutamate Metabolism	0.880729239	-0.183229533	0.204553447	0.420254549
M5738	diphenoxylate	Xenobiotics	Drug - Gastrointestinal	1.368768861	0.452878845	0.203249873	0.420254549
M3126	spingomyelin (d18:1/22:1, d18:2/22:0, d16:1/24:1)*	Lipid	Sphingomyelin	0.9343363	0.493865064	0.205985604	0.421713771
M3125	spingomyelin (d18:2/21:0, d16:2/23:0)*	Lipid	Sphingomyelin	0.896237728	-0.157966152	0.207325467	0.423503033
M4221	pseudouridine	N					

M515	prolylhydroxyproline	Amino Acid	Urea cycle; Arginine and Proline Metabolism	0.867438559	-0.205166521	0.227679297	0.445794562
M1694	tetradecadienediole (C14:2-DC)*	Lipid	Fatty Acid, Dicarboxylate	1.192406489	0.241726092	0.229283873	0.447259939
M4530	4-vinylcadol sulfate	Xenobiotics	Benzoate Metabolism	0.381883111	-1.388796976	0.232036987	0.449254856
M424	alpha-hydroxyisovalerate	Amino Acid	Leucine, Isoleucine and Valine Metabolism	1.116729811	0.159280173	0.231390181	0.449254856
M522	argininate*	Amino Acid	Urea cycle; Arginine and Proline Metabolism	0.830684146	-0.267628075	0.231951207	0.449254856
M455	cysteine	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	1.121743882	0.165743316	0.232972208	0.449254856
M437	N-formylmethionine	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	0.911841552	-0.133144941	0.232376449	0.449254856
M2911	palmitoleyl-linoleoyl-glycerol (16:1/18:2) [1]*	Lipid	Diacetyl/glycerol	0.794177849	-0.332465972	0.232776972	0.449254856
M867	leucylalanine	Peptide	Dipeptidase	0.787159186	-0.345272676	0.23527242	0.452130867
M1447	succinylcarnitine (C4-DC)	Energy	TCA Cycle	1.157262425	0.210716052	0.236286223	0.453131245
M351	isovalerate (CS)	Amino Acid	Leucine, Isoleucine and Valine Metabolism	0.878436313	-0.1869904	0.239630651	0.458577394
M1220	1,5-anhydroglucitol (1,5-AG)	Carbohydrate	Glycolysis, Gluconeogenesis, and Pyruvate Metabolism	0.856878677	-0.222837143	0.242223362	0.462565202
M1671	maleate	Lipid	Fatty Acid, Dicarboxylate	1.454988026	0.54100728	0.244447656	0.465717288
M3123	sphingomyelin (d18:1/20:2, d18:2/20:1, d16:1/22:2)*	Lipid	Sphingomyelin	1.084784643	0.11740866	0.244896274	0.465717288
M2279	1-palmitoyl-2-palmitoleyl-GPC (16:0/16:1)*	Lipid	Phosphatidylcholine (PC)	0.877746889	-0.188123117	0.24751228	0.469450104
M434	methionine	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	0.898561453	-0.154310921	0.247894444	0.469450104
M5129	2-keto-3-deoxy-gluconate	Xenobiotics	Food Component/Plant	0.87112995	-0.199040147	0.250801848	0.472272686
M1576	docosapentaenoate (n6 DPA; 22:5n6)	Lipid	Long Chain Polyunsaturated Fatty Acid (n3 and n6)	1.140806248	0.190053789	0.250036591	0.472272686
M10	serine	Amino Acid	Glycine, Serine and Threonine Metabolism	0.924011975	-0.114016547	0.250944763	0.472272686
M2731	1-arachidonoyl-GPI* (20:4)*	Lipid	Lysophospholipid	0.916900849	-0.125162361	0.25148822	0.473139818
M2262	1-myristoyl-2-palmitoyl-GPC (14:0/16:0)	Lipid	Phosphatidylcholine (PC)	0.846923379	-0.239696639	0.252440303	0.473139209
M3326	cordone glucoseuronide (1)	Lipid	Corticosteroids	1.213822097	0.27955699	0.254436774	0.475891002
M573	cysteine-glutathione disulfide	Amino Acid	Glutathione Metabolism	0.579797959	-0.78637784	0.256658516	0.479067062
M2201	myo-inositol	Lipid	Inositol Metabolism	0.811334101	-0.301631967	0.261768334	0.485581202
M508	N-delta-acetylornithine	Amino Acid	Urea cycle; Arginine and Proline Metabolism	0.772667957	-0.372079526	0.262009231	0.485581202
M2940	oleoyl-arachidonoyl-glycerol (18:1/20:4) [2]*	Lipid	Diacetyl/glycerol	0.855808697	-0.224518385	0.261201283	0.485581202
M3122	sphingomyelin (d18:1/20:1, d18:2/20:0)*	Lipid	Sphingomyelin	0.936163872	-0.095167005	0.262288636	0.485581202
M1837	picolinoloylglycine	Lipid	Fatty Acid Metabolism (Acyl Glycine)	0.843160033	-0.246121612	0.262874888	0.485573784
M1968	2-hydroxyalpimate	Lipid	Fatty Acid, Monohydroxy	1.07444998	0.103598321	0.265245282	0.48938971
M1856	cis-3,4-methylenephantanoylcarnitine	Lipid	Fatty Acid Metabolism (Acyl Carnitine, Medium Chain)	1.114552363	0.156464397	0.266541836	0.490458561
M3106	behenoyl sphingomyelin (d18:1/22:0)*	Lipid	Sphingomyelin	0.935792353	-0.095739655	0.269244532	0.494430867
M2933	linoleoyl-linolenoyl-glycerol (18:2/18:3) [1]*	Lipid	Diacetyl/glycerol	1.414036098	0.49981895	0.272064546	0.498602162
M2539	1-palmitoyl-2-arachidonoyl-GPI (16:0/20:4)*	Lipid	Phosphatidylinositol (PI)	0.843412411	-0.245689844	0.274503414	0.501268888
M1160	fibrinopeptide A (4-15)	Peptide	Fibrinogen Cleavage Peptide	1.218965023	0.285656729	0.274819787	0.501268888
M1187	phenylacetylglutamine	Peptide	Acetylated Peptides	0.778475114	-0.361277175	0.27620129	0.503142026
M642	gamma-glutamylmethionine	Peptide	Gamma-glutamyl Amino Acid	0.867121701	-0.205693604	0.277515329	0.504258669
M4369	gamma-CEHC glucuronide*	Cofactors and Vitamins	Tocopherol Metabolism	1.36650641	0.450492228	0.280198596	0.506166241
M1451	malate	Energy	TCA Cycle	1.138717193	0.18740949	0.27988588	0.506166241
M4593	theophylline	Xenobiotics	Xanthine Metabolism	0.787201889	-0.345194412	0.280646629	0.506166241
M4584	2-methoxyhydroquinone sulfate (1)	Xenobiotics	Benzoate Metabolism	0.727764339	-0.458456735	0.279001698	0.506166241
M1572	dihomolinoleate (20:3n3 or 3n6)	Lipid	Long Chain Polyunsaturated Fatty Acid (n3 and n6)	1.113642423	0.155285842	0.282690782	0.508382788
M426	isobutyrylcarnitine (C4)	Amino Acid	Leucine, Isoleucine and Valine Metabolism	0.829766443	-0.269222795	0.282994159	0.508382788
M2914	palmitoyl-arachidonoyl-glycerol (16:0/20:4) [2]*	Lipid	Diacetyl/glycerol	0.848319242	-0.237320809	0.286301251	0.513309343
M487	ornithine	Amino Acid	Urea cycle; Arginine and Proline Metabolism	0.912326725	-0.132375157	0.290255636	0.51397475
M638	gamma-glutamylsucine*	Peptide	Gamma-glutamyl Amino Acid	0.895076739	-0.159916396	0.292763123	0.528232374
M1750	2-aminoheptanoate	Lipid	Fatty Acid, Amino	0.873932417	-0.194406377	0.294359405	0.52652351
M1566	hexadecadecanoate (16:2n6)	Lipid	Long Chain Polyunsaturated Fatty Acid (n3 and n6)	1.126113732	0.171352539	0.295359504	0.525458042
M6417	glycine conjugate of C10H12O2*	Partially Characterized Molecules	Partially Characterized Molecules	1.212319581	-0.27770059	0.296450282	0.526315052
M3172	galactonate	Carbohydrate	Fructose, Mannose and Galactose Metabolism	0.741339479	-0.431793753	0.297420181	0.526362847
M433	hydroxysarcosagine	Amino Acid	Alanine and Aspartate Metabolism	0.919531303	-0.121029406	0.298214374	0.526362847
M387	N-acetylysucine	Amino Acid	Leucine, Isoleucine and Valine Metabolism	0.858952844	-0.219299281	0.298183139	0.526362847
M4325	N1-Methyl-4-pyridone-3-carboxamide	Cofactors and Vitamins	Nicotinate and Nicotinamide Metabolism	0.708876262	0.496394276	0.299127792	0.527040173
M2913	palmitoyl-arachidonoyl-glycerol (16:0/20:4) [1]*	Lipid	Diacetyl/glycerol	0.858388931	-0.220266623	0.299998125	0.527462855
M2037	3,4-dihydroxybutyrate	Lipid	Fatty Acid, Dihydroxy	0.89774944	0.155615246	0.300801872	0.528502202
M1575	adrenate (22:4n6)	Lipid	Long Chain Polyunsaturated Fatty Acid (n3 and n6)	1.148329074	0.199536131	0.301908892	0.528776845
M1958	alpha-hydroxycaproate	Lipid	Fatty Acid, Monohydroxy	1.373970933	0.458351483	0.304345154	0.530997576
M564	guanidinosuccinate	Amino Acid	Guanidino and Acetamido Metabolism	1.272442421	0.347600375	0.304165855	0.530997576
M399	2-methylbutyryl glycine (C5)	Amino Acid	Leucine, Isoleucine and Valine Metabolism	0.817261002	-0.2911312	0.305799992	0.531495889
M1907	adipoylcarnitine (C6-DC)	Lipid	Fatty Acid Metabolism (Acyl Carnitine, Dicarboxylate)	1.27018034	0.345034133	0.305215804	0.531495889
M2447	1-oleoyl-2-arachidonoyl-GPE (18:1/20:4)*	Lipid	Phosphatidylethanolamine (PE)	1.10201882	0.140148872	0.308281389	0.534785844
M4139	AMP	Nucleotide	Purine Metabolism, Adenine containing	1.039456843	0.05829861	0.310435522	0.53701451
M3129	sphingomyelin (d18:1/24:1, d18:2/24:0)*	Lipid	Sphingomyelin	1.058135421	0.081524277	0.31074767	0.53701451
M4206	dihydroorotate	Nucleotide	Pyrimidine Metabolism, Orotate containing	0.70197541	0.510462118	0.312052982	0.538527851
M159	4-hydroxyphenylacetate	Amino Acid	Phenylalanine Metabolism	1.392371944	0.477544649	0.31340212	0.539502421
M3310	tetrahydrocortisol glucuronide	Lipid	Corticosteroids	1.265518143	0.339800374	0.317717946	0.539502421
M156	2-hydroxyphenylacetate	Amino Acid	Phenylalanine Metabolism	1.229846559	0.298478376	0.318925672	0.546986921
M2852	1-palmitoyl-glycerol (16:1)*	Lipid	Monoacylglycerol	0.661951778	-0.595201972	0.322488471	0.547196731
M2014	13-HODE + 9-HODE	Lipid	Fatty Acid, Monohydroxy	1.113687576	0.155344548	0.323499885	0.547196731
M3248	17alpha-hydroxyprogrenanolone glucuronide	Lipid	Pregnenolone Steroids	1.192230808	0.253663559	0.324549507	0.547196731
M6160	2-acrylamidoglyclic acid	Xenobiotics	Chemical	0.929857623	-0.104918263	0.320558567	0.547196731
M395	2-hydroxy-3-methylvalerate	Amino Acid	Leucine, Isoleucine and Valine Metabolism	1.1404227219	0.189574378	0.324494817	0.547196731
M1679	azelate (C9-DC)	Lipid	Fatty Acid, Dicarboxylate	0.898450605	-0.154488905	0.327434735	0.547196731
M4411	biliverdin	Cofactors and Vitamins	Hemoglobin and Porphyrin Metabolism	1.179617708	0.238319385	0.326778023	0.547196731
M3453	cholate	Lipid	Primary Bile Acid Metabolism	1.1652060829	0.724266808	0.327475272	0.547196731
M332	leucine	Amino Acid	Leucine, Isoleucine and Valine Metabolism	0.952848436	-0.069681343	0.321824264	0.547196731
M139	N-acetyl-2-amino adipate	Amino Acid	Lysine Metabolism	0.890719676	0.166956631	0.31989822	0.547196731
M435	N-acetylmethionine	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	1.119668079	0.163071114	0.326860485	0.547196731
M3031	N-palmitoyl-sphingadine (d18:2/16:0)*	Lipid	Ceramides	1.072104949	0.100464139	0.324019368	0.547196731
M2338	phosphoethanolamine (PE)	Lipid	Phospholipid Metabolism	0.636951002	-0.650723048	0.321113026	0.547196731
M5017	sulfate of piperine metabolite C16H19NO3 (2)*	Xenobiotics	Food Component/Plant	0.725569564	-0.462814155	0.326840402	0.547196731
M2851	1-palmitoylglycerol (16:0)	Lipid	Monocacylglycerol	0.835370206	-0.259552405	0.330237190	0.550979192
M1709	2-hydroxysebacate	Lipid	Fatty Acid, Dicarboxylate	0.834883671	-0.260352902	0.33100025	0.551008656
M1844	hexanoylcarnitine (C6)	Lipid	Fatty Acid Metabolism (Acyl Carnitine, Medium Chain)	1.1092163578	0.149522329	0.3327399	0.552574677
M210	homovanilate (HVA)	Amino Acid	Tyrosine Metabolism	1.171763375	0.228681263	0.333123528	0.552574677
M5210	(S)-a-amino-omega-mega-croplactam	Xenobiotics	Food Component/Plant	0.923245216	-0.115214213	0.336595276	0.55364877
M4223	2'-O-methyluridine	Nucleotide	Priming Metabolism, Uracil containing	1.310288406	0.17669094	0.33731109	0.55364877
M4243	4-methyl-2-oxopentanoate	Amino Acid	Leucine, Isoleucine and Valine Metabolism	1.076062671	0.105762104	0.336895384	0.55364877
M1159	fibrinopeptide A (3-15)	Peptide	Fibrinogen Cleavage Peptide	1.144762834	0.195048739	0.336373453	0.55364877
M1186	phenylacetylglutamate	Peptide	Acetylated Peptides	0.851998225	-0.231077669	0.337427303	0.55364877
M1557	stearylone (18:3n3)	Lipid	Long Chain Polyunsaturated Fatty Acid (n3 and n6)	0.846913236	0.239713918	0.337020014	0.55364877
M4244	3-(3-amino-3-carboxypropyl)uridine*	Nucleotide	Pyrimidine Metabolism, Uracil containing	0.817345412	-0.290982201	0.338089347	0.553735225
M60	2-pyrrrolidinone	Amino Acid	Glutamate Metabolism	0.900699109	-0.150882866	0.341630298	0.556527599
M4256	N4-acetylcytidine	Nucleotide	Pyrimidine Metabolism, Cytidine containing	0.830896094	-0.26760021	0.340665667	0.556527599
M2243	trimethylamine N-oxide	Lipid	Phospholipid Metabolism	0.67220766	-0.573021112	0.341348428	0.556527599
M4905	quinate	Xenobiotics	Food Component/Plant	0.668083091	-0.581900551	0.344354537	0.556896264
M3001	sphinganine-1-phosphate	Lipid	Sphingolipid Synthesis	1.080644981	0.111892639	0.344027996	0.556896264
M6152	dimethyl sulfone	Xenobiotics	Chemical	0.789479402	-0.34102647	0.349198165	0.556813007
M2393	oleoyl-arachidonoyl-glycerol (18:1/20:4) [1]*	Lipid	Diacetyl/glycerol	0.884084965	-0.177740369	0.351159698</	

M1177	Fibrinopeptide B (1-9)	Peptide	Fibrinogen Cleavage Peptide	1.219667732	0.286488175	0.390466556	0.609129304
M4419	inosine	Nucleotide	Purine Metabolism, (Hypo)Xanthine/Inosine containing	0.697475382	-0.519785798	0.392910811	0.611568368
M2310	1-palmitoleoyl-2-linolenoyl-GPC (16:1/18:3)*	Lipid	Phosphatidylcholine (PC)	0.898404737	-0.154562556	0.396571849	0.615160087
M4938	indolin-2-one	Xenobiotics	Food Component/Plant	0.785957561	-0.347476682	0.39609123	0.615160087
M6401	glutamine conjugate of C7H12O2*	Partially Characterized Molecules	Partially Characterized Molecules	1.187866514	0.248372722	0.39102089	0.60979249
M3057	glycosy-N-palmitoyl-phosphogosine (d18:1/16:0)	Lipid	Hexosylceramides (HCEC)	0.904139739	-0.145382333	0.398457248	0.616972949
M2855	1-oleoylglycerol (18:1)	Lipid	Monoaerylglycerol	0.799577937	-0.322689431	0.4021107	0.620183869
M2869	2-palmitoleoylglycerol (16:1)*	Lipid	Monoaerylglycerol	0.68383891	-0.548271581	0.403583824	0.620183869
M1990	3-hydroxyocteate*	Lipid	Fatty Acid, Monohydroxy	1.128052378	0.173834057	0.403904126	0.620183869
M1918	octadecenedioylcarnitine (C18:1-DC)*	Lipid	Fatty Acid Metabolism (Acyl Carnitine, Dicarboxylate)	1.193578464	0.25529341	0.403070605	0.620183869
M2429	1-stearoyl-2-linoleoyl-GPE (18:0/18:2)*	Lipid	Phosphatidylethanolamine (PE)	1.09391192	0.129496579	0.408413992	0.623614276
M4235	2'-deoxyuridine	Nucleotide	Pyrimidine Metabolism, Uracil containing	0.646565287	-0.629132041	0.406850054	0.623614276
M1821	3-hydroxybutyrylglycerine	Lipid	Fatty Acid Metabolism (Acyl Glycine)	1.159340772	0.213304688	0.408882408	0.623614276
M1989	3-hydroxystearate	Lipid	Fatty Acid, Monohydroxy	1.195891624	0.250886653	0.408690862	0.623614276
M1929	3-hydroxyoleylcarnitine	Lipid	Fatty Acid Metabolism (Acyl Carnitine, Hydroxy)	0.858835151	-0.219516618	0.409824168	0.624003632
M3051	ceramide (d16:3/24:1, d18:1/22:1)*	Lipid	Ceramides	1.080963045	0.112317202	0.410905666	0.624604097
M3116	sphingomyelin (d17:2/16:0, d18:2/15:0)*	Lipid	Sphingomyelin	0.913117085	0.131128232	0.412621235	0.628164779
M3271	Salpaha-pregn-3beta,20beta-diol monosulfate (1)	Lipid	Progestin Steroids	1.262882288	0.336720173	0.415046595	0.628759592
M76	N-acetyl-1-methylehistidine	Amino Acid	Histidine Metabolism	0.729303151	0.455409467	0.417575138	0.631573712
M1531	10-heptadecenoate (17:1n7)	Lipid	Long Chain Monounsaturated Fatty Acid	1.107097331	0.146782063	0.420393085	0.637749592
M11	N-acetyleroserine	Amino Acid	Glycine, Serine and Threonine Metabolism	0.890826912	-0.166724652	0.422125649	0.636338665
M146	1-carboxyethylphenylalanine	Amino Acid	Phenylalanine Metabolism	0.861561287	-0.21497467	0.424187011	0.63733222
M2979	1-palmitoyl-2-arachidonoyl-GPC (16:0/20:4n6)	Lipid	Phosphatidylcholine (PC)	0.957898222	-0.062055718	0.423732673	0.63733222
M1325	sucrose	Carbohydrate	Disaccharides and Oligosaccharides	0.56603174	0.821045141	0.427120347	0.640695655
M3380	Salpaha-androstan-3alpha,17beta-diol disulfate	Lipid	Androgenic Steroids	0.711215594	-0.491611137	0.431688907	0.644966837
M6428	carnitine of C10H14O2 (5)*	Lipid	Partially Characterized Molecules	1.093887875	0.129466033	0.425725748	0.644966837
M5224	ethyl beta-glucopyranoside	Xenobiotics	Food Component/Plant	0.764684797	-0.387062903	0.431171122	0.644966837
M282	picolinate	Amino Acid	Tryptophan Metabolism	1.12818053	0.173997944	0.433217718	0.644966837
M2999	3-ketosphinganine	Lipid	Sphingolipid Synthesis	0.658192989	-0.603417437	0.433525564	0.644966837
M6	dimethylglycine	Amino Acid	Glycine, Serine and Threonine Metabolism	0.911125246	-0.134278711	0.435198975	0.645398478
M1563	docosahexanoate (DHA; 22:6n3)	Lipid	Long Chain Polyunsaturated Fatty Acid (n3 and n6)	1.069833575	0.097386387	0.438172001	0.648701778
M6400	glutamine conjugate of C6H10O2 (2)*	Partially Characterized Molecules	Partially Characterized Molecules	1.18836132	0.248973553	0.438890643	0.648701778
M1510	palmitate (16:0)	Lipid	Long Chain Saturated Fatty Acid	1.06598677	0.092205647	0.438412152	0.648701778
M2416	1-palmitoyl-2-arachidonoyl-GPE (16:0/20:4)*	Lipid	Phosphatidylethanolamine (PE)	1.070324947	0.098073123	0.442017566	0.652262934
M62	5-1-pyrroline-5-carboxylate	Amino Acid	Glutamate Metabolism	0.934532174	-0.097683761	0.444782649	0.655727462
M5064	3-hydroxystachydine*	Xenobiotics	Food Component/Plant	0.71472584	-0.484538147	0.450486884	0.661538898
M1189	4-hydroxyphenylacetylglutamine	Peptide	Acetylated Peptides	1.380484682	0.465174788	0.450409096	0.661538898
M3502	taurothiocholate 3-sulfate	Lipid	Secondary Bile Acid Metabolism	1.256616021	0.329537207	0.452118109	0.66283486
M3159	sphingosine	Lipid	Sphingosine	0.644840335	0.632986107	0.453712036	0.664129211
M1921	3-hydroxyhexanoylcarnitine (1)	Lipid	Fatty Acid Metabolism (Acyl Carnitine, Hydroxy)	1.12718848	0.17228772	0.456315916	0.665799417
M1688	dodecanedioate (C12:1-OC)*	Lipid	Fatty Acid, Dicarboxylate	0.896969402	0.156869324	0.455042404	0.665799417
M1560	eicosapentaenoate (EPA; 20:5n3)	Lipid	Long Chain Polyunsaturated Fatty Acid (n3 and n6)	1.098179606	0.135114025	0.464244739	0.667259596
M4368	gamma-CEHC	Cofactors and Vitamins	Tocopherol Metabolism	1.170305379	0.226940508	0.471432342	0.685651198
M3119	sphingomyelin (d18:1/18:1, d18:2/18:0)	Lipid	Sphingomyelins	0.956605421	-0.064004128	0.472735454	0.686484127
M3633	androstenediol (3beta,17beta) disulfate (1)	Lipid	Androgenic Steroids	0.858790849	-0.219621276	0.474433227	0.686574686
M1917	octadecanedioylcarnitine (C18:0-C)*	Lipid	Fatty Acid Metabolism (Acyl Carnitine, Dicarboxylate)	1.144747541	0.195029466	0.473899079	0.686574686
M1980	3-hydroxyoctanoate	Lipid	Fatty Acid, Monohydroxy	1.091400275	0.126180312	0.480861658	0.686625666
M3050	ceramide (d18:1/20:0, d16:1/22:0, d20:1/18:0)*	Lipid	Ceramides	1.057656094	0.080870598	0.480383392	0.686625666
M1439	citrate	Energy	TCA Cycle	1.063519451	0.08884642	0.480599849	0.686625666
M1431	erythronate*	Carbohydrate	Aminosugar Metabolism	0.938433639	0.091673366	0.478971502	0.686625666
M141	N-acetylphenylalanine	Amino Acid	Phenylalanine Metabolism	1.112549171	0.153869099	0.477768721	0.686625666
M109	N2-acetyl,N6-methyllysine	Amino Acid	Lysine Metabolism	0.763313958	0.057948896	0.477723894	0.686625666
M3099	palmitoyl dihydrophingomyelin (d18:0/16:0)*	Lipid	Dihydrophingomyelins	0.960628891	-0.057948896	0.477723894	0.686625666
M4437	retinal	Cofactors and Vitamins	Vitamin A Metabolism	0.840936033	0.249932031	0.481446681	0.686625666
M1550	tetradecanoate (14:2)*	Lipid	Long Chain Polyunsaturated Fatty Acid (n3 and n6)	1.103619613	0.142243001	0.481919909	0.686625666
M1691	tetradecanoate (C12:1-OC)*	Lipid	Fatty Acid, Dicarboxylate	1.10735708	0.147355	0.476364912	0.686625666
M1430	N-acetylglucosaminylidapsagrine	Carbohydrate	Aminosugar Metabolism	0.931606646	-0.10212354	0.484969261	0.68883849
M327	6-bromotryptophan	Amino Acid	Tryptophan Metabolism	0.821638266	-0.28424721	0.49070246	0.691662602
M1703	icosenedioate (C20:1-DC)*	Lipid	Fatty Acid, Dicarboxylate	1.05316475	0.074731134	0.487514004	0.691662602
M3461	glycochenodeoxycholate	Lipid	Primary Bile Acid Metabolism	1.118931623	0.162121877	0.491518625	0.691662602
M1891	linoleylcarnitine (C18:2)*	Lipid	Fatty Acid Metabolism (Acyl Carnitine, Polyunsaturated)	1.075270629	0.104699811	0.487768519	0.691662602
M1526	myristoleate (14:1N5)	Lipid	Long Chain Monounsaturated Fatty Acid	1.101898412	0.139991222	0.491181182	0.691662602
M18	N-acetylthreonine	Amino Acid	Glycine, Serine and Threonine Metabolism	0.935323917	0.096448134	0.489620987	0.691662602
M3283	pregnanediol-3-glucuronide	Lipid	Progesterin Steroids	1.133155364	0.180345679	0.491404416	0.691662602
M3032	N-stearyl-sphingadiene (d18:2/18:0)*	Lipid	Ceramides	1.061014084	0.085443807	0.503601352	0.707325675
M4382	gamma-tocopherol/beta-tocopherol	Cofactors and Vitamins	Tocopherol Metabolism	1.098183737	0.135033579	0.506070301	0.708810329
M3105	stearyl sphingomyelin (d18:1/18:0)	Lipid	Sphingomyelins	0.96340082	-0.053791943	0.505940479	0.708810329
M512	N-methylhydroxyproline	Amino Acid	Urea cycle; Arginine and Proline Metabolism	1.118929973	0.437721341	0.510234563	0.713543412
M4432	carotene diol (2)	Cofactors and Vitamins	Vitamin A Metabolism	0.920411767	-0.119648667	0.514551035	0.718447487
M2866	1-docosahexaenoylglycerol (22:6)	Lipid	Monoaerylglycerol	0.874848781	0.192813578	0.516306597	0.718567861
M4283	3-aminoisobutyrate	Nucleotide	Pyrimidine Metabolism, Thymine containing	1.300254577	0.378794116	0.516076278	0.718567861
M4251	cytidine	Nucleotide	Pyrimidine Metabolism, Cytidine containing	0.885736997	-0.175049713	0.516989289	0.718567861
M498	dimethylarginine (ADMA + SDMA)	Amino Acid	Urea cycle; Arginine and Proline Metabolism	0.89796636	-0.152666696	0.520995815	0.723038333
M397	2-methylbutyrylcarnitine (CS)	Amino Acid	Leucine, Isoleucine and Valine Metabolism	1.136036469	0.184043347	0.525277192	0.725956015
M2033	25,3R-dihydroxybutyrate	Lipid	Fatty Acid, Dihydroxy	1.085602271	0.118495644	0.525373184	0.725956015
M6259	3,5-dichloro-2,6-dihydroxybenzoic acid	Xenobiotics	Chemical	0.943338393	-0.08415271	0.526298145	0.725956015
M1509	pentadecanoate (15:0)	Lipid	Long Chain Saturated Fatty Acid	1.068183631	0.095159681	0.526116827	0.725956015
M2278	1,2-dipalmitoyl-GPC (16:0/16:0)	Lipid	Phosphatidylcholine (PC)	1.047448835	0.066879775	0.540845687	0.743765097
M4785	3-formylindole	Xenobiotics	Food Component/Plant	0.936846931	-0.09114745	0.540507322	0.743765097
M1445	alpha-ketoglutarate	Energy	TCA Cycle	1.064075478	0.089600501	0.544997638	0.747139557
M6443	bilirubin degradation product, C16H18N20S (1)	Partially Characterized Molecules	Partially Characterized Molecules	1.194848406	0.285292088	0.575277056	0.75288314
M2841	glycerol	Lipid	Glycerolipid Metabolism	0.925926802	-0.11029948	0.54952305	0.75288314
M519	benenate (22:0)*	Lipid	Long Chain Saturated Fatty Acid	1.065113888	0.0910077	0.553486207	0.756527288
M4238	3-ureidopropionate	Nucleotide	Pyrimidine Metabolism, Uracil containing	1.161358158	0.215812962	0.559596207	0.757264719
M51	4-hydroxy glutamate	Amino Acid	Glutamate Metabolism	1.065498557	0.091528639	0.559823059	0.757264719
M1573	arachidonate (20:4n6)	Lipid	Long Chain Polyunsaturated Fatty Acid (n3 and n6)	1.061328252	0.085709728	0.557813396	0.757264719
M4410	bilirubin (Z,Z or E,E)*	Cofactors and Vitamins	Hemoglobin and Porphyrin Metabolism	0.921229309	-0.118367783	0.558174477	0.757264719
M4433	carotene diol (3)	Cofactors and Vitamins	Vitamin A Metabolism	0.907811785	-0.139334877	0.559924131	0.757264719
M528	creatine	Amino Acid	Creatine Metabolism	1.133985225	0.181287338	0.559562288	0.757264719
M4544	methyl 4-hydroxybenzoate sulfate	Xenobiotics	Benzoate Metabolism	0.769688574	-0.377653264	0.555516128	0.757264719
M518	N-methylproline	Amino Acid	Urea cycle; Arginine and Proline Metabolism	0.801154059	-0.3198484	0.561336039	0.757354372
M2915	palmitoleyl-archidonylglycerol (16:1/20:4) [2]*	Lipid	Diacylglycerol	0.854520668	0.226812708	0.561558687	0.757354372
M2410	1-palmitoyl-2-linoleoyl-GPE (16:0/18:2)	Lipid	Phosphatidylethanolamine (PE)	1.065455785	0.091470724	0.563877607	0.75701951
M2339	1-stearoyl-2-docosahexaenoyl-GPC (18:0/22:6)	Lipid	Phosphatidylcholine (PC)	1.032284687	-0.102362974	0.590804776	0.774963264
M554	N1,N12-diacylsperrmine	Amino Acid	Polyamine Metabolism	0.716544284	-0.48087227	0.564391552	0.770521951
M2286	1-palmitoyl-2-linoleoyl-GPC (16:0/18:2)	Lipid	Phosphatidylcholine (PC)	0.97818929	-0.201844245	0.567161327	0.78220314
M1960	2-hydroxyoctanoate	Lipid	Fatty Acid, Monohydroxy	1.218635841	0.285267077	0.567205516	0.78220314
M120	5-(galactosylhydroxyl)-L-lysine	Amino Acid					

M2868	2-palmitoylglycerol (16:0)	Lipid	Monoacylglycerol	0.903064865	-0.147098478	0.603619748	0.782382568
M410	methylsuccinate	Amino Acid	Leucine, Isoleucine and Valine Metabolism	0.933693591	-0.098978915	0.604216241	0.782382568
M3000	sphinganine	Lipid	Sphingolipid Synthesis	0.728558545	-0.456883188	0.607576188	0.784564251
M3110	sphingomyelin (d18:2/23:1)*	Lipid	Sphingomyelin	0.96505936	-0.05131041	0.607627319	0.784564251
M3514	glycoscourdeoxycholate	Lipid	Secondary Bile Acid Metabolism	1.412141021	0.497884168	0.608884371	0.785036363
M4153	1-methyladenosine	Nucleotide	Purine Metabolism, Adenine containing	1.070400287	0.098150407	0.609720212	0.785036363
M3012	N-stearoyl-sphinganine (d18:0/18:0)*	Lipid	Dihydroceramides	1.074233648	0.103307817	0.613607337	0.788923719
M3339	16α-hydroxy DHEA 3-sulfate	Lipid	Androgenic Steroids	0.880134789	-0.184203612	0.614516384	0.788976544
M466	lanthionine	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	1.048255276	0.067990091	0.615787938	0.789493986
M2926	oleoyl-linoleoyl-glycerol (18:1/18:2) [1]	Lipid	Diacylglycerol	1.057069292	0.0800695	0.619798841	0.793517108
M2582	1-palmitoyl-GPA (16:0)	Lipid	Lysophospholipid	0.926543457	-0.110069451	0.62484922	0.796877781
M1663	2-hydroxyglutarate	Lipid	Fatty Acid, Dicarboxylate	1.287210716	0.364284242	0.625053749	0.796877781
M417	N-acetyllysine	Amino Acid	Leucine, Isoleucine and Valine Metabolism	0.952337777	-0.070454429	0.624203008	0.786777781
M4192	N2,N2-dimethylguanosine	Nucleotide	Purine Metabolism, Guanine containing	1.066072394	0.092305411	0.628409922	0.80003448
M4525	4-vinylphenol sulfate	Xenobiotics	Benzoate Metabolism	0.813340947	-0.298087807	0.63605507	0.80078935
M3364	androstenediol (3beta,17beta) disulfate (2)	Lipid	Androgenic Steroids	0.941533888	-0.086915073	0.632871407	0.80078935
M3350	androsterone sulfate	Lipid	Androgenic Steroids	0.905120578	-0.143818097	0.635911674	0.80078935
M4959	mannonate*	Xenobiotics	Food Component/Plant	1.049663535	0.069926946	0.635495831	0.80078935
M255	N-acetyltryptophan	Amino Acid	Tryptophan Metabolism	0.937919201	-0.092464451	0.633223756	0.80078935
M116	N6,N6,N6-trimethylsilyne	Amino Acid	Lysine Metabolism	0.944310895	-0.082666179	0.630358847	0.80078935
M4335	pantoate	Cofactors and Vitamins	Panthothene and CoA Metabolism	1.112277306	0.152218869	0.634368511	0.80078935
M3115	sphingomyelin (d17:1/16:0, d18:1/15:0, d16:1/17:0)*	Lipid	Sphingomyelin	0.966289707	-0.049472301	0.632320357	0.80078935
M2358	1-oleoyl-2-docosahexaenoyl-GPC (18:1/22:6)*	Lipid	Phosphatidylcholine (PC)	0.97380837	-0.039772453	0.638266524	0.802467871
M1642	(14 or 15)-methylpalmitate (a17:0 or i17:0)	Lipid	Fatty Acid, Branched	1.060950199	0.08556938	0.645550959	0.804599275
M449	2-hydroxy-4-(methylthio)butanoic acid	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	0.940024222	-0.08923047	0.642643505	0.804599275
M3280	Salpha-pregn-3beta,20alpha-diol disulfate	Lipid	Progestin Steroids	1.096251013	0.132578175	0.641666028	0.804599275
M4186	7-methylguanine	Nucleotide	Purine Metabolism, Guanine containing	1.065691359	0.091789671	0.642405235	0.804599275
M3353	ethocholanolone glucuronide	Lipid	Androgenic Steroids	0.920230683	-0.119932534	0.645243523	0.804599275
M115	N6,N6-dimethyllysine	Amino Acid	Lysine Metabolism	0.839969346	-0.251591416	0.643718418	0.804599275
M1772	propionylglycine (C3)	Lipid	Fatty Acid Metabolism (also BCAA Metabolism)	0.913578574	-0.130399279	0.646157834	0.804599275
M1698	octadecanedioate (C18)	Lipid	Fatty Acid, Dicarboxylate	1.055902191	0.078476202	0.648334030	0.806204969
M448	2,3-dihydroxy-5-methylthio-4-pentenoate (DMTPA)*	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	1.040397018	0.057313417	0.649330405	0.806340681
M1823	N-palmitoylglycine	Lipid	Fatty Acid Metabolism (Acyl Glycine)	0.956134595	-0.064714375	0.651323464	0.806117556
M6190	perfluorooctanesulfonate (PFOS)	Xenobiotics	Chemical	0.915324023	-0.127645549	0.65077082	0.806117556
M6399	glutamine conjugate of C6H10O2 (1)*	Partially Characterized Molecules	Partially Characterized Molecules	0.917310239	0.124518351	0.652608607	0.807103706
M33	N,N-dimethylalanine	Amino Acid	Alanine and Aspartate Metabolism	1.160241098	0.214424628	0.657490495	0.809358553
M538	N-acetylputrescine	Amino Acid	Polyamine Metabolism	1.061386566	0.085950193	0.656812099	0.809358553
M1771	propionylcaritmine (C3)	Lipid	Fatty Acid Metabolism (also BCAA Metabolism)	0.942684996	-0.085152329	0.657406146	0.809358553
M3130	sphingomyelin (d18:2/24:1, d18:1/24:2)*	Lipid	Sphingomyelin	1.016482715	0.023585683	0.658784217	0.810331331
M348	2-ketocaprylate	Amino Acid	Leucine, Isoleucine and Valine Metabolism	1.177342112	0.23533599	0.662263841	0.833962486
M6450	bilirubin degradation product, C16H18N2O5 (3)	Partially Characterized Molecules	Polyamine Metabolism	1.116368116	0.158812826	0.663521978	0.813962486
M556	5-methyladenosine (MTA)	Amino Acid	Corticosteroids	1.065222442	0.091154729	0.666816496	0.816895142
M3297	corticosterone	Lipid	Fatty Acid, Dicarboxylate	1.089325668	0.123435331	0.674320314	0.823867158
M1696	hexadecanedioate (C16:1-DC)*	Lipid	Fibrinopeptide A	1.054855327	0.070745147	0.674293944	0.823867158
M1163	Fibrinopeptide A (7-16)*	Peptide	Fibrinogen Cleavage Peptide	1.049219141	0.069319882	0.679838211	0.824938781
M71	1-methylhistidine	Amino Acid	Histidine Metabolism	0.944333007	0.082632398	0.681756508	0.830719391
M3134	palmitoyl-sphingosine-phosphoethanolamine (d18:1/16:0)	Lipid	Ceramide PEs	1.018802164	0.026873929	0.685205768	0.833010844
M476	succinyltaurine	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	1.105755117	0.145031919	0.685469869	0.833010844
M107	N6-acetylysine	Amino Acid	Lysine Metabolism	0.953834067	-0.061889784	0.687478562	0.834336466
M2872	2-linoleoylglycerol (18:2)	Lipid	Monacylglycerol	0.915237773	-0.1277815	0.691057897	0.837562171
M1504	5-dodecanoate (12:1n)	Lipid	Medium Chain Fatty Acid	1.050852023	0.07159529	0.695339858	0.839528946
M364	beta-hydroxyisovalerylcarnitine	Amino Acid	Leucine, Isoleucine and Valine Metabolism	0.963256248	0.054008457	0.69608736	0.839528946
M1449	fumarate	Energy	TCA Cycle	1.046101167	0.06502238	0.69565772	0.839528946
M427	isobutyrylglycine (C4)	Amino Acid	Leucine, Isoleucine and Valine Metabolism	0.92728917	-0.10890879	0.696374945	0.839528946
M4239	beta-alanine	Nucleotide	Pyrimidine Metabolism, Uracil containing	1.027826525	0.039596789	0.699961434	0.842843025
M6451	bilirubin degradation product, C16H18N2O5 (4)	Partially Characterized Molecules	Partially Characterized Molecules	1.100951418	0.138750808	0.700678952	0.842483025
M1986	3-hydroxymyristate	Lipid	Fatty Acid, Monohydroxy	1.047563897	0.067038245	0.703988686	0.844870999
M1699	octadecenedioate (C18:1-DC)	Lipid	Fatty Acid, Dicarboxylate	0.952579315	-0.070088873	0.704530646	0.844870999
M150	phenylpyruvate	Amino Acid	Phenylalanine Metabolism	1.056030381	0.078651534	0.709665865	0.84666244
M272	kyurenate	Amino Acid	Tryptophan Metabolism	0.958265657	-0.06150243	0.709669895	0.848820545
M6260	3-bromo-5-chloro-2,6-dihydroxybenzoic acid*	Xenobiotics	Chemical	0.966331182	-0.049410379	0.717512521	0.857061839
M1840	acetylcaritmine (C2)	Lipid	Fatty Acid Metabolism (Acyl Carnitine, Short Chain)	1.042797033	0.060458383	0.719125211	0.857851402
M394	3-methyl-2-oxovaleate	Amino Acid	Leucine, Isoleucine and Valine Metabolism	1.027308111	0.038868964	0.72478361	0.863470970
M1562	docosapentaenoate (DPA; 22:5n3)	Lipid	Long Chain Polyunsaturated Fatty Acid (n3 and n6)	1.0404433469	0.051784714	0.726063259	0.863832223
M6177	2,4-di-tert-butylphenol	Xenobiotics	Chemical	0.977941781	-0.032179514	0.728185108	0.865225246
M287	serotonin	Amino Acid	Tryptophan Metabolism	1.093829755	0.129388212	0.730827201	0.867261261
M4349	ascorbic acid 3-sulfate*	Cofactors and Vitamins	Ascorbate and Aldarate Metabolism	0.954272146	-0.067527333	0.732384901	0.867976369
M354	isovalerylcarnitine (C5)	Amino Acid	Leucine, Isoleucine and Valine Metabolism	0.95368	0.068422832	0.734096967	0.868872582
M1852	octanoylcarnitine (C8)	Lipid	Fatty Acid Metabolism (Acyl Carnitine, Medium Chain)	0.961227453	-0.057050242	0.736076758	0.870038994
M3379	Salpha-androstan-3alpha,17beta-diol monosulfate (2)	Lipid	Androgenic Steroids	0.915737081	-0.126994652	0.738193706	0.87452051
M6447	bilirubin degradation product, C17H18N2O4 (3)	Partially Characterized Molecules	Partially Characterized Molecules	1.056174925	0.078848795	0.743609595	0.876770333
M579	5-oxoprolin	Amino Acid	Glutathione Metabolism	1.054857587	0.070088248	0.745039239	0.877524752
M204	3-methoxytyrosine	Lipid	Tyrosine Metabolism	0.958976409	-0.06043277	0.746153725	0.877344048
M439	methionine sulfone	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	0.945333567	0.081104612	0.749801524	0.88058086
M4209	ortotidine	Nucleotide	Pyrimidine Metabolism, Orotate containing	0.882577262	-0.180205516	0.753617222	0.883920071
M3052	ceramide (d18:2/24:1, d18:1/24:2)*	Lipid	Ceramides	1.026682468	0.037995366	0.75480902	0.884177061
M2536	1-palmitoyl-2-linoleoyl-GPI (16:0/18:2)	Lipid	Phosphatidylinositol (PI)	0.96968763	-0.044140237	0.759698227	0.885410445
M36	aspartate	Amino Acid	Fatty Acid, Amino	1.063110647	0.054226543	0.759362068	0.885410445
M4435	beta-cryptoxanthin	Cofactors and Vitamins	Vitamin A Metabolism	1.08685227	0.120155855	0.759758138	0.885410445
M4451	pyridoxate	Cofactors and Vitamins	Vitamin B6 Metabolism	1.047124928	0.066433575	0.757379008	0.885410445
M4963	methyl indole-3-acetate	Xenobiotics	Food Component/Plant	0.921255711	0.052005364	0.762005954	0.886982555
M2322	1-stearoyl-2-oleoyl-GPC (18:0/18:1)	Lipid	Phosphatidylcholine (PC)	0.919459304	0.027804185	0.769903633	0.883776553
M16	2-methylserine	Amino Acid	Glycine, Serine and Threonine Metabolism	0.943396371	0.078651534	0.774482954	0.88741297
M546	N(1')-acetylperimidine	Amino Acid	Polyamine Metabolism	0.892677373	-0.163789237	0.774024121	0.88741297
M1755	2-aminoocanoate	Lipid	Fatty Acid, Amino	1.101723038	0.13976159	0.775584061	0.889338782
M1886	oleoylcarnitine (C18:1)	Lipid	Fatty Acid Metabolism (Acyl Carnitine, Monounsaturated)	0.972098483	-0.040825615	0.778803789	0.900677665
M2861	1-dihomo-linoleoylglycerol (20:3)	Lipid	Monacylglycerol	0.951711633	-0.071403589	0.785397168	0.906498532
M2444	1-oleoyl-2-linoleoyl-GPE (18:1/18:2)*	Lipid	Phosphatidylethanolamine (PE)	1.034514194	0.048953444	0.78737654	0.906498532
M1932	camitine	Lipid	Carnitine Metabolism	0.977914781	-0.032219346	0.787898354	0.906498532
M829	glycylvaline	Peptide	Dipeptide	1.173960144	0.23138343	0.788223255	0.906498532
M2907	palmitoyl-linoleoyl-glycerol (16:0/18:2) [2]*	Lipid	Diacylglycerol	0.967459554	-0.047726746	0.788397547	0.906498532
M3117	spingomyelin (d18:2/16:0, d18:1/16:1)*	Lipid	Sphingomyelins	0.98698946	-0.018879551	0.792045869	0.909055716
M1768	butyrylcarnitine (C4)	Lipid	Fatty Acid Metabolism (also BCAA Metabolism)	0.934485068	-0.097756483	0.79796831	0.914695074
M7	betaine	Amino Acid	Glycine, Serine and Threonine Metabolism	0.982763707	-0.139230842	0.817379883	0.920426849
M428	3-hydroxyisobutyrate	Amino Acid	Leucine, Isoleucine and Valine Metabolism	1.03288729	0.046682833	0.8088102	0.916719608
M119	5-hydroxylsine	Amino Acid	Lysine Metabolism	0.977921194	-0.032209885	0.808206722	0.916719608
M578	cys-gly, oxidized	Amino Acid	Glutathione Metabolism	1.053807976	0.075612004	0.802337147	0.916719608
M385	isoleucine	Amino Acid	Leucine, Isoleucine and Valine Metabolism	0.985329583	-0.021321723	0.807216044	0.916719608
M419	N-carbamoylvaline	Amino Acid	Lysine Metabolism				

M6266	4-chlorobenzoic acid	Xenobiotics	Chemical	1.003658354	0.005268258	0.843580779	0.922554802
M563	4-guanidinobutanoate	Amino Acid	Guanidino and Acetamido Metabolism	0.968488914	-0.04619256	0.83908396	0.922554802
M3206	7-HOCA	Lipid	Sterol	0.984760905	-0.022154606	0.831449951	0.922554802
M56	beta-citrylglutamate	Amino Acid	Glutamate Metabolism	1.049467897	0.069658035	0.846436419	0.922554802
M1179	Fibrinopeptide B (1-12)	Peptide	Fibrinogen Cleavage Peptide	0.968696905	-0.045477509	0.836281034	0.922554802
M1346	fructose	Carbohydrate	Fructose, Mannose and Galactose Metabolism	0.978805412	-0.030906017	0.844963597	0.922554802
M643	gamma-glutamylphenylalanine	Peptide	Gamma-glutamyl Amino Acid	1.022511871	0.032117593	0.845994562	0.922554802
M1243	glycerate	Carbohydrate	Glycolysis, Gluconeogenesis, and Pyruvate Metabolism	0.98727981	-0.018469071	0.833851155	0.922554802
M2241	glycerophosphoserine*	Lipid	Phospholipid Metabolism	0.973524459	-0.038710869	0.833261376	0.922554802
M4501	guaiacol sulfate	Xenobiotics	Benzoate Metabolism	0.864927137	-0.209349492	0.8447945	0.922554802
M4407	heme	Cofactors and Vitamins	Hemoglobin and Porphyrin Metabolism	0.876797373	-0.189684619	0.8392851	0.922554802
M3525	hyocholate	Lipid	Secondary Bile Acid Metabolism	1.049077295	0.069120979	0.838777239	0.922554802
M73	N-acetylhistidine	Amino Acid	Histidine Metabolism	1.061806023	0.086520244	0.840627303	0.922554802
M190	phenol sulfate	Amino Acid	Tyrosine Metabolism	0.894452156	-0.16092378	0.831418562	0.922554802
M4450	pyridoxal	Cofactors and Vitamins	Vitamin B6 Metabolism	0.991746525	-0.011956567	0.845688701	0.922554802
M3109	sphingomyelin (d18:2/18:1)*	Lipid	Sphingomyelin	1.012351496	0.017710292	0.84105909	0.922554802
M1879	3-decenoic carnitine	Lipid	Fatty Acid Metabolism (Acyl Carnitine, Monounsaturated)	1.022306106	0.031827243	0.852238633	0.927763638
M3500	glycothiocholate sulfate*	Lipid	Secondary Bile Acid Metabolism	1.057694314	0.080922732	0.856679582	0.931485335
M1985	3-hydroxylauroate	Lipid	Fatty Acid, Monohydroxy	1.025227637	0.035944275	0.85952	0.932782824
M5328	N-methylpipecolate	Xenobiotics	Bacterial/Fungal	0.932919419	-0.100175622	0.859173447	0.932782824
M91	1-methyl-4-imidazoleacetate	Amino Acid	Histidine Metabolism	0.935549255	-0.069116027	0.863597732	0.935649986
M4360	alpha-tocopherol	Cofactors and Vitamins	Tocopherol Metabolism	1.010724676	0.015390057	0.8646467416	0.935693668
M3504	ursodeoxycholate	Lipid	Secondary Bile Acid Metabolism	0.87720144	-0.189019914	0.866827445	0.936915752
M1564	docosatrienoate (22:3n3)	Lipid	Long Chain Polyunsaturated Fatty Acid (n3 and n6)	0.978350184	0.031577148	0.87225194	0.94165916
M407	ethylmalonate	Amino Acid	Leucine, Isoleucine and Valine Metabolism	0.954559298	-0.067093273	0.876696167	0.945334301
M4408	bilirubin	Cofactors and Vitamins	Hemoglobin and Porphyrin Metabolism	0.983405724	-0.024075327	0.881303418	0.949176311
M2543	1-stearoyl-2-linoleoyl-GPI (18:0/18:2)	Lipid	Phosphatidylinositol (PI)	1.01363764	0.019542004	0.88872803	0.94929389
M1966	2-hydroxylauroate	Lipid	Fatty Acid, Monohydroxy	0.989906796	-0.0146354	0.883941676	0.94929389
M1927	3-hydroxydecanoic carnitine	Lipid	Fatty Acid Metabolism (Acyl Carnitine, Hydroxy)	1.019307387	0.027589182	0.88389277	0.94929389
M6445	bilirubin degradation product, C17H18N2O4 (1)	Partially Characterized Molecules	Partially Characterized Molecules	1.022123006	0.031568827	0.887716158	0.94929389
M2941	linoleyl-arachidonoyl-glycerol (18:2/20:4) [1]*	Lipid	Diacylglycerol	0.982155486	-0.025976658	0.887751933	0.94929389
M227	N-formylphenylalanine	Amino Acid	Tyrosine Metabolism	1.051456037	0.072388529	0.887814411	0.94929389
M3103	palmitoyl sphingomyelin (d18:1/16:0)	Lipid	Sphingomyelin	1.004394007	0.006325325	0.887507518	0.94929389
M3484	deoxycholic acid glucuronide	Lipid	Secondary Bile Acid Metabolism	0.970658812	-0.042965819	0.892751055	0.952773558
M4498	catechol sulfate	Xenobiotics	Benzoate Metabolism	0.904368552	-0.145017269	0.894859746	0.953101743
M647	gamma-glutamylvaline	Peptide	Gamma-glutamyl Amino Acid	0.985861084	-0.020543722	0.89543332	0.953101743
M2862	1-arachidonoylglycerol (20:4)	Lipid	Monoaerylglycerol	0.982289309	-0.025780097	0.898095230	0.953705941
M4304	nicotinamide	Cofactors and Vitamins	Nicotinate and Nicotinamide Metabolism	0.961971114	0.055934482	0.897856822	0.953705941
M1668	3-hydroxyadipate	Lipid	Fatty Acid, Dicarboxylate	0.976030547	0.035001794	0.904082316	0.957821475
M416	valine	Amino Acid	Leucine, Isoleucine and Valine Metabolism	1.006974601	0.010207294	0.903468643	0.957821475
M6444	bilirubin degradation product, C16H18N2O5 (2)	Partially Characterized Molecules	Partially Characterized Molecules	1.025783586	0.036726392	0.9073123109	0.955905635
M1700	octadecadienoate (C18:2-DC)*	Lipid	Fatty Acid, Dicarboxylate	0.969976142	-0.043978833	0.907783109	0.955905635
M519	N,N,N-trimethyl-alanylproline betaine (TMAP)	Amino Acid	Urea cycle: Arginine and Proline Metabolism	0.986576923	-0.019465533	0.910876179	0.961656732
M2906	palmitoyl-linoleoyl-glycerol (16:0/18:2) [1]*	Lipid	Diacylglycerol	1.015859786	0.022701288	0.912337989	0.962082636
M1973	2-hydroxyarachidate*	Lipid	Fatty Acid, Monohydroxy	0.993420131	-0.009524112	0.917358185	0.965137257
M86	N-acetylcarnosine	Amino Acid	Histidine Metabolism	0.986757577	0.019232402	0.917290466	0.965137257
M6446	bilirubin degradation product, C17H18N2O4 (2)	Partially Characterized Molecules	Partially Characterized Molecules	1.015629361	0.022374007	0.924970789	0.965340195
M1860	decanoic carnitine (C10)	Lipid	Fatty Acid Metabolism (Acyl Carnitine, Medium Chain)	1.011231367	0.016113112	0.924020312	0.965340195
M1674	heptenedioate (C7:1-DC)*	Lipid	Fatty Acid, Dicarboxylate	0.985439937	-0.021160153	0.919987858	0.965340195
M4191	N2-methylguanosine	Nucleotide	Purine Metabolism, Guanine containing	0.988637585	-0.016468341	0.924984939	0.965340195
M151	phenylflate (PLA)	Amino Acid	Phenylalanine Metabolism	1.016908472	0.024189834	0.921980537	0.965340195
M1239	pyruvate	Carbohydrate	Glycolysis, Gluconeogenesis, and Pyruvate Metabolism	0.989344536	-0.015455072	0.920157085	0.965340195
M3127	sphingomyelin (d18:1/22:2, d18:2/22:1, d16:1/24:2)*	Lipid	Sphingomyelin	0.994231792	-0.008345858	0.92234292	0.965340195
M1681	sebacate (C10-DC)	Lipid	Fatty Acid, Dicarboxylate	1.019985974	0.028549314	0.926216894	0.965513782
M1920	(S)-3-hydroxybutyrylcarnitine	Lipid	Glutathione Metabolism	1.016556677	0.023690653	0.937486639	0.967411331
M580	2-aminoobutyrate	Amino Acid	Fatty Acid Metabolism (Acyl Carnitine, Medium Chain)	0.993127176	-0.009970625	0.937217255	0.967411331
M1982	3-hydroxydecanoate	Lipid	Fatty Acid, Monohydroxy	1.011250477	0.016140384	0.935402208	0.967411331
M1925	3-hydroxyoctanoylcarnitine (2)	Lipid	Fatty Acid Metabolism (Acyl Carnitine, Hydroxy)	1.0106553	0.015291027	0.937612062	0.967411331
M3368	androstenediol (3 α beta, 17 α) monosulfate (3)	Lipid	Androgenic Steroids	0.984800454	-0.022096668	0.929466478	0.967411331
M1682	decadienoic acid (C10-2-DC)	Lipid	Fatty Acid, Dicarboxylate	0.985764827	-0.02068459	0.933824275	0.967411331
M1136	glu-gly-asn-val	Peptide	Polypeptide	0.979812947	0.029421739	0.936012555	0.967411331
M2129	N,N-dimethyl-pro-pro	Peptide	Modified Peptides	0.987616894	-0.01797658	0.930785764	0.967411331
M3111	sphingomyelin (d18:2/24:2)*	Lipid	Sphingomyelin	0.995819545	0.006043763	0.934041596	0.967411331
M367	3-methylglutaconate	Amino Acid	Leucine, Isoleucine and Valine Metabolism	0.992017959	-0.011561856	0.938907221	0.967649279
M2303	1-palmitoyl-2-docosahexaenoyl-GPC (16:0/22:6)	Lipid	Phosphatidylcholine (PC)	0.996454903	-0.005123581	0.940779986	0.968481322
M1931	deoxycarnitine	Lipid	Carnitine Metabolism	1.00669191	0.009622226	0.947731235	0.973424221
M400	tiglyl carnitine (C5)	Amino Acid	Leucine, Isoleucine and Valine Metabolism	0.987672223	-0.017895759	0.947428582	0.973424221
M1472	malonate	Lipid	Fatty Acid Synthesis	1.003498294	0.005038164	0.949176693	0.97381672
M4164	N6-carbamoylthreonyladenosine	Nucleotide	Purine Metabolism, Adenine containing	0.990349547	-0.013990275	0.952358706	0.973979779
M7075	3-carboxy-4-methyl-5-propyl-2-furanpropanoate (CMFP)	Lipid	Fatty Acid, Dicarboxylate	0.992065208	0.011493143	0.96076318	0.982176545
M1529	palmitoleate (16:1nt)	Lipid	Long Chain Monounsaturated Fatty Acid	1.007337689	0.010547398	0.961094619	0.982176545
M2452	1,2-dilinoleoyl-GPE (18:2/18:2)*	Lipid	Phosphatidylethanolamine (PE)	0.990975204	-0.013079136	0.965419347	0.98381895
M577	cysteinylglycine disulfide*	Amino Acid	Glutathione Metabolism	0.996022224	-0.005750162	0.964479828	0.98381895
M1902	docosahexaenoylcarnitine (C22:6)*	Partially Characterized Molecules	Fatty Acid Metabolism (Acyl Carnitine, Polyunsaturated)	1.005300541	0.007697903	0.965398872	0.98381895
M6449	bilirubin degradation product, C17H20N2O5 (2)	Lipid	Partially Characterized Molecules	1.010048802	0.014425	0.966667968	0.983987887
M1919	(R)-3-hydroxybutyrylcarnitine	Lipid	Fatty Acid Metabolism (Acyl Carnitine, Hydroxy)	1.0120986	0.017349846	0.972103343	0.987309429
M2942	linoleyl-arachidonoyl-glycerol (18:2/20:4) [2]*	Lipid	Diacylglycerol	0.99553168	0.006721743	0.971340305	0.987309429
M2196	N-oleoyserine	Lipid	Endocannabinoid	0.997808447	-0.003165212	0.974769109	0.988911964
M544	N-acetyl-isoputreanine	Amino Acid	Polyamine Metabolism	0.98838894	-0.016849733	0.98018307	0.99301194
M3193	cholesterol sulfate	Lipid	Sterol	0.998129639	-0.002700887	0.965961333	0.994065844
M4364	delta-tocopherol	Cofactors and Vitamins	Tocopherol Metabolism	0.995742615	-0.006155221	0.983944747	0.994065844
M1774	methylmalonate (MMA)	Lipid	Fatty Acid Metabolism (also BCAA Metabolism)	0.997584721	-0.003488726	0.983950463	0.994065844
M4999	phytanate	Xenobiotics	Food Component/Plant	1.002820255	0.004063042	0.987382716	0.994065844
M5073	tartarate	Xenobiotics	Food Component/Plant	1.008141409	0.011698016	0.968686573	0.994065844
M6239	thioproline	Xenobiotics	Chemical	0.99876254	-0.001786384	0.987504353	0.994065844
M110	N2-acetyl,N6,N6-dimethyllysine	Amino Acid	Lysine Metabolism	1.008062907	0.011585672	0.988647453	0.994115636
M2877	1-heptadecenoylglycerol (17:1)*	Lipid	Monoaerylglycerol	1.003279287	0.00473271	0.993270674	0.995460907
M4352	2-O-methylnicotinic acid	Cofactors and Vitamins	Ascorbate and Aldarate Metabolism	0.998959618	-0.001449745	0.992298196	0.995460907
M405	3-hydroxy-2-ethylpropionate	Amino Acid	Leucine, Isoleucine and Valine Metabolism	1.000998019	0.001439119	0.993042798	0.995460907
M3175	3-hydroxy-3-methylgluturate	Lipid	Mevalonate Metabolism	0.999428882	-0.000824185	0.99518751	0.996283531
M6448	bilirubin degradation product, C17H20N2O5 (1)	Partially Characterized Molecules	Partially Characterized Molecules	1.000653923	0.000943103	0.997817261	0.997817261

Supplementary data 4: Serum metabolites associated with gut Akkermansia abundance

Column D: PCM = Partially Characterized Molecules

p values are from mixed effect regression. *q* values are derived from *p* values after FDR correction for multiple testing

Color coding is column E was applied along the regression coefficient gradient, with blue and red representing negative and positive association with Akkermansia abundance, respectively

Color coding in column G was applied along the *q* value gradient, with darker colors indicating more significant values

code	metabolite	pathway	sub_pathway	regression coefficient	<i>p</i>	<i>q</i>
M3342	epiandrosterone sulfate	Lipid	Androgenic Steroids	0.158	0.0000	0.0003
M6422	metabolomic lactone sulfate	Partially Characterized Molecules	PCM	0.100	0.0000	0.0005
M4552	p-cresol sulfate	Xenobiotics	Benzoate Metabolism	0.210	0.0000	0.0005
M4505	4-methylcatechol sulfate	Xenobiotics	Benzoate Metabolism	0.218	0.0000	0.0006
M3368	androstenediol (3 α , 17 α) monosulfate (3)	Lipid	Androgenic Steroids	0.145	0.0001	0.0018
M3500	androsterone sulfate	Lipid	Androgenic Steroids	0.149	0.0001	0.0026
M322	3-indoxyl sulfate	Amino Acid	Tryptophan Metabolism	0.204	0.0003	0.0047
M1187	phenylacetylglutamine	Peptide	Acetylated Peptides	0.151	0.0003	0.0049
M3337	dehydroepiandrosterone sulfate (DHEA-S)	Lipid	Androgenic Steroids	0.130	0.0004	0.0052
M6152	dimethyl sulfone	Xenobiotics	Chemical	0.119	0.0008	0.0096
M1184	phenylacetyl carnitine	Peptide	Acetylated Peptides	0.164	0.0008	0.0104
M6235	6-hydroxyindole sulfate	Xenobiotics	Chemical	0.140	0.0010	0.0116
M4938	indolin-2-one	Xenobiotics	Food Component/Plant	0.130	0.0012	0.0139
M6446	bilirubin degradation product, C17H18N2O4 (2)	Partially Characterized Molecules	PCM	-0.102	0.0015	0.0159
M4462	hippurate	Xenobiotics	Benzoate Metabolism	0.128	0.0017	0.0173
M3502	taurolithocholate 3-sulfate	Lipid	Secondary Bile Acid Metabolism	0.159	0.0017	0.0176
M6447	bilirubin degradation product, C17H18N2O4 (3)	Partially Characterized Molecules	PCM	-0.102	0.0018	0.0178
M576	cysteinylglycine	Amino Acid	Glutathione Metabolism	0.131	0.0022	0.0211
M4498	catechol sulfate	Xenobiotics	Benzoate Metabolism	0.140	0.0025	0.0232
M6449	bilirubin degradation product, C17H20N2O5 (2)	Partially Characterized Molecules	PCM	-0.110	0.0027	0.0251
M6445	bilirubin degradation product, C17H18N2O4 (1)	Partially Characterized Molecules	PCM	-0.098	0.0028	0.0259
M3131	sphingomyelin (d18:1/25:0, d19:0/24:1, d20:1/23:0, d19:1/24:0)*	Lipid	Sphingomyelins	0.059	0.0029	0.0262
M3490	taurodeoxycholic acid 3-sulfate	Lipid	Secondary Bile Acid Metabolism	0.132	0.0029	0.0262
M3107	tricosanoyl sphingomyelin (d18:1/23:0)*	Lipid	Sphingomyelins	0.052	0.0030	0.0269
M56	beta-citrylglutamate	Amino Acid	Glutamate Metabolism	-0.094	0.0031	0.0279
M489	3-amino-2-piperidone	Amino Acid	Urea cycle; Arginine and Proline Metabolism	0.073	0.0040	0.0338
M468	cysteine sulfenic acid	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	-0.079	0.0044	0.0360
M3540	glycodeoxycholate 3-sulfate	Lipid	Secondary Bile Acid Metabolism	0.129	0.0053	0.0410
M4501	guaiacol sulfate	Xenobiotics	Benzoate Metabolism	0.128	0.0054	0.0413
M3500	glycolithocholate sulfate*	Lipid	Secondary Bile Acid Metabolism	0.136	0.0056	0.0424
M6448	bilirubin degradation product, C17H20N2O5 (1)	Partially Characterized Molecules	PCM	-0.105	0.0057	0.0426
M1891	linoleylcarnitine (C18:2)*	Lipid	Fatty Acid Metabolism (Acyl Carnitine, Polyunsaturated)	-0.076	0.0057	0.0426
M3120	sphingomyelin (d18:1/19:0, d19:1/18:0)*	Lipid	Sphingomyelins	0.050	0.0061	0.0452
M3124	sphingomyelin (d18:1/21:0, d17:1/22:0, d16:1/23:0)*	Lipid	Sphingomyelins	0.051	0.0063	0.0460
M1439	citrate	Energy	TCA Cycle	-0.063	0.0064	0.0462
M4435	beta-cryptoxanthin	Cofactors and Vitamins	Vitamin A Metabolism	0.053	0.0075	0.0527
M3113	sphingomyelin (d18:1/14:0, d16:1/16:0)*	Lipid	Sphingomyelins	0.032	0.0085	0.0577
M3050	ceramide (d18:1/20:0, d16:1/22:0, d20:1/18:0)*	Lipid	Ceramides	0.053	0.0086	0.0583
M4433	carotene diol (3)	Cofactors and Vitamins	Vitamin A Metabolism	0.073	0.0088	0.0586
M6261	dibutyl sulfosuccinate	Xenobiotics	Chemical	0.096	0.0090	0.0597
M3119	sphingomyelin (d18:1/18:1, d18:2/18:0)	Lipid	Sphingomyelins	0.047	0.0099	0.0643
M1917	octadecanedioylcarnitine (C18-DC)*	Lipid	Fatty Acid Metabolism (Acyl Carnitine, Dicarboxylate)	-0.084	0.0102	0.0656
M3105	stearoyl sphingomyelin (d18:1/18:0)	Lipid	Sphingomyelins	0.047	0.0105	0.0671
M1679	azelate (C9-DC)	Lipid	Fatty Acid, Dicarboxylate	-0.082	0.0119	0.0734
M4455	cysteine	Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	0.085	0.0126	0.0770
M3118	sphingomyelin (d18:1/17:0, d17:1/18:0, d19:1/16:0)	Lipid	Sphingomyelins	0.045	0.0132	0.0800
M1114	N6-methyllysine	Amino Acid	Lysine Metabolism	-0.066	0.0140	0.0829
M5077	thymol sulfate	Xenobiotics	Food Component/Plant	0.123	0.0154	0.0895
M1750	2-aminoheptanoate	Lipid	Fatty Acid, Amino	-0.070	0.0156	0.0905
M4430	quinolinate	Cofactors and Vitamins	Nicotinate and Nicotinamide Metabolism	-0.070	0.0176	0.0994
M1	glycine	Amino Acid	Glycine, Serine and Threonine Metabolism	-0.057	0.0178	0.0999

Supplementary data 5: Putative metabolites mediating the Akkermansia-NF association

β is the regression coefficient in mixed effect regression predicting metabolite level by Akkermansia abundance

Positive (negative) values of β indicate metabolite rise (decline) after Akkermansia expansion

q values in column C are corrected p values from mixed effect regression, corresponding to β

Fold change is based on serum samples preceding vs. not preceding NF within 24 hours

q values in column E are corrected p values from Welch's t-test comparing serum samples preceding vs. not preceding NF within 24 hours

metabolite	β (metabolite vs. Akkermansia)	q (metabolite vs. Akkermansia)	foldchange	q (NF)
p-cresol sulfate	0.210153264	0.00049063	0.4933	0.0879
3-indoxyl sulfate	0.204089017	0.004662192	0.5498	0.0638
6-hydroxyindole sulfate	0.140246154	0.011644726	0.5451	0.0539
cysteinylglycine	0.130635552	0.021064972	1.6835	0.0137
hippurate	0.127784355	0.017316218	0.4895	0.0299
dibutyl sulfosuccinate	0.096004592	0.059714762	0.4046	0.0197
sphingomyelin (d18:1/25:0, d19:0/24:1, d20:1/23:0, d19:1/24:0)*	0.059086145	0.026239566	0.8227	0.0607
tricosanoyl sphingomyelin (d18:1/23:0)*	0.052243326	0.026938199	0.8397	0.0607
glycine	-0.056601391	0.099927209	0.7412	0.0011