Supplemental Material

Variability of Two Metabolomic Platforms in CKD

Eugene P. Rhee, MD[1,*] Sushrut S. Waikar, MD[2] Casey M. Rebholz, PhD[3,4] Zihe Zheng,[5] Regis Perichon, PhD[6] Clary B. Clish, PhD[7] Anne M. Evans, PhD[6] Julian Avila, PhD[7] Michelle R. Denburg, MD[8] Amanda H. Anderson, PhD[5] Ramachandran Vasan, MD[9] Harold I. Feldman, MD[5,10] Paul L. Kimmel, MD[11] and Josef Coresh MD PhD[3,4,*] on behalf of the CKD Biomarkers Consortium

[1]Nephrology Division and Endocrine Unit, Massachusetts General Hospital, Boston, MA
[2]Renal Division, Brigham and Women's Hospital, Boston, MA
[3]Welch Center for Prevention, Epidemiology, and Clinical Research, Johns Hopkins University, Baltimore, MD
[4]Department of Epidemiology, Johns Hopkins Bloomberg School of Public Health, Baltimore, MD
[5]Department of Biostatistics, Epidemiology, and Informatics, Perelman School of Medicine, University of Pennsylvania, Philadelphia, PA
[6]Metabolon, Inc., Durham, NC
[7]Broad Institute of MIT and Harvard, Cambridge, MA
[8]Division of Nephrology, The Children's Hospital of Philadelphia, Perelman School of Medicine, University of Pennsylvania, Philadelphia, PA
[9]Sections of Preventive Medicine and Epidemiology and Cardiology, Department of Medicine, Boston University School of Medicine, Boston, MA
[10]Department of Medicine, Perelman School of Medicine, University of Pennsylvania, Philadelphia, PA
[11]Division of Kidney Urologic and Hematologic Diseases, National Institutes of Diabetes and Digestive and Kidney Diseases, National Institutes of Health, Bethesda, MD

Supplemental Table of Contents

Detailed Non-targeted Metabolomics Methods

Metabolon

Sample Preparation: All samples were maintained at -80^{o}C until processed. Samples were prepared using the automated MicroLab STAR® system from Hamilton Company. Several recovery standards were added prior to the first step in the extraction process to monitor for consistent extraction for QC purposes. To remove protein, dissociate small molecules bound to protein or trapped in the precipitated protein matrix, and to recover chemically diverse metabolites, proteins were precipitated with methanol under vigorous shaking for 2 min (Glen Mills GenoGrinder 2000) followed by centrifugation. The resulting supernatant extract was divided into five fractions and then placed briefly on a TurboVap® (Zymark) to remove the organic solvent. The sample extracts were stored overnight under nitrogen before preparation for analysis.

Ultrahigh Performance Liquid Chromatography-Tandem Mass Spectroscopy (UPLC-MS/MS): All methods utilized a Waters ACQUITY ultra-performance liquid chromatography (UPLC) system and a ThermoFisher Scientific Q-Exactive high resolution/accurate mass spectrometer interfaced with a heated electrospray ionization (HESI-II) source and Orbitrap mass analyzer operated at 35,000 mass resolution. The respective dried extract samples were reconstituted in solvents compatible for four different LC/MS methods. Each reconstitution solvent contained a series of standards (isotopically labeled compounds) at fixed concentrations to ensure injection and chromatographic consistency. One aliquot was analyzed using acidic positive ion conditions and was eluted from a C18 column (Waters UPLC BEH C18-2.1x100

mm, 1.7 μm) using 0.05% perfluoropentanoic acid (PFPA) and 0.1% formic acid (FA) in water as solvent A and 0.05% PFPA and 0.1% FA in methanol (MeOH) as solvent B in the following gradient; 5 to 80% B in 3.35 min, then rapidly returning to starting conditions (3.5min total MS acquisition time) at a flow rate of 0.35mL/min. Another aliquot was also analyzed using acidic positive ion conditions, however it was chromatographically optimized for more hydrophobic compounds and was eluted from the same aforementioned C18 column using 0.05% PFPA and 0.1% FA in water as solvent A and 0.05% PFPA and 0.01% FA in 1:1 MeOH:acetonitrile (ACN) as solvent B in the following gradient; 40 to 99.5%B in 1min, hold 99.5%B for 2.4 min, then rapidly returning to starting conditions (3.5min total MS acquisition time) at a flow rate of 0.6ml/min. Another aliquot was analyzed using basic negative ion optimized conditions using a separate dedicated LC/MS system using a C18 column (same column type as described above). This extract was gradient eluted using 6.5mM ammonium bicarbonate in water at pH 8 as solvent A and 6.5mM ammonium bicarbonate at pH 8 in 95% MeOH and 5% water as solvent B in the following gradient; 0.5 to 70% B in 4 min, 70 to 98% B in 0.5 min, hold at 98% B for 0.9 min, then rapidly returning to starting conditions (6.5 min total MS acquisition time) at a flow rate of 0.35mL/min. The fourth aliquot was analyzed via negative ionization and was eluted from a HILIC column (Waters UPLC BEH Amide 2.1x150 mm, 1.7 μm) using 80% ACN, 15% water, and 5% MeOH with 10mM ammonium formate, pH 10.8 as solvent A and 50% ACN and 50% water with 10mM ammonium formate as solvent B in the following gradient; 5 to 50% B in 3.5min, 50 to 95% B in 2 min, hold at 95% B for 1 min, then rapidly return to starting conditions (6.5 min total MS acquisition time). All the methods alternated between full scan MS and data-dependent MS^n scans using dynamic exclusion. The scan range varied slighted between methods

but generally covered 70-1000 m/z. Raw data files were archived and data extracted as described below.

Data Extraction, Compound Identification and Quantification: Raw data was extracted, peak-detected and aligned, and QC processed using Metabolon's informatics software. Known compounds were identified from the large list of detected features by comparison to an in-house library of entries of over 3500 authentic standards. Metabolon maintains this library that contains the retention time/index (RI), primary mass to charge (m/z) spectral profile including preferred adduct, in-source fragment, and multimers formation, and fragmentation data (including MS/MS spectral data) on all molecules present in the library per method. Biochemical identifications are therefore based on three criteria: retention index within a narrow retention window of the proposed identification, accurate mass match to the library +/- 10 ppm, and the MS/MS forward and reverse scores between the experimental data and library entry. While there may be similarities between the molecules based on one of these factors, the use of all three data points can be utilized to distinguish and differentiate biochemicals including many structural isomers. Additional mass spectral library entries have been created for structurally unnamed compounds, which have been identified by virtue of their recurrent and reproducible nature (both chromatographic and mass spectral) within the study. These compounds have the potential to be identified by future acquisition of a matching authentic standard or by classical structural analysis. Unnamed compounds were reported by a comparison of the experimental feature data to an in-house spectral library of over 7000 unknowns. Peaks were quantified using area-under-the-curve of a primary MS ion.

Analytical QA/QC: Quality controls measures were utilized throughout the process to ensure data quality: a human plasma technical replicate was run throughout the study to monitor platform precision; extracted water samples served as process blanks to determine compounds introduced as a result of processing and storage; and a cocktail of QC standards (isotopically labeled compounds), which were carefully chosen not to interfere with the measurement of endogenous compounds, were spiked into every analyzed sample. These QC standards were utilized to assess sample extraction, instrument performance and aided chromatographic alignment. Experimental samples were randomized across the platform run with QC samples spaced evenly among the injections.

Informatics QA/QC: A variety of data quality control procedures were carried out to ensure that a high-quality data set was made available for statistical analysis and data interpretation. These QC processes were designed to ensure accurate and consistent identification of true chemical entities, and to remove and/or correct those representing system artifacts, mis-identifications, mis-alignments and background noise. Metabolon data analysts use proprietary visualization and interpretation software to confirm the consistency and accuracy of peak identification and quantification among the various samples. Every reported compound, both known and unnamed, were manually checked and verified for each sample and corrected if necessary.

Broad Institute

Liquid Chromatography-Mass Spectrometry (LC-MS) analyses: A combination of four LC-MS methods were used to profile metabolites in plasma; two methods that measure polar metabolites, a method that measures metabolites of intermediate polarity (e.g. fatty acids and bile acids), and a lipid profiling method. Samples were prepared for each method using extraction procedures that are matched for use with the chromatography conditions. Data were acquired using LC-MS systems comprised of Nexera X2 U-HPLC systems (Shimadzu Scientific Instruments) coupled to Q Exactive/Exactive Plus orbitrap mass spectrometers (Thermo Fisher Scientific). The method details are summarized below:

LC-MS Method 1 – HILIC-pos: positive ion mode MS analyses of polar metabolites. LC-MS samples were prepared from plasma (10 µL) via protein precipitation with the addition of nine volumes of 74.9:24.9:0.2 v/v/v acetonitrile/methanol/formic acid containing stable isotope-labeled internal standards (valine-d8, Isotec; and phenylalanine-d8, Cambridge Isotope Laboratories). The samples were centrifuged (10 min, 9,000 x g, 4°C), and the supernatants injected directly onto a 150 x 2 mm Atlantis HILIC column (Waters). The column was eluted isocratically at a flow rate of 250 µL/min with 5% mobile phase A (10 mM ammonium formate and 0.1% formic acid in water) for 1 minute followed by a linear gradient to 40% mobile phase B (acetonitrile with 0.1% formic acid) over 10 minutes. MS analyses were carried out using electrospray ionization in the positive ion mode using full scan analysis over m/z 70-800 at 70,000 resolution and 3 Hz data acquisition rate. Additional MS settings are: ion spray voltage, 3.5 kV; capillary temperature, 350°C; probe heater temperature, 300 °C; sheath gas, 40; auxiliary gas, 15; and S-lens RF level 40.

LC-MS Method 2 – HILIC-neg: negative ion mode MS analysis of polar metabolites. LC-MS samples were prepared from plasma (30 µL) via protein precipitation with the addition of four

volumes of 80% methanol containing inosine-15N4, thymine-d4 and glycocholate-d4 internal standards (Cambridge Isotope Laboratories). The samples were centrifuged (10 min, 9,000 x g, 4°C) and the supernatants were injected directly onto a 150 x 2.0 mm Luna NH2 column (Phenomenex). The column was eluted at a flow rate of 400 µL/min with initial conditions of 10% mobile phase A (20 mM ammonium acetate and 20 mM ammonium hydroxide in water) and 90% mobile phase B (10 mM ammonium hydroxide in 75:25 v/v acetonitrile/methanol) followed by a 10 min linear gradient to 100% mobile phase A. MS analyses were carried out using electrospray ionization in the negative ion mode using full scan analysis over m/z 60-750 at 70,000 resolution and 3 Hz data acquisition rate. Additional MS settings are: ion spray voltage, -3.0 kV; capillary temperature, 350°C; probe heater temperature, 325 °C; sheath gas, 55; auxiliary gas, 10; and S-lens RF level 40.

LC-MS Method 3 – C18-neg: negative ion mode analysis of metabolites of intermediate polarity (e.g. bile acids and free fatty acids). Plasma samples (30 µL) were extracted using 90 µL of methanol containing PGE2-d4 as an internal standard (Cayman Chemical Co.) and centrifuged (10 min, 9,000 x g, 4°C). The supernatants (10 µL) were injected onto a 150 x 2.1 mm ACQUITY BEH C18 column (Waters). The column was eluted isocratically at a flow rate of 450 µL/min with 20% mobile phase A (0.01% formic acid in water) for 3 minutes followed by a linear gradient to 100% mobile phase B (0.01% acetic acid in acetonitrile) over 12 minutes. MS analyses were carried out using electrospray ionization in the negative ion mode using full scan analysis over m/z 70-850 at 70,000 resolution and 3 Hz data acquisition rate. Additional MS settings are: ion spray voltage, -3.5 kV; capillary temperature, 320°C; probe heater temperature, 300 °C; sheath gas, 45; auxiliary gas, 10; and S-lens RF level 60.

LC-MS Method 4 – C8-pos: Lipids (polar and nonpolar) were extracted from plasma (10 µL) using 190 µL of isopropanol containing 1-dodecanoyl-2-tridecanoyl-sn-glycero-3-phosphocholine as an internal standard (Avanti Polar Lipids). After centrifugation (10 min, 9,000 x g, ambient temperature), supernatants (10 µL) were injected directly onto a 100 x 2.1 mm ACQUITY BEH C8 column (1.7 µm; Waters). The column was eluted at a flow rate of 450 µL/min isocratically for 1 minute at 80% mobile phase A (95:5:0.1 vol/vol/vol 10 mM ammonium acetate/methanol/acetic acid), followed by a linear gradient to 80% mobile-phase B (99.9:0.1 vol/vol methanol/acetic acid) over 2 minutes, a linear gradient to 100% mobile phase B over 7 minutes, and then 3 minutes at 100% mobile-phase B. MS analyses were carried out using electrospray ionization in the positive ion mode using full scan analysis over m/z 200-1100 at 70,000 resolution and 3 Hz data acquisition rate. Additional MS settings are: ion spray voltage, 3.0 kV; capillary temperature, 300°C; probe heater temperature, 300 °C; sheath gas, 50; auxiliary gas, 15; and S-lens RF level 60.

Data processing. Raw LC-MS data were acquired to the data acquisition computer interfaced to each LC-MS system and then stored on a robust and redundant file storage system (Isilon Systems) accessed via the internal network at the Broad Institute. Data processing was conducted using one of five Dell Precision T7600 workstations, each equipped with eight core XEON E5-2687W processors, 32 GB of DDR3 RAM, and 2 TB of storage in RAID 0 array of four 600 GB SAS hard drives. Nontargeted data were processed using Progenesis CoMet software (v 2.0, Nonlinear Dynamics) to detect and de-isotope peaks, perform chromatographic retention time alignment, and integrate peak areas. Peaks of unknown ID were tracked by method, m/z and retention time. Identification of nontargeted metabolite LC-MS peaks were conducted by i)

matching measured retention times and a masses to mixtures of reference metabolites analyzed in each batch, ii) matching an internal database of >600 compounds that have been characterized using the Broad Institute methods, and iii) matching exact masses only to an external database of >40000 metabolites (Human Metabolome Database v3). Compounds matched to the external database were confirmed by analyzing reference standards if they are available.

Supplementary Table 1. Metabolites counts

Step	Known metabolites		Metabolon unnamed compounds	Broad unknown ion features
	Metabolon	Broad		
Original readings	896	681	488*	28630
Exclude metabolites with over 80% missing	837	607	483	28169
Remove metabolites with variance less than 0.01	837	594	483	26180
Cap metabolites to 5+SD above the mean for those over this limit	837	594	483	26180

* 488 unnamed compounds, selected from 44,953 detected unknown ion features

Supplementary Table 2. Technical Variation, Day-to-Day Variation, and Correlation with eGFR for all Metabolon known metabolites

Metabolite	technical replicate CV	day to day variation CV	Pearson correlation with eGFR-Cr	P valu e for correlation
Metabolite	**technical replicate CV**	**day to day variation CV**	**Pearson correlation with eGFR_Cr**	**P value for Pearson correlation with eGFR_Cr**
xylose-MS195.05	0.6491	1.966	-0.2209	1.72E-01
ximenoylcarnitine (C26:1)*-MS538.48	0.0753	0.1347	0.1079	5.10E-01
xanthurenate-MS204.03	0.1649	0.2620	-0.5666	9.32E-05
xanthosine-MS283.06	0.2345	0.3733	-0.3672	1.91E-02
xanthine-MS151.02	0.1026	0.2218	-0.0479	7.70E-01
vanillylmandelate (VMA)-MS197.04	0.1959	0.1349	-0.7175	4.02E-08
vanillic alcohol sulfate-MS233.01	0.0651	6.712	-0.4166	6.97E-03
vanillactate-MS211.06	0.4161	0.1891	-0.8110	6.25E-12
valylleucine-MS231.17	0.1027	0.1753	-0.2259	1.62E-01
valylglycine-MS173.09	0.1531	0.5863	-0.2550	1.13E-01
valine-MS118.08	0.0910	0.1157	0.1907	2.40E-01
ursodeoxycholate-MS391.28	0.2485	2.217	0.2254	1.63E-01
ursodeoxycholate sulfate (1)-MS235.11	0.7832	0.6532	-0.1329	4.16E-01
uridine-MS243.06	0.0785	0.2257	0.4199	6.47E-03
urea-MS121.07	0.0803	0.1296	-0.8382	1.46E-13
urate-MS167.02	0.0931	0.0775	-0.4176	6.81E-03
uracil-MS111.02	0.1634	0.2402	-0.3834	1.40E-02
undecanoate (11:0)-MS185.15	0.1398	0.1672	0.0141	9.32E-01
undecanedioate-MS215.12	0.1924	0.3812	-0.4670	2.07E-03
umbelliferone sulfate-MS240.98	0.0942	16.20	-0.0950	5.62E-01
tyrosine-MS182.08	0.0796	0.1408	0.1795	2.70E-01
tyramine O-sulfate-MS216.03	0.2112	0.8465	-0.4183	6.71E-03
tryptophan-MS205.09	0.0468	0.0838	0.4441	3.69E-03
tryptophan betaine -MS247.14	0.0776	0.5978	-0.0850	6.04E-01
trimethylamine N-oxide-MS76.075	0.0477	0.2982	-0.5547	1.43E-04
trigonelline (N'-methylnicotinate)-MS138.05	0.0726	0.6179	-0.3691	1.85E-02
triethanolamine-MS150.11	0.2481	1.189	-0.0511	7.56E-01
tricosanoyl sphingomyelin (d18:1/23:0)*-MS801.68	0.0873	0.0901	0.1615	3.22E-01
trans-urocanate-MS139.05	0.1458	0.2365	0.0629	7.02E-01
trans-4-hydroxyproline-MS132.06	0.0401	0.1715	-0.5536	1.49E-04
tiglylcarnitine (C5:1-DC)-MS244.15	0.1200	0.1603	-0.6256	7.97E-06
thyroxine-MS775.67	0.0879	0.0790	0.1283	4.32E-01
thymol sulfate-MS229.05	1.550	3.057	0.2511	1.19E-01
threonine-MS120.06	0.0668	0.1382	-0.0748	6.49E-01
threonate-MS135.02	0.0915	0.1855	-0.2509	1.19E-01
thioproline-MS134.02	0.2412	0.1793	0.0051	9.75E-01
theophylline-MS179.05	0.0862	0.5133	0.1307	4.24E-01
theobromine-MS181.07	0.2288	7.224	-0.0680	6.79E-01
theanine-MS175.10	0.0367	205.8	-0.3210	4.30E-02
tetradecanedioate-MS257.17	0.0690	0.4131	-0.0890	5.87E-01
tauroursodeoxycholate-MS498.28	0.3185	1.813	-0.1599	3.26E-01
taurolithocholate 3-sulfate-MS280.62	0.3616	0.7013	-0.4136	7.45E-03

taurodeoxycholate-MS498.28	0.5036	6.967	-0.4130	7.55E-03
taurocholenate sulfate-MS279.61	0.1176	0.3167	-0.2377	1.40E-01
taurocholate-MS514.28	0.2468	2.198	-0.4405	4.02E-03
taurochenodeoxycholate-MS498.28	0.4502	2.161	-0.3733	1.70E-02
tauro-beta-muricholate-MS514.28	0.1197	0.7006	-0.2378	1.40E-01
taurine-MS124.00	0.1000	0.1493	-0.1428	3.82E-01
tartronate (hydroxymalonate)-MS118.99	0.1533	0.3396	0.2136	1.87E-01
tartarate-MS149.00	0.5911	43.92	-0.2893	7.00E-02
sulfate*-MS96.960	0.0989	0.1150	-0.7877	9.20E-11
sucrose-MS341.10	1.554	2.364	-0.5987	2.63E-05
succinylcarnitine (C4-DC)-MS262.12	0.0416	0.1139	-0.6971	1.60E-07
succinimide-MS116.03	0.2210	0.1786	0.0642	6.96E-01
succinate-MS117.01	19.65	58.44	0.1459	3.71E-01
suberoylcarnitine (C8-DC)-MS318.19	0.1317	0.4299	-0.5553	1.40E-04
suberate (octanedioate)-MS173.08	0.3965	0.6561	-0.6658	1.03E-06
stearoylcholine*-MS370.36	0.3934	1.915	0.2421	1.33E-01
stearoylcarnitine (C18)-MS428.37	0.0920	0.1457	0.1513	3.54E-01
stearoyl-arachidonoyl-glycerol (18:0/20:4) [2]*-MS662.57	0.1680	0.2685	0.2290	1.56E-01
stearoyl-arachidonoyl-glycerol (18:0/20:4) [1]*-MS662.57	0.2784	0.2568	-0.0619	7.06E-01
stearoyl sphingomyelin (d18:1/18:0)-MS731.60	0.0562	0.1029	0.2353	1.45E-01
stearidonate (18:4n3)-MS275.20	0.3581	5.734	0.2137	1.87E-01
stearate (18:0)-MS283.26	0.1447	0.2654	0.1689	2.99E-01
stachydrine-MS144.10	0.0621	0.7017	-0.3408	3.08E-02
sphingosine-MS300.28	0.0915	0.2794	0.1165	4.77E-01
sphingosine 1-phosphate-MS380.25	0.0721	0.1639	0.0862	5.99E-01
sphingomyelin (d18:2/24:2)*-MS809.65	0.0726	0.0846	-0.0764	6.41E-01
sphingomyelin (d18:2/24:1, d18:1/24:2)*-MS811.66	0.0558	0.0792	-0.0775	6.37E-01
sphingomyelin (d18:2/23:1)*-MS797.65	0.0790	0.0893	-0.0068	9.67E-01
sphingomyelin (d18:2/23:0, d18:1/23:1, d17:1/24:1)*-MS799.66	0.1185	0.1147	0.0934	5.69E-01
sphingomyelin (d18:2/21:0, d16:2/23:0)*-MS771.63	0.0921	0.1065	0.1310	4.23E-01
sphingomyelin (d18:2/18:1)*-MS727.57	0.0556	0.0995	0.0792	6.29E-01
sphingomyelin (d18:2/16:0, d18:1/16:1)*-MS701.55	0.0586	0.0532	-0.0097	9.53E-01
sphingomyelin (d18:2/14:0, d18:1/14:1)*-MS673.52	0.1432	0.1187	0.2788	8.16E-02
sphingomyelin (d18:1/25:0, d19:0/24:1, d20:1/23:0, d19:1/24:0)*-MS829.71	0.1040	0.1479	0.0687	6.76E-01
sphingomyelin (d18:1/24:1, d18:2/24:0)*-MS813.68	0.0947	0.0902	-0.0463	7.78E-01
sphingomyelin (d18:1/22:2, d18:2/22:1, d16:1/24:2)*-MS783.63	0.0718	0.0990	0.0386	8.14E-01
sphingomyelin (d18:1/22:1, d18:2/22:0, d16:1/24:1)*-MS785.65	0.0538	0.0678	0.1104	5.00E-01
sphingomyelin (d18:1/21:0, d17:1/22:0, d16:1/23:0)*-MS773.65	0.1351	0.1295	0.2329	1.49E-01
sphingomyelin (d18:1/20:2, d18:2/20:1, d16:1/22:2)*-MS755.60	0.1739	0.2065	0.0537	7.44E-01
sphingomyelin (d18:1/20:1, d18:2/20:0)*-MS757.62	0.0601	0.0853	0.0982	5.49E-01
sphingomyelin (d18:1/20:0, d16:1/22:0)*-MS759.63	0.0556	0.0649	0.2393	1.38E-01
sphingomyelin (d18:1/19:0, d19:1/18:0)*-MS745.62	0.0786	0.0830	0.2186	1.77E-01
sphingomyelin (d18:1/18:1, d18:2/18:0)-MS729.59	0.0529	0.0658	0.1931	2.34E-01
sphingomyelin (d18:1/17:0, d17:1/18:0, d19:1/16:0)-MS717.59	0.0665	0.0741	0.0870	5.96E-01
sphingomyelin (d18:1/15:0, d16:1/17:0)*-MS689.55	0.0760	0.1003	-0.0105	9.49E-01

sphingomyelin (d18:1/14:0, d16:1/16:0)*-MS675.54	0.0617	0.0618	0.1784	2.73E-01
sphingomyelin (d18:0/20:0, d16:0/22:0)*-MS761.65	0.1877	0.1828	0.3206	4.33E-02
sphingomyelin (d18:0/18:0, d19:0/17:0)*-MS733.62	0.1101	0.1787	0.3352	3.39E-02
sphingomyelin (d17:2/16:0, d18:2/15:0)*-MS687.54	0.1697	0.1323	0.1199	4.64E-01
sphinganine-MS302.30	0.0677	0.1849	0.2189	1.76E-01
sphinganine-1-phosphate-MS382.27	0.1209	0.2051	0.1267	4.39E-01
spermidine-MS146.16	0.4574	1.124	0.1887	2.45E-01
solanidine-MS398.34	0.1519	0.5902	0.1831	2.60E-01
S-methylmethionine-MS164.07	0.0665	4.246	-0.0933	5.69E-01
S-methylcysteine-MS134.02	0.1078	0.2701	-0.2119	1.91E-01
S-methylcysteine sulfoxide-MS152.03	0.0661	0.4376	-0.3448	2.88E-02
serotonin-MS177.10	0.0674	0.8815	0.0596	7.17E-01
serine-MS106.04	0.0429	0.0936	0.1582	3.32E-01
sedoheptulose-MS209.06	0.3492	0.2573	-0.0529	7.48E-01
sebacate (decanedioate)-MS201.11	0.3838	0.4765	-0.3810	1.47E-02
sarcosine-MS90.054	0.0797	0.1200	-0.0493	7.64E-01
S-allylcysteine-MS162.05	0.1046	11.81	0.0554	7.36E-01
salicyluric glucuronide*-MS370.07	0.6559	29.62	-0.5182	4.81E-04
salicylate-MS137.02	0.1072	834.8	-0.0823	6.16E-01
S-adenosylhomocysteine (SAH)-MS383.11	0.2411	0.1986	-0.8318	3.80E-13
saccharin-MS181.99	0.0890	6.032	-0.1227	4.53E-01
S-1-pyrroline-5-carboxylate-MS114.05	0.0918	0.1930	-0.3542	2.43E-02
S-(3-hydroxypropyl)mercapturic acid (HPMA)-MS220.06	0.3152	0.4884	-0.5725	7.45E-05
ribonate-MS165.04	0.1822	0.1755	-0.8315	3.96E-13
ribitol-MS151.06	0.1311	0.1250	-0.3576	2.29E-02
retinol (Vitamin A)-MS269.22	0.0938	0.1148	-0.2931	6.63E-02
quinolinate-MS168.02	0.0637	0.1870	-0.6807	4.38E-07
quinate-MS191.05	0.0923	5.470	-0.2476	1.24E-01
pyruvate-MS87.008	0.1014	0.2169	0.0063	9.69E-01
pyrraline-MS253.11	0.1886	3.554	-0.0510	7.56E-01
pyroglutamine*-MS129.06	0.0440	0.0934	-0.6084	1.73E-05
pyridoxate-MS182.04	0.2616	0.5467	-0.3655	1.97E-02
pyridoxal-MS168.06	0.3889	23.02	0.0166	9.20E-01
pseudouridine-MS243.06	0.1438	0.1038	-0.8287	5.98E-13
propyl 4-hydroxybenzoate sulfate-MS259.02	0.2775	2.056	0.3467	2.78E-02
propionylglycine-MS130.05	0.2640	0.3913	-0.1820	2.63E-01
propionylcarnitine (C3)-MS218.13	0.0977	0.1761	-0.1285	4.32E-01
prolylglycine-MS173.09	0.2466	0.6870	-0.4807	1.44E-03
proline-MS116.07	0.0455	0.1097	-0.2779	8.26E-02
pro-hydroxy-pro-MS229.11	0.0518	0.2587	-0.6338	5.41E-06
pristanate-MS297.27	0.7459	0.8173	0.1606	3.24E-01
pregnenolone sulfate-MS395.18	0.1538	0.2779	-0.0909	5.79E-01
pregnen-diol disulfate*-MS238.07	0.1562	0.1893	-0.1107	4.99E-01
pregnanolone/allopregnanolone sulfate-MS397.20	0.1559	1.380	-0.0612	7.09E-01
pregnanediol-3-glucuronide-MS495.29	0.2671	0.4689	-0.3203	4.35E-02
pregn steroid monosulfate*-MS397.20	0.1118	0.1874	-0.0521	7.51E-01
prednisolone-MS359.18	0.1904	1.074	-0.0432	7.92E-01
piperine-MS286.14	0.0935	1.239	0.1372	4.01E-01
pipecolate-MS130.08	0.0514	0.2858	-0.1421	3.84E-01
pimeloylcarnitine/3-methyladipoylcarnitine (C7-DC)-MS304.17	0.1501	0.3280	-0.7006	1.27E-07
pimelate (heptanedioate)-MS159.06	0.1917	0.7350	-0.5378	2.56E-04
picolinate-MS124.03	0.0860	0.2567	-0.1268	4.38E-01

phytanate-MS311.29	0.1776	0.5306	0.0765	6.41E-01
phosphoethanolamine-MS142.02	0.1300	0.2658	-0.0109	9.47E-01
phosphate-MS98.984	0.0913	0.1205	-0.2731	8.83E-02
phenylpyruvate-MS163.04	0.1800	0.2492	-0.1256	4.42E-01
phenyllactate (PLA)-MS165.05	0.0952	0.1625	-0.3034	5.67E-02
phenylalanylglycine-MS221.09	0.2159	0.2470	-0.3814	1.46E-02
phenylalanine-MS166.08	0.0540	0.0928	-0.1408	3.89E-01
phenylacetylthreonine-MS236.09	0.1659	0.4183	-0.5287	3.45E-04
phenylacetylmethionine-MS266.08	0.0870	0.4576	-0.5966	2.86E-05
phenylacetylglycine-MS192.06	0.7622	1.218	-0.4582	2.60E-03
phenylacetylglutamine-MS265.11	0.0463	0.3575	-0.6508	2.31E-06
phenylacetylglutamate-MS264.08	0.4294	0.4511	-0.6198	1.04E-05
phenylacetylcarnitine-MS280.15	0.1364	0.7315	0.0320	8.46E-01
phenylacetate-MS135.04	0.4204	0.7803	-0.1194	4.66E-01
phenol sulfate-MS172.99	0.0671	0.2756	-0.3521	2.53E-02
perfluorooctanesulfonic acid (PFOS)-MS498.93	0.1182	0.1191	0.2235	1.67E-01
pentadecanoate (15:0)-MS241.21	0.1386	0.2202	0.1851	2.55E-01
p-cresol-glucuronide*-MS283.08	0.3190	7.414	-0.4472	3.42E-03
p-cresol sulfate-MS187.00	0.1517	1.051	-0.4169	6.93E-03
paraxanthine-MS179.05	0.1314	1.285	0.0265	8.72E-01
pantothenate-MS218.10	0.0877	0.1431	-0.3362	3.33E-02
palmitoyl-palmitoyl-glycerol (16:0/16:0) [2]*-MS586.54	0.3700	0.3775	0.1292	4.30E-01
palmitoyl-palmitoyl-glycerol (16:0/16:0) [1]*-MS586.54	0.4345	0.5499	0.3265	3.92E-02
palmitoyl-oleoyl-glycerol (16:0/18:1) [2]*-MS612.55	0.2576	0.2871	0.1808	2.66E-01
palmitoyl-oleoyl-glycerol (16:0/18:1) [1]*-MS612.55	0.2107	0.2714	0.3464	2.79E-02
palmitoyl-myristoyl-glycerol (16:0/14:0) [2]-MS558.50	0.3088	0.8093	0.2317	1.51E-01
palmitoyl-linoleoyl-glycerol (16:0/18:2) [2]*-MS610.54	0.3146	0.2399	0.2665	9.67E-02
palmitoyl-linoleoyl-glycerol (16:0/18:2) [1]*-MS610.54	0.1680	0.2748	0.1738	2.85E-01
palmitoyl-linolenoyl-glycerol (16:0/18:3) [2]*-MS608.52	0.7117	0.5072	0.1020	5.34E-01
palmitoyl-docosahexaenoyl-glycerol (16:0/22:6) [1]*-MS658.54	0.1503	0.5849	0.2408	1.35E-01
palmitoylcholine-MS342.33	0.2432	1.375	0.2152	1.84E-01
palmitoylcarnitine (C16)-MS400.34	0.0808	0.1678	0.1256	4.43E-01
palmitoyl-arachidonoyl-glycerol (16:0/20:4) [2]*-MS634.54	0.5396	0.9182	0.1485	3.63E-01
palmitoyl-arachidonoyl-glycerol (16:0/20:4) [1]*-MS634.54	3.005	8.569	0.0296	8.57E-01
palmitoyl sphingomyelin (d18:1/16:0)-MS703.57	0.0447	0.0563	-0.0779	6.35E-01
palmitoyl ethanolamide-MS298.27	0.1280	0.2073	0.0541	7.42E-01
palmitoyl dihydrosphingomyelin (d18:0/16:0)*-MS705.59	0.0719	0.0739	0.0931	5.70E-01
palmitoleoyl-linoleoyl-glycerol (16:1/18:2) [1]*-MS608.52	0.1476	0.2988	0.3214	4.27E-02
palmitoleoylcarnitine (C16:1)*-MS398.32	0.0946	0.3418	0.0074	9.64E-01
palmitoleoyl-arachidonoyl-glycerol (16:1/20:4) [2]*-MS632.52	0.2124	0.5467	0.0736	6.54E-01
palmitoleate (16:1n7)-MS253.21	0.1978	6.979	0.2774	8.32E-02
palmitate (16:0)-MS255.23	0.1317	0.3845	0.1936	2.33E-01

oxalate (ethanedioate)-MS88.988	0.0462	0.1824	0.0930	5.70E-01
O-sulfo-L-tyrosine-MS260.02	0.2186	0.1533	-0.8467	3.77E-14
orotidine-MS287.05	0.1114	0.1922	-0.5013	8.02E-04
orotate-MS155.00	0.1329	0.1832	-0.2752	8.58E-02
ornithine-MS133.09	0.0425	0.1025	-0.1116	4.95E-01
O-methylcatechol sulfate-MS203.00	0.1866	0.7519	-0.6132	1.40E-05
oleoyl-oleoyl-glycerol (18:1/18:1) [2]*-MS638.57	0.2253	0.2888	0.1096	5.03E-01
oleoyl-oleoyl-glycerol (18:1/18:1) [1]*-MS638.57	0.1708	0.2409	0.2672	9.58E-02
oleoyl-linoleoyl-glycerol (18:1/18:2) [2]-MS636.55	0.0854	0.2507	0.1698	2.97E-01
oleoyl-linoleoyl-glycerol (18:1/18:2) [1]-MS636.55	0.1281	0.2277	0.0206	9.00E-01
oleoylcholine-MS368.35	0.2602	1.288	0.1773	2.76E-01
oleoylcarnitine (C18:1)-MS426.35	0.0940	0.2638	0.0458	7.80E-01
oleoyl-arachidonoyl-glycerol (18:1/20:4) [2]*-MS660.55	0.1146	0.2927	-0.1169	4.75E-01
oleoyl-arachidonoyl-glycerol (18:1/20:4) [1]*-MS660.55	0.1804	0.2704	-0.0881	5.91E-01
oleoyl ethanolamide-MS326.30	0.0821	0.2833	-0.0614	7.08E-01
oleate/vaccenate (18:1)-MS281.24	0.1720	0.9279	0.1789	2.71E-01
octanoylcarnitine (C8)-MS288.21	0.0928	0.4872	-0.2572	1.10E-01
octadecanedioate-MS313.23	0.0722	0.3298	-0.0802	6.25E-01
o-cresol sulfate-MS187.00	0.2370	0.7291	-0.4719	1.82E-03
O-acetylhomoserine-MS160.06	0.2350	0.3440	-0.7325	1.33E-08
N-stearoyltaurine-MS390.26	0.9129	0.6395	0.1987	2.21E-01
N-stearoyl-sphingosine (d18:1/18:0)*-MS566.55	0.2582	0.1622	0.0236	8.86E-01
N-palmitoyltaurine-MS362.23	0.3746	0.5486	0.0605	7.13E-01
N-palmitoyl-sphingosine (d18:1/16:0)-MS538.51	0.2027	0.1604	0.0009	9.96E-01
N-palmitoyl-sphinganine (d18:0/16:0)-MS540.53	0.0650	0.1894	0.0150	9.27E-01
N-palmitoylglycine-MS312.25	0.1601	0.2852	-0.0065	9.68E-01
nonadecanoate (19:0)-MS297.27	0.1908	0.3083	0.0444	7.87E-01
N-oleoyltaurine-MS388.25	2.688	2.248	-0.0669	6.84E-01
N-methyltaurine-MS138.02	0.0986	1.838	-0.5265	3.70E-04
N-methylproline-MS130.08	0.0712	1.432	-0.1748	2.83E-01
N-methylpipecolate-MS144.10	0.2354	0.3878	-0.4746	1.70E-03
N-linoleoylglycine-MS336.25	0.2742	0.4126	-0.1913	2.39E-01
nicotinamide-MS123.05	0.1046	0.3655	-0.0149	9.28E-01
nicotinamide riboside-MS255.09	0.1598	0.2244	-0.3767	1.60E-02
N-formylphenylalanine-MS192.06	0.1336	0.2418	0.0968	5.55E-01
N-formylmethionine-MS176.03	0.1670	0.0910	-0.8576	5.55E-15
nervonoylcarnitine (C24:1)*-MS510.45	0.1112	0.1733	0.1256	4.42E-01
N-delta-acetylornithine-MS173.09	0.0940	0.1987	-0.3665	1.94E-02
N-behenoyl-sphingadienine (d18:2/22:0)*-MS620.59	0.2024	0.1478	-0.0786	6.32E-01
N-alpha-acetylornithine-MS175.10	0.1669	0.3772	-0.3683	1.87E-02
N-acetylvaline-MS158.08	0.1269	0.1069	-0.8822	0.00E+00
N-acetyltyrosine-MS222.07	0.2786	0.1818	-0.4486	3.31E-03
N-acetyltryptophan-MS245.09	0.1320	0.1781	-0.5509	1.64E-04
N-acetylthreonine-MS160.06	0.1983	0.1384	-0.8196	2.08E-12
N-acetyltaurine-MS166.01	0.1902	0.1481	-0.7297	1.65E-08
N-acetylserine-MS146.04	0.0765	0.0848	-0.8408	9.79E-14
N-acetyl-S-allyl-L-cysteine-MS202.05	0.2687	7.221	-0.0695	6.72E-01
N-acetylputrescine-MS131.11	0.0703	0.1121	-0.6842	3.56E-07
N-acetylphenylalanine-MS206.08	0.1606	0.1774	-0.6442	3.24E-06
N-acetylneuraminate-MS310.11	0.0793	0.2123	-0.8265	8.15E-13
N-acetylmethionine-MS190.05	0.1369	0.1419	-0.7701	5.38E-10
N-acetylleucine-MS172.09	0.1386	0.1403	-0.5017	7.93E-04

N-acetylkynurenine (2)-MS251.10	0.1046	0.3013	-0.4675	2.05E-03
N-acetylisoleucine-MS172.09	0.1256	0.1329	-0.7374	9.10E-09
N-acetylhistidine-MS196.07	0.1768	0.1590	-0.7786	2.34E-10
N-acetylglycine-MS116.03	0.1089	0.1548	-0.4059	8.80E-03
N-acetylglutamine-MS187.07	0.2506	0.1654	-0.6738	6.58E-07
N-acetylglutamate-MS190.07	0.1107	0.2221	-0.4669	2.08E-03
N-acetylglucosaminylasparagine -MS336.14	0.1623	0.2359	-0.7335	1.23E-08
N-acetylglucosamine/N-acetylgalactosamine-MS222.09	0.1214	0.1155	-0.5563	1.35E-04
N-acetylcitrulline-MS216.09	0.5305	0.4060	-0.3163	4.63E-02
N-acetylcarnosine-MS267.10	0.1991	0.2512	-0.4912	1.07E-03
N-acetyl-cadaverine-MS145.13	0.0712	0.6961	-0.1351	4.08E-01
N-acetyl-beta-alanine-MS130.05	0.2248	0.1590	-0.7016	1.19E-07
N-acetyl-aspartyl-glutamate (NAAG)-MS305.09	0.1443	0.2157	-0.6304	6.38E-06
N-acetylaspartate (NAA)-MS174.04	0.1044	0.1224	-0.4038	9.19E-03
N-acetylarginine-MS217.12	0.0597	0.1612	-0.4849	1.28E-03
N-acetylalliin-MS218.04	0.5569	4.849	-0.4477	3.38E-03
N-acetylalanine-MS130.05	0.1219	0.0848	-0.8574	5.77E-15
N-acetyl-3-methylhistidine*-MS210.08	0.0788	1.039	-0.6678	9.23E-07
N-acetyl-1-methylhistidine*-MS212.10	0.0396	0.2401	-0.6177	1.15E-05
N6-succinyladenosine-MS382.10	0.2528	0.2063	-0.7704	5.21E-10
N6-carboxymethyllysine-MS205.11	0.0830	0.2076	-0.6435	3.35E-06
N6-carbamoylthreonyladenosine-MS411.12	0.2603	0.1410	-0.8338	2.82E-13
N6-acetyllysine-MS187.10	0.1468	0.1570	-0.6800	4.56E-07
N6,N6,N6-trimethyllysine-MS189.15	0.0738	0.2304	-0.7325	1.33E-08
N4-acetylcytidine-MS284.08	0.2217	0.1781	-0.7090	7.27E-08
N2-methylguanosine-MS296.10	0.4042	0.4707	-0.0672	6.82E-01
N2-acetyllysine-MS187.10	0.3033	0.2901	-0.4534	2.93E-03
N2,N5-diacetylornithine-MS215.10	0.2314	0.2304	-0.6863	3.13E-07
N2,N2-dimethylguanosine-MS312.13	0.0612	0.1101	-0.8185	2.42E-12
N1-methylinosine-MS283.10	0.0714	0.1090	-0.8577	5.55E-15
N1-methyladenosine-MS282.11	0.1297	0.1154	-0.6698	8.23E-07
N1-Methyl-4-pyridone-3-carboxamide-MS153.06	0.0781	0.2232	-0.6017	2.31E-05
N1-Methyl-2-pyridone-5-carboxamide-MS153.06	0.1014	0.2495	-0.5217	4.32E-04
N1,N12-diacetylspermine-MS287.24	0.1061	0.2615	-0.2774	8.31E-02
N-(2-furoyl)glycine-MS168.03	0.1907	2.522	-0.3509	2.58E-02
myristoyl-linoleoyl-glycerol (14:0/18:2) [1]*-MS582.50	0.1724	0.4327	0.3238	4.11E-02
myristoylcarnitine (C14)-MS372.31	0.1281	0.2400	-0.0555	7.35E-01
myristoyl dihydrosphingomyelin (d18:0/14:0)*-MS677.55	0.0845	0.0968	0.2843	7.53E-02
myristoleoylcarnitine (C14:1)*-MS370.29	0.1160	0.5563	-0.2067	2.02E-01
myristoleate (14:1n5)-MS225.18	0.1738	47.22	0.3014	5.85E-02
myristate (14:0)-MS227.20	0.1432	0.9323	0.2162	1.82E-01
myo-inositol-MS225.06	0.7351	0.4043	-0.6051	2.00E-05
metoprolol acid metabolite*-MS268.15	0.0273	0.0406	-0.1354	4.07E-01
methylsuccinate-MS131.03	1.855	0.7957	-0.3455	2.84E-02
methylmalonate (MMA)-MS117.01	22.64	32.32	-0.5109	6.03E-04
methyl-4-hydroxybenzoate sulfate-MS230.99	0.3150	6.552	0.1008	5.38E-01
methyl indole-3-acetate-MS190.08	0.1263	0.3142	-0.7266	2.08E-08
methyl glucopyranoside (alpha + beta)-MS193.07	0.2552	0.5523	-0.1733	2.87E-01
methionine-MS150.05	0.0692	0.1291	-0.1653	3.10E-01
methionine sulfoxide-MS166.05	0.1072	0.2309	-0.2716	9.01E-02
methionine sulfone-MS182.04	0.0537	0.1213	-0.4294	5.22E-03

margaroylcarnitine*-MS414.35	0.1046	0.1879	0.1458	3.72E-01
margarate (17:0)-MS269.24	0.2277	0.6616	0.1902	2.42E-01
mannose-MS225.06	0.1196	0.1645	0.0609	7.11E-01
mannitol/sorbitol-MS181.07	0.0904	0.7308	-0.2505	1.20E-01
maltotriose-MS549.16	0.2899	0.5664	-0.0419	7.99E-01
maltose-MS387.11	0.3359	2.414	-0.5229	4.16E-04
malonylcarnitine-MS248.11	0.1271	0.1504	-0.7570	1.78E-09
maleate-MS115.00	0.0807	0.3941	-0.3558	2.36E-02
malate-MS133.01	0.0495	0.1630	-0.2475	1.24E-01
lysine-MS147.11	0.0535	0.1008	0.1926	2.35E-01
L-urobilin-MS595.34	0.1039	2.710	-0.3216	4.26E-02
linoleoyl-linoleoyl-glycerol (18:2/18:2) [1]*-MS634.54	0.0900	0.2944	0.0210	8.98E-01
linoleoyl-linolenoyl-glycerol (18:2/18:3) [1]*-MS632.52	0.1568	0.3244	0.0057	9.73E-01
linoleoyl-docosahexaenoyl-glycerol (18:2/22:6) [2]*-MS682.54	0.1716	0.2888	0.0770	6.39E-01
linoleoyl-docosahexaenoyl-glycerol (18:2/22:6) [1]*-MS682.54	0.1256	0.3066	0.1194	4.65E-01
linoleoylcholine*-MS366.33	0.2434	5.687	0.2036	2.09E-01
linoleoylcarnitine (C18:2)*-MS424.34	0.0895	0.2375	-0.0786	6.32E-01
linoleoyl-arachidonoyl-glycerol (18:2/20:4) [2]*-MS658.54	0.1922	0.3169	-0.0316	8.47E-01
linoleoyl-arachidonoyl-glycerol (18:2/20:4) [1]*-MS658.54	0.1494	0.2650	-0.0668	6.84E-01
linoleoyl ethanolamide-MS322.27	0.3045	0.3813	-0.1176	4.72E-01
linolenoylcarnitine (C18:3)*-MS422.32	0.1577	0.3278	-0.1595	3.28E-01
linolenate [alpha or gamma; (18:3n3 or 6)]-MS277.21	0.3348	4.367	0.1542	3.44E-01
linoleate (18:2n6)-MS279.23	0.1766	0.9734	0.1232	4.51E-01
lignoceroylcarnitine (C24)*-MS512.46	0.0831	0.2127	0.0291	8.60E-01
lignoceroyl sphingomyelin (d18:1/24:0)-MS815.70	0.0963	0.1011	0.0301	8.55E-01
levulinate (4-oxovalerate)-MS115.04	1.638	0.5133	-0.0520	7.52E-01
leucylglycine-MS187.10	0.1870	0.1867	-0.2667	9.64E-02
leucine-MS132.10	0.0606	0.1178	0.1123	4.93E-01
laurylcarnitine (C12)-MS344.27	0.1048	0.4831	-0.2557	1.12E-01
laurate (12:0)-MS199.17	0.1661	0.7938	0.0895	5.85E-01
lanthionine-MS209.05	0.1579	0.2977	-0.6925	2.14E-07
lactosyl-N-palmitoyl-sphingosine (d18:1/16:0)-MS862.62	0.0567	0.0741	-0.0472	7.74E-01
lactosyl-N-nervonoyl-sphingosine (d18:1/24:1)*-MS972.73	0.1396	0.1143	-0.1305	4.25E-01
lactate-MS89.024	0.0797	0.2248	-0.0048	9.77E-01
kynurenine-MS209.09	0.1348	0.1596	-0.2487	1.22E-01
kynurenate-MS188.03	0.2494	0.1969	-0.7063	8.70E-08
I-urobilinogen-MS591.31	0.2393	0.9379	-0.0676	6.80E-01
isovalerylglycine-MS158.08	0.1122	0.3326	-0.5109	6.03E-04
isovalerylcarnitine (C5)-MS246.16	0.0728	0.2494	-0.0692	6.73E-01
isovalerate-MS101.06	0.3292	0.4599	0.0684	6.77E-01
isoursodeoxycholate-MS391.28	0.3786	0.6249	0.2184	1.77E-01
isoleucylglycine-MS187.10	0.6367	0.5546	-0.1238	4.49E-01
isoleucine-MS132.10	0.0479	0.1088	0.0317	8.47E-01
isoeugenol sulfate-MS243.03	0.0917	1.021	-0.0367	8.23E-01
isocitrate-MS191.01	2.217	1.718	-0.4268	5.54E-03

isobutyrylglycine-MS144.06	0.2052	0.2604	-0.5098	6.23E-04
isobutyrylcarnitine (C4)-MS232.15	0.0877	0.3051	-0.5760	6.52E-05
inosine-MS267.07	0.1925	0.4104	-0.0977	5.51E-01
indolin-2-one-MS134.06	0.2358	0.4590	-0.5281	3.52E-04
indolepropionylglycine-MS245.09	0.3499	0.5183	-0.2864	7.31E-02
indolepropionate-MS190.08	0.0563	0.3623	0.0240	8.84E-01
indolelactate-MS206.08	0.1238	0.2417	-0.3787	1.53E-02
indolebutyrate-MS202.08	0.2676	0.5934	-0.2968	6.27E-02
indoleacetylglutamine-MS302.11	0.3384	0.5873	-0.7300	1.61E-08
indoleacetate-MS176.07	0.0285	0.2562	-0.4562	2.74E-03
indole-3-carboxylic acid-MS160.04	0.1265	0.2145	-0.3695	1.83E-02
iminodiacetate (IDA)-MS134.04	0.0632	0.1402	0.1750	2.82E-01
imidazole propionate-MS141.06	0.0837	0.2754	-0.5293	3.39E-04
imidazole lactate-MS157.06	0.0892	0.1287	-0.4068	8.64E-03
hypoxanthine-MS135.03	0.1183	0.4082	0.1495	3.60E-01
hypotaurine-MS110.02	0.1381	0.2127	-0.4492	3.26E-03
hyocholate-MS407.28	0.2424	0.4395	0.0189	9.08E-01
hydroquinone sulfate-MS188.98	0.3977	0.4713	-0.6333	5.54E-06
hydantoin-5-propionic acid-MS171.04	0.0896	0.3590	-0.7273	1.97E-08
homovanillate sulfate-MS261.00	0.4604	3.408	-0.6936	2.00E-07
homovanillate (HVA)-MS181.05	0.1869	0.3391	-0.6843	3.54E-07
homostachydrine*-MS158.11	0.2298	0.2913	-0.3861	1.33E-02
homocitrulline-MS190.11	0.3220	0.4738	-0.7661	7.81E-10
homoarginine-MS189.13	0.0627	0.1569	0.1703	2.96E-01
histidine-MS154.06	0.0774	0.0816	0.1692	2.99E-01
hippurate-MS178.05	0.1177	1.145	-0.5444	2.05E-04
hexanoylglycine-MS172.09	0.2800	0.4868	-0.2963	6.31E-02
hexanoylglutamine-MS243.13	0.2040	0.5510	-0.5835	4.86E-05
hexanoylcarnitine (C6)-MS260.18	0.0735	0.3910	-0.1626	3.18E-01
hexadecanedioate-MS285.20	0.0766	0.3395	-0.1391	3.94E-01
heptanoate (7:0)-MS129.09	0.2125	0.2081	0.0359	8.27E-01
heme-MS632.17	0.9739	2.201	-0.1109	4.98E-01
gulonate*-MS195.05	0.4446	0.4672	-0.7773	2.66E-10
guanidinosuccinate-MS174.05	0.5312	0.6872	-0.5771	6.25E-05
guanidinoacetate-MS118.06	0.2487	0.3026	0.0645	6.95E-01
glycoursodeoxycholate-MS448.30	0.0971	152.4	0.1927	2.35E-01
glycosyl-N-stearoyl-sphingosine (d18:1/18:0)-MS728.60	0.2704	0.1584	-0.0166	9.20E-01
glycosyl-N-palmitoyl-sphingosine (d18:1/16:0)-MS700.57	0.1480	0.1281	-0.0537	7.44E-01
glycosyl-N-nervonoyl-sphingosine (d18:1/24:1)*-MS810.68	0.7482	0.2628	-0.2530	1.16E-01
glycosyl-N-behenoyl-sphingadienine (d18:2/22:0)*-MS782.65	0.6707	0.2344	-0.2144	1.85E-01
glycosyl ceramide (d18:2/24:1, d18:1/24:2)*-MS808.66	0.6195	0.2463	-0.2494	1.21E-01
glycolithocholate-MS432.31	0.1117	1.638	-0.0906	5.80E-01
glycolithocholate sulfate*-MS255.63	0.1475	0.5978	-0.2622	1.02E-01
glycohyocholate-MS464.30	0.3544	1.818	-0.3630	2.07E-02
glycodeoxycholate-MS448.30	0.2499	3.204	-0.1823	2.62E-01
glycodeoxycholate sulfate-MS263.62	0.1911	0.5300	-0.3637	2.04E-02
glycodeoxycholate glucuronide (1)-MS624.33	0.1489	0.3803	-0.1787	2.72E-01
glycocholenate sulfate*-MS254.62	0.2189	0.1818	0.0823	6.16E-01
glycocholate-MS464.30	0.0990	1.682	-0.2944	6.50E-02

glycocholate glucuronide (1)-MS640.33	0.4036	0.5231	-0.1273	4.36E-01
glycochenodeoxycholate-MS448.30	0.1473	4.990	-0.1681	3.02E-01
glycochenodeoxycholate sulfate-MS263.62	0.1505	0.5451	-0.3704	1.80E-02
glycochenodeoxycholate glucuronide (1)-MS311.66	0.1271	0.3475	-0.2842	7.55E-02
glycine-MS76.039	0.0543	0.1150	-0.2307	1.53E-01
glycerophosphorylcholine (GPC)-MS258.11	0.0733	0.2405	0.2383	1.39E-01
glycerophosphoinositol*-MS333.05	0.4771	0.4189	-0.0728	6.57E-01
glycerophosphoglycerol-MS245.04	0.8775	0.6398	-0.4660	2.13E-03
glycerophosphoethanolamine-MS216.06	0.0622	0.1727	0.1295	4.28E-01
glycerol-MS91.040	0.1532	0.3579	0.1984	2.21E-01
glycerol 3-phosphate-MS173.02	0.0987	0.2481	-0.0909	5.79E-01
glycerate-MS105.01	0.1138	0.1558	0.1782	2.73E-01
glutarylcarnitine (C5-DC)-MS276.14	0.0744	0.1099	-0.7600	1.36E-09
glutarate (pentanedioate)-MS131.03	0.9897	0.8893	-0.4303	5.12E-03
glutamine-MS147.07	0.0619	0.0678	0.0098	9.52E-01
glutamate-MS148.06	0.0578	0.1510	0.1025	5.32E-01
glutamate, gamma-methyl ester-MS162.07	0.0809	0.1554	0.3028	5.73E-02
glucuronate-MS193.03	1.023	2.627	-0.5365	2.67E-04
glucose-MS225.06	0.0758	0.1283	-0.1461	3.71E-01
gluconate-MS195.05	0.2489	0.5229	-0.7796	2.12E-10
gentisic acid-5-glucoside-MS315.07	0.1311	0.7003	-0.5663	9.42E-05
gentisate-MS153.01	0.1741	0.6159	-0.5180	4.85E-04
gamma-tocopherol/beta-tocopherol-MS416.36	0.1222	0.1193	-0.0983	5.48E-01
gamma-glutamylvaline-MS247.12	0.0689	0.1378	-0.2481	1.23E-01
gamma-glutamyltyrosine-MS311.12	0.3035	0.2398	-0.2562	1.11E-01
gamma-glutamyltryptophan-MS334.13	0.1596	0.1928	-0.3988	1.02E-02
gamma-glutamylthreonine-MS249.10	0.0591	0.1217	-0.4005	9.85E-03
gamma-glutamylphenylalanine-MS293.11	0.1084	0.1531	-0.7315	1.43E-08
gamma-glutamylmethionine-MS279.10	0.0963	0.1857	-0.1072	5.13E-01
gamma-glutamylleucine-MS261.14	0.0686	0.1673	-0.3594	2.21E-02
gamma-glutamylisoleucine*-MS261.14	0.0562	0.1326	-0.5793	5.74E-05
gamma-glutamylhistidine-MS285.11	0.0967	0.1277	-0.5845	4.68E-05
gamma-glutamylglycine-MS205.08	0.0992	0.1466	-0.4623	2.34E-03
gamma-glutamylglutamine-MS276.11	0.0693	0.1120	0.2075	2.00E-01
gamma-glutamylglutamate-MS277.10	0.2224	0.2502	0.0242	8.83E-01
gamma-glutamyl-epsilon-lysine-MS276.15	0.4059	0.2458	-0.3060	5.45E-02
gamma-glutamyl-alpha-lysine-MS276.15	0.0667	0.1330	-0.1100	5.02E-01
gamma-glutamylalanine-MS219.09	0.2196	0.2834	-0.2113	1.92E-01
gamma-glutamyl-2-aminobutyrate-MS233.11	0.5466	0.8107	-0.1015	5.36E-01
gamma-CEHC-MS263.12	0.1625	0.2815	-0.3659	1.96E-02
gamma-CEHC glucuronide*-MS439.16	0.4658	0.3512	-0.7223	2.86E-08
gamma-carboxyglutamate-MS192.05	0.1866	0.2106	-0.6799	4.60E-07
galactonate-MS195.05	5.715	23.72	-0.3030	5.70E-02
furosemide-MS329.00	0.1495	0.7121	-0.3092	5.18E-02
fumarate-MS115.00	3.302	1.674	-0.0618	7.07E-01
fructose-MS225.06	0.4113	0.4183	-0.2846	7.50E-02
flavin mononucleotide (FMN)-MS455.09	0.4823	0.2682	-0.2576	1.09E-01
flavin adenine dinucleotide (FAD)-MS784.14	0.5756	0.2810	0.2761	8.47E-02
ferulic acid 4-sulfate-MS273.00	0.2858	1.728	-0.4193	6.57E-03
eugenol sulfate-MS243.03	0.4242	1.842	-0.2882	7.12E-02
etiocholanolone glucuronide-MS465.24	0.2100	0.2407	-0.5340	2.90E-04
ethylmalonate-MS131.03	0.0554	0.1914	-0.6264	7.69E-06
ethyl glucuronide-MS221.06	0.6537	650.5	-0.2161	1.82E-01

erythronate*-MS135.02	0.0900	0.1087	-0.8357	2.14E-13
erythritol-MS167.05	0.0981	0.1948	-0.8064	1.11E-11
erucoylcarnitine (C22:1)*-MS482.42	0.2073	0.4894	-0.1678	3.03E-01
erucate (22:1n9)-MS337.31	0.1272	0.4788	0.0402	8.07E-01
ergothioneine-MS230.09	0.0732	0.1582	0.0740	6.52E-01
epiandrosterone sulfate-MS369.17	0.1195	0.1651	-0.2167	1.80E-01
eicosenoylcarnitine (C20:1)*-MS454.38	0.0813	0.2281	-0.0740	6.52E-01
eicosenoate (20:1)-MS309.27	0.2492	1.123	0.0603	7.13E-01
eicosapentaenoate (EPA; 20:5n3)-MS301.21	0.4771	0.7372	0.2924	6.70E-02
eicosanodioate-MS341.26	0.1024	0.3316	0.0576	7.26E-01
EDTA-MS291.08	0.0766	0.1218	0.3948	1.11E-02
ectoine-MS143.08	0.1405	1.207	-0.6127	1.44E-05
dopamine 4-sulfate-MS232.02	0.4596	0.5768	-0.2696	9.26E-02
dopamine 3-O-sulfate-MS232.02	0.0810	0.5048	-0.0606	7.12E-01
dodecanedioate-MS229.14	0.1519	0.5090	-0.3624	2.09E-02
docosatrienoate (22:3n3)-MS333.27	0.5267	0.7662	0.3233	4.14E-02
docosapentaenoylcarnitine (C22:5n3)*-MS474.35	0.1295	0.2666	0.1847	2.56E-01
docosapentaenoate (n6 DPA; 22:5n6)-MS329.24	0.2383	0.4242	0.0464	7.77E-01
docosapentaenoate (n3 DPA; 22:5n3)-MS329.24	0.3321	0.8956	0.2026	2.11E-01
docosahexaenoylcholine-MS414.33	0.2478	0.7845	0.2512	1.18E-01
docosahexaenoylcarnitine (C22:6)*-MS472.34	0.1309	0.5043	0.2204	1.73E-01
docosahexaenoate (DHA; 22:6n3)-MS327.23	0.2484	0.4679	0.2643	9.96E-02
docosadioate-MS369.30	0.2445	0.4777	0.1098	5.03E-01
docosadienoate (22:2n6)-MS335.29	0.1744	0.4768	0.0143	9.31E-01
dimethylglycine-MS104.07	0.0511	0.1066	-0.6231	8.95E-06
dimethylarginine (SDMA + ADMA)-MS203.15	0.0737	0.0818	-0.7274	1.96E-08
dimethyl sulfone-MS95.016	0.1409	0.4044	-0.5846	4.66E-05
dihydroorotate-MS157.02	0.1189	0.3092	-0.3921	1.17E-02
dihydroferulic acid-MS195.06	0.1969	0.6799	-0.2976	6.20E-02
dihomo-linoleoylcarnitine (C20:2)*-MS452.37	0.1072	0.2138	-0.0556	7.35E-01
dihomo-linolenoyl-choline-MS392.35	0.2718	0.8010	0.2451	1.28E-01
dihomo-linolenoylcarnitine (20:3n3 or 6)*-MS450.35	0.0954	0.2277	0.1747	2.83E-01
dihomo-linolenate (20:3n3 or n6)-MS305.24	0.2214	0.4301	0.3744	1.67E-02
dihomo-linoleate (20:2n6)-MS307.26	0.2942	0.9833	0.1385	3.96E-01
diacylglycerol (16:1/18:2 [2], 16:0/18:3 [1])*-MS608.52	0.1828	0.2836	0.2961	6.34E-02
diacylglycerol (14:0/18:1, 16:0/16:1) [2]*-MS584.52	0.1831	0.3906	0.2948	6.46E-02
diacylglycerol (14:0/18:1, 16:0/16:1) [1]*-MS584.52	0.1607	0.3633	0.2757	8.52E-02
diacylglycerol (12:0/18:1, 14:0/16:1, 16:0/14:1) [2]*-MS556.49	0.1911	1.494	0.2884	7.10E-02
deoxycholate-MS391.28	0.1264	0.7614	0.0143	9.31E-01
deoxycarnitine-MS146.11	0.0654	0.0919	-0.5142	5.46E-04
dehydroisoandrosterone sulfate (DHEA-S)-MS367.15	0.0803	0.1929	-0.0007	9.97E-01
decanoylcarnitine (C10)-MS316.24	0.2434	0.5966	-0.2477	1.24E-01
cytosine-MS112.05	0.1523	0.5649	-0.3076	5.32E-02
cytidine-MS244.09	0.2174	0.2919	-0.6319	5.91E-06
cystine-MS241.03	0.0621	0.1457	-0.4723	1.80E-03
cysteinylglycine-MS179.04	0.2550	0.4472	-0.0924	5.73E-01
cysteine-MS122.02	0.1562	0.0997	-0.3767	1.60E-02
cysteine-glutathione disulfide-MS427.09	0.0933	0.3059	-0.0936	5.68E-01
cysteine sulfinic acid-MS154.01	0.1598	0.2038	-0.3010	5.88E-02
cysteine s-sulfate-MS199.96	0.1188	0.2630	0.0801	6.25E-01
cystathionine-MS223.07	0.3165	0.3860	-0.7201	3.35E-08

cys-gly, oxidized-MS355.07	0.0612	0.1433	0.0732	6.55E-01
creatinine-MS114.06	0.0374	0.0597	-0.8508	1.89E-14
creatine-MS132.07	0.0367	0.1346	0.4449	3.62E-03
cortisone-MS359.18	0.1419	0.2629	0.0578	7.25E-01
cortisol-MS361.20	0.0899	0.2626	-0.3935	1.14E-02
corticosterone-MS345.20	0.1896	0.5838	-0.0759	6.44E-01
citrulline-MS176.10	0.0601	0.0807	-0.5921	3.45E-05
citrate-MS191.01	0.0443	0.0733	-0.1742	2.84E-01
citraconate/glutaconate-MS129.01	0.0933	0.4739	-0.2668	9.63E-02
cis-urocanate-MS137.03	0.3011	0.5906	-0.1259	4.42E-01
cis-4-decenoylcarnitine (C10:1)-MS314.23	0.0839	0.4124	-0.3857	1.34E-02
cinnamoylglycine-MS204.06	0.3816	1.086	-0.4220	6.18E-03
choline-MS104.10	0.0589	0.1140	-0.7349	1.11E-08
choline phosphate-MS184.07	0.0671	0.1481	-0.1187	4.68E-01
cholesterol-MS369.35	0.1960	0.2180	0.0494	7.64E-01
cholate-MS407.28	0.5350	2.098	0.0917	5.76E-01
chiro-inositol-MS225.06	0.1990	4.821	-0.4865	1.23E-03
chenodeoxycholate-MS391.28	0.3033	0.6966	0.2199	1.74E-01
C-glycosyltryptophan-MS367.14	0.1253	0.1456	-0.7993	2.53E-11
cerotoylcarnitine (C26)*-MS540.49	0.0686	0.1346	0.0871	5.95E-01
ceramide (d18:2/24:1, d18:1/24:2)*-MS646.61	0.2020	0.1448	-0.1289	4.30E-01
ceramide (d18:1/20:0, d16:1/22:0, d20:1/18:0)*-MS594.58	0.2427	0.1221	-0.0956	5.60E-01
ceramide (d18:1/17:0, d17:1/18:0)*-MS552.53	0.1218	0.1567	0.0219	8.94E-01
ceramide (d18:1/14:0, d16:1/16:0)*-MS510.48	0.0866	0.1257	0.1644	3.13E-01
ceramide (d16:1/24:1, d18:1/22:1)*-MS620.59	0.3075	0.3894	-0.0560	7.33E-01
catechol sulfate-MS188.98	0.1787	0.5315	-0.3967	1.07E-02
catechol glucuronide-MS285.06	0.1597	0.6959	-0.3671	1.92E-02
carnitine-MS162.11	0.0406	0.0665	0.2925	6.68E-02
carboxyethyl-GABA-MS176.09	0.1027	0.1710	-0.7390	8.04E-09
caprylate (8:0)-MS143.10	0.2107	0.5705	0.1426	3.82E-01
caproate (6:0)-MS115.07	0.5512	0.3247	0.3054	5.50E-02
caprate (10:0)-MS171.13	0.0601	0.6584	0.1837	2.58E-01
campesterol-MS383.36	0.1778	0.2250	-0.3112	5.03E-02
caffeine-MS195.08	0.1092	2.740	-0.0333	8.39E-01
caffeic acid sulfate-MS258.99	1646	70.76	-0.3557	2.37E-02
butyrylcarnitine (C4)-MS232.15	0.0831	0.1704	0.0072	9.65E-01
biliverdin-MS583.25	0.1725	0.3583	0.2496	1.21E-01
bilirubin (Z,Z)-MS585.27	0.1212	0.1383	0.2961	6.34E-02
bilirubin (E,Z or Z,E)*-MS585.27	0.4497	0.4392	0.3194	4.41E-02
bilirubin (E,E)*-MS585.27	0.7662	0.4101	0.4386	4.21E-03
betonicine-MS160.09	0.0401	15.61	-0.1859	2.53E-01
beta-sitosterol-MS397.38	0.1940	0.3680	-0.1607	3.24E-01
betaine-MS118.08	0.0438	0.0903	-0.2120	1.90E-01
beta-hydroxyisovalerate-MS117.05	0.1384	0.1983	-0.3976	1.05E-02
beta-guanidinopropanoate-MS132.07	0.1847	0.5228	0.0752	6.47E-01
beta-cryptoxanthin-MS552.43	0.0873	0.2165	-0.0609	7.11E-01
beta-citrylglutamate-MS320.06	0.0937	0.1254	-0.2633	1.01E-01
beta-alanine-MS90.054	0.1320	0.2334	-0.1812	2.65E-01
benzoylcarnitine*-MS266.13	0.1999	0.4596	-0.6423	3.55E-06
benzoate-MS121.02	0.3302	0.2610	-0.2334	1.48E-01
behenoylcarnitine (C22)*-MS484.43	0.1248	0.2760	-0.0006	9.97E-01
behenoyl sphingomyelin (d18:1/22:0)*-MS787.66	0.0720	0.0863	0.1680	3.02E-01

behenoyl dihydrosphingomyelin (d18:0/22:0)*-MS789.68	0.1439	0.1582	0.2863	7.32E-02
behenate (22:0)*-MS339.32	1847	43258	-0.0491	7.65E-01
azelate (nonanedioate)-MS187.09	0.1571	1.012	-0.4579	2.62E-03
aspartate-MS134.04	0.0470	0.1737	0.0978	5.51E-01
asparagine-MS133.06	0.0450	0.1017	-0.1301	4.26E-01
arginine-MS175.11	0.0390	0.0996	-0.1537	3.46E-01
argininate*-MS176.10	0.0587	0.1810	-0.4209	6.34E-03
arachidoylcarnitine (C20)*-MS456.40	0.1517	0.2813	-0.1673	3.04E-01
arachidonoylcholine-MS390.33	0.2635	1.991	0.1834	2.59E-01
arachidonoylcarnitine (C20:4)-MS448.34	0.0995	0.2386	0.0365	8.24E-01
arachidonoyl ethanolamide-MS348.28	0.1201	0.3065	0.0251	8.79E-01
arachidonate (20:4n6)-MS303.23	0.2122	0.3110	0.1527	3.49E-01
arachidate (20:0)-MS311.29	0.1024	0.2050	-0.0139	9.33E-01
arabonate/xylonate-MS165.04	0.1547	0.2335	-0.8156	3.53E-12
arabitol/xylitol-MS151.06	0.0844	0.1703	-0.8354	2.24E-13
arabinose-MS195.05	0.5499	0.7529	-0.4169	6.93E-03
anserine-MS241.12	0.1317	16.22	-0.1650	3.11E-01
androsterone sulfate-MS369.17	0.1754	0.1845	-0.1777	2.75E-01
androstenediol (3beta,17beta) monosulfate (2)-MS369.17	0.1230	0.1985	-0.0485	7.68E-01
androstenediol (3beta,17beta) monosulfate (1)-MS369.17	0.0790	0.1920	0.0346	8.33E-01
androstenediol (3beta,17beta) disulfate (2)-MS224.06	0.1431	0.1917	-0.1613	3.22E-01
androstenediol (3beta,17beta) disulfate (1)-MS224.06	0.1675	0.1657	-0.1080	5.09E-01
androstenediol (3alpha, 17alpha) monsulfate (3)-MS369.17	0.0861	0.1608	-0.1841	2.57E-01
androstenediol (3alpha, 17alpha) monsulfate (2)-MS369.17	0.1399	0.3015	0.0417	7.99E-01
andro steroid monosulfate (1)*-MS383.15	0.1557	0.3112	-0.0813	6.20E-01
alpha-tocopherol-MS430.37	0.0681	0.0781	0.1010	5.38E-01
alpha-ketoglutarate-MS145.01	0.3893	1.033	-0.2758	8.51E-02
alpha-ketobutyrate-MS101.02	0.5787	0.6029	-0.0325	8.43E-01
alpha-hydroxymetoprolol-MS284.18	0.0730	0.1588	-0.1040	5.25E-01
alpha-hydroxyisovalerate-MS117.05	0.0937	0.1685	-0.0091	9.56E-01
alpha-hydroxyisocaproate-MS131.07	0.1535	0.2062	0.2025	2.12E-01
alpha-CEHC-MS277.14	0.4009	0.5355	0.1307	4.24E-01
alpha-CEHC sulfate-MS357.10	0.6689	0.5111	-0.1229	4.52E-01
alpha-CEHC glucuronide*-MS453.17	0.7496	0.5088	-0.4053	8.90E-03
alliin-MS178.05	0.1106	6.073	-0.4830	1.35E-03
allantoin-MS157.03	0.0947	0.1326	-0.6156	1.26E-05
alanine-MS90.054	0.0531	0.0955	0.0118	9.43E-01
adrenoylcarnitine (C22:4)*-MS476.37	0.1274	0.2969	0.0282	8.64E-01
adrenate (22:4n6)-MS331.26	0.8671	1.146	0.1488	3.62E-01
adipoylcarnitine (C6-DC)-MS290.15	0.1106	0.3055	-0.6646	1.11E-06
adipate-MS145.05	0.5086	0.4302	-0.4821	1.39E-03
adenosine-MS134.04	0.2418	0.2913	-0.1820	2.63E-01
adenosine 5'-monophosphate (AMP)-MS348.07	0.0913	0.6696	-0.1822	2.62E-01
adenosine 3',5'-cyclic monophosphate (cAMP)-MS328.04	0.1817	0.1529	-0.6256	7.99E-06
adenine-MS136.06	0.1105	0.1726	-0.4500	3.20E-03
aconitate [cis or trans]-MS173.00	0.0597	0.1325	-0.7608	1.27E-09

acisoga-MS183.11	0.1065	0.2471	-0.6058	1.94E-05
acetylcarnitine (C2)-MS204.12	0.0779	0.2205	-0.4765	1.61E-03
acetoacetate-MS103.03	0.1989	0.5351	-0.0191	9.07E-01
acesulfame-MS161.98	0.2516	479585728	-0.1333	4.15E-01
9-hydroxystearate-MS299.25	0.2035	0.7815	0.1962	2.27E-01
9,10-DiHOME-MS313.23	0.1899	0.5463	-0.2500	1.20E-01
7-methylxanthine-MS167.05	0.1045	0.8690	-0.4701	1.91E-03
7-methylurate-MS181.03	0.9508	2.257	-0.3948	1.11E-02
7-methylguanine-MS166.07	0.0428	0.0928	-0.0530	7.47E-01
7-ketolithocholate-MS389.26	0.1849	0.8053	-0.0288	8.61E-01
7-ketodeoxycholate-MS405.26	0.2185	0.7948	-0.1177	4.72E-01
7-hydroxyoctanoate-MS159.10	0.0658	1.901	-0.2625	1.02E-01
7-hydroxyindole sulfate-MS212.00	0.2584	0.3342	-0.2700	9.21E-02
7-alpha-hydroxy-3-oxo-4-cholestenoate (7-Hoca)-MS429.30	0.1066	0.1731	0.3039	5.63E-02
6-oxopiperidine-2-carboxylate-MS142.05	0.1586	0.1881	-0.3260	3.96E-02
6-hydroxyindole sulfate-MS212.00	0.2010	0.3214	-0.5279	3.54E-04
5-oxoproline-MS128.03	0.1143	0.1034	-0.4244	5.86E-03
5-methyluridine (ribothymidine)-MS257.07	0.0991	0.1407	-0.2229	1.68E-01
5-methylthioadenosine (MTA)-MS298.09	0.0963	0.1494	-0.6393	4.13E-06
5-hydroxylysine-MS163.10	0.1159	0.3749	-0.1948	2.30E-01
5-hydroxyindoleacetate-MS190.05	0.2293	0.3965	-0.6964	1.67E-07
5-hydroxyindole sulfate-MS212.00	0.4230	0.3995	-0.4177	6.81E-03
5-hydroxyhexanoate-MS131.07	0.2048	0.2511	-0.4126	7.61E-03
5-dodecenoate (12:1n7)-MS197.15	0.1711	14.03	0.2023	2.12E-01
5-bromotryptophan-MS280.99	0.0974	0.1314	0.4562	2.74E-03
5alpha-pregnan-3beta,20beta-diol monosulfate (1)-MS399.22	0.2006	0.4502	-0.1206	4.61E-01
5alpha-pregnan-3beta,20alpha-diol monosulfate (2)-MS399.22	0.1526	0.5594	-0.0201	9.03E-01
5alpha-pregnan-3beta,20alpha-diol disulfate-MS239.08	0.1606	0.3792	-0.0717	6.62E-01
5alpha-androstan-3beta,17beta-diol monosulfate (2)-MS371.18	0.1915	0.2669	-0.1528	3.49E-01
5alpha-androstan-3beta,17beta-diol disulfate-MS225.06	0.1574	0.1720	-0.1885	2.46E-01
5alpha-androstan-3beta,17alpha-diol disulfate-MS225.06	0.6155	0.2903	-0.2564	1.11E-01
5alpha-androstan-3alpha,17beta-diol monosulfate (2)-MS371.18	0.4808	1.056	-0.1486	3.62E-01
5alpha-androstan-3alpha,17beta-diol monosulfate (1)-MS371.18	0.1209	0.2618	-0.1801	2.68E-01
5alpha-androstan-3alpha,17beta-diol disulfate-MS225.06	0.9653	1.364	-0.2712	9.06E-02
5alpha-androstan-3alpha,17alpha-diol monosulfate-MS371.18	0.1529	0.2840	-0.2851	7.45E-02
5alpha-androstan-3alpha, 17beta-diol 17-glucosiduronate-MS467.26	0.2866	0.7082	-0.0415	8.01E-01
5-acetylamino-6-formylamino-3-methyluracil-MS225.06	0.0759	1.224	-0.3909	1.20E-02
5-acetylamino-6-amino-3-methyluracil-MS197.06	0.0898	0.9075	-0.4933	1.01E-03
5,6-dihydrothymine-MS127.05	0.1100	0.2063	0.0974	5.52E-01
5-(galactosylhydroxy)-L-lysine-MS325.16	0.1186	0.2113	-0.7881	8.82E-11
4-vinylphenol sulfate-MS199.00	0.3756	1.265	-0.3751	1.65E-02

4-vinylguaiacol sulfate-MS229.01	0.1646	11.74	-0.4197	6.51E-03
4-methylcatechol sulfate-MS203.00	0.1585	0.5168	-0.4547	2.84E-03
4-methyl-2-oxopentanoate-MS129.05	0.0982	0.1873	0.2911	6.82E-02
4-imidazoleacetate-MS127.05	1.132	1.350	0.2376	1.41E-01
4-hydroxyphenylpyruvate-MS179.03	0.4332	0.2939	-0.1326	4.17E-01
4-hydroxyphenylacetylglutamine-MS279.09	0.3588	0.3652	-0.8583	4.88E-15
4-hydroxyphenylacetatoylcarnitine-MS296.14	0.1839	0.4500	-0.6936	2.00E-07
4-hydroxyphenylacetate-MS151.04	0.9584	0.6640	-0.6177	1.15E-05
4-hydroxyhippurate-MS194.04	0.1567	0.4186	-0.5665	9.33E-05
4-hydroxyglutamate-MS164.05	0.1514	0.4305	-0.1712	2.93E-01
4-hydroxycoumarin-MS161.02	0.1676	4.606	-0.2704	9.16E-02
4-hydroxycinnamate sulfate-MS242.99	0.1904	0.6315	-0.5710	7.89E-05
4-hydroxychlorothalonil-MS244.90	0.1871	0.1814	-0.0143	9.31E-01
4-hydroxy-2-nonenal-MS155.10	0.3044	0.3462	-0.0196	9.05E-01
4-guanidinobutanoate-MS146.09	0.1076	0.4096	-0.5012	8.04E-04
4-ethylphenylsulfate-MS201.02	0.2060	9.254	-0.4720	1.82E-03
4-cholesten-3-one-MS385.34	0.2246	0.1518	0.0252	8.78E-01
4-allylphenol sulfate-MS213.02	0.2512	0.7169	-0.2384	1.39E-01
4-acetylphenol sulfate-MS215.00	0.2345	0.5131	-0.6100	1.62E-05
4-acetaminophen sulfate-MS230.01	0.3220	28726074	-0.1182	4.70E-01
4-acetamidophenylglucuronide-MS326.08	0.2355	176621	-0.0489	7.66E-01
4-acetamidophenol-MS150.05	3.530	267863	-0.0547	7.39E-01
4-acetamidobutanoate-MS144.06	0.2300	0.1871	-0.6861	3.16E-07
4-acetamidobenzoate-MS178.05	0.3358	0.4474	-0.3106	5.07E-02
3-ureidopropionate-MS133.06	0.3176	0.5636	-0.3272	3.88E-02
3-sialyllactose-MS632.20	0.2087	0.2796	-0.5647	9.99E-05
3-phosphoglycerate-MS187.00	0.1641	0.7863	0.0534	7.45E-01
3-phenylpropionate (hydrocinnamate)-MS149.06	0.1982	0.5384	-0.0524	7.50E-01
3-methylxanthine-MS165.04	0.2039	9.803	-0.5538	1.48E-04
3-methylurate*-MS181.03	0.5262	0.8226	-0.6217	9.56E-06
3-methylhistidine-MS168.07	0.1216	1.947	-0.4074	8.52E-03
3-methylglutarylcarnitine (2)-MS290.15	0.0713	0.5268	-0.6452	3.07E-06
3-methylglutarate/2-methylglutarate-MS145.05	0.3072	0.8025	-0.2657	9.77E-02
3-methylglutaconate-MS143.03	0.1260	0.1903	-0.7354	1.06E-08
3-methylcytidine-MS258.10	0.1719	0.2560	-0.0069	9.66E-01
3-methyladipate-MS159.06	0.2928	0.4577	-0.6515	2.23E-06
3-methyl-2-oxovalerate-MS129.05	0.1126	0.2022	0.2008	2.16E-01
3-methyl-2-oxobutyrate-MS115.04	0.0903	0.1623	0.3965	1.07E-02
3-methyl catechol sulfate (2)-MS203.00	0.1985	2.326	-0.3038	5.64E-02
3-methyl catechol sulfate (1)-MS203.00	0.0863	0.9200	-0.4048	9.01E-03
3-methoxytyrosine-MS212.09	0.0975	0.1749	-0.2525	1.16E-01
3-methoxytyramine sulfate-MS246.04	0.1061	0.3621	-0.4070	8.59E-03
3-methoxycatechol sulfate (2)-MS218.99	0.5830	0.3659	-0.4982	8.79E-04
3-methoxycatechol sulfate (1)-MS218.99	0.0856	0.7430	-0.4644	2.22E-03
3-indoxyl sulfate-MS212.00	0.1794	0.2673	-0.5184	4.78E-04
3-hydroxysebacate-MS217.10	0.2078	0.8559	-0.4719	1.83E-03
3-hydroxypyridine sulfate-MS173.98	0.2255	1.647	-0.3091	5.19E-02
3-hydroxyoctanoate-MS159.10	0.0935	0.4393	-0.1459	3.71E-01
3-hydroxylaurate-MS215.16	0.1477	1.542	0.0345	8.34E-01
3-hydroxyisobutyrate-MS103.04	0.1799	0.2463	-0.2325	1.50E-01
3-hydroxyindolin-2-one sulfate-MS227.99	1.232	0.6509	-0.4858	1.25E-03
3-hydroxyhippurate-MS194.04	0.5162	0.9540	-0.2201	1.74E-01
3-hydroxyhexanoate-MS131.07	0.1058	0.4251	-0.2704	9.16E-02

3-hydroxydecanoate-MS187.13	0.1200	0.9821	0.0897	5.84E-01
3-hydroxybutyrylcarnitine (2)-MS248.14	0.1195	0.3583	-0.5923	3.42E-05
3-hydroxybutyrylcarnitine (1)-MS248.14	0.1540	0.3817	-0.2532	1.15E-01
3-hydroxybutyrate (BHBA)-MS103.04	0.1074	1.804	-0.2289	1.56E-01
3-hydroxy-3-methylglutarate-MS161.04	0.7263	2.979	-0.6778	5.20E-07
3-hydroxy-2-ethylpropionate-MS117.05	0.1045	0.1764	-0.6575	1.62E-06
3-carboxy-4-methyl-5-propyl-2-furanpropanoate (CMPF)-MS239.09	0.3918	0.2751	0.0284	8.63E-01
3b-hydroxy-5-cholenoic acid-MS373.27	0.3195	0.3947	0.2556	1.12E-01
3beta-hydroxy-5-cholestenoate-MS415.32	0.2542	0.1787	0.0783	6.33E-01
3beta,7alpha-dihydroxy-5-cholestenoate-MS431.31	0.1445	0.1256	0.1682	3.02E-01
3-aminoisobutyrate-MS104.07	0.0696	0.2062	-0.5303	3.28E-04
3-acetylphenol sulfate-MS215.00	0.2716	0.5734	-0.4526	2.99E-03
3,7-dimethylurate-MS195.05	0.2826	1.119	-0.4456	3.56E-03
3,4-methyleneheptanoylcarnitine-MS346.18	0.1537	0.4513	-0.3270	3.89E-02
3,4-methyleneheptanoate-MS141.09	0.6928	0.6850	-0.0696	6.71E-01
3,4-methylene heptanoylglycine-MS200.12	0.1134	0.2609	-0.6755	5.94E-07
3-(N-acetyl-L-cystein-S-yl) acetaminophen-MS311.07	0.1140	7.916	0.0126	9.39E-01
3-(4-hydroxyphenyl)lactate-MS181.05	0.1157	0.1312	-0.3561	2.35E-02
3-(3-hydroxyphenyl)propionate-MS165.05	0.1849	1.231	-0.0185	9.11E-01
3-(3-hydroxyphenyl)propionate sulfate-MS245.01	0.3686	5.628	-0.4031	9.34E-03
2-stearoyl-GPE (18:0)*-MS480.30	0.1828	0.1982	0.0901	5.83E-01
2-pyrrolidinone-MS86.060	0.2765	0.3787	-0.7477	3.93E-09
2-piperidinone-MS100.07	0.1237	0.2588	0.1490	3.61E-01
2-palmitoyl-GPC (16:0)*-MS570.34	0.4288	0.4452	0.2094	1.96E-01
2-palmitoleoyl-GPC (16:1)*-MS568.32	0.3289	0.4132	0.2061	2.03E-01
2-oxoarginine*-MS174.08	0.0840	0.2350	-0.2928	6.66E-02
2-oxindole-3-acetate-MS192.06	0.1500	2.001	-0.5429	2.16E-04
2-methylmalonylcarnitine (C4-DC)-MS262.12	0.4890	0.2841	-0.7454	4.79E-09
2-methylcitrate/homocitrate-MS205.03	2.701	2.257	-0.7465	4.37E-09
2-methylbutyrylglycine-MS160.09	0.9758	0.6146	-0.3033	5.68E-02
2-methylbutyrylcarnitine (C5)-MS246.16	0.1117	0.1804	-0.6538	1.97E-06
2-methoxyresorcinol sulfate-MS218.99	0.1047	0.7929	-0.1337	4.13E-01
2-methoxyacetaminophen sulfate*-MS260.02	0.1283	83.38	-0.0417	8.00E-01
2-methoxyacetaminophen glucuronide*-MS356.09	0.0706	24.04	-0.0633	7.00E-01
2-linoleoylglycerol (18:2)-MS279.23	6.799	3.232	0.1117	4.95E-01
2-keto-3-deoxy-gluconate-MS177.04	0.1868	0.1502	-0.7379	8.75E-09
2-isopropylmalate-MS175.06	0.2456	3.650	-0.4899	1.11E-03
2-hydroxystearate-MS299.25	0.1969	0.1878	0.3367	3.30E-02
2-hydroxyphenylacetate-MS151.04	0.1186	0.2693	-0.8279	6.70E-13
2-hydroxypalmitate-MS271.22	0.1319	0.1720	0.1676	3.03E-01
2-hydroxyoctanoate-MS159.10	0.1142	0.2870	-0.1710	2.93E-01
2-hydroxyhippurate (salicylurate)-MS194.04	0.1698	25.66	-0.3405	3.10E-02
2-hydroxyglutarate-MS166.07	0.1240	0.1164	-0.5130	5.66E-04
2-hydroxydecanoate-MS187.13	0.0861	0.4574	-0.2862	7.33E-02
2-hydroxybutyrate/2-hydroxyisobutyrate-MS103.04	0.1321	0.2436	-0.0082	9.60E-01
2-hydroxyadipate-MS161.04	0.5023	0.2817	-0.5821	5.15E-05
2-hydroxyacetaminophen sulfate*-MS246.00	0.6763	5156	-0.1728	2.88E-01
2-hydroxy-3-methylvalerate-MS131.07	0.1165	0.1584	-0.1225	4.54E-01
2-ethylphenylsulfate-MS201.02	0.2200	0.5591	-0.1753	2.81E-01
2'-deoxyuridine-MS111.01	0.2135	0.2704	0.2301	1.54E-01
2-aminophenol sulfate-MS188.00	0.3236	2.274	-0.4918	1.06E-03
2-aminooctanoate-MS158.11	0.1187	0.2671	-0.1235	4.50E-01

2-aminoheptanoate-MS146.11	0.1026	0.1546	-0.4492	3.26E-03
2-aminobutyrate-MS104.07	0.0499	0.1422	0.3779	1.56E-02
2-aminoadipate-MS160.06	0.2008	0.3244	-0.0872	5.95E-01
2-acetamidophenol sulfate-MS230.01	0.1994	1.583	-0.2042	2.08E-01
21-hydroxypregnenolone disulfate-MS245.06	0.1351	0.1984	-0.1967	2.25E-01
2,8-quinolinediol sulfate-MS239.99	0.1552	1.273	-0.4172	6.88E-03
2,3-dihydroxypyridine-MS112.03	0.0838	1.278	-0.0178	9.14E-01
2,3-dihydroxyisovalerate-MS133.05	0.1021	1.114	-0.6787	4.95E-07
1-stearoyl-GPI (18:0)-MS599.32	0.4620	0.4132	0.2314	1.52E-01
1-stearoyl-GPE (18:0)-MS482.32	0.0831	0.1498	0.0529	7.47E-01
1-stearoyl-GPC (18:0)-MS524.37	0.0759	0.1310	0.2567	1.10E-01
1-stearoyl-2-oleoyl-GPS (18:0/18:1)-MS790.55	0.3140	0.3891	-0.0909	5.79E-01
1-stearoyl-2-oleoyl-GPI (18:0/18:1)*-MS882.60	0.1483	0.1924	-0.0325	8.43E-01
1-stearoyl-2-oleoyl-GPE (18:0/18:1)-MS746.56	0.1532	0.2933	-0.0865	5.98E-01
1-stearoyl-2-oleoyl-GPC (18:0/18:1)-MS788.61	0.0636	0.1105	0.1074	5.12E-01
1-stearoyl-2-linoleoyl-GPI (18:0/18:2)-MS880.59	0.0962	0.1362	-0.0031	9.85E-01
1-stearoyl-2-linoleoyl-GPE (18:0/18:2)*-MS744.55	0.0586	0.2148	-0.1146	4.84E-01
1-stearoyl-2-linoleoyl-GPC (18:0/18:2)*-MS786.60	0.0560	0.0647	0.1317	4.20E-01
1-stearoyl-2-arachidonoyl-GPI (18:0/20:4)-MS904.59	0.0887	0.0999	0.2060	2.04E-01
1-stearoyl-2-arachidonoyl-GPE (18:0/20:4)-MS768.55	0.0655	0.1231	-0.1423	3.83E-01
1-stearoyl-2-arachidonoyl-GPC (18:0/20:4)-MS810.60	0.0644	0.0756	0.0676	6.80E-01
1-palmitoyl-GPI (16:0)-MS571.28	0.4937	0.8640	0.1169	4.75E-01
1-palmitoyl-GPG (16:0)*-MS483.27	0.3680	0.4123	0.0414	8.01E-01
1-palmitoyl-GPE (16:0)-MS454.29	0.0840	0.1662	0.0015	9.93E-01
1-palmitoyl-GPC (16:0)-MS496.33	0.0594	0.0967	0.2501	1.20E-01
1-palmitoylglycerol (16:0)-MS255.23	0.1913	0.3117	0.4806	1.44E-03
1-palmitoyl-2-stearoyl-GPE (16:0/18:0)*-MS720.55	0.5186	0.6506	-0.0841	6.08E-01
1-palmitoyl-2-stearoyl-GPC (16:0/18:0)-MS762.60	0.0646	0.0946	0.1113	4.97E-01
1-palmitoyl-2-palmitoleoyl-GPC (16:0/16:1)*-MS732.55	0.0756	0.1998	0.2521	1.17E-01
1-palmitoyl-2-oleoyl-GPI (16:0/18:1)*-MS854.57	0.1186	0.2038	0.0697	6.71E-01
1-palmitoyl-2-oleoyl-GPE (16:0/18:1)-MS718.53	0.0895	0.2729	-0.1439	3.78E-01
1-palmitoyl-2-oleoyl-GPC (16:0/18:1)-MS760.58	0.0423	0.0671	0.1111	4.97E-01
1-palmitoyl-2-linoleoyl-GPI (16:0/18:2)-MS833.51	0.1748	0.1833	0.0541	7.42E-01
1-palmitoyl-2-linoleoyl-GPE (16:0/18:2)-MS716.52	0.0578	0.2329	-0.1455	3.73E-01
1-palmitoyl-2-linoleoyl-GPC (16:0/18:2)-MS758.56	0.0634	0.0635	0.1324	4.18E-01
1-palmitoyl-2-gamma-linolenoyl-GPC (16:0/18:3n6)*-MS756.55	0.0969	0.2525	0.1447	3.75E-01
1-palmitoyl-2-arachidonoyl-GPI (16:0/20:4)*-MS876.55	0.1284	0.2014	0.0579	7.24E-01
1-palmitoyl-2-arachidonoyl-GPE (16:0/20:4)*-MS740.52	0.0594	0.1693	-0.1923	2.36E-01
1-palmitoyl-2-arachidonoyl-GPC (16:0/20:4n6)-MS782.56	0.0623	0.0646	0.1249	4.45E-01
1-palmitoleoyl-GPC (16:1)*-MS494.32	0.0937	0.2262	0.2835	7.62E-02
1-palmitoleoylglycerol (16:1)*-MS253.21	0.3124	0.5509	0.2171	1.80E-01
1-palmitoleoyl-2-linoleoyl-GPC (16:1/18:2)*-MS756.55	0.0604	0.1246	0.1348	4.09E-01
1-palmitoleoyl-2-linolenoyl-GPC (16:1/18:3)*-MS754.53	0.2287	0.2400	0.2169	1.80E-01
1-oleoyl-GPI (18:1)*-MS597.30	0.6599	0.6852	-0.1056	5.19E-01

1-oleoyl-GPG (18:1)*-MS509.28	1.098	0.8710	-0.0033	9.84E-01
1-oleoyl-GPE (18:1)-MS480.30	0.0933	0.2739	-0.1058	5.18E-01
1-oleoyl-GPC (18:1)-MS522.35	0.0786	0.1589	0.1308	4.23E-01
1-oleoylglycerol (18:1)-MS281.24	0.2206	0.3769	0.0601	7.14E-01
1-oleoyl-2-linoleoyl-GPE (18:1/18:2)*-MS742.53	0.0713	0.3338	-0.2504	1.20E-01
1-oleoyl-2-arachidonoyl-GPE (18:1/20:4)*-MS766.53	0.1081	0.1794	-0.2998	5.99E-02
1-myristoylglycerol (14:0)-MS227.20	0.3696	0.6623	0.1509	3.55E-01
1-methylxanthine-MS165.04	0.1347	0.5651	-0.0502	7.60E-01
1-methylurate-MS181.03	3.300	3.620	-0.3674	1.91E-02
1-methylnicotinamide-MS137.07	0.0291	0.3412	-0.2816	7.83E-02
1-methylimidazoleacetate-MS141.06	0.0358	0.1647	-0.8099	7.18E-12
1-methylhistidine-MS168.07	0.1176	0.2051	-0.7600	1.37E-09
1-methylguanidine-MS74.071	0.0961	0.1935	-0.8052	1.28E-11
1-linoleoyl-GPI (18:2)*-MS595.28	0.3231	0.3133	0.0115	9.44E-01
1-linoleoyl-GPG (18:2)*-MS507.27	0.2611	0.1977	-0.1355	4.07E-01
1-linoleoyl-GPE (18:2)*-MS478.29	0.0837	0.2493	0.0021	9.90E-01
1-linoleoyl-GPC (18:2)-MS520.33	0.0772	0.2219	0.1418	3.85E-01
1-linoleoyl-GPA (18:2)*-MS433.23	0.2445	0.3769	-0.0691	6.74E-01
1-linoleoylglycerol (18:2)-MS279.23	0.2436	0.3537	0.1553	3.41E-01
1-linoleoyl-2-linolenoyl-GPC (18:2/18:3)*-MS780.55	0.1685	0.3385	-0.0862	5.99E-01
1-linoleoyl-2-arachidonoyl-GPC (18:2/20:4n6)*-MS806.56	0.0802	0.0855	0.1506	3.56E-01
1-linolenoyl-GPC (18:3)*-MS518.32	0.0910	0.2992	0.1240	4.48E-01
1-linolenoylglycerol (18:3)-MS277.21	0.7952	0.5092	0.0109	9.47E-01
1-docosahexaenoylglycerol (22:6)-MS309.22	0.8246	0.4347	0.2973	6.22E-02
1-dihomo-linolenylglycerol (20:3)-MS305.24	0.5512	0.4689	0.4209	6.34E-03
1-arachidonylglycerol (20:4)-MS303.23	0.6673	0.4786	0.2621	1.03E-01
1-arachidonoyl-GPI (20:4)*-MS619.28	0.3343	0.3061	0.0990	5.46E-01
1-arachidonoyl-GPE (20:4n6)*-MS502.29	0.0760	0.1165	0.0359	8.27E-01
1-arachidonoyl-GPC (20:4n6)*-MS544.33	0.1011	0.2278	0.1516	3.53E-01
17-methylstearate-MS297.27	0.2415	0.4733	0.1338	4.13E-01
17alpha-hydroxypregnenolone 3-sulfate-MS411.18	0.1444	0.3891	0.2536	1.15E-01
17alpha-hydroxypregnanolone glucuronide-MS509.27	0.8267	0.5074	-0.4236	5.96E-03
16-hydroxypalmitate-MS271.22	0.1419	0.3933	0.1027	5.31E-01
16a-hydroxy DHEA 3-sulfate-MS383.15	0.0953	0.2597	0.0239	8.85E-01
15-methylpalmitate-MS269.24	0.1460	0.6560	0.1808	2.66E-01
13-methylmyristate-MS241.21	0.2245	0.9710	0.2318	1.51E-01
13-HODE + 9-HODE-MS295.22	0.2411	1.984	0.0752	6.47E-01
12,13-DiHOME-MS313.23	0.2167	0.6489	-0.1106	4.99E-01
11-ketoetiocholanolone glucuronide-MS479.22	0.3302	0.1936	-0.5233	4.10E-04
10-undecenoate (11:1n1)-MS183.13	0.0767	0.4318	0.1196	4.65E-01
10-nonadecenoate (19:1n9)-MS295.26	0.2929	1.616	0.1819	2.63E-01
10-heptadecenoate (17:1n7)-MS267.23	0.2279	1.649	0.2230	1.68E-01
1,7-dimethylurate-MS195.05	0.3692	1.153	-0.1527	3.49E-01
1,6-anhydroglucose-MS161.04	0.7522	1.031	-0.4611	2.42E-03
1,5-anhydroglucitol (1,5-AG)-MS163.06	0.1321	0.0959	0.4992	8.54E-04
1,3-dimethylurate-MS195.05	0.8089	0.7934	-0.3435	2.94E-02
1,3,7-trimethylurate-MS209.06	0.1652	3.157	-0.3590	2.23E-02
1,2-dipalmitoyl-GPE (16:0/16:0)*-MS692.52	0.2992	0.3699	-0.1162	4.78E-01
1,2-dipalmitoyl-GPC (16:0/16:0)-MS734.56	0.0471	0.0712	-0.0648	6.93E-01
1,2-dilinoleoyl-GPE (18:2/18:2)*-MS740.52	0.1019	0.9863	-0.2769	8.37E-02

1,2-dilinoleoyl-GPC (18:2/18:2)-MS782.56	0.0833	0.1690	-0.0757	6.45E-01
1,2,3-benzenetriol sulfate (2)-MS204.98	18.21	1.834	-0.1858	2.53E-01
1-(1-enyl-stearoyl)-GPE (P-18:0)*-MS466.32	0.1098	0.1724	0.2210	1.72E-01
1-(1-enyl-stearoyl)-2-oleoyl-GPE (P-18:0/18:1)-MS730.57	0.2876	0.2405	0.0165	9.20E-01
1-(1-enyl-stearoyl)-2-linoleoyl-GPE (P-18:0/18:2)*-MS728.55	0.1017	0.1504	-0.1084	5.08E-01
1-(1-enyl-stearoyl)-2-arachidonoyl-GPE (P-18:0/20:4)*-MS752.55	0.0822	0.1303	0.1473	3.67E-01
1-(1-enyl-palmitoyl)-GPE (P-16:0)*-MS438.29	0.1038	0.1776	0.2359	1.44E-01
1-(1-enyl-palmitoyl)-GPC (P-16:0)*-MS480.34	0.1097	0.2012	0.1665	3.07E-01
1-(1-enyl-palmitoyl)-2-palmitoyl-GPC (P-16:0/16:0)*-MS718.57	0.0625	0.0728	-0.1103	5.00E-01
1-(1-enyl-palmitoyl)-2-palmitoleoyl-GPC (P-16:0/16:1)*-MS716.55	0.0712	0.0966	-0.1142	4.85E-01
1-(1-enyl-palmitoyl)-2-oleoyl-GPE (P-16:0/18:1)*-MS702.54	0.0905	0.1255	-0.1282	4.33E-01
1-(1-enyl-palmitoyl)-2-oleoyl-GPC (P-16:0/18:1)*-MS744.59	0.0611	0.0931	-0.3079	5.29E-02
1-(1-enyl-palmitoyl)-2-linoleoyl-GPE (P-16:0/18:2)*-MS700.52	0.0591	0.1269	-0.1376	4.00E-01
1-(1-enyl-palmitoyl)-2-linoleoyl-GPC (P-16:0/18:2)*-MS742.57	0.0441	0.1125	-0.1653	3.10E-01
1-(1-enyl-palmitoyl)-2-arachidonoyl-GPE (P-16:0/20:4)*-MS724.52	0.0763	0.1601	0.1558	3.39E-01
1-(1-enyl-palmitoyl)-2-arachidonoyl-GPC (P-16:0/20:4)*-MS766.57	0.0550	0.0992	0.0408	8.04E-01

Supplementary Table 3. Technical Variation, Day-to-Day Variation, and Correlation with eGFR for all Broad Institute known metabolites

Metabolite	technical replicate CV	day to day variation CV	Pearson correlation with eGFR-Cr	P valu e for correlation
17-Methylstearate_MS297.27	0.1175	0.3417	0.1430	3.81E-01
1-methyladenosine_MS282.11	0.0458	0.1016	-0.6771	5.43E-07
1-methylhistamine_MS126.10	0.0991	0.5717	-0.4749	1.68E-03
1-methylnicotinamide_MS137.07	0.0517	0.3152	-0.1895	2.43E-01
274_51:3 TAG_MS865.72	0.9853	0.4694	0.2184	1.77E-01
276_51:2 TAG_MS867.74	0.6510	0.3370	0.1189	4.67E-01
2-aminoadipate_MS160.06	0.0566	0.2108	-0.0099	9.52E-01
2-furoylglycine_MS168.03	0.0728	1.466	-0.2314	1.52E-01
2-hydroxy-3-methylpentanoic acid_MS131.07	0.0527	0.1685	-0.0197	9.05E-01
2-Hydroxycaprylic acid_MS159.10	0.1311	0.4140	-0.0491	7.65E-01
2-hydroxyglutarate_MS147.02	0.0630	0.0846	-0.5054	7.11E-04
2-phosphoglycerate_MS184.98	0.1307	0.5232	0.0705	6.67E-01
3-dehydroxycarnitine_MS146.11	0.0488	0.0745	-0.6513	2.25E-06
3-hydroxyanthranilic acid_MS154.04	0.1638	0.3039	-0.0472	7.74E-01
3-methyladipate/pimelate_MS159.06	0.0756	0.1462	-0.4873	1.20E-03
3-methylxanthine_MS165.04	0.0513	4.358	-0.6123	1.46E-05
3-phosphoglycerate_MS184.98	0.1224	0.7086	0.1058	5.18E-01
4-hydroxybenzaldehyde_MS121.02	0.1872	0.2386	-0.2831	7.66E-02
4-hydroxymandelate/homogentisate_MS167.03	0.5360	1.023	-0.3829	1.41E-02
4-methylcatechol_MS123.04	0.0878	0.0792	-0.0183	9.12E-01
4-pyridoxate_MS182.04	0.0829	0.5328	-0.4233	6.00E-03
5-aminolevulinic acid_MS132.06	0.3003	0.2466	-0.6881	2.81E-07
5-HIAA_MS192.06	0.7901	0.6796	-0.5646	1.00E-04
5-methyluridine/ribothymidine_MS257.07	0.0599	0.0587	-0.3907	1.21E-02
8.11.14-Eicosatrienoic acid_MS305.24	0.0995	0.5501	0.3771	1.58E-02
acetaminophen_MS152.07	0.4806	50670	-0.0421	7.98E-01
acetylcholine_MS146.11	0.0850	2.184	-0.5686	8.62E-05
acetylglycine_MS118.05	0.2200	0.3828	-0.1943	2.31E-01
acetyl-L-alanine_MS130.05	0.0480	0.0562	-0.8710	4.44E-16
acetyl-L-tyrosine_MS222.07	0.4226	0.7206	-0.5341	2.89E-04
aconitate_MS173.00	0.0374	0.0946	-0.6744	6.35E-07
adenosine_MS268.10	0.7628	0.4598	-0.1820	2.63E-01
adipate_MS145.05	0.0562	0.0924	-0.4647	2.20E-03
ADMA_MS203.15	0.0567	0.0639	-0.4285	5.33E-03
ADP_MS426.02	0.1120	2.512	0.1187	4.68E-01
Adrenic acid_MS331.26	0.0812	0.5230	0.0925	5.72E-01
alanine_MS90.055	0.0296	0.1311	-0.1045	5.23E-01
aldosterone_MS361.20	0.1627	0.3316	0.1185	4.69E-01
allantoin_MS159.05	0.1308	0.2677	-0.5010	8.11E-04
alpha-glycerophosphate_MS171.00	0.0620	0.2950	-0.1968	2.25E-01
alpha-glycerophosphocholine_MS258.11	0.0929	0.2034	-0.1067	5.15E-01
alpha-hydroxybutyrate/beta-hydroxybutyrate_MS103.04	0.0512	0.2897	-0.0607	7.12E-01
alpha-keto-beta-methylvalerate/alpha-ketoisocaproate_MS129.0	0.0508	0.1679	0.3970	1.06E-02
alpha-ketoglutarate_MS145.01	0.1186	0.1652	0.3284	3.80E-02
AMP_MS346.05	0.1373	3.285	-0.1968	2.25E-01

anserine_MS241.12	0.1922	244.5	-0.1545	3.43E-01
anthranilic acid_MS138.05	0.4010	0.3813	-0.6476	2.72E-06
Arachidonic acid_MS303.23	0.0920	0.3882	0.1005	5.39E-01
arginine_MS175.11	0.0398	0.1059	-0.1941	2.32E-01
ascorbate_MS175.02	0.0739	0.2361	-0.5811	5.36E-05
asparagine_MS133.06	0.0453	0.1271	-0.3227	4.18E-02
aspartate_MS132.03	0.0421	0.1092	0.1140	4.86E-01
aspartate_MS134.04	0.3931	0.5410	0.1118	4.95E-01
azelaic acid_MS187.09	0.0642	0.4213	-0.5451	2.00E-04
beta-alanine_MS90.055	0.0931	0.2591	-0.1245	4.46E-01
betaine_MS118.08	0.0337	0.1015	-0.2102	1.94E-01
butyrobetaine_MS147.12	1.066	0.7642	-0.1934	2.34E-01
C10 carnitine_MS316.24	0.0616	0.7017	-0.2834	7.64E-02
C10:2 carnitine_MS312.21	0.0621	0.3122	-0.6072	1.82E-05
C12 carnitine_MS344.27	0.0666	0.5854	-0.2428	1.32E-01
C12:1 carnitine_MS342.26	0.0631	0.5445	-0.2804	7.97E-02
C14 carnitine_MS372.31	0.0619	0.2726	0.0026	9.87E-01
C14:0 CE_MS619.54	0.0404	0.2036	0.2031	2.10E-01
C14:0 LPC_MS468.30	0.0606	0.2496	0.2448	1.28E-01
C14:0 LPC_MS468.30	0.0657	0.2387	0.2869	7.26E-02
C14:0 SM_MS675.54	0.0906	0.1327	0.0849	6.05E-01
C14:0 SM_MS675.54	0.0557	0.0982	0.1755	2.81E-01
C14:1 carnitine_MS370.29	0.0712	0.8024	-0.2073	2.01E-01
C14:2 carnitine_MS368.27	0.0619	0.9029	-0.3073	5.34E-02
C16 carnitine_MS400.34	0.0750	0.1618	0.0603	7.13E-01
C16:0 CE_MS647.57	0.0271	0.0703	-0.0398	8.09E-01
C16:0 Ceramide (d18:1)_MS538.51	0.0969	0.1403	-0.0772	6.38E-01
C16:0 LPC_minor_MS496.33	0.2760	0.2467	0.3186	4.47E-02
C16:0 LPC_MS496.33	0.0565	0.1131	0.1558	3.39E-01
C16:0 LPC_MS496.34	0.0613	0.1169	0.1774	2.75E-01
C16:0 LPE_MS454.29	0.0692	0.1841	0.0129	9.37E-01
C16:0 LPE_MS454.29	0.0884	0.1633	-0.0372	8.21E-01
C16:0 SM_minorA_MS703.57	0.1413	0.1943	-0.1868	2.50E-01
C16:0 SM_minorB_MS703.57	0.2383	1.118	-0.1165	4.76E-01
C16:0 SM_MS703.57	0.1120	0.1229	-0.2025	2.12E-01
C16:0 SM_MS703.57	0.0568	0.0891	-0.0562	7.32E-01
C16:1 CE_MS645.55	0.0254	0.1015	0.1862	2.52E-01
C16:1 LPC_MS494.32	0.0648	0.1579	0.2534	1.15E-01
C16:1 LPC_MS494.32	0.0611	0.1543	0.2428	1.32E-01
C16:1 MAG_MS339.25	0.1530	0.1172	-0.0652	6.91E-01
C16:1 SM_MS701.55	0.0572	0.0843	0.0308	8.51E-01
C16:1 SM_MS701.55	0.0834	0.0770	-0.0125	9.39E-01
C16-OH carnitine_MS416.33	0.5376	1.047	-0.1991	2.20E-01
C18 carnitine_MS428.37	0.1519	0.1952	0.1393	3.94E-01
C18:0 CE_MS675.60	0.0457	0.0798	0.1962	2.27E-01
C18:0 LPC_MS524.37	0.0706	0.1287	0.1717	2.92E-01
C18:0 LPC_MS524.37	0.0739	0.1265	0.1726	2.89E-01
C18:0 LPE_MS482.32	0.0751	0.1545	-0.0202	9.02E-01
C18:0 SM_MS731.60	0.1466	0.1385	-0.0028	9.86E-01
C18:0 SM_MS731.60	0.0559	0.0961	0.2260	1.62E-01
C18:1 carnitine_MS426.35	0.0670	0.2762	0.0602	7.14E-01
C18:1 CE_MS673.58	0.0245	0.1142	-0.1014	5.36E-01
C18:1 LPC_MS522.35	0.0635	0.1483	0.0517	7.53E-01

C18:1 LPE_MS480.30	0.0602	0.3349	-0.1503	3.57E-01
C18:1 LPE_MS480.30	0.0758	0.3201	-0.1328	4.17E-01
C18:1 SM [M+Na]+_MS749.55	0.1628	0.1419	0.2229	1.68E-01
C18:1 SM_MS729.59	0.0868	0.0919	0.1053	5.20E-01
C18:1 SM_MS729.59	0.0544	0.0865	0.1822	2.62E-01
C18:1-OH carnitine_MS442.35	1.260	4.321	-0.3674	1.90E-02
C18:2 carnitine_MS424.34	0.0713	0.3173	-0.1106	4.99E-01
C18:2 CE_MS671.57	0.0175	0.0804	-0.0894	5.86E-01
C18:2 LPC_MS520.33	0.0480	0.2256	0.0454	7.82E-01
C18:2 LPC_MS520.34	0.0616	0.2338	0.0570	7.29E-01
C18:2 LPE_MS478.29	0.0777	0.3011	0.0083	9.60E-01
C18:2 LPE_MS478.29	0.0764	0.2940	-0.0229	8.89E-01
C18:2 SM_MS749.55	0.0710	0.0996	0.0791	6.30E-01
C18:3 CE_MS669.55	0.0315	0.1032	0.0349	8.32E-01
C2 carnitine_MS204.12	0.0458	0.2047	-0.4511	3.11E-03
C20 carnitine_MS456.40	0.1371	0.3117	-0.0103	9.50E-01
C20:0 SM_MS759.63	0.1855	0.1994	-0.1157	4.80E-01
C20:0 SM_MS759.63	0.0582	0.0986	0.1723	2.90E-01
C20:3 CE_MS697.58	0.0317	0.1659	0.1709	2.94E-01
C20:3 LPC_MS518.32	0.0529	0.1008	0.1825	2.62E-01
C20:4 carnitine_MS448.34	0.5792	2.065	0.0175	9.15E-01
C20:4 CE_MS695.57	0.0171	0.1041	-0.0855	6.02E-01
C20:4 LPC_MS544.33	0.0509	0.1387	0.0313	8.49E-01
C20:4 LPC_MS544.34	0.0662	0.1568	0.0639	6.97E-01
C20:4 LPE_MS502.29	0.0797	0.1780	0.0140	9.32E-01
C20:4 LPE_MS502.29	0.0664	0.1595	0.0075	9.64E-01
C20:5 CE_MS693.55	0.0371	0.1808	0.2084	1.98E-01
C20:5 LPC_MS542.32	0.0685	0.2064	0.0951	5.62E-01
C22:0 Ceramide (d18:1)_MS622.61	0.0571	0.1440	0.1119	4.94E-01
C22:0 LPE_MS538.38	0.1149	0.2102	-0.0584	7.22E-01
C22:0 SM_MS787.66	0.3219	0.2286	-0.1564	3.37E-01
C22:0 SM_MS787.66	0.0517	0.0895	0.1393	3.94E-01
C22:1 SM_MS785.65	0.0618	0.0890	0.0783	6.33E-01
C22:4 CE_MS723.60	0.2000	0.5536	-0.2780	8.25E-02
C22:5 CE_MS721.58	0.0709	0.2843	-0.1103	5.01E-01
C22:6 CE_MS719.57	0.0329	0.1496	0.0562	7.32E-01
C22:6 LPC_MS568.33	0.0787	0.2238	0.2808	7.92E-02
C22:6 LPC_MS568.34	0.0632	0.2359	0.2480	1.23E-01
C22:6 LPE_MS526.29	0.0792	0.2660	0.2013	2.14E-01
C22:6 LPE_MS526.29	0.0679	0.2051	0.1574	3.34E-01
C24:0 Ceramide (d18:1)_MS650.64	0.0511	0.1291	0.0784	6.33E-01
C24:0 SM_MS815.70	0.0588	0.0983	0.0667	6.85E-01
C24:1 Ceramide (d18:1)_MS648.62	0.0569	0.1197	-0.0497	7.62E-01
C24:1 SM_MS813.68	0.0520	0.0727	-0.0864	5.98E-01
C26 carnitine_MS540.49	0.0806	0.1207	0.0448	7.85E-01
C3 carnitine_MS218.13	0.0437	0.1839	0.0471	7.74E-01
C30:0 DAG_MS563.46	0.1639	1.352	0.2558	1.12E-01
C30:0 PC_MS706.53	0.0565	0.2786	0.1982	2.22E-01
C30:1 PC_MS704.52	0.0800	0.7581	0.2414	1.34E-01
C32:0 DAG_MS591.49	0.0443	0.4243	0.2750	8.59E-02
C32:0 PC_MS734.56	0.0508	0.0861	-0.0233	8.87E-01
C32:0 PE_MS692.52	0.2622	0.7601	0.2526	1.16E-01
C32:1 DAG_MS589.48	0.0538	0.4431	0.3378	3.25E-02

C32:1 PC_MS732.55	0.0592	0.2236	0.2496	1.21E-01
C32:2 DAG_MS587.46	0.1673	0.6334	0.2962	6.33E-02
C32:2 PC_MS730.53	0.0561	0.2320	0.2402	1.36E-01
C34:0 DAG_MS619.52	0.0417	0.3626	0.2657	9.77E-02
C34:0 PC_MS762.60	0.0646	0.1004	0.1041	5.25E-01
C34:0 PE_MS720.55	0.0591	0.1682	0.1490	3.61E-01
C34:0 PI_MS839.56	0.2139	0.2622	0.1207	4.61E-01
C34:0 PS_MS764.54	0.0803	0.2167	0.2452	1.28E-01
C34:1 DAG_MS617.51	0.0528	0.2836	0.2734	8.80E-02
C34:1 PC plasmalogen-A_MS746.60	0.0575	0.0737	-0.2436	1.31E-01
C34:1 PC plasmalogen-B_MS746.60	0.1041	0.1371	-0.0173	9.16E-01
C34:1 PC_MS760.58	0.0501	0.1097	0.0831	6.12E-01
C34:1 PI_MS837.54	0.0899	0.1625	0.1927	2.35E-01
C34:2 DAG_MS615.49	0.0512	0.2388	0.2283	1.58E-01
C34:2 PC plasmalogen_MS744.59	0.0591	0.1219	-0.1658	3.09E-01
C34:2 PC_MS758.56	0.0487	0.0706	0.0791	6.30E-01
C34:2 PE plasmalogen_MS702.54	0.1339	0.2206	-0.1308	4.23E-01
C34:2 PE_MS716.52	0.0680	0.5080	-0.2244	1.65E-01
C34:2 PI_MS835.53	0.0535	0.1090	0.0339	8.37E-01
C34:3 DAG_MS613.48	0.0434	0.2714	0.1947	2.30E-01
C34:3 PC plasmalogen_MS742.57	0.0525	0.1127	-0.0753	6.46E-01
C34:3 PC_MS756.55	0.0564	0.1586	0.1500	3.58E-01
C34:3 PE plasmalogen_MS700.52	0.1019	0.2525	-0.0728	6.57E-01
C34:4 PC plasmalogen_MS740.55	0.3369	0.3049	0.0263	8.73E-01
C34:4 PC_MS754.53	0.0639	0.2296	0.2549	1.13E-01
C34:5 PC plasmalogen_MS738.54	0.2694	0.4592	0.1643	3.13E-01
C36:0 DAG_MS647.55	0.0425	0.0825	0.2128	1.89E-01
C36:0 PC_MS790.63	0.0761	0.1235	0.1158	4.79E-01
C36:0 PE_MS748.58	0.0522	0.1390	0.1443	3.77E-01
C36:1 DAG_MS645.54	0.0438	0.3461	0.2631	1.01E-01
C36:1 PC plasmalogen_MS774.63	0.0721	0.1026	-0.0139	9.33E-01
C36:1 PC_MS788.61	0.0543	0.1298	0.0760	6.43E-01
C36:1 PE plasmalogen_MS732.59	0.2803	0.2551	0.0718	6.62E-01
C36:1 PE_MS746.57	0.0595	0.3013	-0.1570	3.35E-01
C36:1 PS plasmalogen_MS776.57	0.0766	0.1090	-0.0991	5.45E-01
C36:2 DAG_MS643.52	0.0318	0.2575	0.1994	2.19E-01
C36:2 PC plasmalogen_MS772.62	0.0587	0.0972	-0.1545	3.43E-01
C36:2 PC_MS786.60	0.0559	0.0866	0.1425	3.83E-01
C36:2 PE plasmalogen_MS730.57	0.0700	0.1707	-0.0339	8.36E-01
C36:2 PE_MS744.55	0.0547	0.2855	-0.1164	4.77E-01
C36:2 PI_MS863.56	0.0507	0.0822	-0.0906	5.81E-01
C36:2 PS plasmalogen_MS774.56	0.0738	0.1312	0.0551	7.37E-01
C36:3 DAG_MS641.51	0.0449	0.2188	0.0389	8.13E-01
C36:3 PC plasmalogen_MS770.60	0.0552	0.1213	-0.1079	5.10E-01
C36:3 PC_MS784.58	0.0544	0.1019	0.2048	2.06E-01
C36:3 PE plasmalogen_MS728.55	0.0808	0.1683	-0.1093	5.05E-01
C36:3 PE_MS742.53	0.0761	0.4512	-0.2744	8.67E-02
C36:3 PS plasmalogen_MS772.54	0.2082	0.6202	-0.0416	8.00E-01
C36:4 DAG_MS639.49	0.0496	0.2900	-0.0307	8.52E-01
C36:4 PC plasmalogen_MS768.58	0.0618	0.0735	-0.3242	4.07E-02
C36:4 PC-A_MS782.56	0.0613	0.1802	0.0284	8.63E-01
C36:4 PC-B_MS782.56	0.0470	0.0792	0.0183	9.11E-01
C36:4 PE plasmalogen_MS726.54	0.0827	0.2185	-0.0597	7.16E-01

C36:4 PE_MS740.52	0.0902	0.2497	-0.1424	3.83E-01
C36:4 PI_MS859.52	0.0615	0.1003	0.0533	7.46E-01
C36:5 PC plasmalogen-A_MS766.57	0.0588	0.2931	0.3213	4.28E-02
C36:5 PC plasmalogen-B_MS766.57	0.0519	0.0941	0.0471	7.74E-01
C36:5 PE plasmalogen_MS724.52	0.0618	0.1843	0.1397	3.92E-01
C38:2 PC_MS814.63	0.0624	0.1266	0.1340	4.12E-01
C38:2 PE_MS772.58	0.0599	0.1129	0.0503	7.60E-01
C38:3 PC_MS812.61	0.0620	0.1352	0.4163	7.01E-03
C38:3 PE plasmalogen_MS756.59	0.1095	0.3192	-0.1717	2.92E-01
C38:4 DAG_MS669.54	0.0439	0.2931	0.1502	3.57E-01
C38:4 PC plasmalogen_MS796.62	0.0550	0.0741	0.1824	2.62E-01
C38:4 PC_MS810.59	0.0598	0.0837	0.0579	7.24E-01
C38:4 PE_MS768.55	0.0540	0.1629	-0.1588	3.30E-01
C38:4 PI_MS887.56	0.0538	0.0785	-0.0615	7.08E-01
C38:4 PS_MS812.54	0.1744	0.1762	0.1272	4.37E-01
C38:5 DAG_MS665.51	0.0412	0.1925	-0.1244	4.47E-01
C38:5 PE plasmalogen_MS752.55	0.0678	0.1437	0.1105	5.00E-01
C38:5 PE_MS766.53	0.1223	0.1656	-0.2236	1.66E-01
C38:6 PC plasmalogen_MS792.58	0.0497	0.0943	0.0672	6.82E-01
C38:6 PC_MS806.56	0.0547	0.1078	0.2233	1.67E-01
C38:6 PE plasmalogen_MS750.54	0.0650	0.1474	0.1067	5.15E-01
C38:6 PE_MS764.52	0.0587	0.1794	-0.1169	4.75E-01
C38:6 PS_MS808.50	0.2042	0.8416	0.2563	1.11E-01
C38:7 PC plasmalogen_MS790.57	0.0695	0.1213	0.2323	1.50E-01
C38:7 PE plasmalogen_MS748.52	0.0863	0.1839	0.1882	2.47E-01
C3-DC carnitine_MS248.11	0.2251	0.2510	-0.8614	2.89E-15
C3-DC-CH3 carnitine_MS262.12	0.1385	0.1458	-0.4758	1.65E-03
C4 carnitine_MS232.15	0.0489	0.1831	-0.4665	2.10E-03
C40:10 PC_MS826.53	0.0645	0.1421	0.2839	7.58E-02
C40:6 PC_MS834.59	0.0535	0.1139	0.2442	1.30E-01
C40:6 PE_MS792.55	0.0953	0.7733	0.0135	9.35E-01
C40:6 PS_MS836.53	0.0578	0.1694	0.1491	3.61E-01
C40:7 PC plasmalogen_MS818.60	0.0652	0.0782	0.1284	4.32E-01
C40:7 PE plasmalogen_MS776.55	0.0755	0.1262	0.1636	3.15E-01
C40:9 PC_MS828.55	0.0380	0.0879	0.2145	1.85E-01
C41:0 TAG_MS731.61	0.0717	20.37	0.0772	6.38E-01
C42:0 TAG_MS745.63	0.0741	39.86	0.2352	1.45E-01
C42:11 PE plasmalogen_MS796.52	0.4219	0.4971	0.0117	9.43E-01
C43:0 TAG_MS759.64	0.1553	6.004	0.2345	1.46E-01
C43:1 TAG_MS757.63	0.1113	9.216	0.2067	2.02E-01
C43:2 TAG_MS755.61	0.2216	78.85	0.2125	1.89E-01
C44:0 TAG_MS773.66	0.0428	3.948	0.2595	1.06E-01
C44:1 TAG_MS771.64	0.0339	2.229	0.2579	1.08E-01
C44:13 PE plasmalogen_MS820.52	0.1176	0.3382	-0.0474	7.73E-01
C44:2 TAG_MS769.63	0.0531	3.611	0.2076	2.00E-01
C45:0 TAG_MS787.67	0.1808	10.57	0.2436	1.30E-01
C45:1 TAG_MS785.66	0.1059	1260	0.3293	3.74E-02
C45:2 TAG_MS783.64	0.2047	127.0	0.2315	1.52E-01
C45:3 TAG_MS781.63	0.1568	18.38	0.1545	3.44E-01
C46:0 TAG_MS801.69	0.0515	1.658	0.2753	8.56E-02
C46:1 TAG_MS799.67	0.0286	0.8154	0.2831	7.67E-02
C46:2 TAG_MS797.66	0.0367	0.8191	0.2304	1.53E-01
C46:3 TAG_MS795.64	0.0406	0.8124	0.1957	2.28E-01

C46:4 TAG_MS793.63	0.0511	51.79	0.1283	4.32E-01
C47:0 TAG_MS815.71	0.2322	1.647	0.3015	5.84E-02
C47:1 TAG_MS813.69	0.0413	1.234	0.3792	1.52E-02
C47:2 TAG_MS811.67	0.0491	0.6639	0.2979	6.17E-02
C48:0 TAG_MS829.72	0.0412	0.7309	0.2773	8.32E-02
C48:1 TAG_MS827.70	0.0210	0.4566	0.3389	3.18E-02
C48:2 TAG_MS825.69	0.0256	0.3637	0.3274	3.87E-02
C48:3 TAG_MS823.67	0.0398	0.4215	0.2138	1.87E-01
C48:4 TAG_MS821.66	0.0367	0.5555	0.0757	6.45E-01
C48:5 TAG_MS819.64	0.0475	0.7808	0.0139	9.33E-01
C49:0 TAG_MS843.74	0.2918	1.815	0.3121	4.96E-02
C49:1 TAG_MS841.72	0.0510	0.9045	0.3177	4.53E-02
C49:2 TAG_MS839.71	0.0337	0.3113	0.3614	2.13E-02
C49:3 TAG_MS837.69	0.0359	0.2352	0.2770	8.36E-02
C4-OH carnitine_MS248.14	0.0817	0.4488	-0.4802	1.46E-03
C5 carnitine_MS246.16	0.0454	0.2045	-0.4481	3.35E-03
C5:1 carnitine_MS244.15	0.0616	0.2030	-0.6515	2.22E-06
C50:0 TAG_MS857.75	0.0269	0.5849	0.2849	7.47E-02
C50:1 TAG_MS855.74	0.0262	0.2494	0.3013	5.86E-02
C50:2 TAG_MS853.72	0.0353	0.2000	0.2624	1.02E-01
C50:3 TAG_MS851.70	0.0316	0.1572	0.2884	7.10E-02
C50:4 TAG_MS849.69	0.0316	0.1832	0.1772	2.76E-01
C50:5 TAG_MS847.67	0.0355	0.2537	0.0732	6.56E-01
C50:6 TAG_MS845.66	0.0422	0.3545	0.0159	9.23E-01
C51:0 TAG_MS871.77	32660	471.0	0.1561	3.39E-01
C51:1 TAG_MS869.75	3.307	0.5745	0.0798	6.26E-01
C52:0 TAG_MS885.78	0.0460	0.8000	0.2753	8.57E-02
C52:1 TAG_MS883.77	0.0239	0.2675	0.2957	6.37E-02
C52:2 TAG_MS881.75	0.0180	0.1275	0.2095	1.96E-01
C52:3 TAG_MS879.74	0.0183	0.0758	0.0962	5.57E-01
C52:4 TAG_MS877.72	0.0260	0.1068	-0.0030	9.86E-01
C52:5 TAG_MS875.70	0.0269	0.1288	-0.0221	8.93E-01
C52:6 TAG_MS873.69	0.0322	0.1677	0.0242	8.83E-01
C52:7 TAG_MS871.67	0.0454	0.2262	0.0269	8.70E-01
C53:2 TAG_MS895.77	0.0292	0.1701	0.2207	1.72E-01
C53:3 TAG_MS893.75	0.0387	0.1484	0.0234	8.87E-01
C54:1 TAG_MS911.80	0.0559	0.4763	0.2289	1.56E-01
C54:10 TAG_MS893.66	0.0753	0.0999	0.2913	6.80E-02
C54:2 TAG_MS909.78	0.0436	0.2058	0.1592	3.29E-01
C54:3 TAG_MS907.77	0.0293	0.1326	0.0165	9.20E-01
C54:4 TAG_MS905.75	0.0323	0.1222	-0.1658	3.09E-01
C54:5 TAG_MS903.74	0.0221	0.1797	-0.2432	1.31E-01
C54:6 TAG_MS901.72	0.0276	0.1848	-0.2453	1.28E-01
C54:7 TAG_MS899.70	0.0666	0.1901	0.0063	9.69E-01
C54:8 TAG_MS897.69	0.0577	0.2066	0.0458	7.80E-01
C54:9 TAG_MS895.67	0.1197	0.7597	-0.0470	7.75E-01
C55:2 TAG_MS923.80	0.0593	0.2914	0.1458	3.72E-01
C55:3 TAG_MS921.78	0.0347	0.1892	-0.0045	9.78E-01
C56:1 TAG_MS939.83	0.0682	1.197	0.1101	5.01E-01
C56:10 TAG_MS921.69	0.0572	0.4004	-0.0775	6.36E-01
C56:2 TAG_MS937.81	0.0420	0.3009	0.0948	5.63E-01
C56:3 TAG_MS935.80	0.0386	0.2726	0.0132	9.36E-01
C56:4 TAG_MS933.78	0.0343	0.1466	-0.0834	6.11E-01

C56:5 TAG_MS931.77	0.0258	0.1262	-0.1870	2.50E-01
C56:6 TAG_MS929.75	0.0238	0.0884	-0.2523	1.17E-01
C56:7 TAG_MS927.74	0.0174	0.1312	-0.0890	5.87E-01
C56:8 TAG_MS925.72	0.0325	0.1325	-0.0787	6.31E-01
C56:9 TAG_MS923.70	0.0382	0.1606	-0.0844	6.07E-01
C58:10 TAG_MS949.72	0.0337	0.1943	-0.1550	3.42E-01
C58:11 TAG_MS947.71	0.0549	0.3536	-0.0915	5.77E-01
C58:6 TAG_MS957.78	0.0285	0.1759	-0.1449	3.75E-01
C58:7 TAG_MS955.77	0.0230	0.1661	-0.1191	4.67E-01
C58:8 TAG_MS953.75	0.0574	0.2672	-0.0990	5.46E-01
C58:9 TAG_MS951.73	0.0337	0.1708	-0.1432	3.80E-01
C5-DC carnitine_MS276.14	0.0812	0.1955	-0.7332	1.27E-08
C6 carnitine_MS260.18	0.0422	0.4034	-0.1723	2.90E-01
C60:12 TAG_MS973.72	0.0517	0.4917	-0.0020	9.90E-01
C7 carnitine_MS274.20	0.1254	0.4508	-0.4771	1.59E-03
C8 carnitine_MS288.21	0.1138	1.145	-0.2866	7.29E-02
C9 carnitine_MS302.23	0.0853	0.2761	-0.5261	3.76E-04
Capric acid_MS171.13	0.0481	0.3395	0.1582	3.32E-01
caprylic acid_MS143.10	0.1117	0.7771	0.2184	1.77E-01
Caprylic acid_MS143.10	0.0603	0.4582	0.1919	2.37E-01
carnitine_MS162.11	0.0382	0.0683	0.0382	8.16E-01
chenodeoxycholate/deoxycholate_MS391.28	0.0914	1.015	0.1920	2.37E-01
Chenodeoxycholate_MS391.28	0.2052	1.735	0.1643	3.13E-01
Cholate_MS407.28	0.1272	341.7	0.1272	4.37E-01
choline_MS104.10	0.0379	0.1143	-0.7388	8.17E-09
citrate/isocitrate_MS191.01	0.0306	0.0635	-0.3356	3.37E-02
citrulline_MS176.10	0.0433	0.1461	-0.6755	5.96E-07
CMPF_MS239.09	0.0391	0.2312	0.0478	7.71E-01
cortisol_MS363.21	0.1052	0.3600	-0.3718	1.75E-02
cotinine_MS177.10	1.155	54943	0.2304	1.53E-01
creatine_MS132.07	0.0555	0.1876	0.3704	1.80E-02
creatinine_MS114.06	0.0398	0.0510	-0.8307	4.47E-13
cystathionine_MS221.06	0.1033	0.2400	-0.6781	5.13E-07
cytosine_MS112.05	0.6773	0.9275	0.0489	7.66E-01
Deoxycholate_MS391.28	0.1034	1.475	0.0689	6.75E-01
dihydroorotate_MS157.02	0.4432	0.5615	-0.1664	3.07E-01
dimethylglycine_MS104.07	0.0324	0.1464	-0.5953	3.02E-05
DMGV_MS202.11	0.0386	0.1696	-0.5534	1.50E-04
Docosahexaenoic acid_MS327.23	0.1030	0.4900	0.2713	9.05E-02
Docosapentaenoic acid_MS329.24	0.1065	0.7092	0.1975	2.24E-01
Dodecanedioic acid_MS229.14	0.0630	0.3375	-0.2866	7.29E-02
Dodecanoic acid_MS199.16	0.0616	0.6529	0.1046	5.23E-01
ectoine_MS143.08	0.0543	0.8215	-0.6433	3.39E-06
Eicosadienoic acid_MS307.26	0.0764	0.5949	0.0854	6.02E-01
eicosapentaenoic acid_MS301.21	0.0729	0.8111	0.2826	7.72E-02
Eicosapentaenoic acid_MS301.21	0.0968	0.5359	0.1925	2.36E-01
Erucic acid_MS337.31	0.1094	0.4562	0.0324	8.44E-01
erythronic acid_MS135.02	0.0879	0.1816	-0.3550	2.40E-02
fructose/glucose/galactose_MS179.05	0.0459	0.1327	-0.1559	3.39E-01
fucose_MS163.06	0.0308	0.1211	0.5076	6.66E-04
fumarate/maleate_MS115.00	467.8	5816	-0.1058	5.18E-01
GABA_MS104.07	0.2339	0.2457	-0.2983	6.13E-02
Gamma-Linolenic acid_MS277.21	0.1088	1.638	0.1921	2.37E-01

gentisate_MS153.01	0.1460	0.4791	-0.5124	5.77E-04
gluconolactone_MS177.04	0.1060	0.1476	0.4557	2.77E-03
glucose_MS163.06	0.5136	0.3887	-0.3621	2.11E-02
glucuronate_MS193.03	0.1162	0.1163	-0.7595	1.43E-09
glutamate_MS146.04	0.0373	0.1748	0.0698	6.71E-01
glutamate_MS148.06	0.0327	0.1796	-0.0006	9.97E-01
glutamine_MS147.07	0.0338	0.0965	0.0640	6.97E-01
glyceric acid_MS105.01	0.0526	0.1144	-0.0864	5.98E-01
glycine_MS76.039	0.0381	0.1349	-0.2712	9.06E-02
Glycochenodeoxycholate_MS448.30	0.0837	24.23	0.0130	9.37E-01
Glycocholate_MS464.30	0.0996	17.40	-0.2239	1.66E-01
glycocholate_MS464.30	0.1215	1.430	-0.2575	1.09E-01
glycodeoxycholate/glycochenodeoxycholate_MS448.30	0.1026	11.87	0.0453	7.83E-01
Glycodeoxycholate_MS448.30	0.0943	140.2	-0.0378	8.18E-01
Glycolithocholate_MS432.31	0.1046	7.72E+27	-0.0511	7.56E-01
Glycoursodeoxycholate_MS448.30	0.1127	4296683	0.2371	1.42E-01
guanidoacetic acid_MS118.06	0.0536	0.1518	0.0270	8.70E-01
Hexadecanedioic acid_MS285.20	0.0673	0.2110	-0.1085	5.08E-01
hippurate_MS178.05	0.0534	1.242	-0.5653	9.74E-05
histamine_MS112.08	0.1574	0.2353	-0.0294	8.58E-01
histidine_MS156.07	0.0514	0.1052	-0.0562	7.32E-01
homocysteine_MS136.04	0.2514	0.3528	-0.3500	2.62E-02
homovanillate_MS181.05	0.0611	0.1642	-0.5686	8.63E-05
Hydrocinnamic acid_MS149.05	0.2907	0.8687	0.0655	6.90E-01
hydrocinnamic acid_MS149.06	0.1059	0.7408	-0.0604	7.13E-01
hydroxyphenylacetate_MS151.04	0.0702	0.9745	-0.6772	5.40E-07
hydroxyproline_MS132.06	0.0496	0.2309	-0.6504	2.36E-06
hypoxanthine_MS135.03	0.1396	0.6133	0.1649	3.11E-01
Ibuprofen_MS205.12	0.1477	260.2	0.2868	7.27E-02
Imidazoleacetic acid_MS127.05	0.8465	3.586	-0.6270	7.49E-06
indole-3-propionate_MS188.07	0.0785	1.165	0.0383	8.16E-01
indolelactate_MS204.06	0.0595	0.1657	-0.6432	3.41E-06
indoxylsulfate_MS212.00	0.0552	0.3386	-0.5270	3.65E-04
inosine-15N4_MS271.06	0.0783	0.0820	0.2454	1.28E-01
inositol_MS179.05	0.0818	0.1520	-0.7746	3.49E-10
isovaleric acid_MS101.06	0.1212	0.3766	0.0329	8.41E-01
kynurenic acid_MS190.04	0.1001	0.2279	-0.7543	2.26E-09
kynurenine_MS207.07	0.4353	0.6422	-0.4015	9.65E-03
lactate_MS89.024	0.0357	0.2687	0.1274	4.36E-01
lactose/sucrose/trehalose_MS341.10	0.0980	0.5457	-0.7003	1.30E-07
Linoleic acid_MS279.23	0.0657	0.5403	0.2030	2.10E-01
Lithocholate_MS375.28	0.1782	0.6891	-0.1192	4.66E-01
L-threo-sphingosine_MS300.28	0.3432	0.4771	0.2547	1.13E-01
lysine_MS147.11	0.0322	0.1177	0.1252	4.44E-01
malate_MS133.01	0.0325	0.1476	-0.2448	1.29E-01
MDA_MS71.013	0.1090	0.3553	0.1931	2.34E-01
methionine sulfoxide_MS166.05	0.0665	0.2829	-0.3723	1.74E-02
methionine_MS150.05	0.0460	0.1483	-0.2015	2.14E-01
methylcysteine_MS134.02	0.1876	0.3901	-0.1886	2.46E-01
methylmalonate_MS117.01	0.1080	0.1188	-0.5318	3.12E-04
methylthioadenosine_MS298.09	8.574	0.9440	-0.4854	1.26E-03
Myristic acid_MS227.20	0.0626	0.3987	0.2247	1.64E-01
Myristoleic acid_MS225.18	0.0952	39.13	0.3009	5.90E-02

N6-acetyl-L-lysine_MS187.10	0.0813	0.1142	-0.5839	4.79E-05
N6-Acetyl-L-lysine_MS189.12	0.0435	0.0848	-0.7425	6.07E-09
N-acetylputrescine_MS131.11	0.0506	0.1190	-0.7080	7.78E-08
N-alpha-Acetyl-L-arginine_MS217.12	0.0481	0.1726	-0.4487	3.30E-03
N-alpha-acetyl-L-ornithine_MS175.10	0.0781	116.2	-0.3358	3.36E-02
N-carbamoyl-beta-alanine_MS133.06	0.1270	0.1665	-0.7182	3.83E-08
Ne-Ne dimethyllysine_MS173.12	0.2455	0.4331	-0.3031	5.70E-02
NH4_51:2 TAG_MS862.78	1.635	0.6935	0.1790	2.71E-01
NH4_51:5 TAG_MS860.77	2.498	0.9119	0.2180	1.78E-01
NH4_C14:0 CE_MS614.58	0.0533	0.2180	0.2467	1.25E-01
NH4_C16:0 CE_MS642.61	0.0423	0.0726	0.0785	6.32E-01
NH4_C16:1 CE_MS640.60	0.0256	0.0840	0.2300	1.54E-01
NH4_C18:0 CE_MS670.65	0.0440	0.0800	0.2293	1.56E-01
NH4_C18:1 CE_MS668.63	0.0344	0.0688	0.0187	9.09E-01
NH4_C18:2 CE_MS666.61	0.0341	0.0547	0.0442	7.88E-01
NH4_C18:3 CE_MS664.60	0.0415	0.1052	0.0987	5.47E-01
NH4_C20:3 CE_MS692.63	0.0390	0.0939	0.2630	1.01E-01
NH4_C20:4 CE_MS690.61	0.0252	0.0649	-0.0481	7.70E-01
NH4_C20:5 CE_MS688.60	0.0494	0.1631	0.2347	1.46E-01
NH4_C22:4 CE_MS718.64	0.2079	0.4293	-0.2021	2.13E-01
NH4_C22:5 CE_MS716.63	0.0599	0.1288	-0.0818	6.18E-01
NH4_C22:6 CE_MS714.61	0.0464	0.1061	0.1291	4.30E-01
NH4_C32:0 DAG_MS586.54	0.0637	1.006	0.2859	7.37E-02
NH4_C32:1 DAG_MS584.52	0.0870	0.8565	0.2915	6.78E-02
NH4_C32:2 DAG_MS582.50	0.4882	0.7575	0.1781	2.74E-01
NH4_C34:0 DAG_MS614.57	0.1021	0.5383	0.2781	8.24E-02
NH4_C34:1 DAG_MS612.55	0.0707	0.3227	0.2872	7.23E-02
NH4_C34:2 DAG_MS610.54	0.0595	0.2744	0.2494	1.21E-01
NH4_C34:3 DAG_MS608.52	0.1658	0.6203	0.2496	1.21E-01
NH4_C36:1 DAG_MS640.58	0.0721	0.4337	0.2747	8.64E-02
NH4_C36:2 DAG_MS638.57	0.0505	0.2955	0.2045	2.07E-01
NH4_C36:3 DAG_MS636.55	0.0654	0.2672	0.1005	5.39E-01
NH4_C36:4 DAG_MS634.54	0.0593	0.3271	-0.0103	9.50E-01
NH4_C38:5 DAG_MS660.55	0.0727	0.2588	-0.0538	7.43E-01
NH4_C41:0 TAG_MS726.66	0.4629		0.0897	5.84E-01
NH4_C42:0 TAG_MS740.67	0.1306	3894	0.2391	1.38E-01
NH4_C43:0 TAG_MS754.69	0.2321	166.2	0.1732	2.87E-01
NH4_C43:1 TAG_MS752.67	0.4569	73.33	-0.0391	8.12E-01
NH4_C44:0 TAG_MS768.70	0.0768	62.37	0.2274	1.59E-01
NH4_C44:1 TAG_MS766.69	0.0526	16.13	0.2297	1.55E-01
NH4_C44:2 TAG_MS764.67	0.0763	1909	0.2043	2.08E-01
NH4_C45:0 TAG_MS782.72	0.2223	93.14	0.2759	8.50E-02
NH4_C45:1 TAG_MS780.70	0.1594	3.787	0.2624	1.02E-01
NH4_C45:2 TAG_MS778.69	0.2773	10.05	0.1556	3.40E-01
NH4_C45:3 TAG_MS776.67	0.1676	2.278	-0.1092	5.05E-01
NH4_C46:0 TAG_MS796.73	0.0577	1.463	0.2799	8.02E-02
NH4_C46:1 TAG_MS794.72	0.0630	1.165	0.2543	1.14E-01
NH4_C46:2 TAG_MS792.70	0.0600	1.314	0.2017	2.14E-01
NH4_C46:3 TAG_MS790.69	0.0673	4.986	0.1706	2.95E-01
NH4_C46:4 TAG_MS788.67	0.0947	14.39	0.1470	3.68E-01
NH4_C47:0 TAG_MS810.75	0.1422	1.853	0.3130	4.88E-02
NH4_C47:1 TAG_MS808.73	0.0745	6.657	0.2980	6.16E-02
NH4_C47:2 TAG_MS806.72	0.1054	1.918	0.2430	1.31E-01

NH4_C48:0 TAG_MS824.77	0.0441	0.6554	0.2852	7.44E-02
NH4_C48:1 TAG_MS822.75	0.0269	0.4822	0.3182	4.50E-02
NH4_C48:2 TAG_MS820.73	0.0586	0.4553	0.2743	8.68E-02
NH4_C48:3 TAG_MS818.72	0.0677	0.6457	0.1632	3.17E-01
NH4_C48:4 TAG_MS816.70	0.0562	0.8447	0.0626	7.03E-01
NH4_C48:5 TAG_MS814.69	0.0725	2.056	0.0256	8.76E-01
NH4_C49:0 TAG_MS838.78	0.1209	196177792	0.2721	8.95E-02
NH4_C49:1 TAG_MS836.77	0.0347	0.5172	0.3296	3.73E-02
NH4_C49:2 TAG_MS834.75	0.0486	0.3759	0.3098	5.14E-02
NH4_C49:3 TAG_MS832.73	0.0562	0.4265	0.2305	1.53E-01
NH4_C50:0 TAG_MS852.80	0.0562	0.7121	0.2858	7.37E-02
NH4_C50:1 TAG_MS850.78	0.0444	0.2959	0.2951	6.43E-02
NH4_C50:2 TAG_MS848.77	0.0408	0.2275	0.2700	9.22E-02
NH4_C50:3 TAG_MS846.75	0.0550	0.2435	0.2540	1.14E-01
NH4_C50:4 TAG_MS844.73	0.0660	0.3318	0.1448	3.75E-01
NH4_C50:5 TAG_MS842.72	0.0676	0.3889	0.0735	6.54E-01
NH4_C50:6 TAG_MS840.70	0.0579	0.5626	-0.0050	9.76E-01
NH4_C51:0 TAG_MS866.81	0.6187	0.4415	0.1323	4.18E-01
NH4_C51:1 TAG_MS864.80	1.883	0.7262	0.1339	4.12E-01
NH4_C52:0 TAG_MS880.83	0.0744	1.563	0.2754	8.55E-02
NH4_C52:1 TAG_MS878.81	0.0518	0.4222	0.2865	7.30E-02
NH4_C52:2 TAG_MS876.80	0.0340	0.2180	0.2120	1.90E-01
NH4_C52:3 TAG_MS874.78	0.0378	0.1807	0.1151	4.82E-01
NH4_C52:4 TAG_MS872.76	0.0475	0.1999	0.0376	8.19E-01
NH4_C52:5 TAG_MS870.75	0.0537	0.2220	0.0434	7.92E-01
NH4_C52:6 TAG_MS868.73	0.0659	0.2836	0.0487	7.67E-01
NH4_C52:7 TAG_MS866.72	0.0648	0.3554	-0.0006	9.97E-01
NH4_C53:2 TAG_MS890.81	0.0561	0.2756	0.2428	1.32E-01
NH4_C53:3 TAG_MS888.80	0.0568	0.1893	0.1460	3.71E-01
NH4_C54:1 TAG_MS906.84	0.0743	0.5231	0.2271	1.60E-01
NH4_C54:2 TAG_MS904.83	0.0663	0.3143	0.1836	2.59E-01
NH4_C54:3 TAG_MS902.81	0.0510	0.2547	0.0816	6.19E-01
NH4_C54:4 TAG_MS900.80	0.0532	0.2256	-0.0331	8.40E-01
NH4_C54:5 TAG_MS898.78	0.0354	0.2456	-0.1135	4.88E-01
NH4_C54:6 TAG_MS896.76	0.0535	0.2728	-0.1039	5.26E-01
NH4_C54:7 TAG_MS894.75	0.0488	0.2340	0.0819	6.18E-01
NH4_C54:8 TAG_MS892.73	0.2191	0.3817	0.0936	5.68E-01
NH4_C55:2 TAG_MS918.84	0.1070	1.820	0.1833	2.59E-01
NH4_C55:3 TAG_MS916.83	0.0625	0.3858	0.1463	3.70E-01
NH4_C56:1 TAG_MS934.87	0.1097	768.7	0.2756	8.52E-02
NH4_C56:10 TAG_MS916.74	0.3800	59246664	-0.1192	4.66E-01
NH4_C56:2 TAG_MS932.86	0.0934	0.9138	0.0741	6.52E-01
NH4_C56:3 TAG_MS930.84	0.0722	0.4398	0.0614	7.08E-01
NH4_C56:5 TAG_MS926.81	0.0465	0.1885	-0.0271	8.69E-01
NH4_C56:6 TAG_MS924.80	0.0412	0.1483	-0.0943	5.65E-01
NH4_C56:7 TAG_MS922.78	0.0390	0.1772	-0.0211	8.98E-01
NH4_C56:8 TAG_MS920.77	0.0601	0.2038	0.0033	9.84E-01
NH4_C56:9 TAG_MS918.75	0.0648	0.2662	-0.0545	7.40E-01
NH4_C58:10 TAG_MS944.77	0.0574	0.2483	-0.0866	5.98E-01
NH4_C58:11 TAG_MS942.75	0.1307	0.7317	-0.0701	6.69E-01
NH4_C58:6 TAG_MS952.83	0.0579	0.2585	-0.0458	7.80E-01
NH4_C58:7 TAG_MS950.81	0.0433	0.2176	-0.0482	7.69E-01
NH4_C58:8 TAG_MS948.80	0.0414	0.2213	-0.0670	6.83E-01

NH4_C58:9 TAG_MS946.78	0.0524	0.2062	-0.0726	6.58E-01
NH4_C60:12 TAG_MS968.77	0.0487	0.3334	0.0880	5.92E-01
niacinamide_MS123.05	0.2655	0.3936	0.2537	1.15E-01
N-lauroylglycine_MS258.20	0.3088	0.1289	-0.0896	5.85E-01
NMMA_MS189.13	0.0621	0.1021	-0.3150	4.73E-02
Oleic acid_MS281.24	0.0537	0.3930	0.2087	1.98E-01
ornithine_MS133.09	0.0368	0.1572	-0.1366	4.03E-01
oxalate_MS88.988	0.1475	0.1592	-0.3770	1.59E-02
Palmitic acid_MS255.23	0.0314	0.1494	0.2140	1.86E-01
Palmitoleic acid_MS253.21	0.1081	1.639	0.2655	9.81E-02
pantothenate_MS218.10	0.0404	0.1245	-0.3684	1.87E-02
PEP_MS166.97	0.5724	0.5702	0.0118	9.43E-01
phenylacetate_MS135.04	0.1112	0.2503	-0.5030	7.64E-04
phenylalanine_MS166.08	0.0832	0.1131	-0.2512	1.18E-01
Phenyllactic acid_MS165.05	0.1064	0.3323	0.1082	5.09E-01
phenyllactic acid_MS165.05	0.0719	0.1681	-0.2277	1.59E-01
phosphocholine_MS184.07	0.0684	0.1562	-0.2214	1.71E-01
phosphoethanolamine_MS142.02	0.8161	0.6199	-0.4213	6.28E-03
phytosphingosine_MS318.30	1.415	7.187	0.2921	6.72E-02
pipecolic acid_MS130.08	0.0596	0.3167	-0.1980	2.22E-01
proline_MS116.07	0.0330	0.1207	-0.2624	1.02E-01
proline-betaine_MS144.10	0.0463	0.7541	-0.3616	2.12E-02
propionate_MS73.029	0.0886	0.1310	-0.2426	1.32E-01
putrescine_MS89.107	0.0818	0.1801	0.0070	9.66E-01
pyrocatechol_MS109.02	0.0789	0.0891	-0.1182	4.70E-01
pyroglutamic acid_MS130.04	0.0346	0.1021	0.0184	9.11E-01
pyrrolidonecarboxylic acid_MS130.04	0.1925	0.1920	-0.1856	2.53E-01
pyruvaldehyde_MS71.013	0.0883	0.1604	-0.2520	1.17E-01
pyruvate_MS87.008	0.1992	0.3545	0.2968	6.27E-02
quinic acid_MS191.05	0.0448	1.559	-0.2414	1.34E-01
quinolinate_MS166.01	0.0471	0.2137	-0.7286	1.79E-08
S-adenosylmethionine_MS399.14	0.4027	0.3788	-0.3392	3.17E-02
salicylurate_MS194.04	0.0534	155.1	-0.4005	9.87E-03
sarcosine_MS90.055	0.1012	0.1181	0.1007	5.39E-01
SDMA_MS203.15	0.0673	0.0719	-0.7930	5.19E-11
sebacate_MS201.11	0.7226	0.3346	-0.5360	2.72E-04
serine_MS106.04	0.0386	0.1147	-0.0893	5.86E-01
serotonin_MS177.10	0.1314	0.7877	0.0778	6.36E-01
sorbitol_MS181.07	0.0267	0.7602	-0.3154	4.70E-02
Sphinganine_MS302.30	0.1293	0.2174	0.2836	7.61E-02
Sphingosine 1-Phosphate_MS378.24	0.0834	0.1588	0.0574	7.26E-01
sphingosine_MS300.28	0.0842	0.1186	-0.2567	1.10E-01
Stearic acid_MS283.26	0.0463	0.0949	0.0986	5.47E-01
suberate_MS173.08	0.0543	0.2335	-0.5091	6.36E-04
succinate_MS117.01	0.0355	0.1297	0.2029	2.11E-01
taurine_MS124.00	0.0237	0.1075	-0.0885	5.89E-01
taurine_MS126.02	0.0402	0.1065	-0.2740	8.72E-02
Taurochenodeoxycholate_MS498.28	0.1046	315.8	-0.2502	1.20E-01
Taurocholate_MS514.28	0.1065	53.72	-0.3931	1.15E-02
taurodeoxycholate/taurochenodeoxycholate_MS498.28	0.1985	5.710	-0.3638	2.04E-02
Taurodeoxycholate_MS498.28	0.1273	39384	-0.2276	1.59E-01
Taurohyodeoxycholate/Tauroursodeoxycholate_MS498.28	0.2862	18.66	-0.0909	5.79E-01

Taurolithocholate_MS482.29	0.3165	1.346	-0.2073	2.01E-01
Tetradecanedioic acid_MS257.17	0.0485	0.2242	-0.0805	6.24E-01
theophylline_MS179.05	0.1554	0.7639	0.0147	9.29E-01
thiamine_MS265.11	0.0866	0.4672	-0.2020	2.13E-01
threonine_MS120.06	0.0271	0.1257	-0.1452	3.74E-01
thymine_MS125.03	0.0527	0.0764	-0.8613	2.89E-15
thyroxine_MS777.69	0.0820	0.1259	0.1183	4.70E-01
trimethylamine-N-oxide_MS76.075	0.0383	0.3376	-0.5375	2.59E-04
tryptophan_MS203.08	0.0303	0.0964	0.4391	4.16E-03
tryptophan_MS205.09	0.0314	0.0981	0.4638	2.26E-03
tyrosine_MS182.08	0.0738	0.1239	0.1208	4.60E-01
uracil_MS111.02	0.0323	0.2590	0.2602	1.05E-01
urate_MS167.02	0.0298	0.0371	-0.4128	7.58E-03
uridine_MS243.06	0.0336	0.2801	0.2863	7.32E-02
urocanic acid_MS139.05	0.8022	1.044	0.3325	3.55E-02
valine_MS118.08	0.0333	0.1146	0.1917	2.38E-01
xanthine_MS151.02	0.0940	0.1981	-0.1163	4.77E-01
xanthosine_MS285.08	0.2173	0.3807	-0.3910	1.20E-02
xanthurenate_MS204.03	0.0769	0.2765	-0.6129	1.42E-05
xylose_MS149.04	0.0455	0.1227	-0.2911	6.82E-02

Supplementary Table 4. Interplatform matched metabolites correlation, stratified by super-pathways								
	N	**Mean**	**Median**	**5% tile**	**25% tile**	**75% tile**	**95% tile**	**r>0.8**
Inter-platform correlation	381	0.805	0.889	0.231	0.782	0.936	0.974	274 (71.92)
Amino Acid	102	0.817	0.895	0.376	0.812	0.934	0.968	79 (77.45)
Carbohydrate	12	0.661	0.647	0.044	0.567	0.916	0.971	5 (41.67)
Cofactors and Vitamins	16	0.822	0.904	0.050	0.726	0.960	0.996	10 (62.50)
Energy	7	0.537	0.514	0.090	0.155	0.927	0.955	3 (42.86)
Lipid	184	0.808	0.886	0.359	0.783	0.929	0.960	134 (72.83)
Nucleotide	20	0.708	0.871	0.004	0.619	0.944	0.975	11 (55.00)
Peptide	6	0.850	0.831	0.763	0.790	0.902	0.981	3 (50.00)
Xenobiotics	34	0.901	0.921	0.695	0.855	0.976	0.993	29 (85.29)

r, Pearson correlation coefficient

Supplementary Table 5. Shared metabolites with strong correlation with eGFR			
	Metabolites	**Broad r**	**Metabolon r**
eGFR-Cr	N-acetylalanine	-0.871	-0.857
	creatinine	-0.831	-0.851
	N-acetylserine	-0.854	-0.841
	1-methylguanidine	-0.883	-0.805
	pseudouridine	-0.842	-0.829
eGFR-Cys	N-acetylalanine	-0.812	-0.856
	N-acetylserine	-0.842	-0.851
	homocitrulline	-0.829	-0.823
	N-acetylhistidine	-0.801	-0.821
	pseudouridine	-0.857	-0.845
	C-glycosyltryptophan	-0.896	-0.857
eGFR-CrCys	N-acetylalanine	-0.876	-0.890
	creatinine	-0.837	-0.830
	N-acetylserine	-0.883	-0.879
	1-methylguanidine	-0.885	-0.821
	homocitrulline	-0.845	-0.825
	N-acetylmethionine	-0.803	-0.802
	N-acetylhistidine	-0.810	-0.833
	pseudouridine	-0.883	-0.870
	N2,N2-dimethylguanosine	-0.823	-0.857
	C-glycosyltryptophan	-0.860	-0.859

eGFR, estimated glomerular filtration rate; r, Pearson's correlation coefficient; Cr, creatinine; Cys, cystatin C