# Supplementary Methods

Study Population and sample collection

Chemicals

HPLC-grade acetonitrile (ACN), methanol (MeOH), isopropanol (IPA), and methyl tert-butyl ether (MTBE) were sourced from Merck (Darmstadt, Germany), while HPLC-grade formic acid was purchased from Sigma-Aldrich. Dichloromethane (CH2Cl2) and ammonium formate were obtained from Thermo Scientific, and ultra-pure water was supplied by a Milli-Q system (Millipore, Bedford, MA, USA). Internal standards were added to the quality control (QC) samples, and detailed information about the internal standards used is provided in Table S1.

Sample Preparation

Thawing and Mixing: Samples were taken out of the -80°C freezer and placed on ice to thaw until there were no remaining ice crystals.

Aliquoting: After thawing, the samples were vortexed for 10 seconds, and 50 μL of each sample was transferred into corresponding labeled centrifuge tubes.

Lipid Extraction: 1 mL of lipid extraction solution (MTBE: MeOH = 3:1, V/V), containing internal standards, was added to the tube and vortexed for 15 minutes to extract the lipids.

Water Addition and Vortexing: After vortexing, 200 μL of water was added to the mixture, followed by vortexing for 1 minute. The samples were then centrifuged at 12,000 rpm for 10 minutes at 4°C.

Supernatant Collection: Following centrifugation, the supernatant (200 μL) was collected and concentrated to dryness.

Reconstitution: 200 μL of lipid reconstitution solution (ACN: IPA = 1:1, V/V) was added, followed by vortexing for 3 minutes and centrifuging at 12,000 rpm for 3 minutes. The supernatant was then collected and prepared for LC-MS/MS analysis.

UPLC-MS/MS

HPLC Conditions

Lipidomic analysis was performed using an ExionLC AD Ultra Performance Liquid Chromatography (UPLC) system coupled with a QTRAP®6500+ tandem mass spectrometer (SCIEX, <https://sciex.com.cn/>). Chromatographic separation was carried out on a Thermo Accucore™ C30 column (i.d. 2.1x100 mm, 2.6 μm). The mobile phase consisted of two components: Phase A, which was acetonitrile/water (60/40, V/V) containing 0.1% formic acid and 10 mmol/L ammonium formate, and Phase B, which was acetonitrile/isopropanol (10/90, V/V) with 0.1% formic acid and 10 mmol/L ammonium formate. The gradient for chromatographic separation was set as follows: 0 min (A/B 80:20, V/V), 2 min (A/B 70:30, V/V), 4 min (A/B 40:60, V/V), 9 min (A/B 15:85, V/V), 14 min (A/B 10:90, V/V), 15.5 min (A/B 5:95, V/V), 17.3 min (A/B 5:95, V/V), 17.5 min (A/B 80:20, V/V), and 20 min (A/B 80:20, V/V). The flow rate was maintained at 0.35 mL/min, and the column temperature was set at 45°C. A 2 μL sample volume was injected for analysis.

ESI-QTRAP-MS/MS

LIT and triple quadrupole (QQQ) scans were acquired on a triple quadrupole-linear ion trap mass spectrometer (QTRAP), QTRAP® LC-MS/MS System, equipped with an ESI Turbo Ion-Spray interface, operating in positive and negative ion mode and controlled by Analyst 1.6.3 software (Sciex). The ESI source operation parameters were as follows: ion source, turbo spray; source temperature 500 °C; ion spray voltage (IS) 5500 V（Positive）,-4500 V(Neagtive); ion source gas 1 (GS1), gas 2 (GS2), curtain gas (CUR) were set at 45, 55, and 35 psi, respectively; the collision gas (CAD) was medium. Instrument tuning and mass calibration were performed with 10 and 100 μmol/L polypropylene glycol solutions in QQQ and LIT modes, respectively. QQQ scans were acquired as Multiple Reaction Monitoring (MRM) experiments with collision gas (nitrogen) set to 5 psi. Declustering potential (DP) and collision energy (CE) for individual MRM transitions was done with further DP and CE optimization. A specific set of MRM transitions were monitored for each period according to the metabolites eluted within this period.

Based on the self-built database MWDB (metware database), qualitative analysis is performed on the information according to the retention time RT (Retention time) and parent ions of the detected substances. Lipid quantification is completed by using the MRM mode of triple quadrupole mass spectrometry. In the MRM mode, the quadrupole first screens the precursor ions (parent ions) of the target substance, and excludes the ions corresponding to other molecular weight substances to preliminarily eliminate interference; the precursor ions are induced by the collision chamber and then broken to form many fragment ions, and the fragment ions are then filtered through the triple quadrupole to select the required characteristic fragment ion, eliminating the interference of non-target ions, making the quantification more accurate and more repeatable. After obtaining the lipid mass spectrometry analysis data of different samples, the peak area of ​​the mass spectrum peaks of all substances is integrated, and the mass spectrum peaks of the same lipid in different samples are integrated and corrected.

Raw data processing included peak integration and cross-sample alignment using MultiQuant™ software, with chromatographic peaks manually inspected for retention time consistency and shape. Missing values were imputed as one-fifth of the minimum value per lipid feature. Quality control (QC) samples, analyzed at 10-sample intervals, demonstrated a coefficient of variation (CV) <15% for internal standards, ensuring analytical precision. Lipid species with inter-QC CV >30% were excluded. Total ion chromatogram (TIC) overlays of QC samples (Supplementary Figure S1) confirmed methodological reproducibility.

Statistical analysis

All statistical analyses were performed using R software (version 4.3.4). Baseline characteristics of neonates were summarized as means and standard deviations (mean ± SD) for continuous variables, and group comparisons were performed using the Mann-Whitney U test or Student's t-test. Categorical variables were presented as counts (percentages) and analyzed using the chi-square test. Unsupervised principal component analysis (PCA) was conducted using the prcomp function in R to explore the lipid metabolism profiles of the two groups. Differential lipid identification was based on both univariate and multivariate analyses. was utilized to execute Orthogonal partial least squares discriminant analysis (OPLS-DA) was performed using the MetaboAnalystR package in R to construct a predictive model and calculate Variable Importance in Projection (VIP) scores. Lipids with VIP > 1, fold change (FC)>1.2 or <0.83 and P-value < 0.05 were considered significant differential metabolites. Metabolic pathway enrichment analysis was performed using the Kyoto Encyclopedia of Genes and Genomes (KEGG) database. Spearman’s correlation coefficient was used to evaluate associations between neonatal lipid levels and maternal lipid profiles during early pregnancy , including TC, TG, HDL-C, and LDL-C.

# Supplementary Figures

Figure S1 QC sample TIC overlap detected by mass spectrometry. (A) QC\_MS\_TIC-overlap-N; (B) QC\_MS\_TIC- overlap -P

Figure S2 Principal component analysis (PCA) of the lipidomics data

Figure S3 Radar plots based on the top 10 lipids with the largest absolute value of log2FC



Figure S1 QC sample TIC overlap detected by mass spectrometry. (A) QC\_MS\_TIC-overlap-N; (B) QC\_MS\_TIC- overlap -P



Figure S2 Principal component analysis (PCA) of the lipidomics data



Figure S3 Radar plots based on the top 10 lipids with the largest absolute value of log2FC

# Supplementary table

## Table S1 Details of internal standard in this study

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Name | Class | CAS | Brand name | Product number | m/z | RT (min) | cv |
| LPE(14:0) | LPE | 123060-40-2 | Avanti | 856735P | 426.262064 | 1.5 | 15.99% |
| LPC(16:0)-d31 | LPC | 327178-91-6 | Avanti | 860397P | 527.3 | 2.3 | 6.49% |
| Cer(d18:1/4:0) | Cer | 74713-58-9 | Avanti | 860504P | 352.321 | 3.6 | 3.88% |
| PE(12:0/12:0) | PE | 59752-57-7 | Avanti | 850702P | 578.382182 | 4.81 | 6.62% |
| PG(12:0/12:0) | PG | 322647-27-8 | Avanti | 840435P | 609.376758 | 4.45 | 3.12% |
| PC(13:0/13:0) | PC |  71242-28-9 | Avanti | 850340P | 694.5 | 5.15 | 2.90% |
| DG(12:0/12:0/0:0)  | DG | 60562-15-4 | Avanti | 800812P | 474.425215 | 5.4 | 14.49% |
| PG(16:0-d31/18:1) | PG | 327178-87-0  | Avanti | 860384P | 778.5 | 6.12 | 9.77% |
| PS(16:0-d31/18:1) | PS | 327178-96-1 | Avanti | 860403P | 791.5 | 6.06 | 13.14% |
| PE(16:0-d31/18:1) | PE | 326495-44-7 | Avanti | 860374P | 747.5 | 6.75 | 8.85% |
| TG(12:0/12:0/12:0) | TG | 538-24-9 | Sigma-Aldrich | T4891 | 656.6 | 9.9 | 12.09% |
| TG(17:0/17:0/17:0) | TG | 2438-40-6 | Sigma-Aldrich | T2151 | 866.8 | 12.92 | 8.33% |
| CE(17:0) | CE | 24365-37-5 | Rhawn | R090798  | 656.64392 | 13.7 | 14.24% |
| FFA(16:0)-d31 | FFA | 39756-30-4 | sigma | 68277 | 286.3 | 4.25 | 9.12% |

RT, retention time; m/z, mass-to-charge ratio; CV, Coefficient of Variation

## Table S2 Lipidomic Characterization of 349 Differential Lipids between Late Preterm Neonates with Low Birth Weight and Normal Birth Weight:

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Formula | Compounds | CAS | VIP | *P* value | Fold\_Change | Type |
| C48H75O10P | PG(20:4\_22:6) | - | 4.33  | 5.13E-17 | 7.75E-02 | down |
| C21H38O4 | MG(18:2) | 67968-46-1 | 4.26  | 3.00E-08 | 1.09E+02 | up |
| C45H86NO7P | PE(O-18:0\_22:3) | - | 4.16  | 5.61E-09 | 7.17E+01 | up |
| C59H111NO4 | Cer(d26:3/33:1(2OH)) | - | 4.11  | 3.28E-07 | 1.91E+02 | up |
| C59H111NO4 | Cer(d29:2/30:2(2OH)) | - | 4.09  | 4.53E-07 | 1.51E+02 | up |
| C57H92O6 | TG(18:2\_18:3\_18:4) | - | 3.89  | 1.84E-05 | 3.34E+02 | up |
| C45H84NO8P | PE(18:2\_22:1) | - | 3.84  | 6.54E-07 | 4.74E+02 | up |
| C61H96O6 | TG(18:2\_20:4\_20:5) | - | 3.72  | 5.93E-03 | 9.44E+02 | up |
| C43H84NO7P | PE(O-16:1\_22:1) | - | 2.14  | 3.79E-05 | 7.09E-01 | down |
| C57H96O6 | TG(18:1\_18:2\_18:4) | - | 2.08  | 2.52E-04 | 4.14E+00 | up |
| C59H111NO4 | Cer(d28:3/31:1(2OH)) | - | 2.06  | 1.80E-04 | 3.00E+00 | up |
| C59H111NO4 | Cer(d17:3/42:1(2OH)) | - | 2.03  | 2.82E-04 | 3.18E+00 | up |
| C39H70O5 | DG(18:1\_18:2) | 91125-76-7 | 1.99  | 9.72E-06 | 1.99E+00 | up |
| C53H92O6 | TG(16:1\_18:1\_16:3) | - | 1.99  | 5.95E-05 | 2.29E+00 | up |
| C57H96O6 | TG(18:2\_18:2\_18:3) | - | 1.98  | 6.03E-04 | 3.81E+00 | up |
| C56H107NO5 | Cer(t26:1/30:2(2OH)) | - | 1.96  | 2.40E-05 | 2.30E+00 | up |
| C59H104O6 | TG(18:2\_18:2\_20:1) | - | 1.94  | 7.93E-05 | 2.47E+00 | up |
| C56H94O6 | TG(17:2\_18:2\_18:3) | - | 1.94  | 2.86E-05 | 3.12E+00 | up |
| C59H111NO4 | Cer(d23:2/36:2(2OH)) | - | 1.93  | 1.60E-04 | 3.66E+00 | up |
| C55H96O6 | TG(16:1\_18:2\_18:2) | - | 1.91  | 1.45E-04 | 2.39E+00 | up |
| C57H111NO4 | Cer(d29:1/28:1(2OH)) | - | 1.91  | 3.59E-05 | 2.29E+00 | up |
| C57H94O6 | TG(18:2\_18:3\_18:3) | - | 1.91  | 4.92E-04 | 4.12E+00 | up |
| C61H110O6 | TG(18:1\_22:1\_18:2) | - | 1.91  | 7.46E-04 | 3.36E+00 | up |
| C59H111NO4 | Cer(d19:3/40:1(2OH)) | - | 1.89  | 9.60E-05 | 3.23E+00 | up |
| C55H96O6 | TG(16:0\_18:2\_18:3) | - | 1.89  | 1.04E-04 | 2.36E+00 | up |
| C57H102O6 | TG(16:0\_18:0\_20:4) | - | 1.89  | 1.59E-04 | 2.47E+00 | up |
| C55H94O6 | TG(16:0\_18:2\_18:4) | - | 1.88  | 3.54E-04 | 3.12E+00 | up |
| C57H100O6 | TG(18:1\_17:2\_19:2) | - | 1.88  | 1.01E-05 | 2.14E+00 | up |
| C12H21NO4 | Carnitine C5:1 | 64681-36-3 | 1.88  | 1.20E-04 | 1.21E+00 | up |
| C59H102O6 | TG(20:0\_18:3\_18:3) | - | 1.87  | 7.25E-04 | 2.36E+00 | up |
| C15H29NO4 | Carnitine C8:0 | 25243-95-2 | 1.87  | 1.20E-04 | 1.38E+00 | up |
| C39H76NO8P | LNAPE(16:0/N-18:1) | - | 1.85  | 3.88E-04 | 1.75E+00 | up |
| C63H114O6 | TG(18:1\_24:1\_18:2) | - | 1.84  | 3.08E-05 | 1.95E+00 | up |
| C55H94O6 | TG(16:1\_18:2\_18:3) | - | 1.84  | 1.69E-04 | 2.85E+00 | up |
| C56H105NO5 | Cer(t18:2/38:2(2OH)) | - | 1.84  | 3.20E-05 | 2.40E+00 | up |
| C39H68O5 | DG(18:2\_18:2) | - | 1.83  | 2.13E-04 | 2.71E+00 | up |
| C55H98O6 | TG(16:0\_18:2\_18:2) | - | 1.83  | 5.68E-05 | 1.99E+00 | up |
| C63H106O6 | TG(18:1\_18:2\_24:5) | - | 1.83  | 1.46E-03 | 3.70E+00 | up |
| C57H98O6 | TG(16:0\_18:2\_20:4) | - | 1.83  | 4.43E-04 | 3.12E+00 | up |
| C42H79NO3 | Cer(d18:1/24:2) | - | 1.82  | 2.28E-04 | 1.50E+00 | up |
| C61H98O6 | TG(18:2\_20:4\_20:4) | - | 1.82  | 7.53E-04 | 3.62E+00 | up |
| C57H98O6 | TG(18:1\_18:2\_18:3) | - | 1.82  | 4.72E-05 | 2.59E+00 | up |
| C41H78NO8P | PE(20:2\_16:0) | - | 1.82  | 2.09E-04 | 1.78E+00 | up |
| C41H79NO3 | Cer(d18:1/23:1) | - | 1.82  | 4.93E-04 | 1.73E+00 | up |
| C55H98O6 | TG(16:1\_18:1\_18:2) | - | 1.82  | 8.72E-05 | 1.96E+00 | up |
| C17H29NO4 | Carnitine C10:2 | - | 1.81  | 3.55E-04 | 1.40E+00 | up |
| C13H23NO4 | Carnitine C6:1 | - | 1.81  | 2.52E-03 | 1.81E+00 | up |
| C59H108O6 | TG(18:1\_18:2\_20:0) | - | 1.80  | 2.28E-05 | 2.04E+00 | up |
| C39H76NO8P | PE(16:0\_18:1) | - | 1.80  | 6.90E-04 | 1.82E+00 | up |
| C57H104O6 | TG(18:0\_18:1\_18:2) | - | 1.80  | 1.28E-04 | 1.73E+00 | up |
| C54H94O6 | TG(15:1\_18:1\_18:3) | - | 1.79  | 7.09E-05 | 2.05E+00 | up |
| C61H98O6 | TG(18:2\_18:2\_22:6) | - | 1.79  | 1.17E-03 | 3.53E+00 | up |
| C57H100O6 | TG(18:1\_18:2\_18:2) | - | 1.79  | 3.29E-05 | 2.20E+00 | up |
| C57H102O6 | TG(18:1\_18:1\_18:2) | - | 1.77  | 9.53E-06 | 1.86E+00 | up |
| C42H76NO10P | PS(16:0\_20:3) | - | 1.77  | 7.96E-04 | 1.73E+00 | up |
| C57H111NO4 | Cer(d25:2/32:0(2OH)) | - | 1.77  | 5.12E-05 | 2.13E+00 | up |
| C57H111NO4 | Cer(d24:2/33:0(2OH)) | - | 1.77  | 1.62E-04 | 1.90E+00 | up |
| C57H109NO4 | Cer(d22:2/35:1(2OH)) | - | 1.77  | 7.52E-05 | 2.54E+00 | up |
| C59H113NO4 | Cer(d23:2/36:1(2OH)) | - | 1.77  | 7.80E-05 | 2.29E+00 | up |
| C46H88NO7P | PC(O-18:0\_20:3) | - | 1.77  | 6.84E-04 | 7.84E-01 | down |
| C44H84NO7P | PC(O-18:1\_18:2) | 155575-01-2 | 1.76  | 4.02E-04 | 7.92E-01 | down |
| C55H96O6 | TG(16:1\_18:1\_18:3) | - | 1.76  | 9.20E-05 | 2.24E+00 | up |
| C59H113NO4 | Cer(d28:2/31:1(2OH)) | - | 1.75  | 3.91E-05 | 2.38E+00 | up |
| C40H77NO3 | Cer(d18:1/22:1) | - | 1.75  | 9.66E-04 | 1.67E+00 | up |
| C40H72O4 | DG(O-19:2\_18:2) | - | 1.74  | 1.63E-04 | 2.50E+00 | up |
| C46H87NO8 | HexCer(d18:1/22:1) | - | 1.74  | 1.50E-03 | 1.66E+00 | up |
| C53H92O6 | TG(12:0\_16:0\_22:5) | - | 1.73  | 5.63E-03 | 2.94E+00 | up |
| C61H110O6 | TG(18:1\_18:1\_22:2) | - | 1.73  | 2.98E-04 | 1.82E+00 | up |
| C53H92O6 | TG(16:0\_16:1\_18:4) | - | 1.73  | 2.97E-03 | 2.81E+00 | up |
| C31H58O6 | TG(8:0\_10:0\_10:0) | - | 1.72  | 2.70E-03 | 3.77E+00 | up |
| C56H107NO5 | Cer(t22:1/34:2(2OH)) | - | 1.72  | 4.73E-05 | 1.89E+00 | up |
| C59H113NO4 | Cer(d26:2/33:1(2OH)) | - | 1.72  | 4.52E-05 | 2.28E+00 | up |
| C57H111NO4 | Cer(d26:2/31:0(2OH)) | - | 1.71  | 1.50E-04 | 2.08E+00 | up |
| C57H111NO4 | Cer(d27:1/30:1(2OH)) | - | 1.71  | 5.85E-04 | 1.99E+00 | up |
| C27H56NO6P | LPE(P-22:0) | - | 1.71  | 1.11E-03 | 3.12E+00 | up |
| C59H113NO4 | Cer(d27:2/32:1(2OH)) | - | 1.71  | 9.52E-05 | 2.31E+00 | up |
| C59H110O6 | TG(18:0\_18:2\_20:0) | - | 1.70  | 1.95E-04 | 2.05E+00 | up |
| C59H104O6 | TG(18:0\_18:3\_20:2) | - | 1.69  | 6.89E-04 | 1.95E+00 | up |
| C41H80NO7P | PE(O-18:0\_18:2) | - | 1.69  | 1.37E-03 | 2.96E+00 | up |
| C42H78NO7P | PE(P-17:0\_20:3) | - | 1.69  | 8.45E-04 | 1.67E+00 | up |
| C62H114O6 | TG(23:0\_18:1\_18:2) | - | 1.68  | 4.40E-04 | 2.32E+00 | up |
| C59H106O6 | TG(16:0\_18:1\_22:3) | - | 1.68  | 1.51E-04 | 1.60E+00 | up |
| C57H94O6 | TG(18:1\_16:2\_20:5) | - | 1.68  | 1.27E-02 | 4.83E+00 | up |
| C39H72O5 | DG(18:1\_18:1) | - | 1.68  | 1.58E-04 | 1.64E+00 | up |
| C59H115NO4 | Cer(d17:2/42:0(2OH)) | - | 1.67  | 2.01E-05 | 1.89E+00 | up |
| C59H102O6 | TG(18:2\_18:2\_20:2) | - | 1.66  | 5.08E-04 | 2.04E+00 | up |
| C59H106O6 | TG(18:1\_18:2\_20:1) | - | 1.66  | 2.33E-04 | 1.91E+00 | up |
| C41H82NO7P | PE(P-18:0\_18:0) | - | 1.65  | 1.30E-03 | 2.70E+00 | up |
| C41H82NO7P | PE(O-18:0\_18:1) | - | 1.65  | 1.39E-03 | 2.65E+00 | up |
| C61H112O6 | TG(18:1\_18:2\_22:0) | - | 1.64  | 1.02E-04 | 2.35E+00 | up |
| C15H27NO4 | Carnitine C8:1 | - | 1.64  | 1.55E-03 | 1.41E+00 | up |
| C57H111NO4 | Cer(d17:2/40:0(2OH)) | - | 1.64  | 1.57E-04 | 1.89E+00 | up |
| C63H108O6 | TG(20:0\_18:1\_22:6) | - | 1.64  | 5.38E-03 | 2.52E+00 | up |
| C55H100O6 | TG(16:0\_18:1\_18:2) | - | 1.64  | 1.52E-04 | 1.56E+00 | up |
| C57H92O6 | TG(16:1\_16:2\_22:6) | - | 1.63  | 4.47E-03 | 2.83E+00 | up |
| C59H113NO4 | Cer(d21:1/38:2(2OH)) | - | 1.62  | 3.34E-04 | 2.11E+00 | up |
| C44H78NO8P | PC(18:2\_18:3) | 85046-19-1 | 1.62  | 1.14E-04 | 1.74E+00 | up |
| C56H98O6 | TG(17:1\_18:2\_18:2) | - | 1.62  | 3.38E-04 | 2.58E+00 | up |
| C45H86NO8P | PE(18:1\_22:1) | - | 1.62  | 1.15E-03 | 2.68E+00 | up |
| C56H107NO5 | Cer(t18:1/38:2(2OH)) | - | 1.61  | 1.05E-04 | 1.84E+00 | up |
| C13H25NO4 | Carnitine C6:0 | 6418-78-6 | 1.61  | 1.06E-03 | 1.33E+00 | up |
| C61H102O6 | TG(18:2\_18:2\_22:4) | - | 1.61  | 1.92E-03 | 2.79E+00 | up |
| C59H113NO4 | Cer(d17:2/42:1(2OH)) | - | 1.61  | 7.49E-05 | 2.12E+00 | up |
| C23H45NO4 | Carnitine C16:0 | 2364-67-2 | 1.61  | 2.23E-03 | 7.05E-01 | down |
| C63H104O6 | TG(18:2\_18:2\_24:5) | - | 1.60  | 4.23E-03 | 5.13E+00 | up |
| C21H41NO4 | Carnitine C14:0 | 25597-07-3 | 1.60  | 5.09E-03 | 7.15E-01 | down |
| C57H96O6 | TG(16:0\_18:2\_20:5) | - | 1.60  | 7.14E-03 | 3.49E+00 | up |
| C56H100O6 | TG(17:1\_18:1\_18:2) | - | 1.60  | 2.61E-04 | 1.79E+00 | up |
| C43H70NO10P | PS(17:0\_21:0) | - | 1.60  | 9.12E-04 | 1.21E+00 | up |
| C61H114O6 | TG(18:0\_22:0\_18:2) | - | 1.60  | 9.39E-04 | 2.88E+00 | up |
| C63H116O6 | TG(24:0\_18:1\_18:2) | - | 1.59  | 2.19E-04 | 2.24E+00 | up |
| C59H113NO4 | Cer(d30:2/29:1(2OH)) | - | 1.59  | 1.55E-05 | 2.42E+00 | up |
| C63H106O6 | TG(18:1\_20:3\_22:4) | - | 1.59  | 1.38E-03 | 2.55E+00 | up |
| C43H80NO7P | PE(P-16:0\_22:3) | - | 1.59  | 1.24E-03 | 7.34E-01 | down |
| C61H96O6 | TG(18:2\_18:3\_22:6) | - | 1.59  | 3.15E-03 | 3.91E+00 | up |
| C48H94NO8P | PC(18:1\_22:0) | - | 1.59  | 2.54E-04 | 1.31E+00 | up |
| C40H77NO12S | SHexCer(d18:1/16:0(OH)) | - | 1.59  | 2.64E-03 | 1.96E+00 | up |
| C59H113NO4 | Cer(d24:2/35:1(2OH)) | - | 1.59  | 6.07E-05 | 2.20E+00 | up |
| C43H84NO7P | PE(O-20:0\_18:2) | - | 1.58  | 2.18E-03 | 1.88E+00 | up |
| C45H84NO10P | PS(18:0\_22:0) | - | 1.58  | 4.91E-04 | 1.23E+00 | up |
| C58H102O6 | TG(19:1\_18:2\_18:2) | - | 1.57  | 3.78E-04 | 2.48E+00 | up |
| C59H113NO4 | Cer(d29:1/30:2(2OH)) | - | 1.57  | 1.43E-05 | 2.37E+00 | up |
| C39H78NO7P | PE(O-16:0\_18:1) | - | 1.56  | 2.06E-03 | 2.04E+00 | up |
| C61H104O6 | TG(18:1\_18:2\_22:4) | - | 1.56  | 8.36E-04 | 2.13E+00 | up |
| C61H112O6 | TG(18:1\_18:1\_22:1) | - | 1.55  | 8.81E-04 | 1.95E+00 | up |
| C47H78O2 | CE(20:3) | 7274-08-0 | 1.55  | 1.67E-03 | 8.22E-01 | down |
| C58H109NO5 | Cer(t18:2/40:2(2OH)) | - | 1.55  | 1.14E-04 | 1.74E+00 | up |
| C58H102O6 | TG(18:1\_18:2\_19:2) | - | 1.55  | 7.79E-04 | 2.08E+00 | up |
| C37H68O5 | DG(16:0\_18:2) | 51621-26-2 | 1.55  | 5.91E-04 | 1.61E+00 | up |
| C61H96O6 | TG(18:3\_20:4\_20:4) | - | 1.55  | 1.49E-03 | 3.46E+00 | up |
| C45H88NO8P | PC(19:0\_18:1) | - | 1.55  | 6.65E-04 | 1.23E+00 | up |
| C45H84NO7P | PE(P-18:0\_22:3) | - | 1.54  | 3.03E-03 | 2.26E+00 | up |
| C63H106O6 | TG(16:0\_20:3\_24:5) | - | 1.54  | 4.92E-03 | 3.39E+00 | up |
| C46H84NO10P | PS(18:1\_22:2) | - | 1.54  | 6.99E-04 | 1.25E+00 | up |
| C48H95O10P | PG(20:0\_22:0) | - | 1.53  | 2.97E-04 | 1.32E+00 | up |
| C45H82NO10P | PS(21:0\_18:3) | - | 1.52  | 2.04E-04 | 1.50E+00 | up |
| C26H43NO6 | Glycocholic acid | 475-31-0 | 1.52  | 1.25E-03 | 1.34E+00 | up |
| C56H98O6 | TG(17:0\_18:2\_18:3) | - | 1.52  | 3.89E-04 | 1.96E+00 | up |
| C54H96O6 | TG(15:1\_18:1\_18:2) | - | 1.52  | 6.19E-04 | 1.47E+00 | up |
| C53H92O6 | TG(16:1\_16:1\_18:3) | - | 1.52  | 8.18E-04 | 2.36E+00 | up |
| C59H96O6 | TG(18:1\_18:3\_20:5) | - | 1.52  | 1.39E-02 | 5.47E+00 | up |
| C56H107NO5 | Cer(t24:1/32:2(2OH)) | - | 1.51  | 1.18E-03 | 1.79E+00 | up |
| C45H84NO8P | PE(18:1\_22:2) | - | 1.51  | 1.84E-03 | 1.84E+00 | up |
| C46H91O10P | PG(18:0\_22:0) | - | 1.51  | 8.14E-04 | 1.22E+00 | up |
| C59H94O6 | TG(14:0\_20:4\_22:6) | - | 1.51  | 6.00E-03 | 3.66E+00 | up |
| C45H84NO7P | PE(O-18:0\_22:4) | - | 1.51  | 2.80E-03 | 2.29E+00 | up |
| C44H84NO10P | PS(18:0\_21:0) | - | 1.51  | 8.75E-04 | 1.21E+00 | up |
| C18H32O2 | FFA(18:2) | 60-33-3 | 1.50  | 2.18E-03 | 1.51E+00 | up |
| C41H78NO8P | PE(18:0\_18:2) | 7266-53-7 | 1.50  | 1.05E-03 | 1.57E+00 | up |
| C63H108O6 | TG(18:1\_20:2\_22:4) | - | 1.50  | 9.14E-04 | 2.42E+00 | up |
| C61H114O6 | TG(22:0\_18:1\_18:1) | - | 1.50  | 2.33E-04 | 2.23E+00 | up |
| C43H76NO8P | PE(20:2\_18:3) | - | 1.50  | 6.86E-04 | 1.67E+00 | up |
| C39H78NO7P | PE(P-18:0\_16:0) | - | 1.49  | 3.52E-03 | 1.50E+00 | up |
| C59H108O6 | TG(16:1\_18:1\_22:1) | - | 1.49  | 2.97E-04 | 1.62E+00 | up |
| C44H80NO8P | PC(18:3\_18:1) | - | 1.49  | 3.03E-04 | 1.47E+00 | up |
| C59H96O6 | TG(16:1\_18:2\_22:6) | - | 1.49  | 1.26E-03 | 2.50E+00 | up |
| C39H74NO8P | PE(18:2\_16:0) | - | 1.48  | 1.20E-03 | 1.52E+00 | up |
| C59H96O6 | TG(18:2\_18:3\_20:4) | - | 1.48  | 5.92E-04 | 2.56E+00 | up |
| C61H100O6 | TG(18:1\_18:2\_22:6) | - | 1.48  | 8.51E-04 | 2.33E+00 | up |
| C43H80NO8P | PC(15:0\_20:3) | - | 1.48  | 2.25E-03 | 8.27E-01 | down |
| C63H116O6 | TG(18:1\_18:1\_24:1) | - | 1.47  | 2.68E-04 | 1.67E+00 | up |
| C63H118O6 | TG(24:0\_18:1\_18:1) | - | 1.47  | 1.45E-04 | 2.14E+00 | up |
| C56H107NO5 | Cer(t20:1/36:2(2OH)) | - | 1.47  | 1.72E-03 | 1.65E+00 | up |
| C55H92O6 | TG(16:1\_16:1\_20:5) | - | 1.47  | 2.90E-02 | 4.44E+00 | up |
| C57H111NO4 | Cer(d21:2/36:0(2OH)) | - | 1.46  | 4.90E-04 | 1.79E+00 | up |
| C53H88O6 | TG(12:0\_16:1\_22:6) | - | 1.46  | 1.58E-03 | 2.69E+00 | up |
| C47H92NO10P | PS(20:0\_21:0) | - | 1.46  | 6.57E-04 | 1.31E+00 | up |
| C59H113NO4 | Cer(d25:2/34:1(2OH)) | - | 1.45  | 4.78E-05 | 2.18E+00 | up |
| C59H106O6 | TG(18:0\_18:2\_20:2) | - | 1.45  | 9.58E-04 | 1.45E+00 | up |
| C47H86NO7P | PE(O-18:1\_24:4) | - | 1.45  | 5.12E-03 | 1.56E+00 | up |
| C57H104O6 | TG(18:1\_18:1\_18:1) | 122-32-7 | 1.45  | 2.64E-04 | 1.49E+00 | up |
| C63H116O6 | TG(18:1\_20:1\_22:1) | - | 1.44  | 5.01E-04 | 1.65E+00 | up |
| C61H100O6 | TG(16:0\_20:4\_22:5) | - | 1.44  | 1.95E-03 | 2.32E+00 | up |
| C58H104O6 | TG(17:1\_18:1\_20:2) | - | 1.44  | 5.08E-04 | 1.66E+00 | up |
| C42H77NO3 | Cer(d18:2/24:2) | - | 1.44  | 1.15E-02 | 1.24E+00 | up |
| C56H96O6 | TG(17:1\_18:2\_18:3) | - | 1.43  | 7.72E-04 | 3.30E+00 | up |
| C59H100O6 | TG(18:1\_18:2\_20:4) | - | 1.43  | 3.88E-04 | 1.93E+00 | up |
| C54H98O6 | TG(16:0\_17:1\_18:2) | - | 1.42  | 1.54E-03 | 1.62E+00 | up |
| C57H111NO4 | Cer(d28:2/29:0(2OH)) | - | 1.42  | 4.88E-04 | 1.88E+00 | up |
| C38H73NO3 | Cer(d18:1/20:1) | - | 1.41  | 4.30E-03 | 1.34E+00 | up |
| C45H82NO7P | PE(O-18:0\_22:5) | - | 1.40  | 3.03E-03 | 2.50E+00 | up |
| C58H106O6 | TG(18:1\_18:1\_19:1) | - | 1.40  | 1.46E-03 | 1.49E+00 | up |
| C42H83NO4 | Cer(t16:1/26:0) | - | 1.39  | 9.10E-03 | 1.44E+00 | up |
| C59H102O6 | TG(18:1\_20:2\_18:3) | - | 1.39  | 5.55E-04 | 1.65E+00 | up |
| C55H94O6 | TG(16:0\_16:1\_20:5) | - | 1.39  | 2.10E-02 | 3.49E+00 | up |
| C57H111NO4 | Cer(d23:2/34:0(2OH)) | - | 1.39  | 3.26E-04 | 1.99E+00 | up |
| C43H86NO7P | PE(O-18:0\_20:1) | - | 1.38  | 8.71E-03 | 1.56E+00 | up |
| C56H98O6 | TG(18:1\_17:2\_18:2) | - | 1.38  | 3.36E-04 | 2.23E+00 | up |
| C42H78NO8P | PC(16:1\_18:2) | 182820-31-1 | 1.38  | 3.93E-03 | 1.34E+00 | up |
| C52H99NO4 | Cer(t17:2/35:1) | - | 1.38  | 1.20E-03 | 1.49E+00 | up |
| C39H77NO3 | Cer(d18:1/21:0) | - | 1.38  | 1.32E-03 | 1.60E+00 | up |
| C13H25NO5 | Carnitine C6-OH | 102636-82-8 | 1.37  | 3.76E-03 | 1.30E+00 | up |
| C53H92O6 | TG(16:0\_16:2\_18:3) | - | 1.37  | 5.44E-04 | 1.89E+00 | up |
| C46H89O10P | PG(22:0\_18:1) | - | 1.37  | 1.42E-03 | 1.32E+00 | up |
| C40H73O10P | PG(16:0\_18:3) | - | 1.37  | 4.49E-03 | 1.22E+00 | up |
| C50H97NO8 | HexCer(d18:1/26:0) | - | 1.37  | 2.48E-03 | 1.29E+00 | up |
| C12H23NO5 | Carnitine C5-OH | - | 1.36  | 8.35E-03 | 1.21E+00 | up |
| C51H90O6 | TG(14:0\_16:1\_18:3) | - | 1.36  | 2.47E-03 | 1.92E+00 | up |
| C43H70O5 | DG(18:1\_22:6) | - | 1.36  | 1.37E-03 | 1.82E+00 | up |
| C45H83O13P | PI(18:0\_18:2) | - | 1.35  | 1.12E-03 | 1.49E+00 | up |
| C61H114O6 | TG(16:0\_18:1\_24:1) | - | 1.35  | 2.94E-03 | 1.56E+00 | up |
| C54H94O6 | TG(15:0\_18:2\_18:3) | - | 1.34  | 4.80E-03 | 2.08E+00 | up |
| C48H91NO13 | Hex2Cer(d18:1/18:0) | - | 1.34  | 2.58E-03 | 7.78E-01 | down |
| C41H78NO7P | PE(P-18:0\_18:2) | 205648-90-4 | 1.34  | 6.76E-03 | 1.41E+00 | up |
| C57H94O6 | TG(16:1\_16:1\_22:6) | - | 1.34  | 2.37E-03 | 2.15E+00 | up |
| C59H102O6 | TG(18:0\_18:2\_20:4) | - | 1.34  | 2.88E-04 | 1.65E+00 | up |
| C44H84NO8P | PC(18:1\_18:1) | 68737-67-7 | 1.34  | 1.58E-03 | 1.31E+00 | up |
| C25H49NO5 | Carnitine C18-OH | - | 1.33  | 5.24E-03 | 7.95E-01 | down |
| C44H83NO8 | HexCer(d18:1/20:1) | - | 1.33  | 1.12E-02 | 1.33E+00 | up |
| C11H19NO6 | Carnitine C4:1-2OH | 256928-74-2 | 1.33  | 1.28E-02 | 1.22E+00 | up |
| C62H116O6 | TG(23:0\_18:1\_18:1) | - | 1.33  | 4.16E-04 | 2.05E+00 | up |
| C59H98O6 | TG(16:1\_16:1\_24:6) | - | 1.33  | 7.10E-04 | 1.78E+00 | up |
| C11H21NO4 | Carnitine C4:0 | 25576-40-3 | 1.33  | 1.25E-02 | 1.21E+00 | up |
| C59H104O6 | TG(18:1\_18:2\_20:2) | - | 1.33  | 1.79E-03 | 1.49E+00 | up |
| C61H116O6 | TG(16:0\_20:1\_22:0) | - | 1.33  | 2.19E-03 | 1.89E+00 | up |
| C45H80NO7P | PE(O-18:0\_22:6) | - | 1.32  | 7.21E-03 | 1.86E+00 | up |
| C59H109NO4 | Cer(d21:3/38:2(2OH)) | - | 1.32  | 4.65E-03 | 1.35E+00 | up |
| C47H82O6 | TG(10:0\_16:2\_18:2) | - | 1.32  | 2.25E-02 | 2.67E+00 | up |
| C17H31NO4 | Carnitine C10:1 | - | 1.32  | 7.54E-03 | 1.24E+00 | up |
| C42H79O10P | PG(18:0\_18:2) | - | 1.32  | 2.32E-03 | 1.50E+00 | up |
| C47H84O6 | TG(14:1\_14:1\_16:1) | - | 1.31  | 2.05E-02 | 2.54E+00 | up |
| C60H112O6 | TG(15:0\_18:1\_24:1) | - | 1.31  | 1.55E-03 | 1.73E+00 | up |
| C56H102O6 | TG(17:1\_18:1\_18:1) | - | 1.31  | 1.57E-03 | 1.46E+00 | up |
| C48H80NO8P | PC(20:4\_20:4) | - | 1.31  | 1.82E-02 | 8.17E-01 | down |
| C44H83NO10 | HexCer(t18:2/20:0(2OH)) | - | 1.31  | 6.99E-03 | 8.09E-01 | down |
| C39H76NO7P | PE(O-16:0\_18:2) | - | 1.30  | 4.56E-03 | 2.13E+00 | up |
| C17H33NO4 | Carnitine C10:0 | 1492-27-9 | 1.30  | 7.04E-03 | 1.23E+00 | up |
| C45H81O13P | PI(18:1\_18:2) | - | 1.30  | 1.21E-03 | 1.45E+00 | up |
| C45H80NO7P | PE(P-18:0\_22:5) | - | 1.30  | 7.26E-03 | 1.88E+00 | up |
| C61H106O6 | TG(18:1\_18:1\_22:4) | - | 1.30  | 1.35E-03 | 1.59E+00 | up |
| C57H111NO4 | Cer(d30:1/27:1(2OH)) | - | 1.30  | 1.22E-03 | 1.86E+00 | up |
| C56H102O6 | TG(17:0\_18:1\_18:2) | - | 1.29  | 5.02E-03 | 1.55E+00 | up |
| C54H105NO5 | Cer(t18:1/36:1(2OH)) | - | 1.27  | 4.65E-03 | 1.56E+00 | up |
| C45H82NO7P | PE(P-18:0\_22:4) | - | 1.27  | 2.75E-03 | 2.49E+00 | up |
| C40H75NO8 | HexCer(d18:1/16:1) | - | 1.26  | 1.44E-02 | 1.28E+00 | up |
| C44H83NO10 | HexCer(t22:1/16:1(2OH)) | - | 1.26  | 1.01E-02 | 8.19E-01 | down |
| C65H122O6 | TG(24:0\_18:1\_20:1) | - | 1.26  | 1.13E-03 | 1.64E+00 | up |
| C53H94O6 | TG(16:1\_16:1\_18:2) | - | 1.26  | 4.83E-03 | 1.67E+00 | up |
| C41H77O8P | PA(20:0\_18:2) | - | 1.26  | 8.89E-03 | 1.38E+00 | up |
| C23H45NO5 | Carnitine C16-OH | 195207-76-2 | 1.26  | 1.64E-02 | 7.53E-01 | down |
| C43H80NO8P | PE(20:1\_18:2) | - | 1.25  | 4.11E-03 | 1.88E+00 | up |
| C42H76NO10P | PS(18:2\_18:2) | - | 1.25  | 3.92E-03 | 1.47E+00 | up |
| C59H108O6 | TG(18:1\_18:1\_20:1) | - | 1.25  | 2.12E-03 | 1.58E+00 | up |
| C47H84O6 | TG(8:0\_18:1\_18:2) | - | 1.25  | 2.76E-02 | 2.46E+00 | up |
| C27H49O12P | LPI(18:2/0:0) | - | 1.25  | 6.06E-03 | 1.33E+00 | up |
| C61H106O6 | TG(16:0\_20:0\_22:6) | - | 1.24  | 4.55E-03 | 1.54E+00 | up |
| C43H80NO7P | PE(O-16:0\_22:4) | - | 1.24  | 8.75E-03 | 1.56E+00 | up |
| C61H106O6 | TG(18:1\_18:2\_22:3) | - | 1.23  | 1.67E-03 | 1.54E+00 | up |
| C47H90NO10P | PS(23:0\_18:1) | - | 1.23  | 6.04E-03 | 1.32E+00 | up |
| C41H76NO7P | PE(P-18:1\_18:2) | - | 1.23  | 2.09E-02 | 7.72E-01 | down |
| C42H76NO8P | PC(16:1\_18:3) | - | 1.22  | 1.54E-02 | 1.45E+00 | up |
| C43H83NO3 | Cer(d18:1/25:1) | - | 1.22  | 6.56E-03 | 1.43E+00 | up |
| C53H92O6 | TG(14:1\_18:2\_18:2) | - | 1.22  | 1.05E-02 | 1.84E+00 | up |
| C40H79NO3 | Cer(d18:1/22:0) | 27888-44-4 | 1.21  | 8.55E-03 | 1.30E+00 | up |
| C40H81NO4 | Cer(t18:0/22:0) | - | 1.21  | 7.56E-03 | 1.41E+00 | up |
| C41H76NO8P | PE(18:1\_18:2) | 1188-56-3 | 1.21  | 2.02E-03 | 1.55E+00 | up |
| C59H104O6 | TG(18:0\_20:2\_18:3) | - | 1.21  | 1.42E-03 | 1.44E+00 | up |
| C47H90NO10P | PS(21:0\_20:1) | - | 1.21  | 7.29E-03 | 1.28E+00 | up |
| C25H49NO4 | Carnitine C18:0 | 25597-09-5 | 1.21  | 7.39E-03 | 8.08E-01 | down |
| C18H35NO2 | SPH(d18:2) | - | 1.20  | 1.46E-02 | 7.50E-01 | down |
| C57H94O6 | TG(16:1\_18:3\_20:4) | - | 1.20  | 4.11E-03 | 1.83E+00 | up |
| C55H102O6 | TG(16:0\_18:0\_18:2) | - | 1.20  | 7.76E-03 | 1.41E+00 | up |
| C61H94O6 | TG(14:0\_22:6\_22:6) | - | 1.20  | 1.95E-02 | 5.58E+00 | up |
| C57H106O6 | TG(16:0\_16:1\_22:1) | - | 1.19  | 1.97E-03 | 1.63E+00 | up |
| C61H112O6 | TG(18:1\_20:1\_20:1) | - | 1.19  | 1.92E-03 | 1.68E+00 | up |
| C57H105NO10 | HexCer(t17:2/34:2(2OH)) | - | 1.19  | 4.29E-03 | 1.41E+00 | up |
| C59H106O6 | TG(18:0\_18:1\_20:3) | - | 1.19  | 5.03E-03 | 1.41E+00 | up |
| C49H86O6 | TG(12:0\_16:2\_18:2) | - | 1.18  | 3.77E-02 | 2.71E+00 | up |
| C47H86O6 | TG(14:0\_14:1\_16:1) | - | 1.18  | 1.39E-02 | 1.77E+00 | up |
| C63H98O6 | TG(16:0\_22:6\_22:6) | - | 1.18  | 1.37E-02 | 2.87E+00 | up |
| C53H94O6 | TG(16:0\_16:1\_18:3) | - | 1.18  | 6.27E-03 | 1.49E+00 | up |
| C40H81NO3 | Cer(d18:0/22:0) | - | 1.18  | 1.68E-02 | 1.21E+00 | up |
| C60H114O6 | TG(16:0\_23:0\_18:1) | - | 1.17  | 5.81E-03 | 1.54E+00 | up |
| C59H112O6 | TG(18:0\_18:1\_20:0) | - | 1.17  | 5.15E-03 | 1.54E+00 | up |
| C49H90O6 | TG(14:0\_14:1\_18:1) | - | 1.17  | 1.28E-02 | 2.01E+00 | up |
| C44H83NO3 | Cer(d18:1/26:2) | - | 1.16  | 6.50E-03 | 1.31E+00 | up |
| C54H103NO5 | Cer(t18:1/36:2(2OH)) | - | 1.16  | 5.35E-03 | 1.56E+00 | up |
| C58H111NO5 | Cer(t20:1/38:2(2OH)) | - | 1.16  | 4.37E-03 | 1.40E+00 | up |
| C41H70O5 | DG(18:1\_20:4) | - | 1.16  | 5.89E-03 | 1.60E+00 | up |
| C44H84NO10P | PS(20:0\_18:2) | - | 1.15  | 1.52E-02 | 1.22E+00 | up |
| C61H102O6 | TG(16:0\_20:2\_22:6) | - | 1.15  | 2.35E-03 | 1.67E+00 | up |
| C38H72NO8P | PE(15:0\_18:2) | - | 1.15  | 4.64E-03 | 2.09E+00 | up |
| C53H92O6 | TG(14:0\_18:2\_18:3) | - | 1.15  | 2.95E-03 | 1.82E+00 | up |
| C44H84NO10P | PS(20:0\_18:1) | - | 1.15  | 2.89E-02 | 1.29E+00 | up |
| C21H40O4 | MG(18:1) | - | 1.15  | 5.66E-03 | 1.72E+00 | up |
| C54H96O6 | TG(15:0\_18:2\_18:2) | - | 1.14  | 1.06E-02 | 1.65E+00 | up |
| C23H43NO4 | Carnitine C16:1 | - | 1.14  | 2.20E-02 | 7.55E-01 | down |
| C55H92O6 | TG(14:1\_18:2\_20:4) | - | 1.14  | 7.77E-03 | 2.13E+00 | up |
| C48H93O10P | PG(24:0\_18:1) | - | 1.13  | 1.11E-02 | 1.30E+00 | up |
| C59H98O6 | TG(14:0\_20:2\_22:6) | - | 1.13  | 2.09E-03 | 1.72E+00 | up |
| C28H49O9P | LPG(22:4) | - | 1.13  | 1.41E-02 | 8.23E-01 | down |
| C59H110O6 | TG(16:0\_18:1\_22:1) | - | 1.13  | 1.15E-02 | 1.60E+00 | up |
| C48H85O10P | PG(22:0\_20:5) | - | 1.12  | 3.41E-02 | 1.73E+00 | up |
| C41H78NO8P | PE(18:1\_18:1) | - | 1.12  | 7.26E-03 | 1.59E+00 | up |
| C26H45NO7S | Taurocholic acid | 81-24-3 | 1.12  | 2.01E-02 | 1.25E+00 | up |
| C60H113NO5 | Cer(t20:2/40:2(2OH)) | - | 1.12  | 2.73E-03 | 1.34E+00 | up |
| C41H76NO8P | LNAPE(18:1/N-18:2) | - | 1.11  | 6.52E-03 | 1.46E+00 | up |
| C49H88O6 | TG(10:0\_18:1\_18:2) | - | 1.11  | 2.84E-02 | 2.37E+00 | up |
| C50H97NO4 | Cer(t17:2/33:0) | - | 1.11  | 6.71E-03 | 1.38E+00 | up |
| C49H95NO8 | HexCer(d18:1/25:0) | - | 1.11  | 1.12E-02 | 1.36E+00 | up |
| C57H106O6 | TG(18:0\_18:1\_18:1) | - | 1.11  | 3.82E-03 | 1.34E+00 | up |
| C53H90O6 | TG(14:0\_16:1\_20:5) | - | 1.10  | 1.83E-02 | 2.84E+00 | up |
| C53H90O6 | TG(14:1\_18:2\_18:3) | - | 1.10  | 1.43E-02 | 1.67E+00 | up |
| C39H77NO4 | Cer(d18:1/21:0(2OH)) | - | 1.10  | 1.62E-02 | 1.27E+00 | up |
| C21H41NO5 | Carnitine C14-OH | - | 1.10  | 3.13E-02 | 8.27E-01 | down |
| C45H82O6 | TG(8:0\_16:1\_18:1) | - | 1.09  | 1.03E-02 | 1.72E+00 | up |
| C45H82NO8P | PC(18:2\_19:2) | - | 1.09  | 5.80E-03 | 1.37E+00 | up |
| C41H81NO3 | Cer(d18:1/23:0) | 67605-84-9 | 1.09  | 1.75E-02 | 1.37E+00 | up |
| C47H84O6 | TG(10:0\_16:0\_18:3) | - | 1.09  | 4.12E-02 | 1.88E+00 | up |
| C27H51O12P | LPI(18:1/0:0) | - | 1.08  | 4.38E-02 | 1.40E+00 | up |
| C61H116O6 | TG(16:0\_24:0\_18:1) | - | 1.08  | 6.05E-03 | 1.68E+00 | up |
| C63H110O6 | TG(18:1\_18:1\_24:4) | - | 1.07  | 1.36E-02 | 1.67E+00 | up |
| C63H120O6 | TG(18:0\_20:1\_22:0) | - | 1.07  | 1.04E-02 | 1.56E+00 | up |
| C59H98O6 | TG(16:0\_18:2\_22:6) | - | 1.07  | 3.99E-03 | 1.67E+00 | up |
| C57H100O6 | TG(16:0\_18:1\_20:4) | - | 1.07  | 5.34E-03 | 1.36E+00 | up |
| C20H30O2 | FFA(20:5) | 10417-94-4 | 1.06  | 3.61E-02 | 1.64E+00 | up |
| C51H92O6 | TG(14:0\_16:1\_18:2) | - | 1.06  | 3.15E-02 | 1.38E+00 | up |
| C18H37NO2 | SPH(d18:1) | - | 1.06  | 2.94E-02 | 7.15E-01 | down |
| C46H82NO8P | PC(16:0\_22:5) | - | 1.05  | 1.23E-02 | 1.27E+00 | up |
| C44H84NO10P | PS(18:1\_20:3) | - | 1.05  | 9.72E-03 | 1.50E+00 | up |
| C43H80NO7P | PE(P-18:0\_20:3) | - | 1.05  | 2.97E-02 | 8.22E-01 | down |
| C46H91NO3 | Cer(d20:1/26:0) | - | 1.05  | 3.49E-02 | 1.20E+00 | up |
| C58H109NO5 | Cer(t20:2/38:2(2OH)) | - | 1.05  | 6.75E-03 | 1.43E+00 | up |
| C63H104O6 | TG(20:1\_18:2\_22:6) | - | 1.05  | 3.31E-03 | 1.91E+00 | up |
| C59H108O6 | TG(20:1\_18:2\_18:0) | - | 1.05  | 1.29E-02 | 1.32E+00 | up |
| C44H82NO8P | PC(18:1\_18:2) | - | 1.05  | 9.95E-03 | 1.25E+00 | up |
| C18H39NO2 | SPH(d18:0) | 764-22-7 | 1.05  | 3.38E-02 | 7.55E-01 | down |
| C48H80NO8P | PC(18:2\_22:6) | - | 1.04  | 1.78E-02 | 1.32E+00 | up |
| C43H85NO3 | Cer(d18:1/25:0) | 67492-18-6 | 1.04  | 1.37E-02 | 1.34E+00 | up |
| C57H104O6 | TG(16:0\_18:1\_20:2) | - | 1.04  | 1.54E-02 | 1.28E+00 | up |
| C58H96O6 | TG(16:1\_17:1\_22:6) | - | 1.04  | 1.02E-02 | 2.02E+00 | up |
| C49H86O6 | TG(10:0\_18:1\_18:3) | - | 1.04  | 2.88E-02 | 2.49E+00 | up |
| C43H78NO7P | PE(O-16:0\_22:5) | - | 1.03  | 3.83E-02 | 1.53E+00 | up |
| C60H114O6 | TG(15:0\_24:0\_18:1) | - | 1.03  | 7.29E-03 | 1.51E+00 | up |
| C57H108O6 | TG(16:0\_20:0\_18:1) | - | 1.03  | 1.20E-02 | 1.48E+00 | up |
| C44H85NO3 | Cer(d18:1/26:1) | - | 1.03  | 2.16E-02 | 1.21E+00 | up |
| C19H35NO5 | Carnitine C12:1-OH | - | 1.03  | 2.46E-02 | 1.24E+00 | up |
| C23H48NO7P | LPE(18:0/0:0) | 69747-55-3 | 1.02  | 3.21E-02 | 1.20E+00 | up |
| C59H112O6 | TG(16:0\_18:1\_22:0) | - | 1.02  | 4.86E-03 | 1.70E+00 | up |
| C42H83NO3 | Cer(d18:0/24:1) | - | 1.02  | 1.23E-02 | 1.29E+00 | up |
| C63H106O6 | TG(18:1\_20:1\_22:6) | - | 1.02  | 5.10E-03 | 1.76E+00 | up |
| C34H69NO3 | Cer(d16:0/18:0) | - | 1.02  | 1.17E-02 | 1.24E+00 | up |
| C45H88NO7P | PE(O-18:1\_22:1) | - | 1.01  | 2.38E-02 | 7.85E-01 | down |
| C45H82NO8P | PE(18:0\_22:4) | - | 1.01  | 3.29E-02 | 1.27E+00 | up |
| C43H82NO10P | PS(19:0\_18:1) | - | 1.01  | 1.92E-02 | 1.26E+00 | up |
| C44H80NO8P | PC(18:2\_18:2) | 998-06-1 | 1.01  | 1.31E-02 | 1.31E+00 | up |
| C55H92O6 | TG(12:0\_18:1\_22:6) | - | 1.01  | 9.72E-03 | 1.63E+00 | up |
| C48H93O10P | PG(22:0\_20:1) | - | 1.01  | 1.75E-02 | 1.24E+00 | up |
| C55H100O6 | TG(16:1\_18:1\_18:1) | - | 1.00  | 1.91E-02 | 1.27E+00 | up |

## Table S3 Correlation coefficients (r) and p-values(p) for the correlation analysis between the first 50 differential lipids and maternal lipid metabolism levels

|  |  |  |  |
| --- | --- | --- | --- |
| Maternal Lipids | Neonatal lipids | r | *P* value |
| HDLC | TG(16:0\_18:2\_18:2) | -0.32583595 | 0.001949 |
| HDLC | DG(18:1\_18:2) | -0.32531424 | 0.001984 |
| HDLC | TG(18:1\_18:2\_20:0) | -0.32121175 | 0.002277 |
| HDLC | TG(16:0\_18:2\_18:3) | -0.31574647 | 0.002729 |
| HDLC | TG(18:0\_18:1\_18:2) | -0.31479195 | 0.002816 |
| HDLC | Cer(t18:2/38:2(2OH)) | -0.31468788 | 0.002826 |
| HDLC | Cer(t26:1/30:2(2OH)) | -0.31337674 | 0.002949 |
| HDLC | Cer(d29:2/30:2(2OH)) | -0.3092288 | 0.003373 |
| HDLC | Cer(d19:3/40:1(2OH)) | -0.30765117 | 0.003547 |
| HDLC | Cer(d26:3/33:1(2OH)) | -0.29384282 | 0.005458 |
| HDLC | TG(16:1\_18:1\_16:3) | -0.2927693 | 0.005639 |
| HDLC | TG(18:1\_18:2\_18:3) | -0.29272118 | 0.005647 |
| HDLC | TG(18:1\_17:2\_19:2) | -0.28965772 | 0.006194 |
| HDLC | TG(16:1\_18:1\_18:2) | -0.28889052 | 0.006338 |
| HDLC | Cer(d29:1/28:1(2OH)) | -0.28258138 | 0.007641 |
| HDLC | TG(17:2\_18:2\_18:3) | -0.28087967 | 0.00803 |
| HDLC | Cer(d17:3/42:1(2OH)) | -0.27709492 | 0.008959 |
| HDLC | TG(16:1\_18:2\_18:2) | -0.27068747 | 0.010748 |
| HDLC | TG(18:2\_18:3\_18:4) | -0.2685039 | 0.011426 |
| HDLC | Cer(d23:2/36:2(2OH)) | -0.26476629 | 0.012671 |
| HDLC | Carnitine C10:2 | -0.26445319 | 0.012781 |
| HDLC | TG(16:1\_18:2\_18:3) | -0.26195562 | 0.013684 |
| HDLC | DG(18:2\_18:2) | -0.25717208 | 0.015571 |
| HDLC | Cer(d28:3/31:1(2OH)) | -0.25172465 | 0.017988 |
| HDLC | TG(18:2\_18:2\_18:3) | -0.25093253 | 0.018366 |
| HDLC | TG(16:0\_18:2\_20:4) | -0.24942563 | 0.019102 |
| HDLC | TG(18:2\_18:3\_18:3) | -0.24816236 | 0.019739 |
| HDLC | TG(16:0\_18:0\_20:4) | -0.24773789 | 0.019957 |
| HDLC | TG(18:2\_18:2\_20:1) | -0.24679182 | 0.02045 |
| HDLC | TG(18:1\_22:1\_18:2) | -0.24623631 | 0.020744 |
| HDLC | PE(20:2\_16:0) | -0.23362514 | 0.028475 |
| HDLC | LNAPE(16:0/N-18:1) | -0.22973159 | 0.031307 |
| HDLC | PE(16:0\_18:1) | -0.22312456 | 0.036655 |
| HDLC | TG(18:1\_18:2\_18:4) | -0.2205786 | 0.03891 |
| HDLC | TG(16:0\_18:2\_18:4) | -0.21336428 | 0.045938 |
| HDLC | PE(18:2\_22:1) | -0.20842701 | 0.051329 |
| TC | Cer(t18:2/38:2(2OH)) | -0.20423008 | 0.056311 |
| HDLC | TG(20:0\_18:3\_18:3) | -0.20241817 | 0.05858 |
| TC | Cer(t26:1/30:2(2OH)) | -0.20130638 | 0.06001 |
| TC | TG(20:0\_18:3\_18:3) | -0.1969776 | 0.065848 |
| TC | TG(16:1\_18:2\_18:3) | -0.19539251 | 0.068097 |
| TC | TG(16:0\_18:2\_18:4) | -0.19440718 | 0.069526 |
| HDLC | PE(O-18:0\_22:3) | -0.18938463 | 0.077192 |
| TC | Cer(d19:3/40:1(2OH)) | -0.18824865 | 0.079017 |
| TC | TG(18:1\_18:2\_18:4) | -0.18659604 | 0.081732 |
| HDLC | TG(18:2\_20:4\_20:4) | -0.18613273 | 0.082507 |
| TC | TG(17:2\_18:2\_18:3) | -0.18284314 | 0.088175 |
| TC | Cer(d28:3/31:1(2OH)) | -0.18023599 | 0.092883 |
| TC | TG(16:1\_18:2\_18:2) | -0.17938963 | 0.094454 |
| HDLC | Cer(d18:1/23:1) | -0.17883557 | 0.095493 |
| TC | TG(16:0\_18:2\_18:3) | -0.17697139 | 0.099056 |
| TC | TG(18:1\_18:2\_24:5) | -0.17602726 | 0.100899 |
| TC | TG(18:2\_18:2\_20:1) | -0.1754792 | 0.101982 |
| HDLC | Cer(d18:1/24:2) | -0.17470842 | 0.10352 |
| TC | TG(18:1\_18:2\_18:3) | -0.17372892 | 0.1055 |
| TC | TG(16:1\_18:1\_16:3) | -0.17372206 | 0.105514 |
| TC | PE(20:2\_16:0) | -0.17278103 | 0.107444 |
| TC | Cer(d23:2/36:2(2OH)) | -0.17190409 | 0.109268 |
| TC | PE(16:0\_18:1) | -0.17147289 | 0.110173 |
| TC | DG(18:2\_18:2) | -0.1707903 | 0.111619 |
| TC | LNAPE(16:0/N-18:1) | -0.17053115 | 0.112171 |
| TC | TG(18:0\_18:1\_18:2) | -0.16953198 | 0.114321 |
| LDLC | Cer(d18:1/24:2) | -0.16860239 | 0.11635 |
| HDLC | TG(18:1\_24:1\_18:2) | -0.16781222 | 0.118096 |
| HDLC | TG(18:1\_18:2\_24:5) | -0.16587164 | 0.122471 |
| HDLC | Carnitine C6:1 | -0.16553207 | 0.123249 |
| TC | TG(18:1\_18:2\_20:0) | -0.16506631 | 0.124322 |
| TC | TG(16:0\_18:2\_18:2) | -0.16348502 | 0.12802 |
| TC | TG(18:1\_17:2\_19:2) | -0.16127821 | 0.13332 |
| TC | TG(18:2\_18:3\_18:3) | -0.15905734 | 0.138821 |
| TC | TG(16:1\_18:1\_18:2) | -0.15787331 | 0.141823 |
| TC | TG(18:2\_18:2\_18:3) | -0.15719469 | 0.143565 |
| TC | TG(16:0\_18:2\_20:4) | -0.155988 | 0.146703 |
| TC | Cer(d29:1/28:1(2OH)) | -0.15523465 | 0.148689 |
| HDLC | MG(18:2) | -0.15309505 | 0.154437 |
| TC | PE(18:2\_22:1) | -0.15214454 | 0.157043 |
| TC | TG(18:2\_20:4\_20:4) | -0.15194202 | 0.157602 |
| TC | TG(18:2\_18:3\_18:4) | -0.15094257 | 0.160385 |
| HDLC | TG(18:2\_20:4\_20:5) | -0.15088771 | 0.160539 |
| TC | TG(18:1\_22:1\_18:2) | -0.15006628 | 0.162855 |
| TC | TG(16:0\_18:0\_20:4) | -0.14725066 | 0.170981 |
| LDLC | Carnitine C5:1 | -0.14399374 | 0.180748 |
| TC | Cer(d17:3/42:1(2OH)) | -0.14254655 | 0.185217 |
| LDLC | TG(16:0\_18:2\_18:4) | -0.14211685 | 0.186559 |
| TG | Carnitine C5:1 | -0.13907656 | 0.196257 |
| LDLC | PG(20:4\_22:6) | -0.13774798 | 0.200607 |
| TC | TG(18:1\_24:1\_18:2) | -0.13766682 | 0.200875 |
| LDLC | PE(O-16:1\_22:1) | -0.13678823 | 0.203792 |
| LDLC | TG(18:1\_18:2\_24:5) | -0.1360127 | 0.206392 |
| TC | DG(18:1\_18:2) | -0.13453111 | 0.211424 |
| TC | Cer(d29:2/30:2(2OH)) | -0.13439442 | 0.211893 |
| TG | TG(16:0\_18:2\_18:4) | -0.13239181 | 0.218844 |
| HDLC | PE(O-16:1\_22:1) | -0.1303192 | 0.226205 |
| HDLC | Carnitine C5:1 | -0.12820836 | 0.23388 |
| LDLC | TG(20:0\_18:3\_18:3) | -0.12678376 | 0.23916 |
| LDLC | Cer(t18:2/38:2(2OH)) | -0.12550958 | 0.243953 |
| TC | Cer(d26:3/33:1(2OH)) | -0.12418173 | 0.249017 |
| LDLC | TG(16:1\_18:2\_18:3) | -0.12397426 | 0.249815 |
| TC | Cer(d18:1/24:2) | -0.12340451 | 0.252015 |
| LDLC | TG(18:1\_18:2\_18:4) | -0.12122083 | 0.260569 |
| TC | PG(20:4\_22:6) | -0.12059602 | 0.263052 |
| TC | PE(O-16:1\_22:1) | -0.1191008 | 0.26906 |
| LDLC | PE(16:0\_18:1) | -0.11803157 | 0.273413 |
| TC | Carnitine C10:2 | -0.11705173 | 0.277443 |
| TG | TG(16:1\_18:1\_16:3) | -0.11630748 | 0.280531 |
| LDLC | TG(16:1\_18:1\_16:3) | -0.11547484 | 0.284012 |
| TG | TG(18:1\_18:2\_18:4) | -0.11414629 | 0.289626 |
| LDLC | LNAPE(16:0/N-18:1) | -0.11145416 | 0.301226 |
| TG | Carnitine C10:2 | -0.11095135 | 0.303425 |
| LDLC | Carnitine C10:2 | -0.1108947 | 0.303674 |
| LDLC | Cer(t26:1/30:2(2OH)) | -0.11058539 | 0.305033 |
| LDLC | TG(18:2\_20:4\_20:4) | -0.11031767 | 0.306213 |
| TC | TG(18:2\_20:4\_20:5) | -0.1095509 | 0.309607 |
| LDLC | TG(16:1\_18:2\_18:2) | -0.10946914 | 0.309971 |
| LDLC | DG(18:2\_18:2) | -0.10890827 | 0.312471 |
| LDLC | PE(18:2\_22:1) | -0.10859923 | 0.313854 |
| TG | LNAPE(16:0/N-18:1) | -0.10752741 | 0.318683 |
| TG | Cer(d18:1/24:2) | -0.10747418 | 0.318924 |
| LDLC | Cer(d28:3/31:1(2OH)) | -0.10632364 | 0.324162 |
| TC | PE(O-18:0\_22:3) | -0.10556874 | 0.327629 |
| LDLC | TG(18:2\_18:2\_18:3) | -0.10296821 | 0.339751 |
| TG | TG(18:1\_18:2\_24:5) | -0.10169988 | 0.345765 |
| TC | Carnitine C5:1 | -0.10048613 | 0.351582 |
| TG | PE(16:0\_18:1) | -0.09991627 | 0.354334 |
| TG | Carnitine C6:1 | -0.09969157 | 0.355422 |
| LDLC | TG(18:2\_18:3\_18:3) | -0.09856965 | 0.360889 |
| LDLC | Cer(d23:2/36:2(2OH)) | -0.09744299 | 0.366431 |
| TG | TG(18:2\_20:4\_20:5) | -0.09584349 | 0.374388 |
| TC | Cer(d18:1/23:1) | -0.09524333 | 0.377401 |
| LDLC | Cer(d19:3/40:1(2OH)) | -0.09092029 | 0.399531 |
| LDLC | TG(16:1\_18:1\_18:2) | -0.09054046 | 0.401511 |
| LDLC | Cer(d18:1/23:1) | -0.09050039 | 0.40172 |
| TG | PE(20:2\_16:0) | -0.08777819 | 0.416086 |
| LDLC | TG(18:1\_22:1\_18:2) | -0.0871231 | 0.419587 |
| LDLC | TG(16:0\_18:0\_20:4) | -0.08643397 | 0.423288 |
| TC | MG(18:2) | -0.08643161 | 0.423301 |
| LDLC | TG(16:0\_18:2\_20:4) | -0.08639448 | 0.423501 |
| LDLC | TG(17:2\_18:2\_18:3) | -0.08592992 | 0.426007 |
| LDLC | TG(16:0\_18:2\_18:3) | -0.08488092 | 0.431698 |
| TG | TG(18:2\_20:4\_20:4) | -0.08443125 | 0.434151 |
| TG | PE(18:2\_22:1) | -0.08127587 | 0.451582 |
| LDLC | Cer(d29:1/28:1(2OH)) | -0.08050154 | 0.455918 |
| HDLC | Carnitine C8:0 | -0.08047368 | 0.456075 |
| TG | Cer(t18:2/38:2(2OH)) | -0.08034023 | 0.456824 |
| LDLC | TG(18:2\_18:2\_20:1) | -0.07986722 | 0.459487 |
| TG | TG(16:1\_18:2\_18:3) | -0.07927955 | 0.462808 |
| TC | Carnitine C8:0 | -0.07860764 | 0.46662 |
| LDLC | PE(20:2\_16:0) | -0.07841905 | 0.467693 |
| LDLC | TG(18:1\_24:1\_18:2) | -0.07660023 | 0.478112 |
| LDLC | Carnitine C6:1 | -0.07476878 | 0.488727 |
| LDLC | TG(16:0\_18:2\_18:2) | -0.0741371 | 0.492417 |
| LDLC | Carnitine C8:0 | -0.07361824 | 0.495459 |
| LDLC | TG(18:2\_18:3\_18:4) | -0.07278492 | 0.500365 |
| TG | DG(18:2\_18:2) | -0.0700117 | 0.516873 |
| TG | PE(O-16:1\_22:1) | -0.06897698 | 0.523102 |
| LDLC | Cer(d17:3/42:1(2OH)) | -0.06830057 | 0.527195 |
| LDLC | TG(18:1\_18:2\_18:3) | -0.06795863 | 0.52927 |
| LDLC | TG(18:2\_20:4\_20:5) | -0.06473451 | 0.549033 |
| LDLC | TG(18:0\_18:1\_18:2) | -0.06445766 | 0.550747 |
| LDLC | PE(O-18:0\_22:3) | -0.06201838 | 0.565955 |
| LDLC | MG(18:2) | -0.0588542 | 0.585974 |
| LDLC | TG(18:1\_17:2\_19:2) | -0.05674074 | 0.599522 |
| TG | MG(18:2) | -0.0536368 | 0.619668 |
| TG | TG(18:1\_18:2\_18:3) | -0.0489223 | 0.650807 |
| TG | PE(O-18:0\_22:3) | -0.04778967 | 0.658381 |
| TG | TG(18:2\_18:3\_18:3) | -0.04613011 | 0.669541 |
| TG | TG(17:2\_18:2\_18:3) | -0.04475974 | 0.67881 |
| TG | TG(20:0\_18:3\_18:3) | -0.04365406 | 0.686324 |
| TG | Cer(d18:1/23:1) | -0.04222787 | 0.696061 |
| LDLC | TG(18:1\_18:2\_20:0) | -0.04171906 | 0.699547 |
| TC | Carnitine C6:1 | -0.0406728 | 0.706735 |
| TG | Cer(d17:3/42:1(2OH)) | -0.03731834 | 0.72995 |
| TG | TG(18:2\_18:3\_18:4) | -0.03684668 | 0.733235 |
| TG | TG(18:2\_18:2\_20:1) | -0.03409308 | 0.752503 |
| TG | PG(20:4\_22:6) | -0.03226386 | 0.765389 |
| TG | DG(18:1\_18:2) | 0.030376799 | 0.778749 |
| LDLC | Cer(d26:3/33:1(2OH)) | -0.0293654 | 0.785936 |
| TG | Cer(d29:1/28:1(2OH)) | 0.029078146 | 0.787981 |
| LDLC | Cer(d29:2/30:2(2OH)) | -0.02848646 | 0.792197 |
| HDLC | PG(20:4\_22:6) | 0.02819553 | 0.794272 |
| LDLC | DG(18:1\_18:2) | -0.02811796 | 0.794825 |
| TG | Cer(t26:1/30:2(2OH)) | -0.0277296 | 0.797598 |
| TG | Cer(d28:3/31:1(2OH)) | -0.02693846 | 0.803255 |
| TG | Cer(d23:2/36:2(2OH)) | -0.02529686 | 0.815024 |
| TG | TG(18:1\_17:2\_19:2) | -0.02455536 | 0.820353 |
| TG | TG(16:0\_18:2\_20:4) | -0.0211071 | 0.845242 |
| TG | TG(18:2\_18:2\_18:3) | -0.02067276 | 0.848388 |
| TG | TG(16:1\_18:2\_18:2) | -0.01927312 | 0.858543 |
| TG | TG(18:1\_22:1\_18:2) | -0.01922897 | 0.858864 |
| TG | TG(16:0\_18:2\_18:3) | -0.01794862 | 0.868174 |
| TG | TG(16:0\_18:0\_20:4) | -0.01770997 | 0.869911 |
| TG | Cer(d29:2/30:2(2OH)) | 0.017607945 | 0.870654 |
| TG | Cer(d19:3/40:1(2OH)) | -0.01711607 | 0.874237 |
| TG | TG(18:1\_24:1\_18:2) | -0.0161635 | 0.881184 |
| TG | TG(16:0\_18:2\_18:2) | 0.013398911 | 0.901393 |
| TG | TG(16:1\_18:1\_18:2) | -0.00922261 | 0.932038 |
| TG | TG(18:1\_18:2\_20:0) | -0.00905374 | 0.93328 |
| TG | Cer(d26:3/33:1(2OH)) | 0.008904204 | 0.934379 |
| TG | Carnitine C8:0 | 0.006514446 | 0.951966 |
| TG | TG(18:0\_18:1\_18:2) | -0.00080473 | 0.994063 |