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Nishiumi, Shin
Suzuki, Makoto
Kobayashi, Takashi
Yoshida, Masaru

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Differences in metabolite profiles caused by pre-analytical blood processing procedures

Short title: The influence of blood processing on metabolite profiles

Shin Nishiumi[1], Makoto Suzuki[1], Takashi Kobayashi[1], Masaru Yoshida[1,2,3*]

(1) Division of Gastroenterology, Department of Internal Medicine, Kobe University Graduate School of Medicine, 7-5-1 Kusunoki-cho, Chuo-ku, Kobe, Hyogo 650-0017, Japan

(2) Division of Metabolomics Research, Department of Internal Related, Kobe University Graduate School of Medicine, 7-5-1 Kusunoki-cho, Chuo-ku, Kobe, Hyogo 650-0017, Japan

(3) AMED-CREST, AMED, 7-5-1 Kusunoki-cho, Chuo-ku, Kobe, Hyogo 650-0017, Japan

*Corresponding author: Masaru Yoshida M.D., Ph.D.

E-mail: myoshida@med.kobe-u.ac.jp

TEL: +81-78-382-6305 FAX: +81-78-382-6309

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Metabolomics; Mass spectrometry; Serum; Plasma; Blood processing.

Footnote

Shin Nishiumi and Makoto Suzuki are equally contributed as the first author.

ABSTRACT

Recently, the use of metabolomic analysis of human serum and plasma for biomarker discovery and disease diagnosis in clinical studies has been increasing. The feasibility of using a metabolite biomarker for disease diagnosis is strongly dependent on the metabolite's stability during pre-analytical blood processing procedures, such as serum or plasma sampling and sample storage prior to centrifugation. However, the influence of blood processing procedures on the stability of metabolites has not been fully characterized. In the present study, we compared the levels of metabolites in matched human serum and plasma samples using gas chromatography coupled with mass spectrometry and liquid chromatography coupled with mass spectrometry. In addition, we evaluated the changes in plasma metabolite levels induced by storage at room temperature or at a cold temperature prior to centrifugation. As a result, it was found that 76 metabolites exhibited significant differences between their serum and plasma levels. Furthermore, the pre-centrifugation storage conditions significantly affected the plasma levels of 45 metabolites. These results highlight the importance of blood processing procedures during metabolome analysis, which should be considered during biomarker discovery and the subsequent use of biomarkers for disease diagnosis.

INTRODUCTION

Clinical biomarkers are required for early disease diagnosis and assessing therapeutic responses, especially in the oncological field (1). In clinical studies, human serum or plasma are easy to obtain and are often used for biomarker discovery and disease diagnosis. Metabolomics is a large-scale approach to the acquisition of comprehensive biological information about low-molecular-weight metabolites (<1,000 Da), which can provide snapshots of patients' physiological and pathological states (2). Thus, metabolomic analysis of human serum or plasma is being increasingly applied to clinical studies (3,4).

Many analytical methods based on gas chromatography coupled with mass spectrometry (GC/MS) or liquid chromatography coupled with mass spectrometry (LC/MS) have been extensively used for metabolomic analysis (5,6). These analytical techniques focus on a class of compounds, such as carbohydrates, amino acids, organic acids, lipids, or the metabolites associated with a specific pathway. Furthermore, simple metabolite extraction methods can be applied to the stable analysis of blood metabolites (7,8). In metabolomic analysis of serum or plasma, some metabolites might exhibit aberrant changes caused by their degradation, oxidation, or metabolic reactions induced by pre-analytical blood processing. In serum, varying amounts of blood cell-derived metabolites, such as sphingosine 1-phosphate, are released during the coagulation cascade (9). In addition, the hydrolysis of phospholipids, triacylglycerols, and diacylglycerols by lipases, and the hydrolysis of cholesterol esters by esterases can also occur in serum (10). Therefore, pre-analytical techniques, including serum/plasma sampling methods and storage conditions, can have important effects on data quality.

Carefully following the standard operating procedures (SOP) can reduce the extent to which bias affects the quality of metabolomic data (11). As long as the same blood preparation procedures are used, serum and plasma should generate similar results in clinical and biological studies (12,13). However, the metabolites whose levels were measured in previous studies only represent a small part of the blood metabolome. Accordingly, it is necessary to determine whether serum and plasma analyses produce similar results for a wide variety of metabolites. The storage temperature is another important factor affecting sample stability. In metabolomic analysis, storing blood tubes at 4°C has been shown to be a reliable method for reducing the variability associated with the period prior to sample pre-processing (14). However, many of the currently used SOP have limitations in terms of the intermediate storage period between sample collection and centrifugation. In the clinical setting, the time between the collection of plasma samples and their storage at cold temperatures varies (even though plasma samples should be stored immediately after blood collection). Furthermore, the time for which blood tubes are stored in cold transportation containers prior to centrifugation differs among clinical institutions. The influence of the intermediate storage period on the stability of metabolites should be considered during biomarker discovery and the application of biomarkers to disease diagnosis.

In the present study, we compared the levels of metabolites in matched human serum and plasma samples by using GC/MS to analyze hydrophilic metabolites and LC/MS to analyze lipids, cationic metabolites, and anionic metabolites. In addition, we evaluated the effects of the time for which plasma samples were stored at room temperature or cold temperature on plasma metabolite levels.

MATERIALS AND METHODS

Chemicals

Pyridine, ultrapure water, acetonitrile (LC/MS grade), chloroform, ammonium acetate (1 M solution, high-performance liquid chromatography grade), formic acid (LC/MS grade), and acetic acid (LC/MS grade) were purchased from Wako Pure Chemical Industries, Ltd. (Osaka, Japan), and methanol (LC/MS grade) was obtained from Kanto Chemical Co., Inc. (Tokyo, Japan). Methoxyamine hydrochloride and tributylamine were purchased from Sigma-Aldrich (MO, USA). *N*-methyl-*N*-(trimethylsilyl)trifluoroacetamide (MSTFA) was acquired from GL Sciences, Inc. (Tokyo, Japan). 2-isopropylmalic acid, which was purchased from Sigma-Aldrich (MO, USA), was used as an internal standard for the GC/MS analysis of hydrophilic metabolites. Dilauroylphosphatidylcholine (PC 12:0-12:0), which was purchased from Avanti Polar Lipids (AL, USA), was used as an internal standard for the lipid analysis, whereas 2-bromohypoxanthine and 10-camphorsulfonate, which were purchased from Sigma-Aldrich (MO, USA), were used as internal standards for the analysis of cationic and anionic metabolites, respectively.

Samples

The human samples were collected in accordance with the guidelines of Kobe University Hospital. The serum and plasma samples were prepared from blood samples using the standard venous blood sampling protocol, which has been used for many years in the clinical site. The matched serum and plasma samples that were kept at room temperature before being centrifuged were obtained from 3 healthy volunteers. In addition, plasma samples that were collected from a healthy volunteer were used to

assess the influence of the duration of the cold temperature storage period on the results of metabolomic analysis, as shown in Figure 1. To prepare the serum samples, blood samples were collected in blood tubes containing a clotting activator and separation gel and were gently mixed and kept at room temperature for more than 30 min until they had completely coagulated. To prepare the plasma samples, blood samples were collected in blood tubes containing ethylenediaminetetraacetic acid (EDTA)-2Na and were gently mixed and kept at room temperature for 0, 15, or 30 min or at a cold temperature, which was kept by using Cube Cooler (FORTE GROW MEDICAL, Tochigi, Japan) , for 1, 4, or 8 h. Then, the blood tubes were centrifuged at 2,270 x g for 10 min at 4°C, and the serum and plasma were transferred to clean tubes and stored at -80°C before being used.

Extraction procedure

To extract hydrophilic metabolites prior to the GC/MS analysis, 50 μL of serum or plasma were mixed with 250 μL of methanol and 10 μL of 2-isopropylmalic acid (0.5 mg/mL) as an internal standard. Then, the mixture was shaken at 1,200 rpm for 30 min at 37°C, before being centrifuged at 19,300 ×g for 3 min at 4°C. Two hundred and twenty-five μL of the obtained supernatant were transferred to a clean tube, before being lyophilized using a freeze dryer. For oximation, 80 μL of 20 mg/ml methoxyamine hydrochloride dissolved in pyridine were added to the tube and then sonicated for 20 min, before being shaken at 1,200 rpm for 90 min at 30°C. Then, 40 μL of MSTFA were added, and then the mixture was incubated at 1,200 rpm for 30 min at 37 °C. After the mixture had been centrifuged at 19,300 ×g for 5 min at room temperature, the resultant supernatant was subjected to GC/MS.

For the lipid analysis using LC/MS, 10 μL of serum or plasma were mixed with 80 μL of methanol and 10 μL of 500 ppb PC 12:0-12:0 dissolved in methanol as an internal standard, and then the solution was centrifuged at 16,000 ×g for 5 min at 4°C. The resultant supernatant was subjected to LC/MS analysis.

To extract cationic and anionic metabolites prior to the LC/MS analysis, 50 μL of serum or plasma were mixed with 900 μL of a solvent mixture (methanol : water : chloroform = 2.5:1:1) containing 1 μM 2-bromohypoxanthine and 10-camphorsulfonate as internal standards. The mixture was subsequently shaken at 1,400 rpm for 30 min at 37°C, before being centrifuged at 16,000 ×g for 3 min at 4°C. The resultant supernatant (630 μL) was transferred to a clean tube. Then, 280 μL of water were added, and the mixture was mixed well. After the mixture had been centrifuged at 16,000 ×g for 5 min at 4°C, 500 μL of the resultant supernatant were centrifugally filtrated through a 3-kDa filter device (Millipore, MA, USA) at 14,000 ×g for 1 h to remove any proteins. The filtrate was lyophilized using a freeze dryer, dissolved in water, and analyzed by LC/MS.

GC/MS analysis

The GC/MS analysis was carried out on a GCMS-TQ8040 system (Shimadzu Co.). Each sample was injected at a split ratio of 1:10, and then the separation was performed on a fused silica capillary column (BPX5; inner diameter: 30 m × 0.25 mm, film thickness: 0.25 μm; SGE Analytical Science). The front inlet temperature was 250°C. Helium gas was used as the GC carrier gas, and argon gas was used as a collision-induced dissociation gas. The flow rate of helium gas through the column was 39.0 cm/s. The column temperature was kept at 80°C for 2 min and then raised by

15°C/min to 330°C, before being kept at 330°C for 3 min. The transfer line and ion-source temperatures were 280°C and 200°C, respectively.

LC/MS analysis

The LC/MS/MS analyses were performed using a Nexera LC system (Shimadzu Corp.) equipped with two LC-30AD pumps, a DGU-20A_5 degasser, an SIL-30AC autosampler, a CTO-20AC column oven, and a CBM-20A control module, coupled with an LCMS-8040 triple quadrupole mass spectrometer (Shimadzu Corp.). The mass spectrometer was equipped with an electrospray ionization source under the following conditions: nebulizing gas flow rate, 3 L/min; desolvation line temperature, 250°C; heat block temperature, 400°C; drying gas flow rate, 15 L/min; interface voltage for positive mode, +4.5 kV; and interface voltage for negative mode, -3.5 kV. The collision-induced dissociation gas pressure was set at 230 kPa.

Lipids were separated using an octadecylsilylated silica (ODS) column (InertSustain C18, 100 mm × 2.1 mm, 3 μm; GL Sciences, Tokyo, Japan) and a guard column (10 mm × 3 mm, 5 μm). The mobile phase for hydrophobic metabolites consisted of A: 20 mM ammonium acetate in water and B: methanol. The flow rate was 0.4 mL/min, and the column oven temperature was 40°C. The gradient program for mobile phase B was as follows: 0 min, 80%; 13 min, 98%; 30 min, 98%; 30.1 min, 80%; and 35 min, 80%. Blank runs (involving the injection of isopropanol) between the actual sample runs were employed to remove any carry-over contamination.

The cation analysis was carried out using a pentafluorophenylpropyl column (Discovery HS F5, 150 × 2.1 mm, 3 μm; SUPELCO, PA, USA) and a guard column

(20 × 2.1 mm, 3 μm). The mobile phase for the cation analysis was composed of A: 0.1% formic acid in water and B: acetonitrile. The flow rate was 0.3 mL/min, and the column oven temperature was 40°C. The gradient program for mobile phase B was as follows: 0 min, 0%; 7 min, 0%; 20 min, 40%; 20.1 min, 100%; 25 min, 100%; 25.1 min, 0%; and 35 min, 0%.

The anion analysis was performed using an ODS column (InertSustain C18, 150 × 2.1 mm, 3 μm; GL Sciences, Tokyo, Japan). The mobile phase for the anion analysis consisted of A: water containing 15 mM acetic acid and 10 mM tributylamine, and B: methanol. The flow rate was 0.3 mL/min, and the column oven temperature was 35°C. The gradient program for mobile phase B was as follows: 0 min, 0%; 0.5 min, 0%; 20 min, 75%; 20.1 min, 98%; 24 min, 98%; 24.1 min, 0%; and 30 min, 0%.

Data analysis

Metabolite peaks were extracted from the GC/MS dataset using the Smart Metabolites Database (Shimadzu, Co.), which contained the relevant multiple reaction monitoring (MRM) method file and data regarding the GC analytical conditions, MRM parameters, and the retention index employed for the metabolite measurement. To correct the retention time, the Automatic Adjustment of Retention Time (AART) function of the GCMSsolution software (Shimadzu Co.) and a standard alkane series mixture (C7 to C33) were used. The peak identification was performed automatically, and then the peaks were confirmed manually based on the specific precursor and product ions, and the retention time.

The lipids detected by LC/MS were putatively identified based on multiple reaction monitoring transitions and their retention times using an in-house library, which targeted phospholipids, acylcarnitines (AC), fatty acids (FA), and bile acids (15). The phospholipids included in the library were verified based on the precursor m/z and a head group-specific positive fragment (m/z 184.1) for phosphocholines (PC) or head group-specific neutral loss (NL 141) for phosphoethanolamines (PE). The structural details of the constituent FA were assigned based on the numbers of C-atoms and double bonds in their negative fragments. The AC included in the library were verified based on the precursor m/z and a specific positive fragment (m/z 85.05). The FA and bile acids included in the library were identified using authentic chemical standards. Peak selection and integration were performed automatically using the MRMPROBS (16), and the results were then checked manually.

The cationic and anionic metabolites detected by LC/MS were identified based on the precursor ions, single specific product ions, and retention times produced by authentic chemical standards during analyses involving the same analytical methods (15). Peak selection and integration were carried out automatically using the LabSolutions software (ver. 5.65; Shimadzu Corp.), and the results were then checked manually.

The peak area of each metabolite was normalized to that of the internal standard. Then, the obtained corrected peak area values were statistically evaluated using EZR, which is a graphical user interface for the software R (17). Metabolites whose serum and plasma levels differed significantly were identified using the paired Student's *t* test ($p < 0.05$). Significant changes in the plasma levels of metabolites caused by the storage conditions were identified using one-way repeated measures ANOVA ($p < 0.05$). In

our study, the process of multi comparison was not performed, because our study is the exploratory analysis and, is also needed to avoid the confusion in data evaluation.

RESULTS AND DISCUSSION

To evaluate the disease-specific changes in the serum or plasma levels of metabolites, it is critical to understand the influence of pre-analytical factors, such as degradation, oxidation, or metabolic reactions. Furthermore, serum can contain varying amounts of blood cell-derived metabolites that are released during the coagulation cascade. Plasma separation is carried out along with anticoagulation, and this process is usually able to be performed at the cooling condition. Therefore, the concentrations of metabolites may be less affected by plasma preparation compared with serum preparation. From this viewpoint, collecting procedures of plasma were evaluated in addition to the comparison between serum and plasma metabolite levels.

In our study, serum and plasma were analyzed (using GC/MS to analyze hydrophilic metabolites and LC/MS to analyze lipids, cationic metabolites, and anionic metabolites) to investigate the differences between their metabolite profiles (Figure 1A). As a result, 104, 213, 44, and 37 metabolites were detected during the analyses of hydrophilic metabolites with GC/MS and lipids, cationic metabolites, and anionic metabolites with LC/MS, respectively (Supplementary Table S1). Of these metabolites, 76 exhibited significant differences between their plasma and serum levels (Figure 2). They included carbohydrates, organic acids, amino acids, lyso-PC (LPC), PC, PE, FA, and AC. Most carbohydrates, amino acids, and their derivatives exhibited higher levels in serum than in plasma. In addition, the lipid species, except for LPC, displayed the same tendency. Coagulation is the process by which blood

changes from a liquid to a gel to form a blood clot, which can lead to the enrichment of metabolites, such as carbohydrates, amino acids, and lipid species, in serum due to a reduction in liquid volume compared with that seen in anticoagulated plasma. In the cationic metabolite analysis, guanosine was only detected in the serum samples. This indicated that some metabolites might be released from blood cells via the coagulation cascade during the serum preparation process. On the other hand, the reductions in the serum levels of some metabolites observed in this study might have been caused by the consumption of the metabolites in metabolic reactions by enzymes released from blood cells during clotting. In a previous study, Wedge et al. indicated that the majority of metabolites demonstrated similar levels of inter-subject variation in both serum and plasma, although the levels of specific metabolites displayed different distributions (18). To determine whether metabolite biomarkers found in plasma/serum can be used to obtain clinical diagnoses via analyses of the other fluid (i.e., serum and plasma, respectively), it is crucial to verify the influence of blood processing techniques, as was shown in our study.

The exposure of plasma samples in collection tubes to room temperature or their prolonged storage at cold temperatures before centrifugation is major risks during pre-analytical processing. Thus, we also evaluated the plasma levels of metabolites according to the period for which the samples were stored at room temperature (the room temperature storage period; i.e., for 0, 15, or 30 min, in order to simulate the environment during blood collection in medical check-ups, in which the room temperature storage period varies. In addition, we evaluated the levels of metabolites according to the period for which samples were stored at cold temperatures (the cold temperature storage period); i.e., for 1, 4, or 8 h, in order to simulate the storage of

blood tubes in cold transportation containers prior to centrifugation, which is assumed to differ among clinical institutions (Figure 1B). As a result, 89, 213, 43, and 37 metabolite peaks were commonly detected during the analysis of hydrophilic metabolites with GC/MS and the analysis of lipids, cationic metabolites, and anionic metabolites with LC/MS, respectively (Supplementary Table S2). Of these metabolites, the levels of 45 metabolites were significantly affected by the storage conditions (Figure 3, Supplementary Figure S1). The levels of sucrose and pyruvic acid increased markedly with the room temperature storage period. The level of sucrose did not change when the samples were stored at cold temperatures. In contrast, the level of pyruvic acid fell as the cold temperature storage period increased. Pyruvic acid is involved in primary metabolic pathways, such as glycolysis (19), and the associated metabolic activity in blood cells might affect the production of metabolites in plasma prior to centrifugation. Moreover, the enzymatic consumption or non-enzymatic conversion of metabolites might occur even at cold temperatures. The level of hypoxanthine increased with the duration of the period before centrifugation regardless of whether the samples were stored at room temperature or cold temperature. Yin et al. reported that the plasma level of hypoxanthine increased when freshly collected blood samples were exposed to room temperature before centrifugation (20), which is in line with our results. The high level of hypoxanthine observed in plasma was considered to be derived from blood erythrocytes and platelets (21), which can release hypoxanthine into plasma after blood collection, depending on the duration of the period between sample collection and the removal of blood cells by centrifugation.

In both GC/MS and LC/MS analyses of our study, the internal standards were used in the metabolite extraction step, and then were analyzed along with the blood metabolites. As a result, the internal standards were stably detected among all samples (data not shown). These results indicate the following: Our comprehensive metabolite analyzing system itself is no problem, but some metabolites had the different analytical stability between GC/MS and LC/MS (Supplementary Table S1). For example, threonine, aspartic acid and glutamic acid had the low analytical stability in the LC/MS analysis compared with the GC/MS analysis (Supplementary Table S1). In the case of measuring amino acids by LC/MS, the derivatization step is often selected, although it was not performed in the study due to the comprehensive analysis of blood metabolites including amino acids. LC/MS is relatively weak in analyzing the highly polar molecules, therefore the polarity of the molecules is lowered by derivatization leading to the high separation capacity. The derivatization also leads to an increase in the ionization efficiency. On the other hand, the derivatization step is basically carried out in the GC/MS analysis, although the analytical sensitivity of GC/MS is lower than that of LC/MS. These facts are also important in evaluating our findings and performing exploratory and confirmatory researches about the metabolite biomarkers.

In conclusion, there are significant differences in the metabolite profiles of serum and plasma. In addition, we have shown that the delay between blood collection and centrifugation and the storage temperature during this period have a significant impact on the metabolite profile of plasma. Almost all large clinical trials involving the validation of biomarker candidates are multicenter studies. The validity and confidence of the conclusions drawn from such studies are highly dependent on the quality of the procedures employed. In terms of analytical processes, quality

assurance and quality control processes can ensure the consistency of metabolomic data (22). Most metabolites in plasma are stable at -80°C after centrifugation (23). However, subjecting plasma samples to repeated freeze-thaw cycles affects their metabolite levels (24), which highlights the importance of controlling the experimental conditions using SOP during metabolomic analysis-based biomarker discovery and the subsequent application of the identified biomarkers to disease diagnosis. The current SOP for the blood processing procedures employed before centrifugation in the clinical environment are limited, which might make it difficult to review and make decisions on the quality of metabolomic datasets. Although metabolite profiles are sensitive to pre-analytical blood processing, it is possible to find disease-related biomarker candidates by excluding unstable metabolites from the targets for evaluation. Our findings suggest the following: In the exploratory and confirmatory researches about metabolite biomarkers, it is important to take full account of pre-analytical blood processing procedures. It is preferable to cool immediately after the blood collection and continue the plasma separation promptly, because our study confirmed that some of the metabolites alter depending on the blood treatment time after blood collection. If it is difficult to perform the prompt blood treatment in the clinical practice, the full understandings of the effects of the blood treatment time on the metabolite concentrations are required. Moreover, in the large scale study, stable house hold metabolites may be also important, because stable house hold metabolites are available to evaluate the quality control of each sample and the analytical performance of each analysis batch. The information obtained in this study will contribute to the discovery of reliable biomarker candidates and their application to disease diagnosis. An inter-instrument and inter-laboratory

measurement comparison is also important in determining the reliable metabolite biomarkers.

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Figure legends

Figure 1

Scheme of the pre-analytical blood processing

The differences in metabolite profiles caused by serum or plasma sampling were assessed (A). The changes in metabolite profiles caused by storage at room temperature (RT), which simulated the environment of blood collection during medical check-ups (during which the room temperature storage period varies), or at cold temperature (CT), which simulated blood tube storage in a cold transportation container, were assessed (B).

Figure 2

Differences in the levels of metabolites between serum and plasma

Metabolites whose plasma and serum levels differed significantly are shown (paired Student's *t* test, $p < 0.05$). The columns represent the serum to plasma metabolite level ratios for each subject.

Figure 3

Significant changes in the plasma levels of metabolites caused by the storage conditions

Metabolites whose levels were significantly altered (one-way repeated measures ANOVA, $p < 0.05$) by storage at room temperature or cold temperature are shown. The plots represent the geometric mean ratio of the plasma metabolite level to the level seen at 0 min at room temperature or at 1 h at cold temperature. The results of Figure 3 are also visualized with the heat map in Figure S1.

Supplementary materials

Table S1

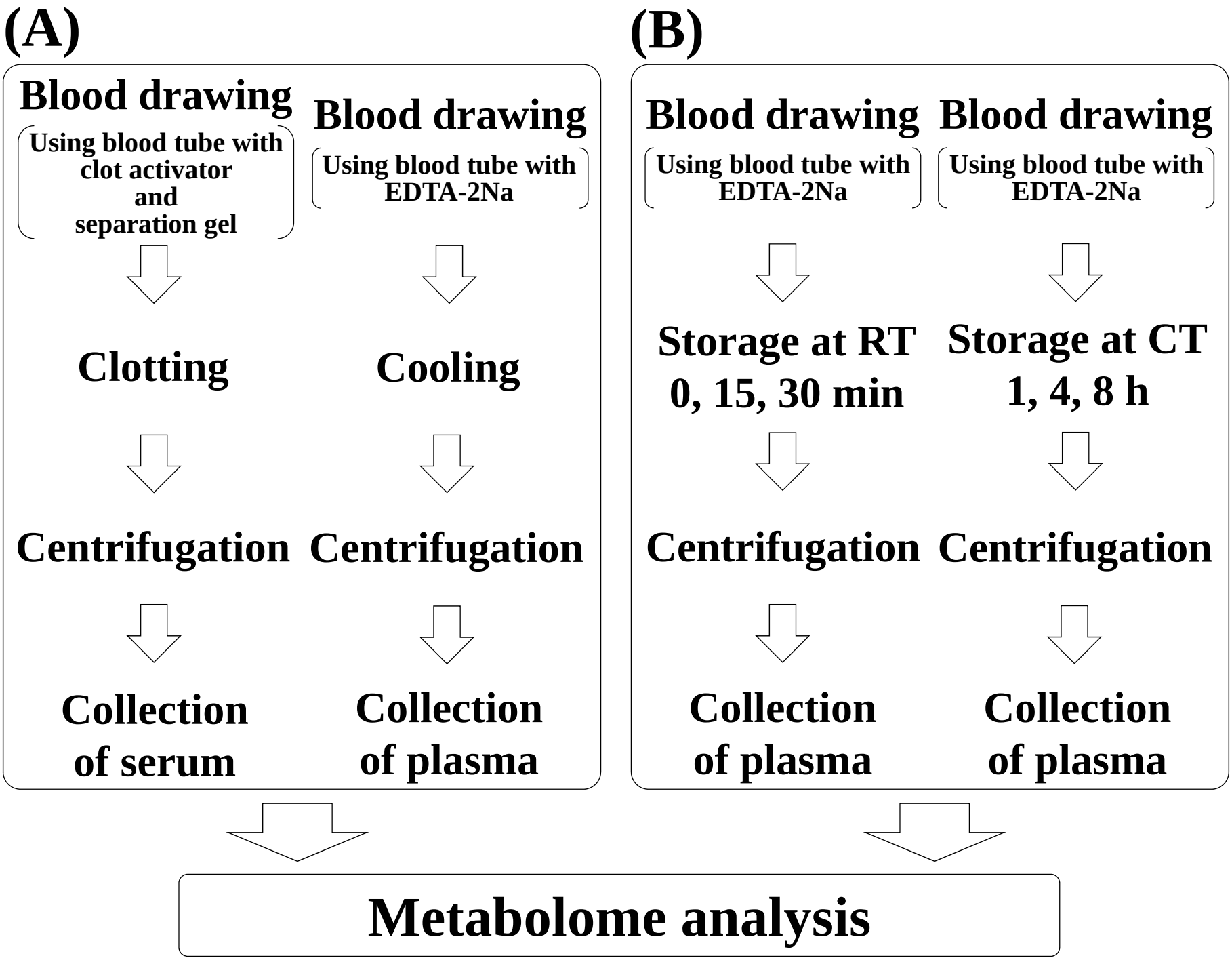
Comparison of the levels of metabolites in serum and plasma according to GC/MS and LC/MS

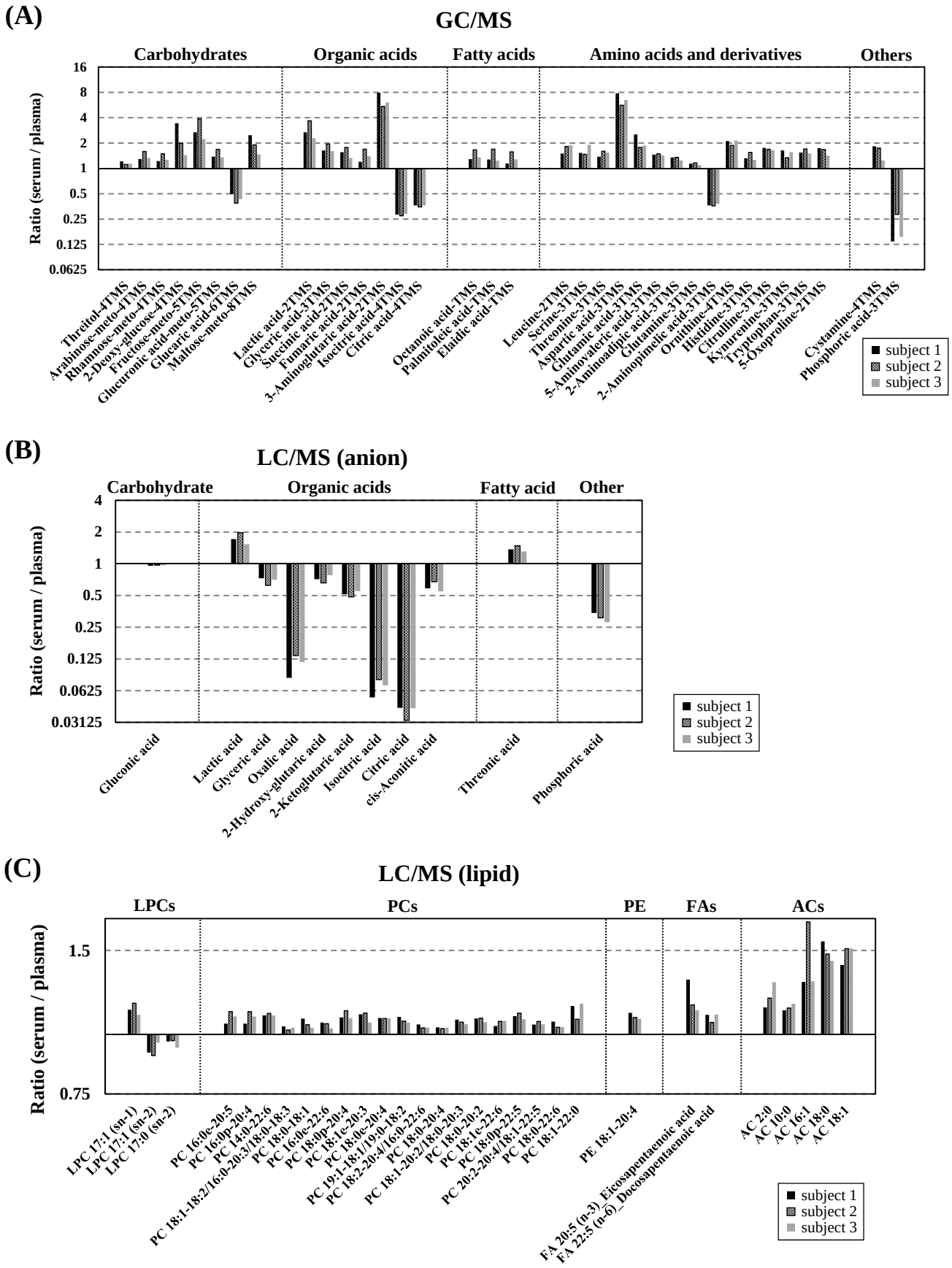
Table S2

Differences in the plasma levels of metabolites caused by storage at room temperature or at cold temperature

Figure S1

Heat map visualization of the significant changes in the plasma levels of metabolites caused by the storage conditions


(A)
Blood drawing
Using blood tube with clot activator and separation gel
Clotting
Centrifugation
Collection of serum
Blood drawing
Using blood tube with EDTA-2Na
Cooling
Centrifugation
Collection of plasma
(B)
Blood drawing
Using blood tube with EDTA-2Na
Storage at RT 0, 15, 30 min
Centrifugation
Collection of plasma
Blood drawing
Using blood tube with EDTA-2Na
Storage at CT 1, 4, 8 h
Centrifugation
Collection of plasma
Metabolome analysis


(A)
GC/MS
Carbohydrates
Organic acids
Fatty acids
Amino acids and derivatives
Others
Ratio (serum / plasma)
16
8
4
2
1
0.5
0.25
0.125
0.0625
ThreitoL-4TMS
Arabinose-meto-4TMS
Rhamnose-meto-4TMS
2-Deoxy-glucose-4TMS
Fructose-meto-5TMS
Glucuronic acid-meto-5TMS
Glucaric acid-6TMS
Maltose-meto-8TMS
Lactic acid-2TMS
Glyceric acid-3TMS
Succinic acid-2TMS
Fumaric acid-2TMS
3-Aminoglutaric acid-2TMS
Isocitric acid-4TMS
Citric acid-4TMS
Octanoic acid-TMS
Palmitoleic acid-TMS
Elaidic acid-TMS
Leucine-2TMS
Serine-3TMS
Threonine-3TMS
Aspartic acid-3TMS
Glutamic acid-3TMS
5-Aminovaleric acid-3TMS
2-Aminoadipic acid-3TMS
2-Aminopimelic acid-3TMS
Glutamine-3TMS
Ornithine-4TMS
Histidine-3TMS
Citrulline-3TMS
Kynurenine-3TMS
Tryptophan-3TMS
5-Oxoproline-2TMS
Cystamine-4TMS
Phosphoric acid-3TMS
subject 1
subject 2
subject 3
(B)
LC/MS (anion)
Carbohydrate
Organic acids
Fatty acid
Other
Ratio (serum / plasma)
4
2
1
0.5
0.25
0.125
0.0625
0.03125
Gluconic acid
Lactic acid
Glyceric acid
Oxalic acid
2-Hydroxy-glutaric acid
2-Ketoglutaric acid
Isocitric acid
Citric acid
cis-Aconitic acid
Threonic acid
Phosphoric acid
subject 1
subject 2
subject 3
(C)
LC/MS (lipid)
LPCs
PCs
PE
FAs
ACs
Ratio (serum / plasma)
1.5
0.75
LPC 17:1 (sn-1)
LPC 17:1 (sn-2)
LPC 17:0 (sn-2)
PC 16:0e-20:5
PC 16:0p-20:4
PC 14:0-22:6
PC 18:1-18:2/16:0-20:3/18:0-18:3
PC 18:0-18:1
PC 16:0e-22:6
PC 18:0p-20:4
PC 18:1e-20:3
PC 18:0e-20:4
PC 19:1-18:1/19:0-18:2
PC 18:2-20:4/16:0-22:6
PC 18:0-20:4
PC 18:1-20:2/18:0-20:3
PC 18:0-20:2
PC 18:1e-22:6
PC 18:0p-22:5
PC 20:2-20:4/18:1-22:5
PC 18:0-22:6
PC 18:1-22:0
PE 18:1-20:4
FA 20:5 (n-3)_Eicosapentaenoic acid
FA 22:5 (n-6)_Docosapentaenoic acid
AC 2:0
AC 10:0
AC 16:1
AC 18:0
AC 18:1
subject 1
subject 2
subject 3

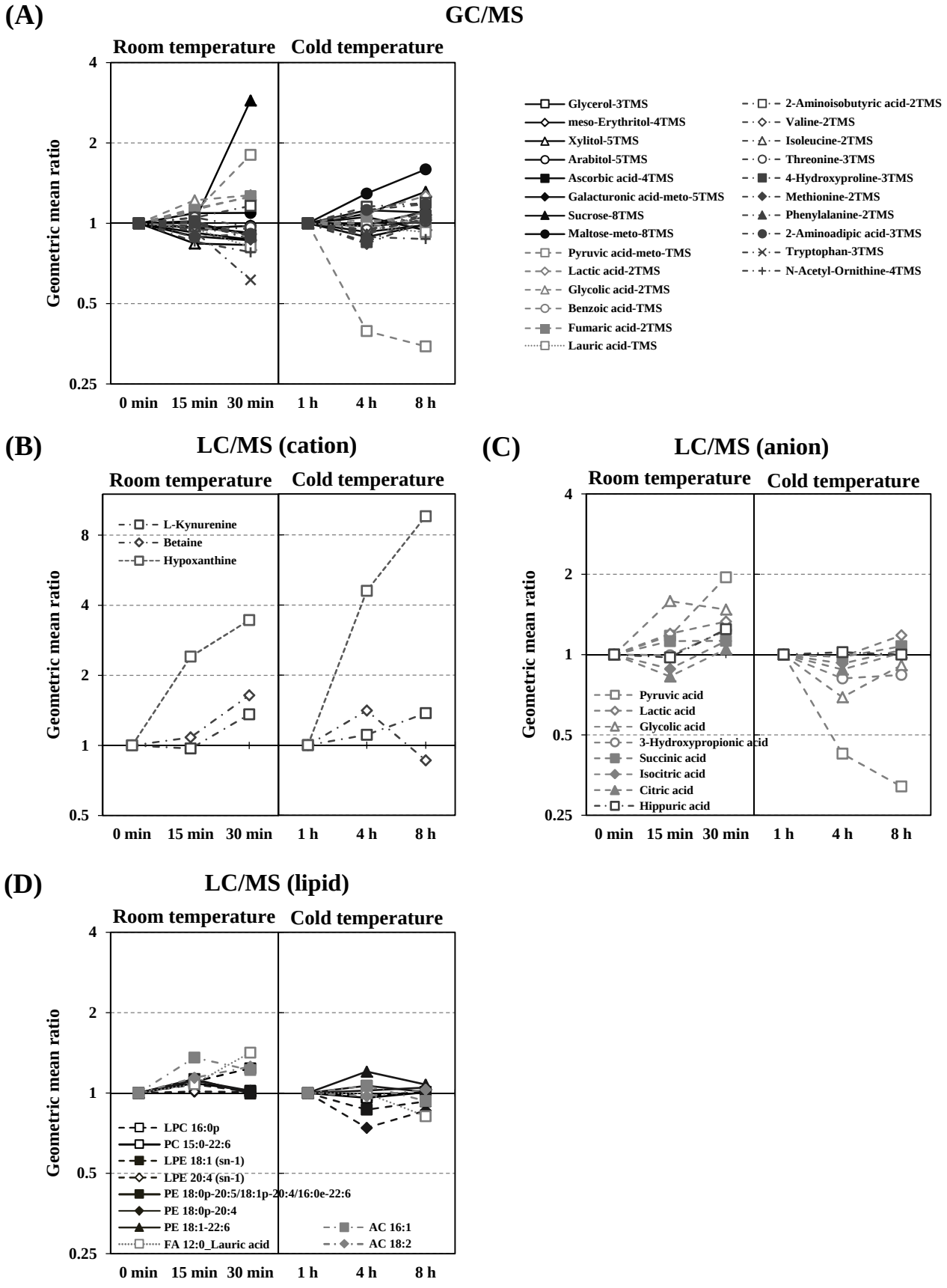

(A)
GC/MS
Room temperature
Cold temperature
Geometric mean ratio
4
2
1
0.5
0.25
0 min
15 min
30 min
1 h
4 h
8 h
Glycerol-3TMS
meso-Erythritol-4TMS
Xylitol-5TMS
Arabitol-5TMS
Ascorbic acid-4TMS
Galacturonic acid-meto-5TMS
Sucrose-8TMS
Maltose-meto-8TMS
Pyruvic acid-meto-TMS
Lactic acid-2TMS
Glycolic acid-2TMS
Benzoic acid-TMS
Fumaric acid-2TMS
Lauric acid-TMS
2-Aminoisobutyric acid-2TMS
Valine-2TMS
Isoleucine-2TMS
Threonine-3TMS
4-Hydroxyproline-3TMS
Methionine-2TMS
Phenylalanine-2TMS
2-Aminoadipic acid-3TMS
Tryptophan-3TMS
N-Acetyl-Ornithine-4TMS
(B)
LC/MS (cation)
Room temperature
Cold temperature
Geometric mean ratio
8
4
2
1
0.5
L-Kynurenine
Betaine
Hypoxanthine
0 min
15 min
30 min
1 h
4 h
8 h
(C)
LC/MS (anion)
Room temperature
Cold temperature
Geometric mean ratio
4
2
1
0.5
0.25
Pyruvic acid
Lactic acid
Glycolic acid
3-Hydroxypropionic acid
Succinic acid
Isocitric acid
Citric acid
Hippuric acid
0 min
15 min
30 min
1 h
4 h
8 h
(D)
LC/MS (lipid)
Room temperature
Cold temperature
Geometric mean ratio
4
2
1
0.5
0.25
LPC 16:0p
PC 15:0-22:6
LPE 18:1 (sn-1)
LPE 20:4 (sn-1)
PE 18:0p-20:5/18:1p-20:4/16:0e-22:6
PE 18:0p-20:4
PE 18:1-22:6
FA 12:0_Lauric acid
AC 16:1
AC 18:2
0 min
15 min
30 min
1 h
4 h
8 h

Table S1
Comparison of the levels of metabolites in serum and plasma by using GC/MS and LC/MS

Metabolite	Method	Corrected peak area						Ratio (Serum level / Plasma level)			*p*-value
		Serum			Plasma						
		subject 1	subect 2	subject 3	subject 1	subject 2	subject 3	subject 1	subject 2	subject 3	
Pyruvic acid-meto-TMS	GC/MS	1.03.E-01	1.60.E-01	3.27.E-01	1.07.E-01	1.52.E-01	2.61.E-01	0.970	1.052	1.254	0.386
Lactic acid-2TMS	GC/MS	5.36.E+00	5.88.E+00	5.97.E+00	2.00.E+00	1.60.E+00	2.61.E+00	2.679	3.679	2.284	0.007
Glycolic acid-2TMS	GC/MS	8.72.E-02	1.02.E-01	8.21.E-02	8.54.E-02	7.20.E-02	8.01.E-02	1.020	1.414	1.026	0.351
Alanine-2TMS	GC/MS	8.69.E-01	8.33.E-01	1.20.E+00	6.59.E-01	4.87.E-01	6.38.E-01	1.319	1.710	1.880	0.068
2-Keto-isovaleric acid-meto-TMS	GC/MS	1.47.E-02	2.15.E-02	1.72.E-02	1.39.E-02	1.44.E-02	1.44.E-02	1.064	1.491	1.198	0.188
Glycine-2TMS	GC/MS	1.70.E-02	1.15.E-02	1.80.E-02	1.79.E-02	1.39.E-02	1.76.E-02	0.947	0.828	1.022	0.343
2-Hydroxybutyric acid-2TMS	GC/MS	1.99.E-01	3.20.E-01	2.15.E-01	1.65.E-01	1.87.E-01	1.65.E-01	1.205	1.718	1.301	0.145
Sarcosine-2TMS	GC/MS	1.06.E-01	1.55.E-01	1.15.E-01	9.26.E-02	9.85.E-02	9.14.E-02	1.143	1.572	1.254	0.141
2-Aminoisobutyric acid-2TMS	GC/MS	6.50.E-02	7.92.E-02	5.89.E-02	4.42.E-02	4.10.E-02	4.52.E-02	1.469	1.931	1.302	0.080
3-Hydroxybutyric acid-2TMS	GC/MS	3.12.E-01	9.35.E-01	3.80.E-01	2.52.E-01	5.44.E-01	2.78.E-01	1.235	1.720	1.369	0.219
2-Aminobutyric acid-2TMS	GC/MS	3.03.E-02	6.02.E-02	2.83.E-02	2.40.E-02	3.66.E-02	1.95.E-02	1.265	1.643	1.451	0.138
3-Hydroxyisovaleric acid-2TMS	GC/MS	5.95.E-02	1.31.E-01	7.15.E-02	5.05.E-02	8.00.E-02	5.94.E-02	1.177	1.634	1.204	0.217
Valine-2TMS	GC/MS	8.76.E+00	1.20.E+01	9.83.E+00	7.13.E+00	7.87.E+00	7.07.E+00	1.230	1.522	1.389	0.058
Urea-2TMS	GC/MS	4.97.E+00	9.28.E+00	4.56.E+00	4.33.E+00	5.93.E+00	3.64.E+00	1.149	1.564	1.252	0.197
2-Aminoethanol-3TMS	GC/MS	3.96.E-01	4.25.E-01	3.79.E-01	3.46.E-01	2.78.E-01	3.39.E-01	1.144	1.529	1.120	0.146
Benzoic acid-TMS	GC/MS	3.19.E-02	4.33.E-02	3.26.E-02	2.96.E-02	2.90.E-02	2.88.E-02	1.078	1.491	1.133	0.212
Glycerol-3TMS	GC/MS	6.22.E-01	8.76.E-01	7.60.E-01	5.74.E-01	6.43.E-01	7.61.E-01	1.083	1.362	1.000	0.319
Leucine-2TMS	GC/MS	5.15.E+00	6.59.E+00	5.45.E+00	3.44.E+00	3.61.E+00	2.89.E+00	1.500	1.824	1.888	0.023
Octanoic acid-TMS	GC/MS	5.76.E-02	6.43.E-02	6.61.E-02	4.47.E-02	3.88.E-02	4.86.E-02	1.288	1.660	1.359	0.037
Phosphoric acid-3TMS	GC/MS	7.76.E-01	1.31.E+00	7.06.E-01	5.72.E+00	4.61.E+00	4.60.E+00	0.136	0.285	0.154	0.014
Isoleucine-2TMS	GC/MS	2.16.E+00	2.97.E+00	2.59.E+00	1.78.E+00	1.91.E+00	1.68.E+00	1.217	1.557	1.540	0.062
Proline-2TMS	GC/MS	3.28.E+00	4.46.E+00	4.05.E+00	2.57.E+00	3.02.E+00	2.17.E+00	1.276	1.476	1.867	0.059
Succinic acid-2TMS	GC/MS	4.26.E-02	3.62.E-02	4.29.E-02	2.74.E-02	2.04.E-02	3.22.E-02	1.557	1.776	1.329	0.014
Glyceric acid-3TMS	GC/MS	9.82.E-02	1.28.E-01	1.08.E-01	6.02.E-02	6.55.E-02	6.74.E-02	1.630	1.951	1.602	0.026
Uracil-2TMS	GC/MS	1.88.E-03	1.61.E-03	2.01.E-03	1.32.E-03	1.99.E-03	1.93.E-03	1.423	0.809	1.039	0.786
Serine-3TMS	GC/MS	1.66.E+00	1.63.E+00	1.70.E+00	1.08.E+00	1.11.E+00	8.91.E-01	1.530	1.472	1.904	0.018
Fumaric acid-2TMS	GC/MS	1.69.E-02	1.48.E-02	1.83.E-02	1.40.E-02	8.77.E-03	1.32.E-02	1.200	1.692	1.388	0.040
Homoserine-2TMS	GC/MS	1.99.E-03	1.35.E-03	1.84.E-03	1.27.E-03	1.37.E-03	1.78.E-03	1.565	0.979	1.034	0.400
Nonanoic acid-TMS	GC/MS	7.86.E-02	7.90.E-02	7.79.E-02	6.75.E-02	4.77.E-02	6.50.E-02	1.165	1.655	1.198	0.104
Threonine-3TMS	GC/MS	3.14.E-01	3.97.E-01	4.62.E-01	2.28.E-01	2.48.E-01	3.00.E-01	1.377	1.597	1.541	0.030
Glutaric acid-2TMS	GC/MS	1.49.E-03	7.89.E-03	2.86.E-03	1.32.E-03	4.61.E-03	2.19.E-03	1.130	1.712	1.305	0.291
Threitol-4TMS	GC/MS	4.45.E-03	3.29.E-03	5.32.E-03	3.67.E-03	2.95.E-03	4.66.E-03	1.214	1.113	1.141	0.047
Malic acid-3TMS	GC/MS	3.86.E-03	2.94.E-03	3.69.E-03	2.50.E-03	2.80.E-03	3.43.E-03	1.548	1.047	1.076	0.274
meso-Erythritol-4TMS	GC/MS	1.12.E-02	2.23.E-02	1.61.E-02	1.04.E-02	1.42.E-02	1.37.E-02	1.078	1.574	1.169	0.234
Aspartic acid-3TMS	GC/MS	2.46.E-02	2.46.E-02	2.53.E-02	3.16.E-03	4.38.E-03	3.88.E-03	7.807	5.634	6.513	0.000
3-Aminoglutaric acid-2TMS	GC/MS	1.45.E-01	1.48.E-01	1.56.E-01	1.82.E-02	2.71.E-02	2.57.E-02	7.964	5.454	6.079	0.001
4-Hydroxyproline-3TMS	GC/MS	3.47.E-01	5.04.E-01	2.69.E-01	2.90.E-01	3.46.E-01	2.09.E-01	1.198	1.453	1.285	0.109
Methionine-2TMS	GC/MS	3.82.E-02	5.01.E-02	4.83.E-02	3.18.E-02	3.18.E-02	3.52.E-02	1.200	1.576	1.373	0.068
4-Aminobutyric acid-3TMS	GC/MS	4.66.E-03	5.46.E-03	5.42.E-03	3.84.E-03	3.34.E-03	6.66.E-03	1.213	1.634	0.814	0.622
5-Oxoproline-2TMS	GC/MS	2.96.E-01	1.96.E-01	2.96.E-01	1.69.E-01	1.17.E-01	2.08.E-01	1.744	1.675	1.419	0.022
Pyrogallol-3TMS	GC/MS	2.00.E-02	4.17.E-03	5.16.E-02	1.64.E-02	2.68.E-03	4.30.E-02	1.219	1.556	1.202	0.164
Cysteine-3TMS	GC/MS	1.85.E-01	2.25.E-01	2.47.E-01	2.41.E-01	2.40.E-01	3.46.E-01	0.770	0.937	0.712	0.146
Creatinine-3TMS	GC/MS	5.08.E-02	7.54.E-02	5.12.E-02	2.57.E-02	2.67.E-02	2.63.E-02	1.976	2.820	1.950	0.053
2-Ketoglutaric acid-meto-2TMS	GC/MS	3.71.E-02	2.96.E-02	5.43.E-02	3.98.E-02	2.94.E-02	4.98.E-02	0.933	1.008	1.091	0.771
Glutamic acid-3TMS	GC/MS	3.93.E-01	3.12.E-01	5.60.E-01	1.55.E-01	1.76.E-01	2.99.E-01	2.536	1.776	1.869	0.031
5-Aminovaleric acid-3TMS	GC/MS	9.13.E-03	6.53.E-03	7.45.E-03	6.26.E-03	4.38.E-03	5.22.E-03	1.458	1.492	1.427	0.009
Phenylalanine-2TMS	GC/MS	1.37.E+00	1.65.E+00	1.42.E+00	1.08.E+00	1.01.E+00	1.10.E+00	1.268	1.637	1.289	0.066
Xylose-meto-4TMS	GC/MS	4.60.E-03	6.52.E-03	5.13.E-03	3.51.E-03	3.91.E-03	3.95.E-03	1.312	1.670	1.299	0.081
Arabinose-meto-4TMS	GC/MS	1.73.E-02	2.17.E-02	2.04.E-02	1.34.E-02	1.36.E-02	1.54.E-02	1.289	1.589	1.326	0.045
Ribulose-meto-4TMS	GC/MS	8.04.E-03	9.56.E-03	8.33.E-03	7.72.E-03	6.39.E-03	7.91.E-03	1.041	1.495	1.053	0.298
Lauric acid-TMS	GC/MS	7.93.E-02	9.93.E-02	5.74.E-02	6.24.E-02	6.19.E-02	4.48.E-02	1.272	1.604	1.281	0.100
Ribose-meto-4TMS	GC/MS	6.52.E-03	1.20.E-02	7.96.E-03	3.94.E-03	3.82.E-03	3.55.E-03	1.657	3.153	2.245	0.092
Homocysteine-3TMS	GC/MS	9.11.E-03	6.44.E-03	7.16.E-03	9.77.E-03	6.50.E-03	7.23.E-03	0.932	0.990	0.990	0.315
Asparagine-3TMS	GC/MS	5.73.E-02	4.98.E-02	6.12.E-02	4.10.E-02	4.76.E-02	4.63.E-02	1.395	1.047	1.324	0.130
Xylitol-5TMS	GC/MS	1.59.E-02	5.20.E-02	2.47.E-02	1.41.E-02	3.29.E-02	2.07.E-02	1.132	1.583	1.192	0.266
Arabitol-5TMS	GC/MS	1.68.E-02	5.52.E-02	2.51.E-02	1.45.E-02	3.40.E-02	2.13.E-02	1.153	1.627	1.181	0.274

Ribitol-5TMS	GC/MS	3.73.E-03	5.04.E-03	4.67.E-03	2.98.E-03	3.14.E-03	3.71.E-03	1.249	1.607	1.257	0.078
1,6-Anhydroglucose-3TMS	GC/MS	3.12.E-03	1.11.E-03	1.51.E-03	2.73.E-03	6.23.E-04	1.47.E-03	1.143	1.782	1.028	0.152
Rhamnose-meto-4TMS	GC/MS	4.57.E-03	3.15.E-03	2.98.E-03	3.74.E-03	2.11.E-03	2.35.E-03	1.222	1.497	1.268	0.020
Fucose-meto-4TMS	GC/MS	4.33.E-03	3.02.E-03	3.09.E-03	4.47.E-03	2.18.E-03	2.61.E-03	0.968	1.387	1.182	0.306
2-Aminoadipic acid-3TMS	GC/MS	9.03.E-03	9.34.E-03	7.88.E-03	6.70.E-03	6.91.E-03	6.35.E-03	1.348	1.353	1.241	0.018
2-Deoxy-glucose-4TMS	GC/MS	6.89.E-03	8.82.E-03	1.02.E-02	2.01.E-03	4.40.E-03	7.06.E-03	3.436	2.002	1.440	0.016
Putrescine-4TMS	GC/MS	1.79.E-02	1.96.E-02	1.77.E-02	1.52.E-02	1.34.E-02	1.47.E-02	1.177	1.465	1.207	0.071
Aconitic acid-3TMS	GC/MS	1.23.E-03	1.31.E-03	1.53.E-03	1.39.E-03	2.18.E-03	2.34.E-03	0.885	0.599	0.656	0.114
Glutamine-3TMS	GC/MS	2.97.E+00	3.10.E+00	3.00.E+00	2.60.E+00	2.66.E+00	2.74.E+00	1.140	1.163	1.097	0.018
Isocitric acid-4TMS	GC/MS	5.28.E-03	4.84.E-03	5.51.E-03	1.86.E-02	1.77.E-02	1.91.E-02	0.283	0.274	0.289	0.000
2-Aminopimelic acid-3TMS	GC/MS	1.27.E-01	1.00.E-01	1.12.E-01	3.50.E-01	2.78.E-01	2.95.E-01	0.363	0.359	0.379	0.005
Citric acid-4TMS	GC/MS	1.81.E-01	1.39.E-01	1.54.E-01	4.98.E-01	3.98.E-01	4.24.E-01	0.363	0.349	0.363	0.004
Ornithine-4TMS	GC/MS	3.31.E+00	3.75.E+00	3.54.E+00	1.57.E+00	2.00.E+00	1.66.E+00	2.114	1.874	2.140	0.001
Psicose-meto-5TMS	GC/MS	6.20.E-03	5.14.E-03	2.26.E-02	5.63.E-03	3.47.E-03	1.90.E-02	1.102	1.479	1.191	0.160
1,5-Anhydro-glucitol-4TMS	GC/MS	3.46.E-01	5.14.E-01	3.71.E-01	2.65.E-01	2.75.E-01	2.89.E-01	1.306	1.872	1.285	0.125
Sorbose-meto-5TMS	GC/MS	1.41.E-01	2.22.E-01	1.81.E-01	8.53.E-02	9.03.E-02	1.08.E-01	1.656	2.459	1.672	0.063
Fructose-meto-5TMS	GC/MS	5.02.E-02	8.64.E-02	6.93.E-02	1.87.E-02	2.23.E-02	3.10.E-02	2.682	3.879	2.234	0.046
Mannose-meto-5TMS	GC/MS	8.16.E-01	1.32.E+00	7.84.E-01	7.65.E-01	9.15.E-01	6.87.E-01	1.067	1.443	1.141	0.239
5-Dehydroquinic acid-meto-4TMS	GC/MS	2.64.E-02	3.83.E-02	2.89.E-02	2.48.E-02	2.50.E-02	2.75.E-02	1.067	1.534	1.051	0.300
Glucose-meto-5TMS	GC/MS	4.10.E+00	5.49.E+00	4.30.E+00	3.72.E+00	3.62.E+00	4.05.E+00	1.105	1.517	1.061	0.249
Hippuric acid-TMS	GC/MS	3.03.E-02	4.37.E-02	3.58.E-02	3.75.E-02	3.46.E-02	3.96.E-02	0.810	1.261	0.903	0.909
Galactose-meto-5TMS	GC/MS	3.98.E+00	5.45.E+00	4.39.E+00	3.73.E+00	3.71.E+00	3.96.E+00	1.066	1.466	1.107	0.229
Glucosamine-5TMS	GC/MS	9.54.E-02	1.32.E-01	1.06.E-01	9.02.E-02	8.78.E-02	9.41.E-02	1.058	1.506	1.121	0.236
Sebacic acid-2TMS	GC/MS	1.34.E-03	1.24.E-03	1.10.E-03	7.96.E-04	7.58.E-04	8.82.E-04	1.688	1.639	1.242	0.056
Lysine-4TMS	GC/MS	3.75.E-01	4.99.E-01	3.06.E-01	2.95.E-01	3.38.E-01	2.39.E-01	1.272	1.474	1.278	0.073
Glucuronic acid-meto-5TMS	GC/MS	4.35.E-02	4.83.E-02	4.01.E-02	3.16.E-02	2.86.E-02	2.96.E-02	1.379	1.687	1.353	0.039
Histidine-3TMS	GC/MS	4.32.E-01	4.88.E-01	4.59.E-01	3.27.E-01	3.15.E-01	3.63.E-01	1.320	1.548	1.264	0.036
Ascorbic acid-4TMS	GC/MS	8.45.E-03	1.21.E-02	9.87.E-03	7.59.E-03	8.63.E-03	9.09.E-03	1.114	1.400	1.086	0.192
Tyrosine-3TMS	GC/MS	3.54.E-01	4.80.E-01	3.65.E-01	2.98.E-01	3.13.E-01	2.96.E-01	1.187	1.536	1.233	0.110
Galacturonic acid-meto-5TMS	GC/MS	1.66.E-02	2.35.E-02	1.90.E-02	1.56.E-02	1.57.E-02	1.81.E-02	1.065	1.496	1.048	0.293
1-Hexadecanol-TMS	GC/MS	4.27.E-03	8.92.E-03	4.44.E-03	3.79.E-03	5.05.E-03	3.93.E-03	1.124	1.767	1.131	0.287
N-Acetyl-Ornithine-4TMS	GC/MS	2.32.E-02	5.25.E-02	3.03.E-02	2.37.E-02	3.39.E-02	2.86.E-02	0.979	1.550	1.061	0.388
Gluconic acid-6TMS	GC/MS	2.01.E-02	2.17.E-02	1.51.E-02	1.68.E-02	1.49.E-02	1.13.E-02	1.195	1.453	1.337	0.051
Glucaric acid-6TMS	GC/MS	4.06.E-03	2.51.E-03	3.32.E-03	8.22.E-03	6.48.E-03	7.70.E-03	0.494	0.387	0.432	0.001
ParaXanthine-TMS	GC/MS	2.56.E-02	3.28.E-01	1.18.E-01	2.31.E-02	2.09.E-01	1.01.E-01	1.107	1.568	1.162	0.338
Palmitoleic acid-TMS	GC/MS	2.18.E-02	1.11.E-02	3.28.E-02	1.71.E-02	6.58.E-03	2.66.E-02	1.275	1.691	1.236	0.011
Inositol-6TMS	GC/MS	7.29.E-02	1.14.E-01	9.22.E-02	5.43.E-02	6.87.E-02	7.15.E-02	1.344	1.652	1.290	0.079
Uric acid-4TMS	GC/MS	2.53.E+00	4.77.E+00	2.59.E+00	2.29.E+00	3.21.E+00	2.27.E+00	1.105	1.487	1.140	0.240
Citrulline-3TMS	GC/MS	3.97.E-03	4.13.E-03	3.93.E-03	2.26.E-03	2.45.E-03	2.39.E-03	1.755	1.690	1.648	0.001
Margaric acid-TMS	GC/MS	3.03.E-02	2.68.E-02	2.37.E-02	2.52.E-02	1.67.E-02	2.16.E-02	1.204	1.602	1.098	0.131
Kynurenine-3TMS	GC/MS	3.94.E-03	5.64.E-03	4.41.E-03	2.41.E-03	4.20.E-03	2.83.E-03	1.639	1.341	1.556	0.001
Cystamine-4TMS	GC/MS	3.23.E-03	2.24.E-03	3.42.E-03	1.76.E-03	1.28.E-03	2.75.E-03	1.830	1.743	1.244	0.047
Tryptophan-3TMS	GC/MS	4.96.E+00	6.22.E+00	4.42.E+00	3.22.E+00	3.65.E+00	2.93.E+00	1.542	1.705	1.506	0.028
Elaidic acid-TMS	GC/MS	1.22.E-01	8.76.E-02	1.56.E-01	1.07.E-01	5.57.E-02	1.22.E-01	1.143	1.574	1.278	0.045
Stearic acid-TMS	GC/MS	1.87.E+00	1.86.E+00	1.84.E+00	1.68.E+00	1.15.E+00	1.63.E+00	1.116	1.624	1.129	0.161
Cystine-4TMS	GC/MS	2.95.E-02	3.72.E-02	2.78.E-02	9.77.E-03	3.60.E-02	9.98.E-03	3.021	1.032	2.781	0.160
Sucrose-8TMS	GC/MS	1.16.E-02	1.23.E-02	2.54.E-02	7.43.E-03	8.73.E-03	3.61.E-02	1.560	1.410	0.703	0.857
Maltose-meto-8TMS	GC/MS	4.40.E-03	3.09.E-03	7.12.E-03	1.78.E-03	1.62.E-03	4.85.E-03	2.477	1.907	1.469	0.025
Betaine	LC/MS_Cation	3.66.E+00	4.67.E+00	1.14.E+01	3.40.E+00	2.87.E+00	3.67.E+00	1.076	1.624	3.117	0.289
Carnitine	LC/MS_Cation	1.30.E+01	1.68.E+01	3.11.E+01	1.26.E+01	8.63.E+00	7.81.E+00	1.031	1.951	3.986	0.255
Choline	LC/MS_Cation	6.36.E-01	8.16.E-01	1.55.E+00	4.34.E-01	3.15.E-01	2.47.E-01	1.466	2.593	6.256	0.178
Creatine	LC/MS_Cation	8.88.E+00	1.14.E+01	1.99.E+01	8.15.E+00	6.44.E+00	4.81.E+00	1.090	1.768	4.134	0.245
Creatinine	LC/MS_Cation	6.04.E+00	8.04.E+00	1.81.E+01	7.47.E+00	2.84.E+00	3.68.E+00	0.808	2.833	4.921	0.318
Glycine	LC/MS_Cation	3.67.E+00	3.55.E+00	1.11.E+01	3.99.E+00	9.87.E-01	1.97.E+00	0.918	3.598	5.665	0.309
Guanosine	LC/MS_Cation	2.49.E+00	1.16.E+00	3.21.E+00	N.D.	N.D.	N.D.	N.A.	N.A.	N.A.	N.A.
4-Hydroxy-L-proline	LC/MS_Cation	1.98.E+00	3.24.E+00	3.56.E+00	2.09.E+00	1.52.E+00	8.40.E-01	0.946	2.133	4.238	0.224
Hypoxanthine	LC/MS_Cation	6.18.E-01	4.66.E-01	1.15.E+00	5.39.E-02	7.06.E-03	8.83.E-03	11.470	65.975	130.319	0.077
L-Alanine; Sarcosine	LC/MS_Cation	8.57.E+00	9.09.E+00	2.68.E+01	8.11.E+00	3.06.E+00	5.09.E+00	1.057	2.970	5.264	0.278
L-Arginine	LC/MS_Cation	9.16.E+00	1.83.E+01	2.59.E+01	8.31.E+00	9.38.E+00	7.45.E+00	1.102	1.952	3.477	0.206
L-Aspartate	LC/MS_Cation	6.50.E-01	1.04.E+00	1.54.E+00	2.87.E-01	1.36.E-01	9.43.E-02	2.263	7.666	16.317	0.102
L-Asparagine	LC/MS_Cation	5.23.E+00	6.85.E+00	1.48.E+01	4.44.E+00	2.63.E+00	2.86.E+00	1.179	2.600	5.162	0.228

L-Citrulline	LC/MS	Cation	1.57.E+00	1.46.E+00	3.59.E+00	1.12.E+00	8.41.E-01	9.37.E-01	1.406	1.738	3.829	0.221
L-Cysteine	LC/MS	Cation	4.54.E-01	7.00.E-01	1.00.E+00	3.82.E-01	2.33.E-01	2.31.E-01	1.187	2.999	4.339	0.164
L-Lysine	LC/MS	Cation	4.23.E+00	7.75.E+00	7.79.E+00	3.97.E+00	3.73.E+00	1.93.E+00	1.065	2.077	4.039	0.177
L-Glutamine	LC/MS	Cation	1.69.E+02	2.09.E+02	3.99.E+02	1.38.E+02	1.04.E+02	9.46.E+01	1.228	2.007	4.217	0.213
L-Glutamate	LC/MS	Cation	8.20.E+00	1.00.E+01	2.21.E+01	5.63.E+00	3.91.E+00	4.35.E+00	1.458	2.571	5.083	0.194
L-Histidine	LC/MS	Cation	5.03.E+00	7.22.E+00	1.23.E+01	4.41.E+00	4.42.E+00	3.71.E+00	1.142	1.633	3.323	0.234
L-Homoserine; D-Homoserine	LC/MS	Cation	5.64.E+00	8.65.E+00	1.78.E+01	5.22.E+00	3.37.E+00	3.75.E+00	1.081	2.567	4.744	0.240
L-Isoleucine	LC/MS	Cation	3.02.E+01	3.72.E+01	7.32.E+01	3.25.E+01	1.58.E+01	1.47.E+01	0.929	2.349	4.993	0.281
L-Leucine	LC/MS	Cation	5.47.E+01	6.28.E+01	1.21.E+02	5.56.E+01	2.52.E+01	2.31.E+01	0.984	2.494	5.251	0.259
L-Methionine	LC/MS	Cation	4.34.E+00	5.87.E+00	1.09.E+01	4.54.E+00	3.29.E+00	2.83.E+00	0.956	1.784	3.859	0.288
L-Ornithine	LC/MS	Cation	1.12.E+00	1.71.E+00	3.45.E+00	5.57.E-01	5.85.E-01	3.85.E-01	2.014	2.925	8.961	0.171
L-Phenylalanine	LC/MS	Cation	1.50.E+01	2.01.E+01	3.41.E+01	1.41.E+01	1.00.E+01	8.18.E+00	1.070	2.000	4.167	0.233
L-Proline	LC/MS	Cation	5.92.E+00	9.44.E+00	1.30.E+01	5.54.E+00	3.95.E+00	2.49.E+00	1.067	2.387	5.234	0.204
L-Serine	LC/MS	Cation	9.25.E+00	1.05.E+01	2.06.E+01	8.95.E+00	3.73.E+00	3.83.E+00	1.033	2.807	5.377	0.240
L-Threonine	LC/MS	Cation	4.56.E+00	7.05.E+00	1.53.E+01	4.28.E+00	2.56.E+00	2.94.E+00	1.065	2.748	5.188	0.248
L-Tryptophan	LC/MS	Cation	3.79.E+00	4.65.E+00	9.05.E+00	3.50.E+00	1.95.E+00	2.01.E+00	1.082	2.380	4.498	0.233
L-Tyrosine	LC/MS	Cation	1.08.E+01	1.76.E+01	2.52.E+01	9.37.E+00	1.06.E+01	6.90.E+00	1.154	1.662	3.656	0.214
L-Valine	LC/MS	Cation	5.07.E+01	6.63.E+01	1.28.E+02	5.68.E+01	2.81.E+01	2.73.E+01	0.894	2.358	4.714	0.289
DMG	LC/MS	Cation	8.82.E-02	1.26.E-01	1.84.E-01	1.88.E-01	7.52.E-02	6.96.E-02	0.470	1.673	2.645	0.763
Uridine	LC/MS	Cation	1.33.E+00	2.60.E+00	2.32.E+00	8.21.E-01	1.50.E+00	4.94.E-01	1.619	1.732	4.694	0.095
L-Cystathionine	LC/MS	Cation	3.27.E-02	3.01.E-02	4.46.E-02	3.31.E-02	1.19.E-02	1.63.E-02	0.990	2.530	2.733	0.208
L-Cystine	LC/MS	Cation	3.87.E+01	7.95.E+01	9.41.E+01	2.52.E+01	3.63.E+01	1.97.E+01	1.535	2.187	4.786	0.131
N-Acetylglycine	LC/MS	Cation	8.85.E-02	1.34.E-01	3.64.E-01	1.54.E-01	4.08.E-02	4.53.E-02	0.576	3.279	8.018	0.409
L-Pyroglutamic acid	LC/MS	Cation	3.42.E+00	5.38.E+00	1.34.E+01	3.29.E+00	2.03.E+00	2.58.E+00	1.040	2.647	5.201	0.272
S-Methyl-L-cysteine	LC/MS	Cation	1.15.E-01	1.20.E-01	7.37.E-01	1.24.E-01	6.76.E-02	8.10.E-02	0.933	1.782	9.101	0.386
N-Acetyl-DL-alanine	LC/MS	Cation	2.03.E-01	3.78.E-01	1.05.E+00	2.76.E-01	1.31.E-01	1.30.E-01	0.734	2.899	8.056	0.339
L-Kynurenine	LC/MS	Cation	1.81.E-01	4.08.E-01	3.55.E-01	2.39.E-01	2.07.E-01	1.44.E-01	0.759	1.971	2.455	0.311
Phosphocholine	LC/MS	Cation	8.99.E-02	7.91.E-02	3.64.E-01	7.71.E-02	1.08.E-01	8.64.E-02	1.166	0.735	4.217	0.459
Acetyl-L-glutamine	LC/MS	Cation	7.39.E-01	1.13.E+00	1.99.E+00	8.89.E-01	7.95.E-01	6.52.E-01	0.831	1.421	3.052	0.367
L-2-Aminobutyric acid	LC/MS	Cation	3.25.E-01	3.15.E-01	5.46.E-01	4.01.E-01	2.64.E-01	2.63.E-01	0.810	1.190	2.079	0.501
Uric Acid	LC/MS	Cation	1.38.E+00	2.76.E+00	3.40.E+00	1.35.E+00	1.55.E+00	9.08.E-01	1.026	1.778	3.741	0.221
Glycolic acid	LC/MS	Anion	3.13.E-03	3.48.E-03	2.51.E-03	4.20.E-03	1.69.E-03	4.07.E-03	0.746	2.064	0.617	0.816
Lactic acid	LC/MS	Anion	6.47.E-01	5.65.E-01	6.81.E-01	3.77.E-01	2.85.E-01	4.45.E-01	1.713	1.980	1.532	0.002
Benzoic acid	LC/MS	Anion	2.14.E-02	2.31.E-02	1.66.E-02	2.58.E-02	1.82.E-02	2.36.E-02	0.830	1.271	0.702	0.612
Ethyl-malonic acid	LC/MS	Anion	7.96.E-02	8.35.E-02	1.65.E-01	7.94.E-02	9.27.E-02	1.79.E-01	1.004	0.900	0.921	0.210
o-Toluic acid	LC/MS	Anion	3.10.E-03	1.54.E-03	1.75.E-03	1.75.E-03	6.05.E-04	1.84.E-03	1.772	2.542	0.956	0.226
2-Hydroxy-phenylacetic acid	LC/MS	Anion	7.47.E-03	7.62.E-03	7.61.E-03	6.61.E-03	5.66.E-03	9.31.E-03	1.130	1.347	0.817	0.764
3-Hydroxy-3-methyl-glutaric acid	LC/MS	Anion	5.42.E-03	2.67.E-03	3.99.E-03	4.90.E-03	6.36.E-03	7.15.E-03	1.108	0.420	0.558	0.253
Uric acid	LC/MS	Anion	1.09.E-01	1.55.E-01	1.27.E-01	1.17.E-01	1.32.E-01	9.98.E-02	0.928	1.172	1.270	0.342
Glucuronic acid	LC/MS	Anion	1.45.E-02	1.79.E-02	1.28.E-02	1.98.E-02	1.43.E-02	1.98.E-02	0.731	1.252	0.644	0.469
N-Acetyl-neuraminic acid	LC/MS	Anion	4.54.E-03	3.05.E-03	5.34.E-03	7.25.E-03	4.13.E-03	4.81.E-03	0.626	0.739	1.110	0.366
Pyruvic acid	LC/MS	Anion	9.42.E-03	1.66.E-02	3.36.E-02	2.72.E-02	2.37.E-02	4.27.E-02	0.347	0.700	0.786	0.074
Oxalic acid	LC/MS	Anion	3.00.E-03	4.31.E-03	4.66.E-03	3.63.E-02	3.19.E-02	3.99.E-02	0.083	0.135	0.117	0.005
Fumaric acid	LC/MS	Anion	3.00.E-02	3.33.E-02	3.74.E-02	3.21.E-02	3.19.E-02	3.13.E-02	0.932	1.046	1.196	0.529
3-Hydroxy-3-methyl-butanoic acid (3-Hydroxyisovaleric acid	LC/MS	Anion	3.97.E-02	6.39.E-02	5.01.E-02	4.09.E-02	5.82.E-02	4.16.E-02	0.970	1.099	1.204	0.273
4-Methyl-2-oxovaleric acid	LC/MS	Anion	1.12.E-01	1.18.E-01	1.04.E-01	1.31.E-01	1.14.E-01	1.12.E-01	0.857	1.039	0.927	0.379
2-Hydroxy-isocaproic acid	LC/MS	Anion	4.45.E-02	4.77.E-02	5.64.E-02	4.51.E-02	3.67.E-02	5.31.E-02	0.985	1.298	1.063	0.313
2-Hydroxy-glutaric acid	LC/MS	Anion	4.44.E-03	5.36.E-03	8.73.E-03	6.21.E-03	8.13.E-03	1.12.E-02	0.715	0.660	0.778	0.016
4-Hydroxy-phenyl-lactic acid	LC/MS	Anion	9.36.E-03	9.71.E-03	2.00.E-02	8.65.E-03	4.61.E-03	1.26.E-02	1.082	2.108	1.586	0.154
Isocitric acid	LC/MS	Anion	2.62.E-03	3.36.E-03	3.45.E-03	4.87.E-02	4.22.E-02	4.91.E-02	0.054	0.080	0.070	0.003
Phosphoric acid	LC/MS	Anion	2.32.E-01	1.65.E-01	1.61.E-01	6.81.E-01	5.38.E-01	5.76.E-01	0.341	0.307	0.279	0.003
Malic acid	LC/MS	Anion	1.38.E-02	1.35.E-02	2.88.E-02	9.29.E-02	4.60.E-02	6.91.E-02	0.148	0.293	0.417	0.072
β-Phenyl-lactic acid	LC/MS	Anion	7.62.E-03	6.39.E-03	1.28.E-02	8.21.E-03	9.75.E-03	1.39.E-02	0.929	0.655	0.921	0.188
Hippuric acid	LC/MS	Anion	6.27.E-03	1.73.E-02	5.91.E-03	8.93.E-03	1.46.E-02	5.36.E-03	0.702	1.181	1.102	0.918
Citric acid	LC/MS	Anion	1.11.E-01	7.67.E-02	1.10.E-01	2.59.E+00	2.35.E+00	2.59.E+00	0.043	0.033	0.043	0.001
2-Hydroxy-hippuric acid	LC/MS	Anion	7.53.E-04	7.51.E-04	5.22.E-03	2.91.E-03	2.87.E-03	4.58.E-03	0.259	0.262	1.140	0.321
3-Hydroxy-propionic acid	LC/MS	Anion	6.29.E-03	4.29.E-03	4.66.E-03	4.75.E-03	4.24.E-03	4.79.E-03	1.322	1.012	0.974	0.452
3-Hydroxy-isobutyric acid	LC/MS	Anion	6.32.E-02	9.16.E-02	8.26.E-02	7.12.E-02	8.37.E-02	6.93.E-02	0.888	1.095	1.191	0.563
Glyceric acid	LC/MS	Anion	6.31.E-02	4.97.E-02	5.65.E-02	8.67.E-02	7.96.E-02	8.01.E-02	0.728	0.625	0.706	0.007
Succinic acid	LC/MS	Anion	2.81.E-01	2.82.E-01	3.57.E-01	2.51.E-01	2.02.E-01	2.55.E-01	1.121	1.395	1.402	0.079
2-Hydroxy-3-methyl-butyric acid (2-Hydroxyisovaleric acid	LC/MS	Anion	2.84.E-01	4.21.E-01	4.95.E-01	2.70.E-01	3.26.E-01	4.27.E-01	1.052	1.294	1.158	0.133

Glutaric acid	LC/MS	Anion	2.65.E-02	3.41.E-02	2.59.E-02	2.29.E-02	3.28.E-02	2.18.E-02	1.159	1.038	1.190	0.077
Threonic acid	LC/MS	Anion	1.08.E+00	9.85.E-01	1.16.E+00	7.84.E-01	6.63.E-01	8.88.E-01	1.374	1.486	1.311	0.002
Acetyl-salicylic acid	LC/MS	Anion	1.20.E-02	1.64.E-02	2.76.E-02	8.43.E-03	1.50.E-02	2.18.E-02	1.420	1.096	1.267	0.104
2-Ketoglutaric acid	LC/MS	Anion	5.78.E-02	4.94.E-02	7.71.E-02	1.12.E-01	1.02.E-01	1.40.E-01	0.514	0.485	0.551	0.003
cis-Aconitic acid	LC/MS	Anion	1.32.E-01	1.24.E-01	1.30.E-01	2.26.E-01	1.84.E-01	2.37.E-01	0.585	0.677	0.547	0.026
Quinic acid	LC/MS	Anion	3.46.E-03	3.91.E-02	7.05.E-03	6.70.E-03	3.51.E-02	2.84.E-03	0.517	1.114	2.479	0.568
Gluconic acid	LC/MS	Anion	7.62.E-02	6.89.E-02	5.98.E-02	7.95.E-02	7.08.E-02	6.18.E-02	0.958	0.973	0.967	0.034
LPC 14:0 (sn-1)	LC/MS	Lipid	4.90.E-02	1.05.E-01	1.14.E-01	4.26.E-02	1.12.E-01	1.16.E-01	1.150	0.942	0.980	0.849
LPC 14:0 (sn-2)	LC/MS	Lipid	1.26.E-01	2.75.E-01	2.77.E-01	1.19.E-01	2.81.E-01	2.81.E-01	1.059	0.982	0.986	0.865
LPC 16:0p	LC/MS	Lipid	2.44.E-02	1.83.E-02	2.70.E-02	2.38.E-02	1.74.E-02	2.72.E-02	1.025	1.049	0.991	0.360
LPC 15:0 (sn-1)	LC/MS	Lipid	5.43.E-02	6.10.E-02	3.89.E-02	4.74.E-02	6.07.E-02	5.03.E-02	1.146	1.005	0.772	0.816
LPC 15:0 (sn-2)	LC/MS	Lipid	1.14.E-01	1.19.E-01	9.04.E-02	1.03.E-01	1.31.E-01	9.69.E-02	1.109	0.911	0.933	0.767
LPC 16:0e	LC/MS	Lipid	2.15.E-02	1.41.E-02	2.00.E-02	2.32.E-02	1.65.E-02	1.90.E-02	0.928	0.851	1.055	0.434
LPC 16:1 (sn-1)	LC/MS	Lipid	1.46.E-01	2.12.E-01	3.14.E-01	1.22.E-01	2.11.E-01	3.55.E-01	1.199	1.003	0.886	0.809
LPC 16:1 (sn-2)	LC/MS	Lipid	3.59.E-01	5.23.E-01	8.11.E-01	3.61.E-01	5.16.E-01	8.79.E-01	0.996	1.013	0.922	0.470
LPC 16:0 (sn-1)	LC/MS	Lipid	9.23.E+00	1.20.E+01	1.28.E+01	8.66.E+00	1.22.E+01	1.43.E+01	1.066	0.980	0.898	0.588
LPC 16:0 (sn-2)	LC/MS	Lipid	2.02.E+01	2.50.E+01	2.80.E+01	1.93.E+01	2.47.E+01	2.85.E+01	1.048	1.012	0.981	0.641
LPC 17:1 (sn-1)	LC/MS	Lipid	2.28.E-02	2.72.E-02	3.54.E-02	2.02.E-02	2.34.E-02	3.22.E-02	1.127	1.163	1.100	0.012
LPC 17:1 (sn-2)	LC/MS	Lipid	4.34.E-02	4.50.E-02	7.04.E-02	4.74.E-02	4.99.E-02	7.33.E-02	0.916	0.903	0.961	0.021
LPC 17:0 (sn-1)	LC/MS	Lipid	1.91.E-01	1.76.E-01	1.49.E-01	2.25.E-01	1.55.E-01	1.60.E-01	0.848	1.136	0.932	0.667
LPC 17:0 (sn-2)	LC/MS	Lipid	2.37.E-01	1.99.E-01	1.95.E-01	2.45.E-01	2.05.E-01	2.08.E-01	0.966	0.971	0.939	0.045
LPC 18:3 (sn-1)	LC/MS	Lipid	2.95.E-02	3.90.E-02	9.24.E-02	2.46.E-02	4.36.E-02	9.76.E-02	1.201	0.894	0.946	0.668
LPC 18:3 (sn-2)	LC/MS	Lipid	4.62.E-02	4.94.E-02	1.38.E-01	3.77.E-02	5.30.E-02	1.64.E-01	1.223	0.931	0.845	0.559
LPC 18:2 (sn-1)	LC/MS	Lipid	5.06.E+00	5.03.E+00	6.73.E+00	4.69.E+00	5.60.E+00	8.10.E+00	1.079	0.899	0.832	0.408
LPC 18:2 (sn-2)	LC/MS	Lipid	7.92.E+00	7.31.E+00	1.17.E+01	7.81.E+00	8.10.E+00	1.31.E+01	1.014	0.903	0.897	0.251
LPC 18:1 (sn-1)	LC/MS	Lipid	2.60.E+00	2.60.E+00	4.44.E+00	2.49.E+00	2.57.E+00	4.56.E+00	1.044	1.013	0.975	0.900
LPC 18:1 (sn-2)	LC/MS	Lipid	4.48.E+00	4.32.E+00	8.00.E+00	4.70.E+00	4.67.E+00	8.95.E+00	0.953	0.926	0.893	0.155
LPC 18:0 (sn-1)	LC/MS	Lipid	3.71.E+00	3.19.E+00	3.83.E+00	3.47.E+00	3.13.E+00	4.06.E+00	1.071	1.019	0.943	0.878
LPC 18:0 (sn-2)	LC/MS	Lipid	7.29.E+00	6.48.E+00	7.78.E+00	7.17.E+00	6.51.E+00	8.15.E+00	1.017	0.996	0.955	0.594
LPC 19:0 (sn-1)	LC/MS	Lipid	1.54.E-02	1.65.E-02	1.59.E-02	1.46.E-02	1.65.E-02	2.13.E-02	1.054	1.003	0.743	0.516
LPC 19:0 (sn-2)	LC/MS	Lipid	2.40.E-02	2.00.E-02	2.64.E-02	2.19.E-02	1.99.E-02	2.52.E-02	1.093	1.004	1.045	0.195
LPC 20:5 (sn-1)	LC/MS	Lipid	6.70.E-02	1.82.E-01	1.71.E-01	6.14.E-02	1.88.E-01	2.01.E-01	1.091	0.967	0.847	0.431
LPC 20:5 (sn-2)	LC/MS	Lipid	9.17.E-02	2.30.E-01	2.63.E-01	7.31.E-02	2.22.E-01	3.02.E-01	1.255	1.039	0.871	0.846
LPC 20:4 (sn-1)	LC/MS	Lipid	7.18.E-01	1.02.E+00	1.10.E+00	6.30.E-01	1.07.E+00	1.29.E+00	1.140	0.948	0.853	0.583
LPC 20:4 (sn-2)	LC/MS	Lipid	9.27.E-01	1.18.E+00	1.58.E+00	8.54.E-01	1.21.E+00	1.67.E+00	1.086	0.979	0.950	0.820
LPC 20:3 (sn-1)	LC/MS	Lipid	2.48.E-01	2.56.E-01	3.08.E-01	2.29.E-01	2.71.E-01	3.49.E-01	1.081	0.943	0.882	0.541
LPC 20:3 (sn-2)	LC/MS	Lipid	2.62.E-01	2.93.E-01	4.28.E-01	2.44.E-01	2.71.E-01	4.57.E-01	1.073	1.080	0.936	0.855
LPC 20:2 (sn-1)	LC/MS	Lipid	3.65.E-02	4.06.E-02	4.64.E-02	3.64.E-02	3.99.E-02	6.10.E-02	1.003	1.016	0.761	0.453
LPC 20:2 (sn-2)	LC/MS	Lipid	5.20.E-02	4.61.E-02	7.71.E-02	4.71.E-02	4.54.E-02	8.39.E-02	1.104	1.015	0.918	0.913
LPC 20:1 (sn-1)	LC/MS	Lipid	3.57.E-02	3.09.E-02	5.40.E-02	3.14.E-02	2.79.E-02	5.95.E-02	1.136	1.105	0.907	0.870
LPC 20:1 (sn-2)	LC/MS	Lipid	5.76.E-02	4.61.E-02	9.45.E-02	5.40.E-02	4.73.E-02	1.13.E-01	1.066	0.975	0.834	0.506
LPC 20:0 (sn-1)	LC/MS	Lipid	2.59.E-02	1.52.E-02	2.49.E-02	1.89.E-02	1.76.E-02	3.00.E-02	1.371	0.860	0.830	0.963
LPC 20:0 (sn-2)	LC/MS	Lipid	4.12.E-02	3.11.E-02	4.94.E-02	4.26.E-02	3.40.E-02	5.02.E-02	0.966	0.915	0.983	0.107
LPC 22:6 (sn-1)	LC/MS	Lipid	2.60.E-01	4.03.E-01	4.06.E-01	2.30.E-01	4.30.E-01	5.08.E-01	1.129	0.938	0.801	0.479
LPC 22:6 (sn-2)	LC/MS	Lipid	3.04.E-01	4.03.E-01	5.51.E-01	2.61.E-01	4.23.E-01	5.83.E-01	1.164	0.951	0.946	0.907
LPC 22:4 (sn-1)	LC/MS	Lipid	1.39.E-02	1.67.E-02	1.72.E-02	9.76.E-03	1.93.E-02	2.23.E-02	1.420	0.863	0.773	0.703
LPC 22:4 (sn-2)	LC/MS	Lipid	1.27.E-02	1.64.E-02	1.83.E-02	1.09.E-02	1.49.E-02	2.17.E-02	1.160	1.106	0.843	0.987
LPC 22:0 (sn-1)	LC/MS	Lipid	5.88.E-03	3.56.E-03	6.36.E-03	5.75.E-03	4.40.E-03	5.38.E-03	1.022	0.810	1.182	0.879
LPC 22:0 (sn-2)	LC/MS	Lipid	1.14.E-02	8.04.E-03	9.87.E-03	9.19.E-03	7.88.E-03	1.30.E-02	1.242	1.020	0.757	0.882
PC 14:0-16:1	LC/MS	Lipid	3.90.E+01	3.11.E+01	3.20.E+01	3.49.E+01	3.01.E+01	3.04.E+01	1.117	1.033	1.052	0.146
PC 16:0-14:0	LC/MS	Lipid	2.15.E+00	2.93.E+00	3.27.E+00	1.94.E+00	2.96.E+00	3.25.E+00	1.109	0.991	1.005	0.458
PC 15:0-16:1	LC/MS	Lipid	8.25.E-02	1.26.E-01	1.01.E-01	7.19.E-02	1.33.E-01	1.18.E-01	1.148	0.948	0.856	0.640
PC 16:0p-16:0	LC/MS	Lipid	9.28.E-01	6.85.E-01	7.81.E-01	8.04.E-01	6.62.E-01	8.16.E-01	1.154	1.034	0.957	0.507
PC 16:0-15:0	LC/MS	Lipid	2.41.E-01	3.32.E-01	1.56.E-01	2.25.E-01	3.27.E-01	1.68.E-01	1.069	1.014	0.928	0.772
PC 16:0e-16:0	LC/MS	Lipid	1.78.E+00	1.46.E+00	1.84.E+00	1.60.E+00	1.42.E+00	1.85.E+00	1.114	1.028	0.996	0.338
PC 14:0-18:2/16:1-16:1	LC/MS	Lipid	3.37.E+00	4.96.E+00	4.73.E+00	2.87.E+00	4.92.E+00	5.07.E+00	1.175	1.008	0.933	0.812
PC 14-0:18-1/16:0-16:1	LC/MS	Lipid	1.18.E+01	2.01.E+01	2.46.E+01	1.03.E+01	1.94.E+01	2.57.E+01	1.148	1.039	0.959	0.644
PC 16:0-16:0	LC/MS	Lipid	7.94.E+00	9.76.E+00	1.03.E+01	7.18.E+00	1.02.E+01	1.05.E+01	1.106	0.957	0.986	0.887
PC 15:0-18:2	LC/MS	Lipid	2.56.E+00	2.50.E+00	1.51.E+00	2.26.E+00	2.56.E+00	1.59.E+00	1.131	0.978	0.954	0.690
PC 16:0e-18:2	LC/MS	Lipid	4.75.E+00	4.64.E+00	4.09.E+00	4.17.E+00	4.74.E+00	4.27.E+00	1.139	0.980	0.958	0.710
PC 16:1e-18:1	LC/MS	Lipid	2.46.E+00	2.54.E+00	3.34.E+00	2.16.E+00	2.61.E+00	3.45.E+00	1.142	0.975	0.969	0.767
PC 15:0-18:1/16:0-17:1	LC/MS	Lipid	9.43.E-01	1.36.E+00	1.08.E+00	8.89.E-01	1.38.E+00	1.06.E+00	1.060	0.986	1.019	0.477

PC 18:1e-16:0/18:0e-16:1	LC/MS Lipid	8.04.E+00	7.53.E+00	8.76.E+00	6.96.E+00	7.48.E+00	9.14.E+00	1.155	1.006	0.958	0.626
PC 17:0-16:0/18:0-15:0	LC/MS Lipid	7.47.E-01	7.10.E-01	8.05.E-01	6.32.E-01	7.08.E-01	8.18.E-01	1.181	1.003	0.984	0.478
PC 18:0e-16:0	LC/MS Lipid	8.43.E-01	5.72.E-01	5.00.E-01	7.54.E-01	5.78.E-01	5.10.E-01	1.118	0.991	0.981	0.522
PC 14:0-20:5	LC/MS Lipid	6.65.E-02	2.60.E-01	2.52.E-01	7.60.E-02	2.91.E-01	2.71.E-01	0.876	0.892	0.931	0.089
PC 16:1-18:3/14:0-20:4	LC/MS Lipid	1.15.E+00	2.50.E+00	2.70.E+00	1.01.E+00	2.32.E+00	2.76.E+00	1.141	1.078	0.979	0.352
PC 14:0-20:3	LC/MS Lipid	1.43.E+01	2.08.E+01	2.51.E+01	1.27.E+01	2.16.E+01	2.59.E+01	1.128	0.967	0.968	0.975
PC 16:1-18:2/16:0-18:3	LC/MS Lipid	1.43.E+01	2.08.E+01	2.51.E+01	1.27.E+01	2.16.E+01	2.59.E+01	1.127	0.964	0.971	0.975
PC 16:0-18:2/16:1-18:1	LC/MS Lipid	1.52.E+02	1.64.E+02	1.50.E+02	1.43.E+02	1.66.E+02	1.55.E+02	1.065	0.989	0.973	0.823
PC 16:0-18:1	LC/MS Lipid	1.17.E+02	1.58.E+02	1.50.E+02	1.09.E+02	1.61.E+02	1.52.E+02	1.078	0.982	0.983	0.816
PC 16:0-18:0	LC/MS Lipid	5.10.E+00	6.53.E+00	5.17.E+00	4.58.E+00	6.61.E+00	5.13.E+00	1.114	0.989	1.007	0.472
PC 15:0-20:5	LC/MS Lipid	1.04.E-01	2.93.E-01	1.58.E-01	9.68.E-02	2.78.E-01	1.59.E-01	1.073	1.055	0.992	0.282
PC 16:0e-20:5	LC/MS Lipid	8.05.E+00	8.55.E+00	8.90.E+00	7.64.E+00	7.66.E+00	8.16.E+00	1.054	1.116	1.091	0.041
PC 16:0p-20:4	LC/MS Lipid	8.05.E+00	8.55.E+00	8.90.E+00	7.64.E+00	7.66.E+00	8.16.E+00	1.054	1.116	1.091	0.041
PC 15:0-20:4	LC/MS Lipid	6.68.E-01	1.02.E+00	6.73.E-01	5.89.E-01	1.05.E+00	6.88.E-01	1.134	0.972	0.978	0.765
PC 16:1e-20:3	LC/MS Lipid	1.18.E+01	1.43.E+01	1.21.E+01	1.09.E+01	1.43.E+01	1.20.E+01	1.085	1.003	1.007	0.345
PC 17:1-18:2	LC/MS Lipid	1.60.E+00	1.68.E+00	1.53.E+00	1.45.E+00	1.61.E+00	1.52.E+00	1.108	1.043	1.002	0.230
PC 18:1e-18:2	LC/MS Lipid	3.17.E+00	2.65.E+00	2.92.E+00	2.98.E+00	2.56.E+00	2.84.E+00	1.062	1.033	1.028	0.076
PC 18:2e-18:1	LC/MS Lipid	3.62.E+00	3.18.E+00	3.89.E+00	3.29.E+00	3.23.E+00	3.91.E+00	1.099	0.984	0.993	0.565
PC 17:1-18:1/17:0-18:2	LC/MS Lipid	8.52.E+00	7.18.E+00	5.03.E+00	8.04.E+00	7.14.E+00	5.13.E+00	1.060	1.007	0.981	0.498
PC 18:0p-18:1/18:1e-18:1	LC/MS Lipid	5.37.E+00	4.27.E+00	4.68.E+00	4.86.E+00	3.92.E+00	4.55.E+00	1.106	1.089	1.028	0.098
PC 16:0e-20:2	LC/MS Lipid	1.10.E+00	7.99.E-01	1.11.E+00	1.00.E+00	6.69.E-01	1.07.E+00	1.096	1.194	1.041	0.070
PC 17:0-18:1/17:1-18:0/16:0-19:1	LC/MS Lipid	3.15.E+00	4.12.E+00	3.10.E+00	2.91.E+00	4.02.E+00	3.12.E+00	1.084	1.025	0.993	0.297
PC 16:1-20:5	LC/MS Lipid	9.16.E-02	3.10.E-01	4.95.E-01	9.51.E-02	2.24.E-01	4.51.E-01	0.964	1.385	1.096	0.247
PC 14:0-22:6	LC/MS Lipid	6.00.E-01	1.26.E+00	1.26.E+00	5.47.E-01	1.14.E+00	1.15.E+00	1.097	1.107	1.096	0.047
PC 18:2-18:3	LC/MS Lipid	2.83.E+00	3.67.E+00	5.85.E+00	2.35.E+00	3.35.E+00	5.76.E+00	1.202	1.096	1.016	0.118
PC 14:0-22:5/16:1-20:4/16:0-20:5	LC/MS Lipid	1.54.E+01	4.54.E+01	3.45.E+01	1.39.E+01	4.47.E+01	3.41.E+01	1.108	1.016	1.011	0.120
PC 18:2-18:2/18:1-18:3	LC/MS Lipid	4.00.E+01	3.73.E+01	4.05.E+01	3.59.E+01	3.58.E+01	4.06.E+01	1.111	1.043	0.997	0.272
PC 16:0-20:4/16:1-20:3	LC/MS Lipid	4.97.E+01	7.19.E+01	6.54.E+01	4.82.E+01	7.14.E+01	6.39.E+01	1.031	1.007	1.023	0.078
PC 18:1-18:2/16:0-20:3/18:0-18:3	LC/MS Lipid	8.38.E+01	9.05.E+01	9.23.E+01	8.06.E+01	8.86.E+01	8.93.E+01	1.039	1.022	1.033	0.019
PC 18:1-18:1/18:0-18:2	LC/MS Lipid	1.63.E+02	1.62.E+02	1.63.E+02	1.55.E+02	1.59.E+02	1.59.E+02	1.050	1.019	1.020	0.095
PC 18:0-18:1	LC/MS Lipid	4.88.E+01	6.27.E+01	6.49.E+01	4.52.E+01	5.98.E+01	6.28.E+01	1.080	1.048	1.033	0.023
PC 16:0p-22:6	LC/MS Lipid	1.44.E+00	2.12.E+00	1.94.E+00	1.32.E+00	2.05.E+00	1.76.E+00	1.088	1.031	1.105	0.073
PC 18:0-18:0	LC/MS Lipid	2.37.E-01	3.20.E-01	2.21.E-01	1.60.E-01	3.70.E-01	1.35.E-01	1.485	0.864	1.635	0.484
PC 15:0-22:6	LC/MS Lipid	4.76.E-01	6.02.E-01	3.19.E-01	4.38.E-01	5.82.E-01	3.51.E-01	1.086	1.035	0.910	0.714
PC 18:1e-20:5	LC/MS Lipid	5.27.E-01	9.20.E-01	6.74.E-01	5.28.E-01	8.16.E-01	6.36.E-01	0.999	1.128	1.061	0.262
PC 16:0e-22:6	LC/MS Lipid	4.61.E+00	5.86.E+00	4.97.E+00	4.35.E+00	5.56.E+00	4.83.E+00	1.059	1.054	1.030	0.038
PC 17:0-20:5/17:1-20:4	LC/MS Lipid	6.83.E-01	1.21.E+00	8.09.E-01	6.42.E-01	1.15.E+00	7.97.E-01	1.063	1.054	1.015	0.119
PC 16:0e-22:5/18:0e-20:5	LC/MS Lipid	8.78.E+00	8.06.E+00	8.12.E+00	8.02.E+00	7.56.E+00	7.86.E+00	1.094	1.066	1.033	0.072
PC 18:0p-20:4	LC/MS Lipid	4.00.E+00	4.46.E+00	3.61.E+00	3.69.E+00	3.98.E+00	3.33.E+00	1.086	1.122	1.083	0.030
PC 17:0-20:4	LC/MS Lipid	2.01.E+00	2.44.E+00	1.45.E+00	1.93.E+00	2.35.E+00	1.46.E+00	1.037	1.041	0.999	0.201
PC 18:1e-20:3	LC/MS Lipid	2.09.E+00	1.97.E+00	1.94.E+00	1.89.E+00	1.78.E+00	1.83.E+00	1.103	1.109	1.059	0.029
PC 18:0e-20:4	LC/MS Lipid	9.87.E+00	8.02.E+00	5.95.E+00	9.12.E+00	7.43.E+00	5.50.E+00	1.082	1.080	1.081	0.021
PC 17:0-20:3/19:1-18:2	LC/MS Lipid	9.48.E-01	9.19.E-01	6.37.E-01	9.24.E-01	8.55.E-01	5.96.E-01	1.026	1.075	1.069	0.066
PC 19:1-18:1/19:0-18:2	LC/MS Lipid	1.83.E+00	1.74.E+00	1.67.E+00	1.68.E+00	1.63.E+00	1.58.E+00	1.088	1.067	1.059	0.020
PC 19:0-18:1/18:0-19:1	LC/MS Lipid	7.43.E-01	8.01.E-01	7.61.E-01	7.12.E-01	7.38.E-01	6.69.E-01	1.043	1.085	1.138	0.073
PC 18:2-20:5/16:1-22:6	LC/MS Lipid	1.90.E+00	4.11.E+00	3.90.E+00	1.73.E+00	4.08.E+00	3.79.E+00	1.098	1.008	1.031	0.121
PC 18:2-20:4/16:0-22:6	LC/MS Lipid	6.12.E+01	7.93.E+01	6.63.E+01	5.84.E+01	7.68.E+01	6.42.E+01	1.049	1.033	1.034	0.007
PC 18:1-20:4	LC/MS Lipid	1.44.E+01	1.52.E+01	1.34.E+01	1.18.E+01	1.48.E+01	1.25.E+01	1.225	1.029	1.071	0.191
PC 18:0-20:5	LC/MS Lipid	8.09.E+00	1.50.E+01	1.31.E+01	8.20.E+00	1.47.E+01	1.31.E+01	0.987	1.019	1.003	0.598
PC 18:1-20:3	LC/MS Lipid	4.72.E+00	4.57.E+00	5.13.E+00	4.54.E+00	4.70.E+00	4.95.E+00	1.040	0.972	1.037	0.543
PC 18:0-20:4	LC/MS Lipid	3.35.E+01	4.48.E+01	3.86.E+01	3.24.E+01	4.36.E+01	3.73.E+01	1.035	1.029	1.034	0.001
PC 18:1-20:2/18:0-20:3	LC/MS Lipid	2.97.E+01	3.28.E+01	3.00.E+01	2.77.E+01	3.09.E+01	2.86.E+01	1.074	1.061	1.051	0.010
PC 16:0-22:2	LC/MS Lipid	3.27.E+00	3.54.E+00	3.12.E+00	2.98.E+00	3.35.E+00	3.00.E+00	1.097	1.058	1.038	0.059
PC 18:0-20:2	LC/MS Lipid	6.16.E+00	6.47.E+00	7.33.E+00	5.71.E+00	5.98.E+00	6.91.E+00	1.080	1.082	1.061	0.002
PC 20:0-18:1	LC/MS Lipid	1.28.E+01	1.12.E+01	1.37.E+01	1.21.E+01	9.92.E+00	1.15.E+01	1.057	1.125	1.191	0.089
PC 18:1e-22:6	LC/MS Lipid	1.70.E+00	1.76.E+00	1.72.E+00	1.64.E+00	1.65.E+00	1.61.E+00	1.042	1.065	1.068	0.019
PC 17:0-22:6	LC/MS Lipid	9.78.E-01	1.06.E+00	7.04.E-01	8.90.E-01	1.02.E+00	6.71.E-01	1.098	1.044	1.050	0.079
PC 18:1e-22:5	LC/MS Lipid	5.65.E-01	3.50.E-01	4.73.E-01	4.75.E-01	4.48.E-01	3.79.E-01	1.190	0.782	1.248	0.694
PC 18:0p-22:5	LC/MS Lipid	2.39.E+00	2.27.E+00	1.56.E+00	2.18.E+00	2.05.E+00	1.45.E+00	1.093	1.109	1.076	0.035
PC 19:0-20:3	LC/MS Lipid	4.68.E-01	3.41.E-01	3.78.E-01	4.32.E-01	3.30.E-01	3.00.E-01	1.084	1.035	1.260	0.163
PC 20:4-20:4	LC/MS Lipid	1.04.E+00	1.60.E+00	1.39.E+00	9.26.E-01	1.51.E+00	1.41.E+00	1.121	1.060	0.980	0.317
PC 20:3-20:4	LC/MS Lipid	5.05.E-01	5.62.E-01	4.79.E-01	4.41.E-01	5.29.E-01	4.67.E-01	1.146	1.062	1.025	0.141

PC 18:1-22:6	LC/MS Lipid	1.22.E+00	1.49.E+00	1.67.E+00	1.22.E+00	1.43.E+00	1.59.E+00	1.004	1.036	1.047	0.167
PC 20:2-20:4/18:1-22:5	LC/MS Lipid	9.36.E-01	1.12.E+00	1.20.E+00	8.92.E-01	1.05.E+00	1.14.E+00	1.049	1.065	1.050	0.016
PC 18:0-22:6	LC/MS Lipid	1.07.E+01	1.44.E+01	1.24.E+01	1.00.E+01	1.39.E+01	1.20.E+01	1.064	1.036	1.037	0.012
PC 18:0-22:5	LC/MS Lipid	4.67.E+00	5.93.E+00	5.30.E+00	4.32.E+00	5.71.E+00	5.15.E+00	1.083	1.038	1.029	0.060
PC 20:1-20:3/18:0-22:4	LC/MS Lipid	2.12.E+00	2.48.E+00	2.05.E+00	1.90.E+00	2.28.E+00	2.03.E+00	1.117	1.087	1.008	0.156
PC 18:1-22:0	LC/MS Lipid	5.21.E-02	5.87.E-02	4.97.E-02	4.54.E-02	5.46.E-02	4.28.E-02	1.147	1.076	1.161	0.021
PC 19:0-22:6	LC/MS Lipid	1.07.E-01	1.40.E-01	1.09.E-01	8.63.E-02	1.13.E-01	1.01.E-01	1.242	1.238	1.080	0.078
LPE 16:0 (sn-1)	LC/MS Lipid	4.85.E-02	4.40.E-02	7.15.E-02	5.24.E-02	4.96.E-02	8.49.E-02	0.926	0.886	0.842	0.121
LPE 16:0 (sn-2)	LC/MS Lipid	7.47.E-02	5.98.E-02	1.00.E-01	7.96.E-02	7.33.E-02	1.08.E-01	0.938	0.815	0.925	0.072
LPE 18:2 (sn-1)	LC/MS Lipid	1.01.E-01	7.91.E-02	1.25.E-01	1.01.E-01	1.12.E-01	1.63.E-01	0.993	0.706	0.769	0.178
LPE 18:2 (sn-2)	LC/MS Lipid	1.33.E-01	1.04.E-01	1.52.E-01	1.43.E-01	1.28.E-01	1.91.E-01	0.932	0.812	0.795	0.105
LPE 18:1 (sn-1)	LC/MS Lipid	4.71.E-02	4.67.E-02	8.50.E-02	5.16.E-02	5.12.E-02	1.07.E-01	0.914	0.912	0.796	0.218
LPE 18:1 (sn-2)	LC/MS Lipid	9.84.E-02	8.97.E-02	1.81.E-01	9.99.E-02	1.06.E-01	2.12.E-01	0.985	0.849	0.851	0.200
LPE 18:0 (sn-1)	LC/MS Lipid	1.11.E-01	9.75.E-02	1.23.E-01	1.01.E-01	1.13.E-01	1.70.E-01	1.099	0.861	0.725	0.398
LPE 18:0 (sn-2)	LC/MS Lipid	1.70.E-01	1.55.E-01	1.81.E-01	1.57.E-01	1.76.E-01	2.27.E-01	1.079	0.880	0.797	0.394
LPE 20:4 (sn-1)	LC/MS Lipid	4.21.E-02	4.60.E-02	6.03.E-02	4.35.E-02	5.94.E-02	7.48.E-02	0.968	0.774	0.806	0.146
LPE 20:4 (sn-2)	LC/MS Lipid	4.34.E-02	4.80.E-02	5.33.E-02	4.77.E-02	5.98.E-02	7.55.E-02	0.909	0.804	0.706	0.133
LPE 22:6 (sn-1)	LC/MS Lipid	3.36.E-02	5.46.E-02	5.57.E-02	4.15.E-02	6.60.E-02	8.71.E-02	0.810	0.827	0.640	0.147
LPE 22:6 (sn-2)	LC/MS Lipid	3.57.E-02	4.07.E-02	6.07.E-02	3.21.E-02	5.01.E-02	6.72.E-02	1.110	0.811	0.904	0.403
PE 16:0-16:1/14:0-18:1	LC/MS Lipid	1.45.E-02	1.71.E-02	2.42.E-02	1.69.E-02	1.86.E-02	3.07.E-02	0.858	0.923	0.787	0.158
PE 16:0p-18:1	LC/MS Lipid	1.08.E-02	1.01.E-02	1.08.E-02	1.16.E-02	9.87.E-03	1.20.E-02	0.934	1.024	0.895	0.310
PE 16:0e-18:1	LC/MS Lipid	3.88.E-02	3.29.E-02	6.16.E-02	3.79.E-02	3.47.E-02	6.03.E-02	1.023	0.948	1.022	0.909
PE 16:0-18:3	LC/MS Lipid	2.89.E-02	2.39.E-02	2.77.E-02	2.27.E-02	2.51.E-02	3.41.E-02	1.275	0.955	0.814	0.920
PE 16:1-18:1/16:0-18:2	LC/MS Lipid	1.03.E-01	7.41.E-02	7.33.E-02	1.02.E-01	6.37.E-02	7.03.E-02	1.019	1.163	1.043	0.197
PE 16:0-18:1	LC/MS Lipid	7.48.E-02	5.26.E-02	6.34.E-02	7.20.E-02	5.81.E-02	5.56.E-02	1.038	0.905	1.140	0.707
PE 16:0p-20:4	LC/MS Lipid	3.47.E-02	4.94.E-02	4.19.E-02	3.37.E-02	4.71.E-02	4.28.E-02	1.030	1.049	0.980	0.473
PE 16:0p-20:3/16:0e-20:4	LC/MS Lipid	5.68.E-02	7.00.E-02	7.26.E-02	5.14.E-02	6.66.E-02	7.15.E-02	1.103	1.051	1.016	0.115
PE 18:1p-18:1/18:0p-18:2/18:0e-18:3	LC/MS Lipid	9.14.E-02	6.26.E-02	5.86.E-02	9.32.E-02	5.96.E-02	6.01.E-02	0.980	1.051	0.975	0.962
PE 17:0-18:2	LC/MS Lipid	1.18.E-02	2.23.E-03	2.90.E-03	7.32.E-03	4.03.E-03	1.37.E-03	1.612	0.553	2.114	0.520
PE 18:0e-18:2	LC/MS Lipid	5.20.E-02	4.64.E-02	6.21.E-02	5.36.E-02	4.96.E-02	5.24.E-02	0.971	0.935	1.185	0.725
PE 18:0p-18:1	LC/MS Lipid	4.89.E-02	4.24.E-02	4.16.E-02	4.12.E-02	3.70.E-02	4.12.E-02	1.185	1.145	1.008	0.175
PE 18:0e-18:1	LC/MS Lipid	2.11.E-02	3.17.E-02	1.88.E-02	2.22.E-02	3.10.E-02	2.24.E-02	0.952	1.024	0.840	0.408
PE 18:2-18:3	LC/MS Lipid	5.71.E-03	8.52.E-03	1.71.E-02	6.06.E-03	6.67.E-03	2.00.E-02	0.942	1.278	0.856	0.767
PE 16:0-20:5	LC/MS Lipid	2.91.E-02	5.95.E-02	4.33.E-02	2.41.E-02	5.58.E-02	4.81.E-02	1.204	1.067	0.898	0.726
PE 18:2-18:2	LC/MS Lipid	6.99.E-02	6.64.E-02	9.17.E-02	5.82.E-02	5.48.E-02	9.65.E-02	1.202	1.212	0.950	0.378
PE 16:0-20:4	LC/MS Lipid	9.40.E-02	7.05.E-02	5.81.E-02	7.99.E-02	6.95.E-02	5.41.E-02	1.176	1.014	1.074	0.249
PE 18:1-18:2	LC/MS Lipid	1.60.E-01	1.03.E-01	1.44.E-01	1.71.E-01	9.56.E-02	1.29.E-01	0.936	1.078	1.116	0.669
PE 18:1-18:1/18:0-18:2	LC/MS Lipid	5.09.E-01	4.02.E-01	3.86.E-01	5.69.E-01	3.77.E-01	3.48.E-01	0.894	1.066	1.111	0.979
PE 16:0-20:1/18:0-18:1	LC/MS Lipid	2.25.E-01	2.15.E-01	2.20.E-01	2.23.E-01	2.04.E-01	1.96.E-01	1.010	1.056	1.118	0.179
PE 16:0p-22:6	LC/MS Lipid	1.63.E-02	3.08.E-02	2.56.E-02	1.88.E-02	2.85.E-02	2.32.E-02	0.868	1.083	1.100	0.693
PE 18:0p-20:5/18:1p-20:4/16:0e-22:6	LC/MS Lipid	1.00.E-01	1.25.E-01	1.40.E-01	9.11.E-02	1.25.E-01	1.40.E-01	1.099	0.994	1.000	0.472
PE 18:1p-20:3/16:0p-22:4	LC/MS Lipid	3.67.E-02	5.50.E-02	4.99.E-02	3.60.E-02	5.05.E-02	5.57.E-02	1.018	1.090	0.895	0.952
PE 18:0p-20:4	LC/MS Lipid	1.42.E-01	2.19.E-01	1.74.E-01	1.32.E-01	2.31.E-01	1.74.E-01	1.079	0.946	0.998	0.917
PE 18:1e-20:3	LC/MS Lipid	1.35.E-01	2.15.E-01	1.76.E-01	1.20.E-01	2.17.E-01	1.58.E-01	1.127	0.992	1.111	0.231
PE 16:1-22:6/18:2-20:5	LC/MS Lipid	1.08.E-02	1.46.E-02	1.65.E-02	7.94.E-03	1.45.E-02	1.48.E-02	1.358	1.003	1.114	0.201
PE 18:2-20:4/18:1-20:5	LC/MS Lipid	3.81.E-01	2.91.E-01	2.64.E-01	3.39.E-01	2.99.E-01	2.71.E-01	1.123	0.972	0.973	0.650
PE 16:0-22:6/16:1-22:5/20:2-18:4	LC/MS Lipid	3.81.E-01	2.91.E-01	2.64.E-01	3.39.E-01	2.99.E-01	2.71.E-01	1.123	0.972	0.973	0.651
PE 18:1-20:4	LC/MS Lipid	1.02.E-01	6.87.E-02	7.07.E-02	9.19.E-02	6.33.E-02	6.56.E-02	1.110	1.086	1.078	0.050
PE 18:0-20:5	LC/MS Lipid	3.58.E-02	5.29.E-02	5.15.E-02	4.11.E-02	5.41.E-02	4.58.E-02	0.871	0.977	1.124	0.940
PE 18:0-20:4	LC/MS Lipid	3.33.E-01	2.76.E-01	2.34.E-01	3.15.E-01	2.85.E-01	2.22.E-01	1.057	0.965	1.052	0.518
PE 20:1-18:2	LC/MS Lipid	2.76.E-02	2.24.E-02	2.11.E-02	2.56.E-02	2.03.E-02	2.31.E-02	1.078	1.106	0.914	0.651
PE 18:0-20:3	LC/MS Lipid	9.02.E-02	7.20.E-02	7.07.E-02	8.53.E-02	8.04.E-02	6.63.E-02	1.058	0.896	1.067	0.946
PE 18:1-20:1	LC/MS Lipid	7.54.E-03	6.40.E-03	3.14.E-03	1.04.E-02	5.36.E-03	4.59.E-03	0.727	1.192	0.684	0.439
PE 20:0-18:2	LC/MS Lipid	2.47.E-02	3.44.E-02	2.59.E-02	2.50.E-02	3.67.E-02	3.24.E-02	0.989	0.938	0.800	0.240
PE 18:0-20:1	LC/MS Lipid	1.39.E-02	1.78.E-02	1.56.E-02	1.21.E-02	2.11.E-02	1.34.E-02	1.147	0.843	1.164	0.913
PE 18:0p-22:6/18:1p-22:5	LC/MS Lipid	6.22.E-02	9.33.E-02	6.68.E-02	5.59.E-02	9.35.E-02	6.48.E-02	1.113	0.998	1.031	0.293
PE 17:0-22:6	LC/MS Lipid	5.31.E-03	2.93.E-03	5.26.E-03	6.29.E-03	4.31.E-03	2.03.E-03	0.845	0.681	2.596	0.859
PE 18:0p-22:5/18:1p-22:4	LC/MS Lipid	8.32.E-02	1.31.E-01	9.07.E-02	8.39.E-02	1.20.E-01	9.01.E-02	0.992	1.088	1.007	0.430
PE 18:1-22:6	LC/MS Lipid	2.07.E-02	2.04.E-02	2.18.E-02	2.03.E-02	1.71.E-02	2.19.E-02	1.019	1.195	0.996	0.374
PE 18:0-22:6	LC/MS Lipid	9.63.E-02	1.00.E-01	7.19.E-02	9.16.E-02	9.84.E-02	7.39.E-02	1.051	1.018	0.972	0.531
PE 18:0-22:5	LC/MS Lipid	5.15.E-02	4.72.E-02	4.10.E-02	5.68.E-02	5.17.E-02	3.90.E-02	0.906	0.913	1.051	0.376
FA 12:0 Lauric acid	LC/MS Lipid	6.76.E-02	3.28.E-02	4.34.E-02	5.43.E-02	3.09.E-02	4.17.E-02	1.244	1.061	1.042	0.278

FA 14:1 (n-5) Myristoleic acid	LC/MS	Lipid	8.58.E-02	2.23.E-02	3.83.E-02	2.35.E-02	1.97.E-02	3.98.E-02	3.647	1.129	0.961	0.414
FA 14:0 Myristic acid	LC/MS	Lipid	2.45.E-01	9.56.E-02	1.51.E-01	9.24.E-02	9.23.E-02	1.36.E-01	2.651	1.036	1.108	0.358
FA 16:1 (n-7) Palmitoleic acid	LC/MS	Lipid	2.13.E+00	3.25.E-01	1.12.E+00	5.65.E-01	2.73.E-01	9.88.E-01	3.765	1.189	1.130	0.359
FA 16:0 Palmitic acid	LC/MS	Lipid	4.81.E+00	3.07.E+00	4.51.E+00	3.37.E+00	2.90.E+00	3.72.E+00	1.429	1.059	1.213	0.160
FA 17:1 (n-7) cis-10-Heptadecanoic acid	LC/MS	Lipid	2.80.E-01	3.56.E-02	7.40.E-02	4.82.E-02	3.92.E-02	5.61.E-02	5.807	0.908	1.320	0.389
FA 18:4 (n-3) Stearidonic acid	LC/MS	Lipid	7.47.E-03	8.65.E-03	1.37.E-02	4.94.E-03	5.54.E-03	1.29.E-02	1.512	1.563	1.060	0.093
FA 18:3 (n-3) Alpha-linolenic acid (n-6) gamma-Linolenic aci	LC/MS	Lipid	2.84.E-01	2.00.E-01	4.95.E-01	1.95.E-01	1.70.E-01	4.50.E-01	1.453	1.174	1.099	0.092
FA 18:2 (n-6) Linoleic acid	LC/MS	Lipid	2.10.E+00	1.31.E+00	2.16.E+00	1.45.E+00	1.16.E+00	1.94.E+00	1.448	1.125	1.111	0.166
FA 18:1 (n-9) cis-Oleic acid (n-7) cis-Vaccenic acid	LC/MS	Lipid	5.92.E+00	3.24.E+00	6.75.E+00	4.24.E+00	2.79.E+00	5.87.E+00	1.398	1.158	1.151	0.110
FA 18:0 Stearic acid	LC/MS	Lipid	3.46.E+00	2.85.E+00	2.43.E+00	2.89.E+00	2.92.E+00	2.03.E+00	1.199	0.978	1.195	0.253
FA 20:5 (n-3) Eicosapentaenoic acid	LC/MS	Lipid	2.02.E-02	4.52.E-02	3.16.E-02	1.55.E-02	3.91.E-02	2.81.E-02	1.304	1.154	1.124	0.023
FA 20:4 (n-6) Arachidonic acid	LC/MS	Lipid	6.78.E-01	5.56.E-01	4.94.E-01	2.62.E-01	3.86.E-01	3.04.E-01	2.588	1.438	1.626	0.082
FA 20:3 (n-6) Dihomo-gamma-linolenic acid (n-9) Mead aci	LC/MS	Lipid	5.92.E-02	4.51.E-02	6.27.E-02	4.80.E-02	4.81.E-02	5.83.E-02	1.235	0.938	1.077	0.412
FA 20:2 (n-6) cis-11-14-Eicosadienoic acid	LC/MS	Lipid	1.44.E-01	7.53.E-02	8.76.E-02	6.09.E-02	7.23.E-02	8.46.E-02	2.371	1.042	1.035	0.382
FA 20:1 (n-9) cis-11-Eicosenoic acid	LC/MS	Lipid	2.56.E-01	1.24.E-01	2.56.E-01	1.41.E-01	1.11.E-01	2.24.E-01	1.809	1.124	1.145	0.226
FA 22:6 (n-3) Docosahexaenoic acid	LC/MS	Lipid	1.01.E-01	1.81.E-01	1.36.E-01	8.65.E-02	1.72.E-01	1.37.E-01	1.168	1.053	0.993	0.238
FA 22:5 (n-6) Docosapentaenoic acid	LC/MS	Lipid	7.97.E-02	1.10.E-01	1.11.E-01	7.25.E-02	1.04.E-01	1.01.E-01	1.099	1.060	1.100	0.022
FA 22:4 (n-6) Docosatetraenoic acid	LC/MS	Lipid	4.09.E-02	4.16.E-02	4.00.E-02	2.76.E-02	4.29.E-02	3.97.E-02	1.483	0.970	1.008	0.468
FA 23:0 Tricosanoic acid	LC/MS	Lipid	7.96.E-02	9.14.E-02	1.02.E-01	6.97.E-02	8.95.E-02	1.00.E-01	1.141	1.022	1.016	0.240
FA 24:1 (n-9) Nervonic acid	LC/MS	Lipid	1.53.E-01	1.49.E-01	1.67.E-01	1.20.E-01	1.46.E-01	1.47.E-01	1.283	1.015	1.140	0.175
FA 25:0 Pentacosanoic acid	LC/MS	Lipid	2.50.E-01	2.13.E-01	2.19.E-01	1.98.E-01	2.31.E-01	2.17.E-01	1.267	0.923	1.010	0.615
AC 2:0	LC/MS	Lipid	4.59.E+00	4.11.E+00	4.34.E+00	4.03.E+00	3.45.E+00	3.37.E+00	1.140	1.192	1.287	0.027
AC 4:0	LC/MS	Lipid	2.41.E-02	1.74.E-02	5.81.E-02	2.02.E-02	1.28.E-02	4.62.E-02	1.190	1.361	1.257	0.118
AC 6:0	LC/MS	Lipid	8.46.E-03	8.09.E-03	1.09.E-02	8.28.E-03	4.23.E-03	6.99.E-03	1.021	1.911	1.554	0.166
AC 8:0	LC/MS	Lipid	4.84.E-02	4.99.E-02	5.96.E-02	3.72.E-02	4.91.E-02	4.90.E-02	1.300	1.016	1.217	0.155
AC 10:0	LC/MS	Lipid	9.56.E-02	1.05.E-01	1.28.E-01	8.51.E-02	9.25.E-02	1.10.E-01	1.124	1.137	1.159	0.023
AC 12:0	LC/MS	Lipid	2.04.E-02	2.96.E-02	2.71.E-02	2.04.E-02	2.63.E-02	2.67.E-02	1.000	1.124	1.013	0.364
AC 14:0	LC/MS	Lipid	7.13.E-03	7.64.E-03	9.01.E-03	4.92.E-03	9.51.E-03	8.27.E-03	1.447	0.804	1.090	0.791
AC 14:1	LC/MS	Lipid	2.60.E-02	3.24.E-02	5.33.E-02	2.69.E-02	2.84.E-02	5.25.E-02	0.963	1.138	1.014	0.482
AC 16:0	LC/MS	Lipid	5.13.E-02	4.60.E-02	5.39.E-02	3.84.E-02	4.11.E-02	3.76.E-02	1.333	1.121	1.431	0.077
AC 16:1	LC/MS	Lipid	1.13.E-02	1.26.E-02	1.73.E-02	8.74.E-03	7.34.E-03	1.34.E-02	1.289	1.723	1.293	0.040
AC 18:0	LC/MS	Lipid	3.11.E-02	2.12.E-02	1.78.E-02	1.98.E-02	1.44.E-02	1.25.E-02	1.568	1.475	1.427	0.048
AC 18:1	LC/MS	Lipid	9.07.E-02	5.60.E-02	1.09.E-01	6.49.E-02	3.70.E-02	7.19.E-02	1.399	1.514	1.517	0.035
AC 18:2	LC/MS	Lipid	4.26.E-02	3.13.E-02	4.73.E-02	2.80.E-02	2.56.E-02	3.33.E-02	1.522	1.223	1.421	0.058

Derivatized metabolites are labeled with 'TMS' (trimethylsilylation) and/or 'meto' (methoximation

Ether-linked lipid species are labeled with 'e' (plasmanyl) or 'p' (plasmenyl).

Four types of methods, which targeted hydrophilic metabolites (GC/MS), cationic metabolites (LC/MS_Cation), anionic metabolites (LC/MS_Anion) and lipids (LC/MS_Lipid), were employed, and they were shown in the column of 'Method'.

P-values were calculated using the paired Student's *t*-test.

N.D. indicates that the metabolite peak was not detected.

N.A. indicates that statistical test is not available due to insufficiency of the metabolite data.

Abbreviations: LPC, lysophosphatidylcholine; PC, phosphatidylcholine; LPE, lysophosphatidylethanolamine; PE, phosphatidylethanolamine; FA, fatty acid; AC, acylcarnitine

Table S2

Differences in the levels of metabolites in plasma by the influence of storage at room temperature or at cold temperature before centrifugation process

Metabolite	Method	Room temperature																Cold temperature															
		Corrected peak area									Ratio						*p*-value	Corrected peak area									Ratio						*p*-value
		0 min			15 min			30 min			15 min / 0 min			30 min / 0 min				1 h			4 h			8 h			4 h / 1 h			8 h / 1 h			
		sample 1	sample 2	sample 3	sample 1	sample 2	sample 3	sample 1	sample 2	sample 3	sample 1	sample 2	sample 3	sample 1	sample 2	sample 3		sample A	sample B	sample C	sample A	sample B	sample C	sample A	sample B	sample C	sample A	sample B	sample C	sample A	sample B	sample C	
Pyruvic acid-meto-TMS	GC/MS	8.92.E-02	1.43.E-01	2.04.E-01	9.91.E-02	1.51.E-01	2.33.E-01	2.00.E-01	2.08.E-01	3.67.E-01	1.110	1.056	1.141	2.246	1.452	1.799	0.012	6.45.E-01	5.43.E-01	5.72.E-01	2.22.E-01	2.26.E-01	2.45.E-01	1.99.E-01	1.98.E-01	2.11.E-01	0.344	0.416	0.428	0.308	0.364	0.368	0.000
Lactic acid-2TMS	GC/MS	2.00.E+00	1.79.E+00	2.48.E+00	2.30.E+00	2.08.E+00	2.73.E+00	2.57.E+00	2.18.E+00	3.13.E+00	1.150	1.160	1.101	1.283	1.216	1.263	0.004	3.85.E+00	3.66.E+00	3.97.E+00	4.21.E+00	4.16.E+00	4.17.E+00	5.10.E+00	4.62.E+00	4.82.E+00	1.094	1.137	1.052	1.325	1.263	1.214	0.002
Glycolic acid-2TMS	GC/MS	1.26.E-01	1.23.E-01	1.21.E-01	1.57.E-01	1.49.E-01	1.45.E-01	1.60.E-01	1.50.E-01	1.62.E-01	1.247	1.211	1.200	1.269	1.222	1.336	0.002	1.59.E-01	1.51.E-01	1.63.E-01	1.50.E-01	1.64.E-01	1.59.E-01	1.79.E-01	1.64.E-01	1.77.E-01	0.944	1.083	0.975	1.121	1.086	1.080	0.105
Alanine-2TMS	GC/MS	7.48.E-01	8.67.E-01	1.03.E+00	7.28.E-01	8.12.E-01	9.72.E-01	8.34.E-01	8.25.E-01	1.23.E+00	0.973	0.937	0.945	1.115	0.951	1.196	0.208	1.03.E+00	1.22.E+00	1.11.E+00	9.91.E-01	1.06.E+00	1.00.E+00	1.27.E+00	1.11.E+00	1.17.E+00	0.965	0.871	0.906	1.235	0.908	1.052	0.202
2-Keto-isovaleric acid-meto-TMS	GC/MS	1.38.E-02	1.56.E-02	1.43.E-02	1.32.E-02	1.38.E-02	1.38.E-02	1.32.E-02	1.32.E-02	1.55.E-02	0.956	0.882	0.969	0.956	0.844	1.088	0.516	2.81.E-02	2.37.E-02	2.95.E-02	2.55.E-02	2.61.E-02	2.55.E-02	2.75.E-02	2.69.E-02	2.67.E-02	0.906	1.102	0.864	0.979	1.137	0.908	0.608
Glycine-2TMS	GC/MS	3.35.E-02	3.00.E-02	2.98.E-02	2.60.E-02	2.29.E-02	3.42.E-02	2.60.E-02	2.77.E-02	2.70.E-02	0.775	0.761	1.149	0.775	0.921	0.906	0.446	1.86.E-02	1.85.E-02	1.85.E-02	1.20.E-02	3.29.E-02	1.88.E-02	2.29.E-02	1.33.E-02	1.72.E-02	0.644	1.774	1.021	1.230	0.715	0.931	0.857
2-Hydroxybutyric acid-2TMS	GC/MS	2.02.E-01	2.49.E-01	1.99.E-01	1.94.E-01	2.32.E-01	1.96.E-01	1.92.E-01	2.20.E-01	2.05.E-01	0.965	0.934	0.983	0.954	0.884	1.031	0.383	4.41.E-01	3.80.E-01	4.43.E-01	4.42.E-01	4.49.E-01	4.58.E-01	4.37.E-01	4.60.E-01	4.33.E-01	1.003	1.180	1.033	0.991	1.210	0.978	0.456
Oxalic acid-2TMS	GC/MS	2.54.E-02	1.75.E-02	2.30.E-02	2.47.E-02	1.86.E-02	1.68.E-02	2.73.E-02	2.50.E-02	2.60.E-02	0.970	1.060	0.730	1.076	1.427	1.130	0.078	2.55.E-02	2.67.E-02	2.58.E-02	1.18.E-02	2.07.E-02	3.08.E-02	2.22.E-02	2.22.E-02	3.25.E-02	0.465	0.774	1.197	0.870	0.833	1.261	0.485
Sarcosine-2TMS	GC/MS	7.91.E-02	1.24.E-01	9.32.E-02	8.31.E-02	1.18.E-01	8.15.E-02	9.12.E-02	1.20.E-01	1.12.E-01	1.051	0.951	0.874	1.153	0.969	1.202	0.245	2.08.E-01	2.34.E-01	2.43.E-01	2.13.E-01	2.25.E-01	2.28.E-01	2.56.E-01	2.45.E-01	2.40.E-01	1.024	0.964	0.940	1.230	1.047	0.987	0.175
2-Aminoisobutyric acid-2TMS	GC/MS	3.73.E-02	4.35.E-02	4.00.E-02	4.27.E-02	4.16.E-02	4.23.E-02	4.49.E-02	4.79.E-02	4.73.E-02	1.145	0.955	1.058	1.204	1.102	1.184	0.031	9.54.E-02	1.04.E-01	1.23.E-01	1.45.E-01	1.07.E-01	1.21.E-01	1.41.E-01	1.19.E-01	1.23.E-01	1.519	1.028	0.984	1.481	1.138	1.001	0.329
3-Hydroxybutyric acid-2TMS	GC/MS	3.07.E-01	7.24.E-01	3.30.E-01	3.01.E-01	6.96.E-01	3.28.E-01	3.09.E-01	6.65.E-01	3.57.E-01	0.978	0.961	0.995	1.007	0.920	1.082	0.794	1.69.E+00	1.31.E+00	1.52.E+00	1.54.E+00	1.49.E+00	1.57.E+00	1.41.E+00	1.54.E+00	1.39.E+00	0.910	1.138	1.033	0.833	1.176	0.913	0.740
2-Aminobutyric acid-2TMS	GC/MS	2.64.E-02	4.49.E-02	2.54.E-02	2.65.E-02	3.93.E-02	2.26.E-02	2.39.E-02	3.51.E-02	2.20.E-02	1.002	0.875	0.891	0.903	0.782	0.866	0.091	3.01.E-02	3.21.E-02	3.08.E-02	2.86.E-02	2.77.E-02	2.69.E-02	3.31.E-02	2.96.E-02	3.08.E-02	0.950	0.863	0.873	1.099	0.923	1.000	0.066
3-Hydroxyisovaleric acid-2TMS	GC/MS	6.97.E-02	1.11.E-01	7.83.E-02	6.66.E-02	1.04.E-01	7.52.E-02	6.57.E-02	9.52.E-02	7.72.E-02	0.954	0.936	0.960	0.942	0.858	0.985	0.210	2.00.E-01	1.84.E-01	2.05.E-01	1.96.E-01	1.93.E-01	1.96.E-01	2.13.E-01	2.01.E-01	2.02.E-01	0.981	1.049	0.957	1.063	1.092	0.987	0.196
Valine-2TMS	GC/MS	9.74.E+00	1.02.E+01	8.89.E+00	9.32.E+00	1.00.E+01	8.16.E+00	8.87.E+00	9.12.E+00	8.46.E+00	0.957	0.979	0.918	0.911	0.893	0.952	0.074	1.96.E+01	1.99.E+01	2.09.E+01	1.85.E+01	1.93.E+01	1.92.E+01	2.25.E+01	2.21.E+01	2.08.E+01	0.941	0.969	0.918	1.148	1.107	0.996	0.035
Urea-2TMS	GC/MS	3.21.E+00	4.88.E+00	2.52.E+00	2.97.E+00	4.30.E+00	2.46.E+00	2.77.E+00	4.13.E+00	2.77.E+00	0.926	0.880	0.977	0.865	0.845	1.099	0.360	3.19.E+01	2.89.E+01	2.99.E+01	2.91.E+01	2.88.E+01	2.86.E+01	3.22.E+01	2.95.E+01	3.07.E+01	0.914	0.997	0.957	1.010	1.021	1.026	0.071
2-Aminoethanol-3TMS	GC/MS	4.76.E-01	4.48.E-01	4.64.E-01	4.70.E-01	3.97.E-01	4.58.E-01	4.71.E-01	3.86.E-01	4.40.E-01	0.988	0.887	0.986	0.990	0.862	0.947	0.180	5.16.E-01	5.56.E-01	5.63.E-01	5.00.E-01	5.42.E-01	5.26.E-01	6.57.E-01	5.65.E-01	6.52.E-01	0.970	0.975	0.935	1.273	1.016	1.158	0.073
Benzoic acid-TMS	GC/MS	5.11.E-02	5.05.E-02	4.86.E-02	4.84.E-02	5.12.E-02	4.69.E-02	4.57.E-02	4.54.E-02	4.45.E-02	0.947	1.013	0.963	0.894	0.898	0.915	0.012	6.35.E-02	6.26.E-02	6.48.E-02	6.89.E-02	5.13.E-02	6.49.E-02	6.34.E-02	6.70.E-02	7.15.E-02	1.086	0.819	1.001	0.998	1.071	1.103	0.538
Glycerol-3TMS	GC/MS	9.29.E+00	1.04.E+01	1.02.E+01	9.75.E+00	9.97.E+00	1.02.E+01	8.72.E+00	9.24.E+00	9.07.E+00	1.049	0.960	0.998	0.938	0.889	0.886	0.012	1.04.E+00	1.12.E+00	1.13.E+00	9.51.E-01	8.59.E-01	1.14.E+00	1.15.E+00	1.04.E+00	1.07.E+00	0.914	0.765	1.004	1.101	0.925	0.948	0.332
Leucine-2TMS	GC/MS	4.68.E+00	4.63.E+00	3.72.E+00	4.56.E+00	4.65.E+00	3.43.E+00	4.09.E+00	4.24.E+00	3.79.E+00	0.975	1.004	0.922	0.873	0.916	1.019	0.396	8.81.E+00	9.80.E+00	9.68.E+00	8.42.E+00	8.64.E+00	8.96.E+00	1.11.E+01	1.16.E+01	9.45.E+00	0.956	0.881	0.926	1.258	1.178	0.976	0.080
Octanoic acid-TMS	GC/MS	4.22.E-02	4.96.E-02	5.00.E-02	4.56.E-02	4.84.E-02	5.54.E-02	4.45.E-02	4.61.E-02	4.97.E-02	1.079	0.976	1.109	1.054	0.930	0.994	0.268	8.61.E-02	9.56.E-02	1.02.E-01	9.38.E-02	8.35.E-02	9.50.E-02	1.11.E-01	1.11.E-01	9.74.E-02	1.090	0.873	0.931	1.291	1.162	0.954	0.202
Phosphoric acid-3TMS	GC/MS	7.14.E+00	5.78.E+00	5.57.E+00	6.68.E+00	5.53.E+00	4.92.E+00	6.11.E+00	5.61.E+00	5.23.E+00	0.936	0.957	0.885	0.856	0.970	0.939	0.153	8.33.E+00	8.99.E+00	8.42.E+00	8.19.E+00	9.01.E+00	8.95.E+00	8.50.E+00	8.12.E+00	8.61.E+00	0.983	1.002	1.063	1.021	0.903	1.022	0.644
Isoleucine-2TMS	GC/MS	2.15.E+00	2.18.E+00	1.91.E+00	2.11.E+00	2.23.E+00	1.77.E+00	1.87.E+00	2.03.E+00	2.02.E+00	0.980	1.023	0.930	0.872	0.932	1.059	0.685	3.43.E+00	3.83.E+00	3.80.E+00	3.30.E+00	3.38.E+00	3.45.E+00	4.23.E+00	4.41.E+00	3.76.E+00	0.961	0.883	0.908	1.234	1.151	0.989	0.049
Proline-2TMS	GC/MS	4.07.E+00	4.11.E+00	2.82.E+00	4.01.E+00	4.38.E+00	2.55.E+00	3.23.E+00	3.92.E+00	3.18.E+00	0.985	1.066	0.904	0.794	0.955	1.129	0.774	7.95.E+00	9.12.E+00	8.22.E+00	7.12.E+00	7.47.E+00	7.53.E+00	9.52.E+00	1.06.E+01	8.04.E+00	0.895	0.819	0.916	1.198	1.166	0.978	0.064
Succinic acid-2TMS	GC/MS	5.35.E-02	3.68.E-02	5.21.E-02	4.41.E-02	3.41.E-02	4.75.E-02	3.72.E-02	3.38.E-02	4.50.E-02	0.824	0.926	0.911	0.696	0.918	0.863	0.078	1.36.E-02	1.92.E-02	1.92.E-02	1.81.E-02	1.74.E-02	1.54.E-02	1.82.E-02	1.40.E-02	1.92.E-02	1.331	0.905	0.799	1.336	0.728	0.999	0.987
Glyceric acid-3TMS	GC/MS	1.22.E-01	1.25.E-01	1.26.E-01	1.32.E-01	1.24.E-01	1.30.E-01	1.34.E-01	1.24.E-01	1.37.E-01	1.082	0.995	1.033	1.096	0.994	1.090	0.178	1.07.E-01	1.03.E-01	1.09.E-01	1.14.E-01	1.13.E-01	1.08.E-01	1.10.E-01	1.18.E-01	1.03.E-01	1.064	1.092	0.993	1.027	1.145	0.950	0.501
Uracil-2TMS	GC/MS	1.13.E-03	2.21.E-03	9.62.E-04	9.95.E-04	3.12.E-03	1.34.E-03	2.19.E-03	3.11.E-03	1.00.E-03	0.878	1.407	1.390	1.933	1.404	1.044	0.301	3.63.E-03	5.12.E-03	3.34.E-03	3.52.E-03	3.71.E-03	4.53.E-03	3.25.E-03	3.44.E-03	3.44.E-03	0.968	0.724	1.358	0.896	0.672	1.030	0.514
Serine-3TMS	GC/MS	1.61.E+00	1.32.E+00	1.23.E+00	1.65.E+00	1.66.E+00	1.16.E+00	1.31.E+00	1.47.E+00	1.31.E+00	1.024	1.259	0.939	0.815	1.114	1.065	0.658	1.61.E+00	1.78.E+00	1.64.E+00	1.49.E+00	1.63.E+00	1.68.E+00	1.38.E+00	1.81.E+00	1.59.E+00	0.926	0.917	1.021	0.857	1.021	0.966	0.548
Fumaric acid-2TMS	GC/MS	1.14.E-02	1.10.E-02	1.33.E-02	1.23.E-02	1.33.E-02	1.43.E-02	1.34.E-02	1.45.E-02	1.72.E-02	1.082	1.215	1.075	1.178	1.327	1.290	0.011	1.10.E-02	1.14.E-02	1.40.E-02	1.15.E-02	1.34.E-02	1.22.E-02	1.12.E-02	1.20.E-02	1.37.E-02	1.048	1.178	0.874	1.022	1.056	0.978	0.946
Nonanoic acid-TMS	GC/MS	5.67.E-02	5.16.E-02	5.51.E-02	5.40.E-02	5.91.E-02	7.03.E-02	5.09.E-02	5.71.E-02	5.01.E-02	0.952	1.145	1.276	0.898	1.107	0.909	0.314	9.16.E-02	9.53.E-02	1.03.E-01	1.03.E-01	9.27.E-02	9.30.E-02	1.14.E-01	1.03.E-01	1.01.E-01	1.127	0.972	0.906	1.249	1.080	0.982	0.246
Threonine-3TMS	GC/MS	7.94.E-01	7.73.E-01	9.52.E-01	8.11.E-01	9.33.E-01	8.99.E-01	6.99.E-01	7.76.E-01	9.68.E-01	1.021	1.207	0.944	0.881	1.004	1.017	0.556	9.55.E-01	9.96.E-01	1.01.E+00	9.05.E-01	9.62.E-01	9.34.E-01	9.35.E-01	1.06.E+00	1.02.E+00	0.948	0.966	0.927	0.979	1.062	1.013	0.047
Threitol-4TMS	GC/MS	3.21.E-03	4.55.E-03	4.02.E-03	3.94.E-03	3.58.E-03	5.05.E-03	3.19.E-03	4.58.E-03	4.83.E-03	1.229	0.787	1.256	0.995	1.007	1.201	0.827	5.31.E-03	5.92.E-03	5.91.E-03	5.54.E-03	6.55.E-03	4.68.E-03	5.28.E-03	4.84.E-03	6.46.E-03	1.043	1.107	0.792	0.995	0.818	1.093	0.967
Malic acid-3TMS	GC/MS	2.85.E-03	3.06.E-03	3.54.E-03	2.62.E-03	3.10.E-03	3.50.E-03	2.53.E-03	3.38.E-03	3.87.E-03	0.919	1.012	0.990	0.889	1.107	1.093	0.529	1.30.E-03	1.60.E-03	1.78.E-03	1.46.E-03	2.18.E-03	1.40.E-03	2.41.E-03	1.84.E-03	1.89.E-03	1.129	1.368	0.787	1.856	1.152	1.063	0.389
meso-Erythritol-4TMS	GC/MS	9.99.E-03	1.45.E-02	1.40.E-02	1.02.E-02	1.36.E-02	1.31.E-02	1.02.E-02	1.24.E-02	1.26.E-02	1.018	0.941	0.935	1.016	0.855	0.904	0.190	1.34.E-02	1.36.E-02	1.39.E-02	1.26.E-02	1.41.E-02	1.37.E-02	1.54.E-02	1.50.E-02	1.49.E-02	0.940	1.035	0.985	1.152	1.103	1.068	0.040
Aspartic acid-3TMS	GC/MS	4.31.E-03	4.36.E-03	5.20.E-03	4.80.E-03	5.27.E-03	4.75.E-03	3.80.E-03	5.72.E-03	5.45.E-03	1.113	1.209	0.912	0.881	1.312	1.047	0.745	5.80.E-03	4.23.E-03	4.40.E-03	4.59.E-03	5.48.E-03	5.28.E-03	5.12.E-03	6.41.E-03	5.81.E-03	0.792	1.297	1.200	0.882	1.516	1.321	0.418
4-Hydroxyproline-3TMS	GC/MS	3.61.E-01	4.36.E-01	2.65.E-01	3.74.E-01	4.61.E-01	2.55.E-01	3.41.E-01	3.63.E-01	2.37.E-01	1.038	1.057	0.963	0.946	0.833	0.898	0.105	5.85.E-01	5.24.E-01	4.71.E-01	4.49.E-01	4.94.E-01	4.00.E-01	5.40.E-01	6.02.E-01	5.48.E-01	0.768	0.942	0.847	0.923	1.148	1.163	0.046
Methionine-2TMS	GC/MS	3.40.E-02	3.65.E-02	3.46.E-02	3.37.E-02	3.67.E-02	3.61.E-02	3.02.E-02	2.68.E-02	3.48.E-02	0.992	1.005	1.044	0.890	0.734	1.006	0.171	3.74.E-02	3.72.E-02	3.61.E-02	2.99.E-02	3.33.E-02	2.95.E-02	3.54.E-02	4.01.E-02	3.78.E-02	0.800	0.897	0.817	0.946	1.079	1.047	0.008
5-Oxoproline-2TMS	GC/MS	4.63.E-01	2.91.E-01	3.17.E-01	3.83.E-01	3.72.E-01	2.73.E-01	3.96.E-01	3.51.E-01	3.39.E-01	0.828	1.280	0.863	0.854	1.209	1.069	0.881	2.13.E-01	1.98.E-01	2.13.E-01	2.17.E-01	2.89.E-01	1.59.E-01	2.20.E-01	2.41.E-01	2.41.E-01	1.022	1.463	0.747	1.037	1.221	1.132	0.744
Pyrogallol-3TMS	GC/MS	1.66.E-02	3.05.E-03	4.35.E-02	1.67.E-02	3.19.E-03	4.18.E-02	1.67.E-02	3.30.E-03	4.30.E-02	1.006	1.049	0.961	1.005	1.084	0.988	0.534	1.39.E-02	1.37.E-02	1.64.E-02	1.39.E-02	1.35.E-02	1.37.E-02	1.49.E-02	1.61.E-02	1.39.E-02	0.997	0.987	0.834	1.068	1.179	0.849	0.513
Cysteine-3TMS	GC/MS	1.55.E-01	1.74.E-01	2.12.E-01	1.52.E-01	1.63.E-01	1.98.E-01	1.59.E-01	1.31.E-01	1.77.E-01	0.976	0.935	0.935	1.020	0.754	0.834	0.175	3.44.E-01	2.84.E-01	2.62.E-01	1.80.E-01	2.32.E-01	2.38.E-01	2.69.E-01	2.56.E-01	2.84.E-01	0.522	0.817	0.907	0.780	0.901	1.084	0.141
2-Ketoglutaric acid-meto-2TMS	GC/MS	3.76.E-02	2.97.E-02	4.72.E-02	3.43.E-02	2.79.E-02	4.71.E-02	3.60.E-02	2.88.E-02	5.21.E-02	0.912	0.940	0.998	0.959	0.969	1.104	0.325	3.91.E-02	4.04.E-02	4.06.E-02	3.60.E-02	4.51.E-02	3.60.E-02	3.80.E-02	3.36.E-02	4.20.E-02	0.921	1.116	0.886	0.971	0.832	1.034	0.849
3-Aminoglutaric acid-3TMS	GC/MS	4.16.E-02	4.91.E-02	4.33.E-02	4.20.E-02	4.04.E-02	4.38.E-02	3.71.E-02	3.66.E-02	3.13.E-02	1.009	0.821	1.013	0.892	0.744	0.723	0.058	7.09.E-02	8.13.E-02	9.51.E-02	9.44.E-02	8.95.E-02	8.84.E-02	9.62.E-02	9.86.E-02	8.73.E-02	1.331	1.101	0.929	1.357	1.212	0.918	0.400
Glutamic acid-3TMS	GC/MS	1.25.E-01	1.75.E-01	3.27.E-01	1.57.E-01	1.42.E-01	3.35.E-01	1.53.E-01	1.62.E-01	2.85.E-01	1.262	0.810	1.024	1.225	0.923	0.871	0.836	5.20.E-01	3.49.E-01	3.38.E-01	4.49.E-01	4.64.E-01	4.56.E-01	3.35.E-01	4.73.E-01	3.19.E-01	0.862	1.328	1.349	0.643	1.355	0.943	0.538
5-Aminovaleric acid-3TMS	GC/MS	5.71.E-03	7.29.E-03	6.32.E-03	6.35.E-03	6.83.E-03	7.25.E-03	6.06.E-03	6.48.E-03	5.76.E-03	1.112	0.936	1.147	1.061	0.888	0.910	0.299	1.70.E-02	2.06.E-02	2.13.E-02	2.35.E-02	2.27.E-02	2.30.E-02	2.43.E-02	2.10.E-02	2.33.E-02	1.387	1.103	1.079	1.430	1.020	1.093	0.155
Phenylalanine-2TMS	GC/MS	8.94.E-01	1.06.E+00	1.04.E+00	1.04.E+00	9.11.E-01	1.07.E+00	1.00.E+00	8.07.E-01	9.00.E-01	1.158	0.857	1.024	1.119	0.760	0.864	0.450	1.65.E+00	1.61.E+00	1.61.E+00	1.45.E+00	1.55.E+00	1.42.E+00	1.76.E+00	1.81.E+00	1.66.E+00	0.880	0.964	0.882	1.065	1.127	1.031	0.006
Xylose-meto-4TMS	GC/MS	4.41.E-03	4.91.E-03	4.14.E-03	4.47.E-03	4.07.E-03	4.92.E-03	4.59.E-03	4.39.E-03	4.96.E-03	1.012	0.830	1.188	1.041	0.894	1.197	0.876	3.71.E-03	4.92.E-03	6.11.E-03	5.16.E-03	4.85.E-03	5.78.E-03	5.72.E-03	5.13.E-03	5.35.E-03	1.390	0.985	0.946	1.542	1.041	0.876	0.719
Arabinose-meto-4TMS	GC/MS	1.45.E-02	1.56.E-02	1.67.E-02	1.38.E-02	1.40.E-02	1.63.E-02	1.46.E-02	1.46.E-02	1.66.E-02	0.946	0.897	0.977	1.005	0.937	0.997	0.082	1.41.E-02	1.32.E-02	1.18.E-02	1.36.E-02	1.42.E-02	1.30.E-02	1.39.E-02	1.60.E-02	1.43.E-02	0.966	1.078	1.098	0.987	1.215	1.212	0.143
Ribulose-meto-4TMS	GC/MS	9.69.E-03	9.50.E-03	9.60.E-03	9.71.E-03	8.57.E-03	8.97.E-03	9.13.E-03	8.02.E-03	8.98.E-03	1.002	0.902	0.934	0.941	0.845	0.935	0.064	1.00.E-02	1.05.E-02	8.70.E-03	6.84.E-03	9.24.E-03	6.50.E-03	9.13.E-03	7.76.E-03	8.33.E-03	0.684	0.877	0.747	0.912	0.736	0.958	0.139
Lauric acid-TMS	GC/MS	1.66.E-01	1.51.E-01	1.60.E-01	1.69.E-01	1.47.E-01	1.40.E-01	1.45.E-01	1.19.E-01	1.25.E-01	1.021	0.974	0.877	0.873	0.791	0.782	0.010	2.93.E-01	2.86.E-01	3.30.E-01	3.07.E-01	2.83.E-01	2.91.E-01	2.88.E-01	2.64.E-01	2.90.E-01	1.047	0.989	0.882	0.982	0.924	0.877	0.247
Asparagine-3TMS	GC/MS	4.10.E-02	4.72.E-02	6.49.E-02	4.30.E-02	3.23.E-02	6.06.E-02	3.38.E-02	3.74.E-02	4.29.E-02	1.048	0.684	0.934	0.824	0.792	0.662	0.169	7.91.E-02	7.79.E-02	6.17.E-02	5.75.E-02	7.50.E-02	6.70.E-02	8.09.E-02	6.34.E-02	6.85.E-02	0.727	0.962	1.086	1.023	0.814	1.111	0.749
Xylitol-5TMS	GC/MS	4.76.E-03	5.52.E-03	5.09.E-03	4.25.E-03	4.52.E-03	4.12.E-03	4.08.E-03	4.21.E-03	4.44.E-03	0.893	0.819	0.810	0.856	0.763	0.872	0.016	5.34.E-03	5.20.E-03	5.41.E-03	5.33.E-03	4.56.E-03	4.94.E-03	6.55.E-03	4.17.E-03	5.25.E-03	0.997	0.878	0.913	1.226	0.803	0.971	0.682
Arabitol-5TMS	GC/MS	1.62.E-02	4.13.E-02	2.35.E-02	1.57.E-02	3.92.E-02	2.25.E-02	1.64.E-02	3.78.E-02	2.38.E-02	0.964	0.949	0.959	1.007	0.914	1.015	0.435	1.60.E-02	1.70.E-02	1.69.E-02	1.75.E-02	1.85.E-02	2.00.E-02	1.72.E-02	1.84.E-02	1.92.E-02	1.091	1.086	1.182	1.076	1.083	1.136	0.013
Ribitol-5TMS	GC/MS	3.93.E-03	3.80.E-03	4.51.E-03	3.82.E-03	3.35.E-03	4.22.E-03	4.09.E-03	3.21.E-03	4.31.E-03	0.974	0.881	0.937	1.041	0.843	0.957	0.282	3.53.E-03	3.47.E-03	3.65.E-03	3.70.E-03	4.43.E-03	3.26.E-03	3.89.E-03	3.12.E-03	4.03.E-03	1.048	1.279	0.892	1.102	0.901	1.103	0.862
2-Aminoadipic acid-3TMS	GC/MS	4.24.E-03	3.35.E-03	2.70.E-03	3.38.E-03	2.95.E-03	2.68.E-03	3.19.E-03	3.27.E-03	2.80.E-03	0.798	0.880	0.995	0.754	0.975	1.037	0.332	3.73.E-03	3.79.E-03	3.89.E-03	4.56.E-03	3.92.E-03	4.35.E-03	4.71.E-03	4.19.E-03	4.56.E-03	1.221	1.034	1.118	1.262	1.106	1.173	0.025
2-Deoxy-glucose-4TMS	GC/MS	3.35.E-03	2.77.E-03	3.17.E-03	3.76.E-03	2.71.E-03	4.19.E-03	4.45.E-03	3.22.E-03	3.97.E-03	1.123	0.980	1.322	1.330	1.163	1.253	0.096	1.48.E-02	1.30.E-02	1.30.E-02	1.10.E-02	1.27.E-02	1.22.E-02	1.32.E-02	1.32.E-02	1.62.E-02	0.745	0.976	0.939	0.894	1.014	1.247	0.260
Glutamine-3TMS	GC/MS	1.78.E-02	4.46.E-02	4.16.E-02	1.81.E-02	1.26.E-02	1.02.E-01	1.80.E-02	1.41.E-02	2.29.E-02	1.017	0.282	2.445	1.016	0.317	0.551	0.560	1.01.E+00	9.94.E-01	8.97.E-01	8.51.E-01	9.27.E-01	8.43.E-01	1.11.E+00	8.26.E-01	9.60.E-01	0.844	0.932	0.939	1.100	0.831	1.069	0.476
Isocitric acid-4TMS	GC/MS	2.50.E-02	2.26.E-02	2.84.E-02	2.48.E-02	2.14.E-02	2.87.E-02	2.22.E-02	2.43.E-02	2.75.E-02	0.991	0.948	1.009	0.887	1.075	0.969	0.867	2.22.E-02	3.00.E-02	2.37.E-02	2.78.E-02	3.28.E-02	2.78.E-02	2.53.E-02	2.21.E-02	2.60.E-02	1.250	1.094	1.170	1.138	0.738	1.094	0.247
2-Aminopimelic acid-3TMS	GC/MS	4.30.E-01	3.24.E-01	3.90.E-01	4.21.E-01	3.08.E-01	3.70.E-01	3.78.E-01	3.38.E-01	3.64.E-01	0.979	0.949	0.949	0.878	1.042	0.934	0.478	3.44.E-01	4.00.E-01	3.14.E-01	3.42.E-01	3.88.E-01	3.60.E-01	3.21.E-01	3.02.E-01	3.35.E-01	0.994	0.970	1.149	0.933	0.754	1.067	0.306
Citric acid-4TMS	GC/MS	6.00.E-01	4.49.E-01	5.42.E-01	5.85.E-01	4.31.E-01	5.12.E-01	5.27.E-01	4.70.E-01	5.07.E-01	0.975	0.960	0.945	0.879	1.047	0.935	0.485	3.37.E-01	3.99.E-01	3.07.E-01	3.35.E-01	3.80.E-01	3.58.E-01	3.29.E-01	2.99.E-01	3.24.E-01	0.995	0.952	1.169	0.976	0.748	1.057	0.388
Ornithine-4TMS	GC/MS	5.78.E-01	1.04.E+00	8.30.E-01	7.82.E-01	7.94.E-01	1.43.E+00	8.76.E-01	8.32.E-01	1.02.E+00	1.351	0.761	1.717	1.514	0.798	1.224	0.659	3.20.E+00	2.73.E+00	2.86.E+00	2.73.E+00	3.10.E+00	2.71.E+00	3.15.E+00	2.79.E+00	2.99.E+00	0.851	1.134	0.946	0.984	1.022	1.045	0.787
1,5-Anhydro-glucitol-4TMS	GC/MS	4.11.E+00	4.63.E+00	4.14.E+00	3.99.E+00	4.31.E+00	4.05.E+00	4.03.E+00	4.08.E+00	4.17.E+00	0.972	0.930	0.980	0.981	0.881	1.007	0.331	7.79.E+00	7.19.E+00	7.99.E+00	7.22.E+00	7.51.E+00	7.21.E+00	8.09.E+00	7.65.E+00	7.79.E+00	0.928	1.044	0.902	1.038	1.064	0.975	0.228
Sorbose-meto-5TMS	GC/MS	9.17.E-02	1.15.E-01	1.10.E-01	9.94.E-02	1.19.E-01	1.23.E-01	1.02.E-01	1.09.E-01	1.17.E-01	1.084	1.039	1.123	1.110	0.947	1.060	0.205	1.32.E-01	1.22.E-01	1.56.E-01	1.35.E-01	1.21.E-01	1.13.E-01	1.51.E-01	1.59.E-01	1.45.E-01	1.026	0.994	0.720	1.149	1.304	0.927	0.185
Fructose-meto-5TMS	GC/MS	2.41.E-02	3.67.E-02	3.57.E-02	2.95.E-02	3.91.E-02	4.42.E-02	3.32.E-02	3.73.E-02	3.74.E-02	1.223	1.065	1.238	1.379	1.016	1.047	0.210	3.02.E-02	3.25.E-02	4.20.E-02	4.03.E-02	2.61.E-02	2.62.E-02	4.31.E-02	4.89.E-02	3.93.E-02	1.334	0.805	0.625	1.426	1.506	0.937	0.238
Mannose-meto-5TMS	GC/MS	7.40.E-01	1.01.E+00	6.72.E-01	7.14.E-01	9.27.E-01	6.42.E-01	7.24.E-01	8.86.E-01	6.51.E-01	0.965	0.921	0.955	0.978	0.881	0.968	0.171	9.07.E-01	8.72.E-01	9.47.E-01	8.09.E-01	8.88.E-01	8.64.E-01	9.03.E-01	8.57.E-01	8.94.E-01	0.893	1.019	0.913	0.996	0.983	0.944	0.306
5-Dehydroquinic acid-meto-4TMS	GC/MS	3.58.E-02	3.91.E-02	3.55.E-02	3.47.E-02	3.61.E-02	3.45.E-02	3.46.E-02	3.17.E-02	3.43.E-02	0.970	0.923	0.972	0.967	0.811	0.964	0.203	2.16.E-01	2.14.E-01	2.28.E-01	2.21.E-01	2.18.E-01	2.06.E-01	2.36.E-01	2.18.E-01	2.32.E-01	1.023	1.021	0.905	1.093	1.018	1.019	0.288
Glucose-meto-5TMS	GC/MS	4.64.E+00	5.04.E+00	4.66.E+00	4.56.E+00	4.62.E+00	4.49.E+00	4.50.E+00	4.29.E+00	4.55.E+00	0.982	0.917	0.963	0.969	0.852	0.976	0.185	3.78.E+01	3.49.E+01	3.81.E+01	3.52.E+01	3.71.E+01	3.49.E+01	3.88.E+01	3.62.E+01	3.79.E+01	0.932	1.064	0.917	1.026	1.038	0.995	0.430
Hippuric acid-TMS	GC/MS	4.27.E-02	4.58.E-02	4.51.E-02	4.11.E-02	4.04.E-02	4.62.E-02	4.77.E-02	3.89.E-02	4.71.E-02	0.962	0.883	1.025	1.119	0.850	1.043	0.726	4.44.E-01	3.95.E-01	4.22.E-01	4.18.E-01	4.38.E-01	3.96.E-01	4.88.E-01	4.35.E-01	4.52.E-01	0.943	1.110	0.939	1.100	1.102	1.072	0.158
Galactose-meto-5TMS	GC/MS	5.09.E+00	5.38.E+00	5.21.E+00	4.80.E+00	4.86.E+00	4.92.E+00	4.67.E+00	4.56.E+00	5.04.E+00	0.942	0.905	0.944	0.918	0.847	0.967	0.055	1.48.E+01	1.35.E+01	1.44.E+01	1.33.E+01	1.38.E+01	1.35.E+01	1.41.E+01	1.35.E+01	1.39.E+01	0.899	1.020	0.936	0.958	0.994	0.963	0.275
Glucosamine-5TMS	GC/MS	1.15.E-01	1.21.E-01	1.19.E-01	1.09.E-01	1.11.E-01	1.11.E-01	1.05.E-01	1.04.E-01	1.16.E-01	0.950	0.919	0.935	0.912	0.860	0.974	0.070	3.48.E-01	3.23.E-01	3.31.E-01	3.25.E-01	3.35.E-01	3.25.E-01	3.46.E-01	3.09.E-01	3.08.E-01	0.935	1.038	0.984	0.995	0.958	0.932	0.549
Lysine-4TMS	GC/MS	1.28.E-01	4.05.E-01	1.58.E-01	1.33.E-01	1.80.E-01	4.14.E-01	1.28.E-01	1.69.E-01	1.01.E-01	1.041	0.445	2.611	0.999	0.417	0.637	0.578	6.77.E-01	6.03.E-01	6.29.E-01	5.69.E-01	6.57.E-01	5.57.E-01	6.65.E-01	5.98.E-01	6.66.E-01	0.841	1.089	0.885	0.981	0.993	1.058	0.527
Glucuronic acid-meto-5TMS	GC/MS	4.05.E-02	3.80.E-02	3.67.E-02	3.99.E-02	3.80.E-02	3.47.E-02	3.93.E-02	3.57.E-02	3.46.E-02	0.985	1.000	0.944	0.972	0.942	0.943	0.075	4.23.E-02	4.53.E-02	4.39.E-02	4.46.E-02	4.78.E-02	4.05.E-02	4.97.E-02	4.94.E-02	4.26.E-02	1.054	1.057	0.924	1.176	1.091	0.972	0.272
Histidine-3TMS	GC/MS	1.90.E-01	4.53.E-01	4.77.E-01	2.59.E-01	2.02.E-01	9.88.E-01	2.44.E-01	1.90.E-01	2.14.E-01	1.360	0.446	2.072	1.279	0.420	0.449	0.485	1.24.E+00	8.05.E-01	5.11.E-01	7.69.E-01	8.25.E-01	3.26.E-01	1.14.E+00	5.62.E-01	6.41.E-01	0.621	1.025	0.639	0.919	0.698	1.255	0.460
Ascorbic acid-4TMS	GC/MS	9.79.E-03	1.11.E-02	1.08.E-02	9.56.E-03	9.75.E-03	9.87.E-03	8.84.E-03	9.01.E-03	9.68.E-03	0.976	0.879	0.911	0.903	0.812	0.893	0.022	9.23.E-03	1.07.E-02	6.61.E-03	8.10.E-03	8.85.E-03	8.39.E-03	9.05.E-03	8.98.E-03	8.38.E-03	0.878	0.828	1.270	0.980	0.839	1.269	0.890
Tyrosine-3TMS	GC/MS	8.09.E-02	1.84.E-01	1.08.E-01	7.63.E-02	9.33.E-02	2.24.E-01	7.16.E-02	8.90.E-02	6.99.E-02	0.942	0.507	2.084	0.885	0.483	0.649	0.518	3.60.E-01	3.38.E-01	3.53.E-01	3.22.E-01	3.42.E-01	3.15.E-01	3.58.E-01	3.33.E-01	3.51.E-01	0.894	1.013	0.892	0.994	0.985	0.995	0.208
Galacturonic acid-meto-5TMS	GC/MS	1.62.E-02	1.94.E-02	1.90.E-02	1.50.E-02	1.67.E-02	1.70.E-02	1.48.E-02	1.53.E-02	1.68.E-02	0.926	0.859	0.895	0.918	0.790	0.887	0.026	1.89.E-02	1.14.E-02	1.80.E-02	1.73.E-02	1.55.E-02	1.70.E-02	1.54.E-02	1.40.E-02	1.49.E-02	0.920	1.359	0.943	0.818	1.230	0.829	0.533
N-Acetyl-Ornithine-4TMS	GC/MS	3.73.E-02	4.01.E-02	3.96.E-02	3.26.E-02	3.32.E-02	3.43.E-02	3.05.E-02	2.89.E-02	3.18.E-02	0.873	0.827	0.865	0.818	0.720	0.803	0.002	3.89.E-02	3.37.E-02	3.34.E-02	3.33.E-02	3.25.E-02	2.83.E-02	3.06.E-02	3.49.E-02	2.73.E-02	0.856	0.966	0.848	0.788	1.036	0.816	0.171
Gluconic acid-6TMS	GC/MS	2.24.E-02	1.95.E-02	1.78.E-02	2.28.E-02	1.86.E-02	1.68.E-02	1.79.E-02	1.74.E-02	1.75.E-02	1.016	0.955	0.948	0.797	0.895	0.987	0.259	1.33.E-02	1.38.E-02	1.44.E-02	1.31.E-02	1.25.E-02	1.30.E-02	1.46.E-02	1.36.E-02	1.26.E-02	0.985	0.904	0.901	1.101	0.987	0.875	0.386
Glucaric acid-6TMS	GC/MS	8.14.E-03	7.06.E-03	6.89.E-03	8.61.E-03	6.75.E-03	6.80.E-03	7.47.E-03	6.69.E-03	6.42.E-03	1.058	0.955	0.988	0.919	0.947	0.932	0.145	5.11.E-03	4.92.E-03	5.50.E-03	6.38.E-03	5.65.E-03	5.54.E-03	4.62.E-03	5.33.E-03	5.16.E-03	1.248	1.148	1.007	0.904	1.083	0.938	0.181
Palmitoleic acid-TMS	GC/MS	1.64.E-02	8.07.E-03	2.58.E-02	1.55.E-02	6.17.E-03	2.42.E-02	1.81.E-02	6.81.E-03	2.59.E-02	0.946	0.764	0.938	1.107	0.843	1.003	0.106	1.35.E-02	1.15.E-02	1.30.E-02	9.86.E-03	1.19.E-02	1.28.E-02	9.74.E-03	1.43.E-02	9.96.E-03	0.729	1.038	0.983	0.720	1.246	0.768	0.709
Inositol-6TMS	GC/MS	1.55.E-01	2.12.E-01	2.09.E-01	1.54.E-01	1.99.E-01	2.01.E-01	1.56.E-01	1.95.E-01	2.05.E-01	0.997	0.939	0.960	1.009	0.920	0.977	0.241	2.28.E-01	2.18.E-01	2.33.E-01	2.10.E-01	2.30.E-01	2.14.E-01	2.37.E-01	2.26.E-01	2.32.E-01	0.920	1.057	0.920	1.036	1.036	0.996	0.365
Uric acid-4TMS	GC/MS	1.75.E+00	3.21.E+00	2.34.E+00	1.82.E+00	2.37.E+00	2.05.E+00	1.31.E+00	2.54.E+00	1.47.E+00	1.042	0.737	0.876	0.749	0.792	0.629	0.095	2.05.E+00	2.66.E+00	1.94.E+00	1.88.E+00	1.75.E+00	2.63.E+00	2.15.E+00	1.63.E+00	2.05.E+00	0.917	0.660	1.355	1.050	0.612	1.058	0.779
Margaric acid-TMS	GC/MS	2.46.E-02	3.05.E-02	2.42.E-02	2.84.E-02	2.41.E-02	2.51.E-02	3.11.E-02	2.34.E-02	2.16.E-02	1.154	0.790	1.037	1.263	0.768	0.892	0.942	2.53.E-02	2.28.E-02	2.65.E-02	2.49.E-02	2.49.E-02	2.45.E-02	2.68.E-02	2.51.E-02	2.53.E-02	0.982	1.089	0.924	1.058	1.099	0.952	0.597
Kynurenine-3TMS	GC/MS	9.60.E-04	5.09.E-03	3.45.E-03	1.19.E-03	1.83.E-03	5.22.E-03	1.30.E-03	1.51.E-03	1.27.E-03	1.238	0.359	1.512	1.349	0.297	0.367	0.434	2.36.E-03	2.11.E-03	1.95.E-03	2.01.E-03	1.91.E-03	1.41.E-03	1.67.E-03	2.51.E-03	1.85.E-03	0.854	0.904	0.722	0.706	1.187	0.949	0.432
Cystamine-4TMS	GC/MS	3.04.E-03	5.60.E-03	3.39.E-03	3.28.E-03	3.39.E-03	3.59.E-03	3.49.E-03	3.71.E-03	2.79.E-03	1.077	0.605	1.060	1.148	0.663	0.825	0.566	4.21.E-03	6.44.E-03	6.96.E-03	5.58.E-03	6.97.E-03	8.85.E-03	5.12.E-03	7.47.E-03	7.08.E-03	1.326	1.082	1.270	1.216	1.161	1.016	0.129
Tryptophan-3TMS	GC/MS	9.41.E-01	3.15.E+00	2.36.E+00	1.25.E+00	1.31.E+00	3.49.E+00	1.21.E+00	1.14.E+00	1.18.E+00	1.330	0.416	1.479	1.283	0.362	0.499	0.460	7.57.E+00	6.52.E+00	6.82.E+00	6.96.E+00	6.36.E+00	5.98.E+00	7.85.E+00	6.90.E+00	6.98.E+00	0.918	0.976	0.877	1.037	1.058	1.023	0.013
Elaidic acid-TMS	GC/MS	9.31.E-02	1.06.E-01	1.52.E-01	1.10.E-01	8.43.E-02	1.42.E-01	1.24.E-01	8.42.E-02	1.23.E-01	1.182	0.794	0.935	1.329	0.793	0.811	0.886	6.64.E-02	6.22.E-02	7.52.E-02	5.92.E-02	6.99.E-02	7.03.E-02	7.28.E-02	7.11.E-02	6.93.E-02	0.892	1.124	0.936	1.096	1.142	0.922	0.632
Stearic acid-TMS	GC/MS	1.44.E+00	1.87.E+00	1.65.E+00	1.68.E+00	1.44.E+00	1.76.E+00	1.95.E+00	1.46.E+00	1.49.E+00	1.168	0.773	1.066	1.357	0.783	0.901	0.993	1.90.E+00	1.65.E+00	1.97.E+00	1.68.E+00	1.98.E+00	1.83.E+00	2.01.E+00	1.95.E+00	1.88.E+00	0.887	1.196	0.930	1.058	1.182	0.954	0.653
Cystine-4TMS	GC/MS	7.40.E-04	3.75.E-02	2.06.E-02	2.83.E-03	4.56.E-03	4.03.E-02	3.20.E-03	1.11.E-03	4.76.E-03	3.821	0.121	1.955	4.323	0.030	0.231	0.469	3.96.E-02	2.62.E-02	2.24.E-02	3.56.E-02	2.13.E-02	2.11.E-02	2.78.E-02	2.11.E-02	2.04.E-02	0.898	0.811	0.942	0.703	0.806	0.909	0.116
Sucrose-8TMS	GC/MS	3.33.E-03	3.68.E-03	2.08.E-02	2.47.E-03	4.67.E-03	2.34.E-02	1.51.E-02	1.05.E-02	3.86.E-02	0.741	1.270	1.124	4.515	2.859	1.859	0.015	3.46.E-03	2.43.E-03	2.99.E-03	3.05.E-03	3.89.E-03	2.70.E-03	3.83.E-03	4.36.E-03	3.39.E-03	0.881	1.603	0.903	1.108	1.795	1.136	0.246
Maltose-meto-8TMS	GC/MS	3.14.E-03	6.22.E-03	7.09.E-03	3.19.E-03	8.32.E-03	6.79.E-03	3.46.E-03	7.36.E-03	7.14.E-03	1.015	1.337	0.957	1.100	1.182	1.006	0.529	7.67.E-04	7.55.E-04	8.49.E-04	9.54.E-04	1.11.E-03	9.99.E-04	1.08.E-03	1.35.E-03	1.36.E-03	1.243	1.476	1.176	1.407	1.790	1.602	0.008
Betaine	LC/MS_Cation	3.40.E+00	2.87.E+00	3.67.E+00	2.90.E+00	4.70.E+00	3.35.E+00	4.91.E+00	6.15.E+00	5.26.E+00	0.853	1.635	0.911	1.444	2.141	1.433	0.036	9.07.E+00	6.95.E+00	2.84.E+01	2.18.E+01	1.78.E+01	1.29.E+01	1.03.E+01	1.19.E+01	9.31.E+00	2.407	2.561	0.453	1.136	1.716	0.328	0.633
Carnitine	LC/MS_Cation	1.26.E+01	8.63.E+00	7.81.E+00	7.61.E+00	1.69.E+01	8.21.E+00	1.63.E+01	2.05.E+01	1.33.E+01	0.604	1.959	1.051	1.292	2.369	1.701	0.128	1.25.E+01	8.81.E+00	1.16.E+01	1.08.E+01	1.23.E+01	1.06.E+01	1.13.E+01	1.12.E+01	1.16.E+01	0.860	1.395	0.910	0.900	1.266	0.997	0.956
Choline	LC/MS_Cation	4.34.E-01	3.15.E-01	2.47.E-01	2.69.E-01	6.60.E-01	3.17.E-01	6.89.E-01	7.98.E-01	5.92.E-01	0.620	2.097	1.284	1.589	2.535	2.395	0.055	9.46.E-01	6.02.E-01	9.34.E-01	7.72.E-01	9.74.E-01	8.93.E-01	8.17.E-01	8.71.E-01	8.65.E-01	0.817	1.620	0.956	0.864	1.447	0.927	0.912
Creatine	LC/MS_Cation	8.15.E+00	6.44.E+00	4.81.E+00	5.04.E+00	1.21.E+01	5.27.E+00	9.58.E+00	1.49.E+01	8.36.E+00	0.618	1.877	1.095	1.176	2.318	1.739	0.160	1.19.E+01	9.21.E+00	1.08.E+01	1.07.E+01	1.20.E+01	1.04.E+01	1.04.E+01	1.22.E+01	1.07.E+01	0.901	1.300	0.964	0.873	1.321	0.994	0.893
Creatinine	LC/MS_Cation	7.47.E+00	2.84.E+00	3.68.E+00	2.65.E+00	1.00.E+01	4.92.E+00	9.33.E+00	9.43.E+00	7.80.E+00	0.354	3.529	1.335	1.248	3.321	2.118	0.322	1.69.E+01	9.10.E+00	1.57.E+01	1.16.E+01	1.67.E+01	1.28.E+01	1.50.E+01	1.26.E+01	1.66.E+01	0.689	1.837	0.812	0.887	1.381	1.057	0.933
Glycine	LC/MS_Cation	3.99.E+00	9.87.E-01	1.97.E+00	1.58.E+00	5.50.E+00	2.37.E+00	5.60.E+00	3.73.E+00	4.09.E+00	0.395	5.572	1.207	1.402	3.779	2.080	0.440	3.00.E+00	1.31.E+00	2.86.E+00	2.03.E+00	3.18.E+00	2.11.E+00	2.40.E+00	2.19.E+00	2.82.E+00	0.674	2.423	0.737	0.800	1.665	0.987	0.993
4-Hydroxy-L-proline	LC/MS_Cation	2.09.E+00	1.52.E+00	8.40.E-01	1.27.E+00	3.40.E+00	8.42.E-01	2.68.E+00	3.68.E+00	1.79.E+00	0.610	2.234	1.002	1.284	2.416	2.130	0.198	2.73.E+00	1.60.E+00	2.38.E+00	2.30.E+00	2.80.E+00	2.10.E+00	2.52.E+00	2.05.E+00	2.53.E+00	0.843	1.755	0.882	0.921	1.283	1.062	0.906
Hypoxanthine	LC/MS_Cation	5.39.E-02	7.06.E-03	8.83.E-03	4.29.E-02	4.14.E-02	2.64.E-02	4.51.E-02	3.44.E-02	8.91.E-02	0.796	5.861	2.989	0.836	4.875	10.095	0.380	3.62.E-02	3.51.E-02	3.53.E-02	1.72.E-01	2.00.E-01	1.27.E-01	2.85.E-01	3.50.E-01	4.01.E-01	4.763	5.681	3.601	7.879	9.978	11.336	0.003
L-Alanine; Sarcosine	LC/MS_Cation	8.11.E+00	3.06.E+00	5.09.E+00	3.30.E+00	1.03.E+01	5.94.E+00	1.09.E+01	9.41.E+00	1.05.E+01	0.407	3.366	1.167	1.342	3.074	2.060	0.251	1.85.E+01	1.00.E+01	1.92.E+01	1.39.E+01	2.05.E+01	1.33.E+01	1.78.E+01	1.62.E+01	1.83.E+01	0.749	2.049	0.690	0.964	1.619	0.952	0.895
L-Arginine	LC/MS_Cation	8.31.E+00	9.38.E+00	7.45.E+00	5.42.E+00	1.52.E+01	6.41.E+00	9.24.E+00	1.73.E+01	1.07.E+01	0.652	1.622	0.860	1.111	1.846	1.439	0.205	1.27.E+01	1.23.E+01	1.23.E+01	1.11.E+01	1.29.E+01	1.16.E+01	1.32.E+01	1.26.E+01	1.35.E+01	0.875	1.051	0.946	1.040	1.024	1.098	0.246
L-Aspartate	LC/MS_Cation	2.87.E-01	1.36.E-01	9.43.E-02	1.08.E-01	1.87.E+00	1.73.E-01	2.25.E-01	4.91.E-01	3.23.E-01	0.378	13.808	1.830	0.784	3.620	3.429	0.533	2.70.E-01	2.11.E-01	2.52.E-01	2.95.E-01	4.03.E-01	2.85.E-01	4.80.E-01	3.00.E-01	3.48.E-01	1.096	1.913	1.130	1.780	1.424	1.379	0.213
L-Asparagine	LC/MS_Cation	4.44.E+00	2.63.E+00	2.86.E+00	2.48.E+00	5.94.E+00	3.48.E+00	5.57.E+00	6.61.E+00	5.46.E+00	0.558	2.256	1.216	1.255	2.510	1.909	0.155	3.23.E+00	2.57.E+00	3.17.E+00	3.64.E+00	3.63.E+00	2.90.E+00	3.33.E+00	3.28.E+00	3.37.E+00	1.127	1.412	0.913	1.031	1.273	1.062	0.426
L-Citrulline	LC/MS_Cation	1.12.E+00	8.41.E-01	9.37.E-01	9.66.E-01	1.39.E+00	7.46.E-01	1.51.E+00	1.43.E+00	1.38.E+00	0.865	1.654	0.796	1.356	1.704	1.468	0.105	3.12.E+00	2.70.E+00	3.98.E+00	4.27.E+00	3.76.E+00	3.18.E+00	3.28.E+00	5.26.E+00	2.73.E+00	1.371	1.396	0.800	1.052	1.953	0.686	0.818
L-Cysteine	LC/MS_Cation	3.82.E-01	2.33.E-01	2.31.E-01	1.93.E-01	9.94.E-01	2.55.E-01	6.63.E-01	8.07.E-01	5.26.E-01	0.505	4.258	1.106	1.733	3.458	2.277	0.293	8.00.E-01	3.54.E-01	8.79.E-01	5.39.E-01	8.56.E-01	7.18.E-01	7.09.E-01	6.37.E-01	7.85.E-01	0.673	2.416	0.817	0.886	1.799	0.893	0.980
L-Lysine	LC/MS_Cation	3.97.E+00	3.73.E+00	1.93.E+00	2.29.E+00	7.35.E+00	1.99.E+00	4.75.E+00	8.74.E+00	3.50.E+00	0.576	1.969	1.031	1.198	2.342	1.814	0.218	1.05.E+01	7.17.E+00	1.07.E+01	9.11.E+00	1.09.E+01	9.31.E+00	9.63.E+00	8.69.E+00	1.13.E+01	0.869	1.520	0.870	0.919	1.212	1.060	0.940
L-Glutamine	LC/MS_Cation	1.38.E+02	1.04.E+02	9.46.E+01	9.30.E+01	1.81.E+02	1.01.E+02	1.74.E+02	2.27.E+02	1.62.E+02	0.676	1.734	1.066	1.265	2.177	1.708	0.083	1.22.E+02	1.04.E+02	1.28.E+02	1.33.E+02	1.31.E+02	1.11.E+02	1.27.E+02	1.32.E+02	1.23.E+02	1.089	1.259	0.870	1.046	1.272	0.967	0.613
L-Glutamate	LC/MS_Cation	5.63.E+00	3.91.E+00	4.35.E+00	3.61.E+00	8.20.E+00	4.29.E+00	7.38.E+00	8.82.E+00	7.14.E+00	0.642	2.099	0.986	1.311	2.258	1.641	0.152	7.78.E+00	5.05.E+00	7.37.E+00	8.05.E+00	8.12.E+00	6.88.E+00	6.78.E+00	8.67.E+00	6.64.E+00	1.035	1.607	0.934	0.872	1.716	0.901	0.706
L-Histidine	LC/MS_Cation	4.41.E+00	4.42.E+00	3.71.E+00	3.59.E+00	7.14.E+00	3.45.E+00	5.62.E+00	8.29.E+00	5.70.E+00	0.814	1.616	0.932	1.274	1.875	1.537	0.089	7.11.E+00	6.98.E+00	7.06.E+00	6.72.E+00	6.93.E+00	6.77.E+00	6.46.E+00	6.68.E+00	7.59.E+00	0.945	0.993	0.960	0.909	0.957	1.076	0.730
L-Homoserine; D-Homoserine	LC/MS_Cation	5.22.E+00	3.37.E+00	3.75.E+00	2.56.E+00	9.69.E+00	4.10.E+00	6.93.E+00	8.88.E+00	7.70.E+00	0.491	2.878	1.095	1.326	2.636	2.055	0.253	6.86.E+00	4.15.E+00	6.36.E+00	5.89.E+00	6.95.E+00	5.39.E+00	6.24.E+00	5.65.E+00	6.41.E+00	0.859	1.673	0.847	0.909	1.362	1.008	0.931
L-Isoleucine	LC/MS_Cation	3.25.E+01	1.58.E+01	1.47.E+01	1.42.E+01	5.19.E+01	1.86.E+01	4.01.E+01	4.50.E+01	3.20.E+01	0.438	3.276	1.268	1.236	2.841	2.185	0.365	4.82.E+01	2.47.E+01	4.22.E+01	3.22.E+01	4.92.E+01	3.64.E+01	4.11.E+01	3.34.E+01	4.72.E+01	0.667	1.993	0.863	0.854	1.352	1.119	0.970
L-Leucine	LC/MS_Cation	5.56.E+01	2.52.E+01	2.31.E+01	2.47.E+01	7.86.E+01	2.82.E+01	6.85.E+01	7.48.E+01	5.03.E+01	0.444	3.124	1.221	1.232	2.971	2.179	0.315	7.72.E+01	3.79.E+01	6.77.E+01	5.13.E+01	7.87.E+01	5.79.E+01	6.64.E+01	5.29.E+01	7.47.E+01	0.664	2.077	0.855	0.860	1.396	1.103	0.969
L-Methionine	LC/MS_Cation	4.54.E+00	3.29.E+00	2.83.E+00	2.57.E+00	6.50.E+00	3.00.E+00	5.13.E+00	7.07.E+00	4.67.E+00	0.567	1.974	1.058	1.130	2.148	1.649	0.244	5.38.E+00	4.18.E+00	5.47.E+00	5.25.E+00	5.61.E+00	4.81.E+00	5.54.E+00	5.31.E+00	5.57.E+00	0.976	1.342	0.880	1.030	1.268	1.019	0.622
L-Ornithine	LC/MS_Cation	5.57.E-01	5.85.E-01	3.85.E-01	4.42.E-01	3.13.E+00	4.53.E-01	1.21.E+00	1.58.E+00	1.23.E+00	0.793	5.345	1.176	2.177	2.706	3.189	0.435	2.05.E+00	1.22.E+00	1.67.E+00	1.57.E+00	1.88.E+00	1.48.E+00	1.66.E+00	1.52.E+00	1.97.E+00	0.767	1.548	0.884	0.811	1.248	1.180	0.956
L-Phenylalanine	LC/MS_Cation	1.41.E+01	1.00.E+01	8.18.E+00	8.85.E+00	2.10.E+01	9.04.E+00	1.73.E+01	2.36.E+01	1.44.E+01	0.630	2.093	1.105	1.231	2.347	1.757	0.181	1.71.E+01	1.32.E+01	1.65.E+01	1.55.E+01	1.79.E+01	1.54.E+01	1.69.E+01	1.59.E+01	1.85.E+01	0.903	1.363	0.932	0.987	1.209	1.122	0.656
L-Proline	LC/MS_Cation	5.54.E+00	3.95.E+00	2.49.E+00	2.91.E+00	9.06.E+00	2.87.E+00	7.23.E+00	1.01.E+01	4.98.E+00	0.526	2.292	1.154	1.304	2.550	2.002	0.207	3.32.E+01	2.08.E+01	2.94.E+01	2.48.E+01	3.08.E+01	2.49.E+01	2.89.E+01	2.64.E+01	3.12.E+01	0.746	1.480	0.847	0.870	1.268	1.063	0.889
L-Serine	LC/MS_Cation	8.95.E+00	3.73.E+00	3.83.E+00	3.83.E+00	1.89.E+01	4.67.E+00	1.09.E+01	1.17.E+01	8.04.E+00	0.428	5.071	1.217	1.223	3.132	2.097	0.577	1.04.E+01	5.22.E+00	9.23.E+00	8.11.E+00	1.04.E+01	7.44.E+00	8.75.E+00	7.84.E+00	9.43.E+00	0.778	1.988	0.806	0.839	1.503	1.022	0.971
L-Threonine	LC/MS_Cation	4.28.E+00	2.56.E+00	2.94.E+00	2.08.E+00	7.90.E+00	3.47.E+00	5.47.E+00	7.35.E+00	6.07.E+00	0.487	3.080	1.182	1.278	2.866	2.065	0.263	5.56.E+00	3.31.E+00	5.28.E+00	4.51.E+00	6.00.E+00	4.28.E+00	5.10.E+00	4.64.E+00	5.36.E+00	0.812	1.811	0.810	0.918	1.400	1.013	0.938
L-Tryptophan	LC/MS_Cation	3.50.E+00	1.95.E+00	2.01.E+00	1.93.E+00	4.81.E+00	2.17.E+00	4.73.E+00	5.47.E+00	3.61.E+00	0.551	2.461	1.077	1.352	2.800	1.795	0.167	3.10.E+00	2.03.E+00	2.78.E+00	2.52.E+00	3.20.E+00	2.61.E+00	2.77.E+00	2.56.E+00	3.10.E+00	0.814	1.581	0.938	0.892	1.266	1.115	0.897
L-Tyrosine	LC/MS_Cation	9.37.E+00	1.06.E+01	6.90.E+00	7.48.E+00	1.66.E+01	7.18.E+00	1.15.E+01	2.15.E+01	1.13.E+01	0.799	1.565	1.040	1.228	2.027	1.645	0.097	9.58.E+00	9.65.E+00	9.69.E+00	1.05.E+01	9.96.E+00	9.35.E+00	9.95.E+00	1.05.E+01	9.97.E+00	1.094	1.032	0.965	1.039	1.089	1.029	0.372
L-Valine	LC/MS_Cation	5.68.E+01	2.81.E+01	2.73.E+01	2.45.E+01	8.12.E+01	3.23.E+01	7.06.E+01	7.80.E+01	5.53.E+01	0.431	2.889	1.184	1.245	2.775	2.027	0.306	1.04.E+02	5.98.E+01	9.43.E+01	7.80.E+01	1.02.E+02	8.14.E+01	9.20.E+01	8.23.E+01	9.94.E+01	0.748	1.703	0.862	0.883	1.376	1.054	0.937
DMG	LC/MS_Cation	1.88.E-01	7.52.E-02	6.96.E-02	9.62.E-02	1.87.E-01	9.77.E-02	2.34.E-01	2.13.E-01	1.32.E-01	0.512	2.487	1.403	1.247	2.828	1.897	0.245	5.56.E-01	3.35.E-01	6.65.E-01	4.32.E-01	7.27.E-01	5.69.E-01	6.34.E-01	6.04.E-01	6.76.E-01	0.778	2.174	0.856	1.142	1.806	1.017	0.641
Uridine	LC/MS_Cation	8.21.E-01	1.50.E+00	4.94.E-01	7.24.E-01	2.12.E+00	5.98.E-01	9.33.E-01	3.33.E+00	8.14.E-01	0.882	1.416	1.209	1.136	2.217	1.648	0.247	5.79.E-01	7.81.E-01	6.44.E-01	7.90.E-01	6.86.E-01	6.37.E-01	6.66.E-01	7.83.E-01	6.54.E-01	1.364	0.878	0.989	1.149	1.003	1.016	0.840
L-Cystathionine	LC/MS_Cation	3.31.E-02	1.19.E-02	1.63.E-02	1.05.E-02	5.16.E-02	2.03.E-02	3.37.E-02	2.75.E-02	1.23.E-02	0.318	4.333	1.247	1.020	2.310	0.755	0.877	3.67.E-03	1.32.E-02	8.29.E-03	1.40.E-02	4.79.E-03	5.54.E-03	1.10.E-02	1.22.E-02	1.15.E-02	3.829	0.364	0.668	2.999	0.924	1.389	0.658
L-Cystine	LC/MS_Cation	2.52.E+01	3.63.E+01	1.97.E+01	2.18.E+01	5.26.E+01	2.61.E+01	3.08.E+01	7.64.E+01	3.35.E+01	0.866	1.448	1.328	1.223	2.102	1.703	0.124	1.89.E+01	1.92.E+01	1.85.E+01	2.69.E+01	2.07.E+01	1.92.E+01	1.97.E+01	2.16.E+01	1.83.E+01	1.423	1.078	1.038	1.042	1.120	0.987	0.315
N-Acetylglycine	LC/MS_Cation	1.54.E-01	4.08.E-02	4.53.E-02	2.75.E-02	1.95.E-01	7.24.E-02	9.31.E-02	2.07.E-01	1.60.E-01	0.179	4.784	1.597	0.606	5.067	3.526	0.533	1.94.E-01	6.27.E-02	1.71.E-01	9.10.E-02	2.22.E-01	1.55.E-01	1.63.E-01	1.44.E-01	2.53.E-01	0.468	3.537	0.905	0.838	2.295	1.478	0.761
L-Pyroglutamic acid	LC/MS_Cation	3.29.E+00	2.03.E+00	2.58.E+00	1.40.E+00	1.15.E+01	3.22.E+00	4.64.E+00	6.89.E+00	5.62.E+00	0.425	5.685	1.248	1.411	3.390	2.176	0.478	8.91.E-01	3.80.E-01	6.89.E-01	6.32.E-01	6.03.E-01	3.81.E-01	6.67.E-01	4.45.E-01	6.53.E-01	0.709	1.588	0.553	0.749	1.170	0.948	0.703
S-Methyl-L-cysteine	LC/MS_Cation	1.24.E-01	6.76.E-02	8.10.E-02	3.59.E-02	1.32.E-01	1.04.E-01	1.18.E-01	1.23.E-01	1.40.E-01	0.290	1.959	1.283	0.953	1.812	1.732	0.506	3.32.E-01	1.97.E-01	2.86.E-01	2.83.E-01	3.11.E-01	2.66.E-01	3.24.E-01	2.63.E-01	3.29.E-01	0.851	1.580	0.931	0.974	1.337	1.151	0.690
N-Acetyl-DL-alanine	LC/MS_Cation	2.76.E-01	1.31.E-01	1.30.E-01	1.12.E-01	4.02.E-01	1.61.E-01	3.50.E-01	4.28.E-01	3.32.E-01	0.407	3.077	1.236	1.266	3.279	2.552	0.198	3.50.E-01	1.72.E-01	2.94.E-01	1.77.E-01	3.71.E-01	2.51.E-01	2.90.E-01	2.38.E-01	2.73.E-01	0.506	2.160	0.855	0.829	1.387	0.930	0.997
L-Kynurenine	LC/MS_Cation	2.39.E-01	2.07.E-01	1.44.E-01	1.18.E-01	3.52.E-01	1.56.E-01	1.78.E-01	4.19.E-01	2.40.E-01	0.496	1.704	1.080	0.748	2.024	1.661	0.452	1.74.E-01	2.12.E-01	1.68.E-01	2.07.E-01	2.21.E-01	1.84.E-01	2.50.E-01	2.43.E-01	2.63.E-01	1.192	1.042	1.096	1.437	1.148	1.566	0.025
Phosphocholine	LC/MS_Cation	7.71.E-02	1.08.E-01	8.64.E-02	6.87.E-02	1.64.E-01	1.11.E-01	8.28.E-02	1.44.E-01	1.68.E-01	0.891	1.526	1.279	1.074	1.335	1.944	0.263	2.51.E-02	4.58.E-02	6.01.E-02	1.77.E-02	4.76.E-02	2.49.E-02	3.63.E-02	7.51.E-02	3.38.E-02	0.706	1.041	0.414	1.444	1.641	0.563	0.370
Acetyl-L-glutamine	LC/MS_Cation	8.89.E-01	7.95.E-01	6.52.E-01	5.72.E-01	1.61.E+00	7.39.E-01	1.24.E+00	1.64.E+00	1.08.E+00	0.643	2.024	1.135	1.392	2.064	1.658	0.181	8.92.E-01	6.40.E-01	8.11.E-01	8.04.E-01	8.35.E-01	7.19.E-01	8.16.E-01	6.30.E-01	7.76.E-01	0.901	1.306	0.887	0.915	0.984	0.957	0.803
L-2-Aminobutyric acid	LC/MS_Cation	4.01.E-01	2.64.E-01	2.63.E-01	2.95.E-01	4.32.E-01	2.23.E-01	5.53.E-01	5.74.E-01	3.42.E-01	0.735	1.633	0.849	1.379	2.171	1.299	0.089	9.63.E-01	7.54.E-01	1.17.E+00	8.35.E-01	1.10.E+00	8.93.E-01	9.49.E-01	1.14.E+00	9.35.E-01	0.867	1.455	0.764	0.985	1.509	0.800	0.907
Uric Acid	LC/MS_Cation	1.35.E+00	1.55.E+00	9.08.E-01	8.13.E-01	2.35.E+00	8.69.E-01	1.69.E+00	3.33.E+00	1.43.E+00	0.603	1.514	0.957	1.253	2.148	1.571	0.118	1.80.E+00	1.56.E+00	1.62.E+00	1.77.E+00	1.91.E+00	1.62.E+00	1.75.E+00	1.93.E+00	1.82.E+00	0.982	1.224	0.997	0.976	1.234	1.119	0.358
Glycolic acid	LC/MS_Anion	4.20.E-03	1.69.E-03	4.07.E-03	5.87.E-03	3.75.E-03	5.23.E-03	6.11.E-03	3.25.E-03	4.66.E-03	1.399	2.223	1.285	1.457	1.924	1.144	0.013	5.34.E-03	3.36.E-03	5.16.E-03	4.00.E-03	2.94.E-03	2.62.E-03	3.98.E-03	5.10.E-03	3.48.E-03	0.748	0.874	0.507	0.745	1.517	0.673	0.299
Lactic acid	LC/MS_Anion	3.77.E-01	2.85.E-01	4.45.E-01	3.93.E-01	4.00.E-01	5.24.E-01	4.84.E-01	4.54.E-01	5.13.E-01	1.040	1.402	1.177	1.282	1.591	1.153	0.042	4.10.E-01	4.14.E-01	3.73.E-01	4.26.E-01	3.59.E-01	3.93.E-01	4.62.E-01	4.74.E-01	4.76.E-01	1.039	0.867	1.054	1.127	1.146	1.275	0.038
Benzoic acid	LC/MS_Anion	2.58.E-02	1.82.E-02	2.36.E-02	1.74.E-02	1.72.E-02	2.03.E-02	2.00.E-02	1.73.E-02	1.99.E-02	0.676	0.942	0.858	0.775	0.952	0.842	0.108	3.40.E-02	1.90.E-02	2.40.E-02	2.70.E-02	2.73.E-02	2.11.E-02	3.84.E-02	2.58.E-02	3.06.E-02	0.793	1.436	0.879	1.130	1.357	1.272	0.244
Ethyl-malonic acid	LC/MS_Anion	7.94.E-02	9.27.E-02	1.79.E-01	9.18.E-02	9.55.E-02	2.09.E-01	9.01.E-02	1.02.E-01	1.79.E-01	1.157	1.029	1.165	1.135	1.104	0.997	0.295	7.18.E-02	9.49.E-02	9.14.E-02	8.49.E-02	8.86.E-02	8.61.E-02	9.28.E-02	9.25.E-02	8.84.E-02	1.183	0.935	0.941	1.292	0.975	0.966	0.658
o-Toluic acid	LC/MS_Anion	1.75.E-03	6.05.E-04	1.84.E-03	N.D.	1.24.E-03	1.83.E-03	1.54.E-03	1.01.E-03	1.42.E-03	N.A.	2.044	0.995	0.883	1.665	0.773	0.849	7.81.E-04	1.45.E-03	N.D.	N.D.	1.56.E-03	1.06.E-03	3.93.E-04	5.25.E-04	1.60.E-03	N.A.	1.072	N.A.	0.503	0.361	N.A.	0.971
2-Hydroxy-phenylacetic acid	LC/MS_Anion	6.61.E-03	5.66.E-03	9.31.E-03	5.37.E-03	8.80.E-03	8.88.E-03	7.34.E-03	6.92.E-03	9.31.E-03	0.812	1.554	0.954	1.110	1.223	0.999	0.811	2.28.E-02	2.02.E-02	2.74.E-02	2.10.E-02	2.49.E-02	2.49.E-02	2.89.E-02	2.54.E-02	2.54.E-02	0.921	1.231	0.908	1.264	1.256	0.927	0.435
3-Hydroxy-3-methyl-glutaric acid	LC/MS_Anion	4.90.E-03	6.36.E-03	7.15.E-03	7.19.E-03	6.16.E-03	7.77.E-03	7.09.E-03	7.03.E-03	6.77.E-03	1.468	0.969	1.087	1.447	1.105	0.947	0.419	1.87.E-02	1.02.E-02	1.07.E-02	9.68.E-03	1.07.E-02	1.04.E-02	1.03.E-02	1.37.E-02	1.53.E-02	0.519	1.046	0.975	0.554	1.347	1.430	0.591
Uric acid	LC/MS_Anion	1.17.E-01	1.32.E-01	9.98.E-02	8.88.E-02	1.35.E-01	1.18.E-01	1.02.E-01	1.80.E-01	1.06.E-01	0.759	1.024	1.182	0.874	1.360	1.062	0.631	3.04.E-01	2.83.E-01	2.77.E-01	2.87.E-01	2.75.E-01	3.32.E-01	3.03.E-01	2.99.E-01	3.30.E-01	0.944	0.971	1.199	0.995	1.057	1.194	0.467
Glucuronic acid	LC/MS_Anion	1.98.E-02	1.43.E-02	1.98.E-02	2.00.E-02	1.95.E-02	2.01.E-02	2.24.E-02	2.00.E-02	1.73.E-02	1.006	1.364	1.010	1.127	1.396	0.873	0.570	1.40.E-02	9.81.E-03	1.43.E-02	1.18.E-02	1.33.E-02	1.46.E-02	9.72.E-03	1.51.E-02	1.02.E-02	0.843	1.357	1.027	0.697	1.541	0.714	0.800

N-Acetyl-neuraminic acid	LC/MS_Anion	7.25.E-03	4.13.E-03	4.81.E-03	4.52.E-03	4.38.E-03	5.37.E-03	4.68.E-03	8.06.E-03	5.99.E-03	0.624	1.060	1.116	0.646	1.953	1.245	0.605	3.17.E-03	2.12.E-03	2.56.E-03	2.25.E-03	2.42.E-03	1.55.E-03	3.99.E-04	2.54.E-03	1.61.E-03	0.709	1.137	0.608	0.126	1.194	0.630	0.376
Pyruvic acid	LC/MS_Anion	2.72.E-02	2.37.E-02	4.27.E-02	2.81.E-02	2.88.E-02	5.54.E-02	4.42.E-02	6.12.E-02	7.53.E-02	1.035	1.213	1.296	1.628	2.578	1.761	0.009	4.47.E-02	4.06.E-02	4.61.E-02	1.49.E-02	1.77.E-02	2.44.E-02	1.12.E-02	1.56.E-02	1.58.E-02	0.334	0.436	0.529	0.250	0.385	0.342	0.000
Oxalic acid	LC/MS_Anion	3.63.E-02	3.19.E-02	3.99.E-02	4.20.E-02	3.31.E-02	4.12.E-02	4.25.E-02	3.94.E-02	3.92.E-02	1.158	1.037	1.034	1.172	1.234	0.983	0.256	4.84.E-02	2.87.E-02	3.43.E-02	2.72.E-02	4.08.E-02	3.83.E-02	4.26.E-02	3.45.E-02	3.93.E-02	0.561	1.423	1.116	0.881	1.201	1.145	0.899
Fumaric acid	LC/MS_Anion	3.21.E-02	3.19.E-02	3.13.E-02	2.95.E-02	3.48.E-02	3.78.E-02	3.50.E-02	3.73.E-02	3.62.E-02	0.919	1.093	1.208	1.090	1.172	1.156	0.200	3.02.E-02	3.52.E-02	3.57.E-02	3.55.E-02	3.59.E-02	2.78.E-02	3.15.E-02	3.33.E-02	3.06.E-02	1.177	1.021	0.779	1.045	0.946	0.858	0.797
3-Hydroxy-3-methyl-butanoic acid (3-Hydroxyisovaleric acid)	LC/MS_Anion	4.09.E-02	5.82.E-02	4.16.E-02	4.25.E-02	6.24.E-02	4.58.E-02	4.05.E-02	6.31.E-02	4.58.E-02	1.039	1.072	1.101	0.990	1.085	1.100	0.091	9.77.E-02	8.42.E-02	1.01.E-01	8.73.E-02	8.51.E-02	8.95.E-02	8.45.E-02	8.50.E-02	9.30.E-02	0.893	1.011	0.888	0.865	1.010	0.923	0.187
4-Methyl-2-oxovaleric acid	LC/MS_Anion	1.31.E-01	1.14.E-01	1.12.E-01	1.23.E-01	1.28.E-01	1.16.E-01	1.42.E-01	1.38.E-01	1.20.E-01	0.939	1.125	1.032	1.085	1.212	1.067	0.115	1.22.E-01	1.47.E-01	1.37.E-01	1.46.E-01	1.36.E-01	1.38.E-01	1.59.E-01	1.48.E-01	1.46.E-01	1.195	0.927	1.003	1.299	1.003	1.060	0.309
2-Hydroxy-isocaproic acid	LC/MS_Anion	4.51.E-02	3.67.E-02	5.31.E-02	3.70.E-02	4.17.E-02	5.15.E-02	3.96.E-02	3.90.E-02	5.02.E-02	0.819	1.135	0.970	0.877	1.062	0.946	0.749	4.87.E-02	5.17.E-02	4.52.E-02	5.02.E-02	4.52.E-02	5.20.E-02	5.50.E-02	4.64.E-02	4.70.E-02	1.030	0.875	1.150	1.130	0.898	1.041	0.959
2-Hydroxy-glutaric acid	LC/MS_Anion	6.21.E-03	8.13.E-03	1.12.E-02	4.24.E-03	1.19.E-02	2.18.E-02	8.94.E-03	1.13.E-02	1.45.E-02	0.682	1.465	1.947	1.440	1.387	1.293	0.419	2.13.E-02	1.26.E-02	2.12.E-02	1.71.E-02	1.92.E-02	1.85.E-02	1.97.E-02	1.84.E-02	2.44.E-02	0.801	1.517	0.874	0.926	1.457	1.151	0.567
4-Hydroxy-phenyl-lactic acid	LC/MS_Anion	8.65.E-03	4.61.E-03	1.26.E-02	5.66.E-03	7.88.E-03	1.01.E-02	6.32.E-03	9.42.E-03	1.12.E-02	0.654	1.712	0.799	0.731	2.045	0.886	0.822	7.30.E-03	1.19.E-02	1.39.E-02	1.39.E-02	8.23.E-03	1.44.E-02	1.21.E-02	1.07.E-02	1.10.E-02	1.905	0.689	1.031	1.657	0.896	0.786	0.890
Isocitric acid	LC/MS_Anion	4.87.E-02	4.22.E-02	4.91.E-02	3.82.E-02	4.00.E-02	4.56.E-02	4.91.E-02	5.34.E-02	5.46.E-02	0.784	0.947	0.929	1.008	1.265	1.113	0.027	7.80.E-02	7.19.E-02	8.36.E-02	6.49.E-02	7.63.E-02	7.51.E-02	8.59.E-02	8.03.E-02	7.65.E-02	0.831	1.061	0.898	1.101	1.116	0.914	0.367
Phosphoric acid	LC/MS_Anion	6.81.E-01	5.38.E-01	5.76.E-01	6.50.E-01	5.67.E-01	5.28.E-01	6.54.E-01	5.75.E-01	5.22.E-01	0.953	1.055	0.916	0.960	1.070	0.905	0.703	4.25.E-01	5.40.E-01	4.72.E-01	5.09.E-01	4.38.E-01	4.68.E-01	5.02.E-01	5.68.E-01	5.31.E-01	1.196	0.811	0.991	1.180	1.052	1.124	0.328
Malic acid	LC/MS_Anion	9.29.E-02	4.60.E-02	6.91.E-02	3.87.E-02	6.18.E-02	1.41.E-01	6.03.E-02	9.52.E-02	6.64.E-02	0.416	1.342	2.033	0.649	2.067	0.961	0.943	8.80.E-02	7.68.E-02	9.23.E-02	7.89.E-02	8.44.E-02	8.40.E-02	1.23.E-01	7.71.E-02	1.23.E-01	0.896	1.100	0.910	1.400	1.004	1.331	0.180
β-Phenyl-lactic acid	LC/MS_Anion	8.21.E-03	9.75.E-03	1.39.E-02	7.53.E-03	8.34.E-03	8.64.E-03	6.95.E-03	6.57.E-03	8.38.E-03	0.918	0.855	0.623	0.847	0.673	0.605	0.087	2.14.E-02	1.57.E-02	1.75.E-02	2.16.E-02	1.66.E-02	2.20.E-02	1.61.E-02	1.99.E-02	1.80.E-02	1.011	1.056	1.259	0.751	1.265	1.030	0.655
Hippuric acid	LC/MS_Anion	8.93.E-03	1.46.E-02	5.36.E-03	7.87.E-03	1.49.E-02	5.53.E-03	9.96.E-03	1.66.E-02	8.15.E-03	0.882	1.021	1.031	1.116	1.138	1.520	0.012	5.05.E-02	5.51.E-02	6.32.E-02	5.74.E-02	5.88.E-02	5.54.E-02	5.57.E-02	5.50.E-02	5.73.E-02	1.137	1.068	0.876	1.103	0.999	0.907	0.930
Citric acid	LC/MS_Anion	2.59.E+00	2.35.E+00	2.59.E+00	2.37.E+00	1.88.E+00	2.01.E+00	3.16.E+00	2.27.E+00	2.53.E+00	0.915	0.799	0.777	1.224	0.966	0.976	0.047	6.84.E+00	6.60.E+00	7.11.E+00	4.96.E+00	6.98.E+00	6.29.E+00	7.24.E+00	6.04.E+00	7.69.E+00	0.725	1.059	0.885	1.059	0.915	1.082	0.453
2-Hydroxy-hippuric acid	LC/MS_Anion	2.91.E-03	2.87.E-03	4.58.E-03	1.21.E-03	1.12.E-03	5.17.E-03	1.61.E-03	1.50.E-03	2.15.E-03	0.416	0.390	1.130	0.552	0.524	0.470	0.232	2.29.E-03	3.42.E-03	3.35.E-03	N.D.	1.49.E-03	2.46.E-03	9.42.E-04	2.17.E-03	3.89.E-03	N.A.	0.437	0.732	0.411	0.635	1.160	0.048
3-Hydroxy-propionic acid	LC/MS_Anion	4.75.E-03	4.24.E-03	4.79.E-03	4.91.E-03	3.98.E-03	4.85.E-03	5.77.E-03	5.52.E-03	5.64.E-03	1.033	0.940	1.013	1.214	1.303	1.178	0.005	5.21.E-03	3.57.E-03	3.69.E-03	4.72.E-03	2.54.E-03	3.09.E-03	3.69.E-03	3.56.E-03	3.09.E-03	0.905	0.710	0.837	0.709	0.995	0.838	0.280
3-Hydroxy-isobutyric acid	LC/MS_Anion	7.12.E-02	8.37.E-02	6.93.E-02	6.69.E-02	8.01.E-02	7.42.E-02	6.92.E-02	8.67.E-02	6.23.E-02	0.939	0.956	1.071	0.972	1.035	0.899	0.885	1.30.E-01	1.26.E-01	1.30.E-01	1.39.E-01	1.32.E-01	1.34.E-01	1.22.E-01	1.34.E-01	1.51.E-01	1.067	1.047	1.037	0.938	1.065	1.166	0.610
Glyceric acid	LC/MS_Anion	8.67.E-02	7.96.E-02	8.01.E-02	9.15.E-02	7.69.E-02	9.31.E-02	9.08.E-02	8.97.E-02	9.09.E-02	1.055	0.967	1.163	1.047	1.128	1.135	0.225	5.29.E-02	4.99.E-02	5.39.E-02	5.71.E-02	6.43.E-02	5.19.E-02	5.40.E-02	6.18.E-02	6.31.E-02	1.080	1.288	0.962	1.022	1.238	1.170	0.306
Succinic acid	LC/MS_Anion	2.51.E-01	2.02.E-01	2.55.E-01	2.54.E-01	2.31.E-01	3.11.E-01	2.93.E-01	2.44.E-01	2.57.E-01	1.013	1.144	1.222	1.170	1.208	1.009	0.337	3.45.E-01	3.38.E-01	3.34.E-01	3.43.E-01	3.30.E-01	3.23.E-01	3.79.E-01	3.43.E-01	3.71.E-01	0.996	0.977	0.967	1.099	1.015	1.113	0.041
2-Hydroxy-3-methyl-butyric acid (2-Hydroxyisovaleric acid)	LC/MS_Anion	2.70.E-01	3.26.E-01	4.27.E-01	2.53.E-01	3.77.E-01	4.80.E-01	2.71.E-01	3.87.E-01	4.12.E-01	0.934	1.158	1.122	1.001	1.188	0.963	0.562	3.89.E-01	3.97.E-01	4.09.E-01	4.45.E-01	3.91.E-01	4.19.E-01	4.11.E-01	4.02.E-01	4.24.E-01	1.143	0.985	1.025	1.056	1.013	1.037	0.409
Glutaric acid	LC/MS_Anion	2.29.E-02	3.28.E-02	2.18.E-02	2.73.E-02	3.33.E-02	2.86.E-02	2.24.E-02	3.85.E-02	2.75.E-02	1.191	1.015	1.312	0.978	1.172	1.264	0.285	4.83.E-02	4.83.E-02	4.77.E-02	6.13.E-02	5.10.E-02	4.91.E-02	4.69.E-02	5.40.E-02	5.91.E-02	1.268	1.057	1.029	0.969	1.120	1.237	0.528
Threonic acid	LC/MS_Anion	7.84.E-01	6.63.E-01	8.88.E-01	7.69.E-01	6.97.E-01	9.95.E-01	8.37.E-01	7.60.E-01	9.05.E-01	0.981	1.052	1.121	1.067	1.147	1.020	0.406	8.29.E-01	8.54.E-01	8.79.E-01	1.05.E+00	8.87.E-01	8.58.E-01	9.01.E-01	9.16.E-01	8.28.E-01	1.269	1.038	0.977	1.087	1.072	0.943	0.456
Acetyl-salicylic acid	LC/MS_Anion	8.43.E-03	1.50.E-02	2.18.E-02	7.62.E-03	1.73.E-02	2.91.E-02	1.16.E-02	1.67.E-02	2.47.E-02	0.904	1.154	1.339	1.381	1.111	1.134	0.366	1.40.E-02	1.35.E-02	1.57.E-02	1.94.E-02	1.34.E-02	1.49.E-02	1.60.E-02	1.42.E-02	1.41.E-02	1.386	0.992	0.950	1.145	1.055	0.897	0.607
2-Ketoglutaric acid	LC/MS_Anion	1.12.E-01	1.02.E-01	1.40.E-01	1.16.E-01	9.84.E-02	1.44.E-01	1.29.E-01	1.09.E-01	1.42.E-01	1.029	0.967	1.031	1.146	1.074	1.016	0.164	1.03.E-01	9.81.E-02	9.84.E-02	9.92.E-02	1.17.E-01	1.17.E-01	1.07.E-01	9.97.E-02	1.05.E-01	0.965	1.196	1.184	1.042	1.017	1.062	0.298
cis-Aconitic acid	LC/MS_Anion	2.26.E-01	1.84.E-01	2.37.E-01	2.32.E-01	2.30.E-01	2.99.E-01	2.91.E-01	2.70.E-01	2.75.E-01	1.024	1.253	1.258	1.285	1.468	1.157	0.073	2.92.E-01	3.05.E-01	3.25.E-01	2.90.E-01	3.22.E-01	3.23.E-01	3.37.E-01	3.33.E-01	3.15.E-01	0.996	1.057	0.994	1.156	1.091	0.969	0.366
Quinic acid	LC/MS_Anion	6.70.E-03	3.51.E-02	2.84.E-03	1.95.E-03	4.45.E-02	1.81.E-03	2.81.E-03	4.86.E-02	1.40.E-03	0.292	1.268	0.635	0.420	1.386	0.491	0.806	4.06.E-02	2.72.E-02	3.90.E-02	3.89.E-02	4.48.E-02	3.87.E-02	3.96.E-02	3.46.E-02	4.00.E-02	0.958	1.646	0.992	0.974	1.270	1.024	0.555
Gluconic acid	LC/MS_Anion	7.95.E-02	7.08.E-02	6.18.E-02	8.57.E-02	7.89.E-02	8.85.E-02	8.49.E-02	8.65.E-02	6.86.E-02	1.077	1.113	1.431	1.068	1.222	1.109	0.205	9.73.E-02	8.37.E-02	8.82.E-02	9.78.E-02	8.84.E-02	1.02.E-01	1.03.E-01	1.09.E-01	9.25.E-02	1.006	1.056	1.160	1.056	1.303	1.049	0.330
LPC 14:0 (sn-1)	LC/MS_Lipid	4.26.E-02	1.12.E-01	1.16.E-01	5.56.E-02	1.07.E-01	1.07.E-01	6.45.E-02	1.14.E-01	1.17.E-01	1.304	0.955	0.922	1.514	1.017	1.007	0.323	1.83.E-01	1.69.E-01	1.79.E-01	1.73.E-01	1.68.E-01	1.71.E-01	1.55.E-01	1.65.E-01	1.77.E-01	0.944	0.995	0.954	0.849	0.973	0.991	0.322
LPC 14:0 (sn-2)	LC/MS_Lipid	1.19.E-01	2.81.E-01	2.81.E-01	1.53.E-01	2.67.E-01	2.85.E-01	1.58.E-01	2.62.E-01	3.05.E-01	1.287	0.951	1.012	1.330	0.934	1.085	0.591	3.75.E-01	3.62.E-01	3.60.E-01	3.54.E-01	3.73.E-01	3.47.E-01	3.57.E-01	3.52.E-01	3.78.E-01	0.944	1.030	0.962	0.953	0.972	1.050	0.813
LPC 16:0p	LC/MS_Lipid	2.38.E-02	1.74.E-02	2.72.E-02	2.70.E-02	1.79.E-02	3.14.E-02	2.80.E-02	2.16.E-02	3.53.E-02	1.134	1.031	1.152	1.175	1.241	1.298	0.021	1.18.E-02	1.23.E-02	1.11.E-02	1.07.E-02	1.13.E-02	1.25.E-02	1.04.E-02	1.18.E-02	1.36.E-02	0.908	0.914	1.118	0.883	0.956	1.223	0.864
LPC 15:0 (sn-1)	LC/MS_Lipid	4.74.E-02	6.07.E-02	5.03.E-02	6.00.E-02	6.77.E-02	4.58.E-02	6.26.E-02	6.09.E-02	4.82.E-02	1.265	1.115	0.911	1.321	1.003	0.958	0.548	7.68.E-02	7.49.E-02	6.00.E-02	7.97.E-02	6.87.E-02	6.56.E-02	6.54.E-02	6.86.E-02	8.18.E-02	1.037	0.917	1.093	0.851	0.916	1.363	0.986
LPC 15:0 (sn-2)	LC/MS_Lipid	1.03.E-01	1.31.E-01	9.69.E-02	1.18.E-01	1.23.E-01	9.28.E-02	1.25.E-01	1.27.E-01	1.04.E-01	1.148	0.942	0.958	1.215	0.972	1.078	0.391	1.27.E-01	1.23.E-01	1.28.E-01	1.24.E-01	1.18.E-01	1.17.E-01	1.17.E-01	1.21.E-01	1.43.E-01	0.971	0.954	0.914	0.919	0.981	1.115	0.555
LPC 16:0e	LC/MS_Lipid	2.32.E-02	1.65.E-02	1.90.E-02	2.12.E-02	1.39.E-02	2.58.E-02	2.75.E-02	2.22.E-02	2.21.E-02	0.914	0.841	1.358	1.185	1.344	1.162	0.350	1.10.E-02	1.09.E-02	1.30.E-02	1.20.E-02	1.43.E-02	9.61.E-03	1.01.E-02	1.10.E-02	1.23.E-02	1.095	1.306	0.742	0.917	1.010	0.950	0.869
LPC 16:1 (sn-1)	LC/MS_Lipid	1.22.E-01	2.11.E-01	3.55.E-01	1.61.E-01	2.20.E-01	3.16.E-01	1.62.E-01	2.04.E-01	3.64.E-01	1.318	1.039	0.891	1.324	0.967	1.028	0.746	2.55.E-01	2.64.E-01	2.60.E-01	2.56.E-01	2.51.E-01	2.41.E-01	2.34.E-01	2.41.E-01	2.59.E-01	1.001	0.951	0.926	0.916	0.912	0.996	0.301
LPC 16:1 (sn-2)	LC/MS_Lipid	3.61.E-01	5.16.E-01	8.79.E-01	4.32.E-01	5.45.E-01	8.98.E-01	4.32.E-01	5.17.E-01	9.30.E-01	1.197	1.056	1.021	1.198	1.001	1.058	0.147	5.30.E-01	5.28.E-01	5.14.E-01	5.52.E-01	5.09.E-01	5.05.E-01	5.09.E-01	5.15.E-01	5.71.E-01	1.040	0.963	0.983	0.960	0.976	1.111	0.912
LPC 16:0 (sn-1)	LC/MS_Lipid	8.66.E+00	1.22.E+01	1.43.E+01	1.10.E+01	1.27.E+01	1.36.E+01	1.11.E+01	1.18.E+01	1.51.E+01	1.272	1.039	0.952	1.282	0.965	1.058	0.531	8.40.E+00	9.45.E+00	8.51.E+00	8.90.E+00	8.55.E+00	8.10.E+00	8.10.E+00	8.58.E+00	9.03.E+00	1.060	0.905	0.952	0.964	0.908	1.061	0.818
LPC 16:0 (sn-2)	LC/MS_Lipid	1.93.E+01	2.47.E+01	2.85.E+01	2.24.E+01	2.60.E+01	2.93.E+01	2.29.E+01	2.50.E+01	3.06.E+01	1.158	1.053	1.028	1.188	1.010	1.072	0.124	1.89.E+01	1.91.E+01	1.85.E+01	1.86.E+01	1.85.E+01	1.78.E+01	1.79.E+01	1.86.E+01	1.94.E+01	0.986	0.965	0.963	0.950	0.970	1.053	0.625
LPC 17:1 (sn-1)	LC/MS_Lipid	2.02.E-02	2.34.E-02	3.22.E-02	2.33.E-02	2.63.E-02	3.12.E-02	2.39.E-02	1.93.E-02	3.25.E-02	1.154	1.125	0.970	1.181	0.825	1.010	0.685	2.18.E-02	2.40.E-02	2.05.E-02	2.33.E-02	2.01.E-02	2.05.E-02	2.02.E-02	2.16.E-02	2.04.E-02	1.069	0.839	0.996	0.923	0.901	0.992	0.585
LPC 17:1 (sn-2)	LC/MS_Lipid	4.74.E-02	4.99.E-02	7.33.E-02	4.52.E-02	5.26.E-02	8.02.E-02	5.05.E-02	5.05.E-02	7.85.E-02	0.954	1.055	1.094	1.066	1.013	1.072	0.420	4.46.E-02	4.31.E-02	5.07.E-02	4.16.E-02	4.50.E-02	4.36.E-02	4.19.E-02	4.17.E-02	4.76.E-02	0.933	1.045	0.860	0.940	0.968	0.938	0.403
LPC 17:0 (sn-1)	LC/MS_Lipid	2.25.E-01	1.55.E-01	1.60.E-01	2.34.E-01	2.08.E-01	1.85.E-01	2.22.E-01	2.05.E-01	1.72.E-01	1.037	1.336	1.154	0.987	1.318	1.074	0.157	1.08.E-01	8.81.E-02	7.08.E-02	8.26.E-02	7.84.E-02	6.11.E-02	6.08.E-02	6.20.E-02	8.31.E-02	0.768	0.889	0.863	0.565	0.703	1.174	0.374
LPC 17:0 (sn-2)	LC/MS_Lipid	2.45.E-01	2.05.E-01	2.08.E-01	2.79.E-01	2.06.E-01	2.19.E-01	3.05.E-01	2.35.E-01	2.20.E-01	1.139	1.005	1.056	1.243	1.147	1.061	0.085	1.30.E-01	1.37.E-01	1.25.E-01	1.26.E-01	1.17.E-01	1.25.E-01	1.22.E-01	1.30.E-01	1.40.E-01	0.966	0.853	0.995	0.937	0.950	1.120	0.419
LPC 18:3 (sn-1)	LC/MS_Lipid	2.46.E-02	4.36.E-02	9.76.E-02	3.30.E-02	3.94.E-02	9.72.E-02	3.07.E-02	3.75.E-02	9.86.E-02	1.340	0.905	0.995	1.250	0.862	1.010	0.917	4.99.E-02	5.84.E-02	5.58.E-02	5.59.E-02	4.76.E-02	4.96.E-02	4.59.E-02	5.06.E-02	4.97.E-02	1.121	0.815	0.889	0.919	0.866	0.891	0.367
LPC 18:3 (sn-2)	LC/MS_Lipid	3.77.E-02	5.30.E-02	1.64.E-01	4.71.E-02	5.26.E-02	1.42.E-01	4.39.E-02	5.42.E-02	1.51.E-01	1.248	0.991	0.868	1.163	1.021	0.922	0.817	5.45.E-02	5.73.E-02	5.61.E-02	6.28.E-02	4.90.E-02	5.15.E-02	5.57.E-02	4.84.E-02	5.53.E-02	1.152	0.856	0.918	1.022	0.845	0.986	0.779
LPC 18:2 (sn-1)	LC/MS_Lipid	4.69.E+00	5.60.E+00	8.10.E+00	6.13.E+00	5.43.E+00	7.21.E+00	5.54.E+00	4.79.E+00	7.66.E+00	1.305	0.969	0.890	1.182	0.856	0.946	0.894	4.55.E+00	5.31.E+00	4.65.E+00	4.96.E+00	4.66.E+00	4.43.E+00	4.25.E+00	4.67.E+00	4.79.E+00	1.091	0.877	0.953	0.934	0.878	1.030	0.668
LPC 18:2 (sn-2)	LC/MS_Lipid	7.81.E+00	8.10.E+00	1.31.E+01	9.19.E+00	8.07.E+00	1.28.E+01	8.59.E+00	7.64.E+00	1.29.E+01	1.177	0.996	0.980	1.100	0.943	0.984	0.619	7.26.E+00	7.70.E+00	7.26.E+00	7.28.E+00	7.27.E+00	6.85.E+00	6.97.E+00	7.14.E+00	7.69.E+00	1.003	0.945	0.943	0.960	0.928	1.059	0.655
LPC 18:1 (sn-1)	LC/MS_Lipid	2.49.E+00	2.57.E+00	4.56.E+00	2.77.E+00	2.62.E+00	4.57.E+00	2.69.E+00	2.71.E+00	4.32.E+00	1.115	1.021	1.003	1.082	1.057	0.948	0.591	2.51.E+00	2.92.E+00	2.53.E+00	2.69.E+00	2.54.E+00	2.51.E+00	2.27.E+00	2.50.E+00	2.72.E+00	1.073	0.872	0.992	0.903	0.858	1.074	0.696
LPC 18:1 (sn-2)	LC/MS_Lipid	4.70.E+00	4.67.E+00	8.95.E+00	5.12.E+00	4.67.E+00	9.83.E+00	5.39.E+00	5.20.E+00	9.01.E+00	1.090	1.001	1.098	1.146	1.114	1.007	0.351	4.26.E+00	4.56.E+00	4.16.E+00	4.13.E+00	4.15.E+00	4.19.E+00	4.02.E+00	4.22.E+00	4.47.E+00	0.969	0.910	1.006	0.942	0.926	1.074	0.573
LPC 18:0 (sn-1)	LC/MS_Lipid	3.47.E+00	3.13.E+00	4.06.E+00	4.12.E+00	3.28.E+00	4.12.E+00	4.17.E+00	3.50.E+00	4.09.E+00	1.188	1.046	1.015	1.202	1.118	1.007	0.169	2.11.E+00	2.47.E+00	2.09.E+00	2.27.E+00	2.15.E+00	2.12.E+00	1.97.E+00	2.14.E+00	2.29.E+00	1.075	0.873	1.016	0.931	0.867	1.095	0.824
LPC 18:0 (sn-2)	LC/MS_Lipid	7.17.E+00	6.51.E+00	8.15.E+00	8.09.E+00	6.72.E+00	8.76.E+00	8.60.E+00	7.24.E+00	8.32.E+00	1.128	1.033	1.075	1.199	1.113	1.020	0.132	4.35.E+00	4.72.E+00	4.27.E+00	4.37.E+00	4.33.E+00	4.34.E+00	4.20.E+00	4.36.E+00	4.55.E+00	1.004	0.918	1.015	0.964	0.925	1.064	0.785
LPC 19:0 (sn-1)	LC/MS_Lipid	1.46.E-02	1.65.E-02	2.13.E-02	1.96.E-02	1.90.E-02	1.49.E-02	1.83.E-02	1.76.E-02	2.00.E-02	1.339	1.151	0.697	1.250	1.069	0.935	0.899	7.75.E-03	1.00.E-02	7.81.E-03	1.49.E-02	1.11.E-02	1.11.E-02	9.79.E-03	1.15.E-02	6.65.E-03	1.923	1.102	1.418	1.263	1.141	0.851	0.137
LPC 19:0 (sn-2)	LC/MS_Lipid	2.19.E-02	1.99.E-02	2.52.E-02	2.61.E-02	1.69.E-02	2.38.E-02	2.82.E-02	2.02.E-02	2.37.E-02	1.192	0.848	0.944	1.288	1.016	0.941	0.618	1.29.E-02	1.59.E-02	1.28.E-02	1.45.E-02	1.38.E-02	1.57.E-02	1.36.E-02	1.40.E-02	1.50.E-02	1.119	0.866	1.223	1.055	0.876	1.171	0.807
LPC 20:5 (sn-1)	LC/MS_Lipid	6.14.E-02	1.88.E-01	2.01.E-01	7.58.E-02	1.82.E-01	1.51.E-01	7.11.E-02	1.41.E-01	1.76.E-01	1.234	0.966	0.751	1.158	0.748	0.874	0.554	1.46.E-01	1.69.E-01	1.47.E-01	1.71.E-01	1.49.E-01	1.46.E-01	1.39.E-01	1.41.E-01	1.60.E-01	1.169	0.885	0.994	0.952	0.838	1.086	0.769
LPC 20:5 (sn-2)	LC/MS_Lipid	7.31.E-02	2.22.E-01	3.02.E-01	9.91.E-02	2.31.E-01	2.66.E-01	8.61.E-02	2.16.E-01	2.73.E-01	1.356	1.043	0.878	1.178	0.972	0.901	0.828	1.90.E-01	1.96.E-01	1.93.E-01	1.93.E-01	1.92.E-01	1.76.E-01	1.92.E-01	1.82.E-01	2.06.E-01	1.014	0.976	0.912	1.008	0.927	1.065	0.730
LPC 20:4 (sn-1)	LC/MS_Lipid	6.30.E-01	1.07.E+00	1.29.E+00	8.39.E-01	1.08.E+00	1.10.E+00	7.26.E-01	9.46.E-01	1.21.E+00	1.333	1.003	0.854	1.153	0.881	0.942	0.879	9.27.E-01	1.07.E+00	9.01.E-01	9.91.E-01	9.24.E-01	8.84.E-01	8.05.E-01	9.06.E-01	9.23.E-01	1.068	0.867	0.981	0.869	0.850	1.025	0.437
LPC 20:4 (sn-2)	LC/MS_Lipid	8.54.E-01	1.21.E+00	1.67.E+00	1.05.E+00	1.22.E+00	1.60.E+00	9.04.E-01	1.20.E+00	1.58.E+00	1.227	1.011	0.963	1.060	0.994	0.950	0.545	1.05.E+00	1.14.E+00	1.06.E+00	1.06.E+00	1.09.E+00	1.01.E+00	9.87.E-01	1.05.E+00	1.13.E+00	1.016	0.956	0.956	0.944	0.920	1.067	0.812
LPC 20:3 (sn-1)	LC/MS_Lipid	2.29.E-01	2.71.E-01	3.49.E-01	2.77.E-01	2.70.E-01	3.23.E-01	2.55.E-01	2.80.E-01	3.48.E-01	1.207	0.994	0.927	1.114	1.032	0.998	0.772	2.21.E-01	2.67.E-01	2.32.E-01	2.26.E-01	2.13.E-01	2.00.E-01	1.85.E-01	2.17.E-01	2.20.E-01	1.022	0.799	0.860	0.837	0.814	0.949	0.204
LPC 20:3 (sn-2)	LC/MS_Lipid	2.44.E-01	2.71.E-01	4.57.E-01	2.96.E-01	2.94.E-01	4.46.E-01	2.72.E-01	2.85.E-01	4.18.E-01	1.216	1.087	0.975	1.115	1.050	0.915	0.408	2.30.E-01	2.69.E-01	2.30.E-01	2.37.E-01	2.35.E-01	2.28.E-01	2.35.E-01	2.30.E-01	2.49.E-01	1.031	0.876	0.991	1.023	0.856	1.081	0.784
LPC 20:2 (sn-1)	LC/MS_Lipid	3.64.E-02	3.99.E-02	6.10.E-02	4.45.E-02	4.49.E-02	5.57.E-02	3.63.E-02	4.09.E-02	5.48.E-02	1.224	1.125	0.914	0.999	1.026	0.899	0.411	3.44.E-02	4.31.E-02	3.49.E-02	3.22.E-02	3.37.E-02	3.29.E-02	3.19.E-02	3.04.E-02	3.21.E-02	0.936	0.784	0.943	0.929	0.706	0.920	0.146
LPC 20:2 (sn-2)	LC/MS_Lipid	4.71.E-02	4.54.E-02	8.39.E-02	4.98.E-02	4.65.E-02	8.17.E-02	5.25.E-02	4.54.E-02	8.17.E-02	1.058	1.025	0.974	1.114	1.001	0.974	0.823	3.68.E-02	4.23.E-02	3.56.E-02	3.29.E-02	4.07.E-02	3.69.E-02	3.50.E-02	3.81.E-02	4.21.E-02	0.895	0.962	1.036	0.952	0.902	1.182	0.788
LPC 20:1 (sn-1)	LC/MS_Lipid	3.14.E-02	2.79.E-02	5.95.E-02	4.14.E-02	2.76.E-02	5.33.E-02	3.42.E-02	2.68.E-02	5.58.E-02	1.318	0.989	0.895	1.088	0.961	0.937	0.864	2.20.E-02	2.49.E-02	1.79.E-02	2.50.E-02	2.16.E-02	2.02.E-02	1.94.E-02	2.10.E-02	2.04.E-02	1.135	0.869	1.130	0.881	0.844	1.138	0.598
LPC 20:1 (sn-2)	LC/MS_Lipid	5.40.E-02	4.73.E-02	1.13.E-01	6.73.E-02	4.87.E-02	1.05.E-01	6.74.E-02	4.92.E-02	1.10.E-01	1.246	1.029	0.926	1.247	1.040	0.971	0.721	3.02.E-02	3.45.E-02	2.99.E-02	3.31.E-02	3.51.E-02	3.32.E-02	3.31.E-02	3.49.E-02	3.64.E-02	1.098	1.017	1.112	1.097	1.011	1.219	0.144
LPC 20:0 (sn-1)	LC/MS_Lipid	1.89.E-02	1.76.E-02	3.00.E-02	2.74.E-02	1.51.E-02	2.42.E-02	2.89.E-02	1.49.E-02	2.95.E-02	1.451	0.854	0.807	1.529	0.843	0.983	0.778	1.13.E-02	1.59.E-02	1.14.E-02	1.22.E-02	1.04.E-02	7.97.E-03	1.01.E-02	1.04.E-02	1.16.E-02	1.080	0.658	0.702	0.898	0.658	1.023	0.374
LPC 20:0 (sn-2)	LC/MS_Lipid	4.26.E-02	3.40.E-02	5.02.E-02	4.27.E-02	2.90.E-02	4.82.E-02	4.77.E-02	2.93.E-02	4.73.E-02	1.002	0.852	0.961	1.119	0.861	0.942	0.611	2.18.E-02	2.04.E-02	2.01.E-02	2.12.E-02	2.04.E-02	2.13.E-02	2.21.E-02	2.23.E-02	2.11.E-02	0.974	0.999	1.062	1.014	1.091	1.049	0.233
LPC 22:6 (sn-1)	LC/MS_Lipid	2.30.E-01	4.30.E-01	5.08.E-01	3.11.E-01	4.10.E-01	4.09.E-01	2.69.E-01	3.43.E-01	4.62.E-01	1.353	0.955	0.805	1.172	0.797	0.910	0.776	3.77.E-01	4.35.E-01	3.67.E-01	4.00.E-01	3.69.E-01	3.47.E-01	3.32.E-01	3.66.E-01	3.60.E-01	1.060	0.849	0.945	0.879	0.841	0.980	0.314
LPC 22:6 (sn-2)	LC/MS_Lipid	2.61.E-01	4.23.E-01	5.83.E-01	3.45.E-01	4.21.E-01	5.52.E-01	2.87.E-01	3.89.E-01	5.47.E-01	1.320	0.994	0.948	1.100	0.919	0.939	0.504	3.59.E-01	3.95.E-01	3.50.E-01	3.65.E-01	3.66.E-01	3.39.E-01	3.29.E-01	3.61.E-01	3.89.E-01	1.015	0.928	0.969	0.916	0.914	1.111	0.855
LPC 22:4 (sn-1)	LC/MS_Lipid	9.76.E-03	1.93.E-02	2.23.E-02	1.66.E-02	1.90.E-02	1.67.E-02	1.39.E-02	1.59.E-02	2.02.E-02	1.704	0.985	0.750	1.428	0.822	0.908	0.962	1.45.E-02	1.47.E-02	1.65.E-02	1.62.E-02	1.68.E-02	1.52.E-02	1.49.E-02	1.23.E-02	1.46.E-02	1.116	1.141	0.919	1.028	0.836	0.881	0.243
LPC 22:4 (sn-2)	LC/MS_Lipid	1.09.E-02	1.49.E-02	2.17.E-02	1.29.E-02	1.42.E-02	2.02.E-02	1.30.E-02	1.46.E-02	1.96.E-02	1.181	0.956	0.927	1.184	0.980	0.901	0.988	8.03.E-03	1.04.E-02	9.28.E-03	1.11.E-02	1.01.E-02	8.64.E-03	9.97.E-03	9.97.E-03	9.89.E-03	1.384	0.971	0.931	1.241	0.963	1.065	0.673
LPC 22:0 (sn-1)	LC/MS_Lipid	5.75.E-03	4.40.E-03	5.38.E-03	7.20.E-03	4.94.E-03	5.07.E-03	6.88.E-03	3.27.E-03	7.51.E-03	1.252	1.124	0.943	1.196	0.743	1.396	0.745	4.23.E-03	4.91.E-03	3.63.E-03	6.16.E-03	3.49.E-03	2.21.E-03	4.14.E-03	4.20.E-03	4.52.E-03	1.458	0.711	0.610	0.980	0.856	1.246	0.938
LPC 22:0 (sn-2)	LC/MS_Lipid	9.19.E-03	7.88.E-03	1.30.E-02	8.98.E-03	6.49.E-03	1.16.E-02	1.10.E-02	7.10.E-03	1.08.E-02	0.977	0.824	0.887	1.201	0.901	0.829	0.542	7.22.E-03	8.25.E-03	6.61.E-03	5.49.E-03	6.37.E-03	5.40.E-03	7.59.E-03	6.64.E-03	7.60.E-03	0.761	0.773	0.818	1.051	0.805	1.151	0.091
PC 14:0-16:1	LC/MS_Lipid	3.49.E+01	3.01.E+01	3.04.E+01	3.60.E+01	3.02.E+01	3.19.E+01	3.48.E+01	3.12.E+01	2.85.E+01	1.032	1.001	1.046	0.998	1.035	0.937	0.486	3.12.E+01	2.90.E+01	3.06.E+01	3.09.E+01	3.16.E+01	2.89.E+01	2.99.E+01	2.97.E+01	3.02.E+01	0.990	1.089	0.944	0.959	1.024	0.987	0.870
PC 16:0-14:0	LC/MS_Lipid	1.94.E+00	2.96.E+00	3.25.E+00	2.10.E+00	2.93.E+00	3.24.E+00	2.06.E+00	2.71.E+00	3.11.E+00	1.083	0.989	0.997	1.062	0.916	0.958	0.344	5.45.E+00	5.44.E+00	5.44.E+00	5.84.E+00	5.33.E+00	4.96.E+00	5.59.E+00	5.68.E+00	5.33.E+00	1.072	0.980	0.912	1.026	1.045	0.980	0.741
PC 15:0-16:1	LC/MS_Lipid	7.19.E-02	1.33.E-01	1.18.E-01	9.33.E-02	1.22.E-01	1.10.E-01	8.82.E-02	1.03.E-01	1.19.E-01	1.299	0.922	0.930	1.227	0.775	1.009	0.887	3.01.E-01	3.11.E-01	2.92.E-01	3.45.E-01	2.94.E-01	2.69.E-01	3.04.E-01	3.18.E-01	2.88.E-01	1.146	0.946	0.920	1.010	1.021	0.987	0.994
PC 16:0p-16:0	LC/MS_Lipid	8.04.E-01	6.62.E-01	8.16.E-01	9.44.E-01	6.60.E-01	7.92.E-01	9.26.E-01	6.05.E-01	7.54.E-01	1.175	0.997	0.970	1.152	0.913	0.924	0.675	7.63.E-01	7.29.E-01	7.46.E-01	7.60.E-01	7.26.E-01	6.97.E-01	7.31.E-01	7.40.E-01	7.27.E-01	0.996	0.996	0.934	0.958	1.014	0.974	0.518
PC 16:0-15:0	LC/MS_Lipid	2.25.E-01	3.27.E-01	1.68.E-01	2.76.E-01	3.41.E-01	1.35.E-01	2.60.E-01	2.91.E-01	1.63.E-01	1.225	1.041	0.803	1.151	0.888	0.970	0.839	8.25.E-01	8.18.E-01	8.52.E-01	9.19.E-01	7.96.E-01	7.34.E-01	9.54.E-01	9.13.E-01	8.16.E-01	1.114	0.973	0.861	1.157	1.117	0.957	0.327
PC 16:0e-16:0	LC/MS_Lipid	1.60.E+00	1.42.E+00	1.85.E+00	1.84.E+00	1.43.E+00	1.84.E+00	1.75.E+00	1.29.E+00	1.75.E+00	1.154	1.006	0.994	1.100	0.909	0.944	0.397	2.02.E+00	1.88.E+00	2.02.E+00	2.06.E+00	1.96.E+00	1.91.E+00	1.98.E+00	1.96.E+00	1.99.E+00	1.021	1.040	0.948	0.978	1.041	0.986	0.995
PC 14:0-18:2/16:1-16:1	LC/MS_Lipid	2.87.E+00	4.92.E+00	5.07.E+00	3.54.E+00	4.73.E+00	4.45.E+00	3.49.E+00	3.92.E+00	4.94.E+00	1.236	0.961	0.878	1.217	0.798	0.975	0.918	7.02.E+00	7.88.E+00	7.37.E+00	7.87.E+00	6.76.E+00	6.76.E+00	7.28.E+00	7.73.E+00	7.01.E+00	1.121	0.859	0.917	1.037	0.982	0.951	0.802
PC 14-0:18-1/16:0-16:1	LC/MS_Lipid	1.03.E+01	1.94.E+01	2.57.E+01	1.20.E+01	1.97.E+01	2.29.E+01	1.20.E+01	1.68.E+01	2.40.E+01	1.167	1.017	0.892	1.172	0.868	0.937	0.821	3.34.E+01	3.19.E+01	3.32.E+01	3.46.E+01	3.30.E+01	3.01.E+01	3.49.E+01	3.34.E+01	3.35.E+01	1.036	1.037	0.908	1.046	1.049	1.010	0.439
PC 16:0-16:0	LC/MS_Lipid	7.18.E+00	1.02.E+01	1.05.E+01	8.81.E+00	9.45.E+00	1.06.E+01	8.82.E+00	9.03.E+00	1.03.E+01	1.227	0.926	1.015	1.228	0.885	0.984	0.858	1.26.E+01	1.23.E+01	1.29.E+01	1.36.E+01	1.24.E+01	1.15.E+01	1.32.E+01	1.33.E+01	1.25.E+01	1.081	1.002	0.892	1.048	1.077	0.974	0.627
PC 15:0-18:2	LC/MS_Lipid	2.26.E+00	2.56.E+00	1.59.E+00	2.83.E+00	2.40.E+00	1.47.E+00	2.74.E+00	2.16.E+00	1.52.E+00	1.253	0.938	0.927	1.214	0.845	0.956	0.872	3.08.E+00	3.11.E+00	3.24.E+00	3.40.E+00	3.01.E+00	2.80.E+00	3.35.E+00	3.37.E+00	3.03.E+00	1.101	0.969	0.866	1.088	1.082	0.935	0.605
PC 16:0e-18:2	LC/MS_Lipid	4.17.E+00	4.74.E+00	4.27.E+00	5.54.E+00	4.43.E+00	4.13.E+00	5.48.E+00	3.92.E+00	4.16.E+00	1.327	0.935	0.966	1.314	0.828	0.973	0.827	3.97.E+00	3.74.E+00	3.93.E+00	4.11.E+00	3.93.E+00	3.69.E+00	4.01.E+00	3.90.E+00	3.92.E+00	1.035	1.050	0.938	1.010	1.042	0.997	0.842
PC 16:1e-18:1	LC/MS_Lipid	2.16.E+00	2.61.E+00	3.45.E+00	2.85.E+00	2.51.E+00	3.39.E+00	2.82.E+00	2.17.E+00	3.45.E+00	1.325	0.961	0.982	1.307	0.832	1.000	0.781	2.80.E+00	2.61.E+00	2.73.E+00	2.78.E+00	2.72.E+00	2.54.E+00	2.75.E+00	2.83.E+00	2.82.E+00	0.992	1.045	0.930	0.980	1.088	1.030	0.454
PC 15:0-18:1/16:0-17:1	LC/MS_Lipid	8.89.E-01	1.38.E+00	1.06.E+00	1.10.E+00	1.33.E+00	1.10.E+00	1.10.E+00	1.21.E+00	1.07.E+00	1.234	0.965	1.033	1.233	0.879	1.009	0.714	2.31.E+00	2.19.E+00	2.30.E+00	2.42.E+00	2.24.E+00	2.17.E+00	2.38.E+00	2.36.E+00	2.26.E+00	1.046	1.022	0.942	1.029	1.080	0.981	0.561
PC 18:1e-16:0/18:0e-16:1	LC/MS_Lipid	6.96.E+00	7.48.E+00	9.14.E+00	9.14.E+00	7.18.E+00	8.68.E+00	9.13.E+00	6.11.E+00	9.20.E+00	1.312	0.959	0.949	1.312	0.816	1.007	0.852	7.84.E+00	7.21.E+00	7.75.E+00	8.04.E+00	7.58.E+00	7.18.E+00	7.81.E+00	7.73.E+00	7.88.E+00	1.026	1.051	0.927	0.996	1.072	1.018	0.651
PC 17:0-16:0/18:0-15:0	LC/MS_Lipid	6.32.E-01	7.08.E-01	8.18.E-01	8.20.E-01	6.99.E-01	7.88.E-01	8.42.E-01	5.91.E-01	8.11.E-01	1.298	0.988	0.963	1.332	0.835	0.991	0.801	7.06.E-01	6.67.E-01	6.85.E-01	7.56.E-01	6.51.E-01	6.34.E-01	7.06.E-01	7.00.E-01	7.05.E-01	1.072	0.977	0.926	1.001	1.050	1.030	0.708
PC 18:0e-16:0	LC/MS_Lipid	7.54.E-01	5.78.E-01	5.10.E-01	8.75.E-01	5.95.E-01	4.78.E-01	9.01.E-01	4.71.E-01	5.02.E-01	1.160	1.030	0.938	1.195	0.815	0.985	0.827	6.02.E-01	5.61.E-01	5.93.E-01	5.71.E-01	5.72.E-01	5.39.E-01	5.77.E-01	6.19.E-01	6.16.E-01	0.948	1.021	0.909	0.959	1.104	1.038	0.242
PC 14:0-20:5	LC/MS_Lipid	7.60.E-02	2.91.E-01	2.71.E-01	8.80.E-02	2.69.E-01	2.37.E-01	8.40.E-02	2.38.E-01	2.90.E-01	1.159	0.923	0.875	1.106	0.816	1.072	0.791	3.16.E-01	3.29.E-01	3.21.E-01	3.49.E-01	3.08.E-01	2.89.E-01	3.20.E-01	3.20.E-01	3.06.E-01	1.104	0.936	0.901	1.012	0.973	0.953	0.875
PC 16:1-18:3/14:0-20:4	LC/MS_Lipid	1.01.E+00	2.32.E+00	2.76.E+00	1.14.E+00	2.42.E+00	2.34.E+00	1.14.E+00	2.04.E+00	2.56.E+00	1.130	1.041	0.847	1.130	0.878	0.929	0.785	2.92.E+00	2.96.E+00	2.84.E+00	2.83.E+00	2.79.E+00	2.74.E+00	2.68.E+00	2.90.E+00	2.94.E+00	0.967	0.942	0.965	0.915	0.978	1.036	0.436
PC 14:0-20:3	LC/MS_Lipid	1.27.E+01	2.16.E+01	2.59.E+01	1.58.E+01	2.03.E+01	2.45.E+01	1.58.E+01	1.81.E+01	2.53.E+01	1.251	0.941	0.945	1.250	0.839	0.978	0.956	1.50.E+01	1.44.E+01	1.56.E+01	1.60.E+01	1.51.E+01	1.40.E+01	1.55.E+01	1.53.E+01	1.51.E+01	1.067	1.047	0.893	1.030	1.064	0.968	0.868
PC 16:1-18:2/16:0-18:3	LC/MS_Lipid	1.27.E+01	2.16.E+01	2.59.E+01	1.58.E+01	2.02.E+01	2.44.E+01	1.58.E+01	1.81.E+01	2.54.E+01	1.248	0.939	0.943	1.244	0.841	0.980	0.963	1.50.E+01	1.44.E+01	1.56.E+01	1.60.E+01	1.51.E+01	1.40.E+01	1.55.E+01	1.53.E+01	1.51.E+01	1.067	1.047	0.893	1.030	1.064	0.968	0.868
PC 16:0-18:2/16:1-18:1	LC/MS_Lipid	1.43.E+02	1.66.E+02	1.55.E+02	1.75.E+02	1.59.E+02	1.50.E+02	1.68.E+02	1.40.E+02	1.54.E+02	1.222	0.960	0.972	1.173	0.845	0.997	0.790	1.18.E+02	1.15.E+02	1.22.E+02	1.28.E+02	1.14.E+02	1.06.E+02	1.25.E+02	1.25.E+02	1.15.E+02	1.089	0.989	0.870	1.058	1.088	0.945	0.662
PC 16:0-18:1	LC/MS_Lipid	1.09.E+02	1.61.E+02	1.52.E+02	1.31.E+02	1.55.E+02	1.54.E+02	1.31.E+02	1.41.E+02	1.49.E+02	1.207	0.962	1.011	1.209	0.878	0.979	0.754	1.24.E+02	1.19.E+02	1.26.E+02	1.31.E+02	1.21.E+02	1.18.E+02	1.27.E+02	1.30.E+02	1.25.E+02	1.060	1.025	0.934	1.023	1.100	0.990	0.574
PC 16:0-18:0	LC/MS_Lipid	4.58.E+00	6.61.E+00	5.13.E+00	5.48.E+00	6.66.E+00	5.09.E+00	5.61.E+00	5.75.E+00	5.03.E+00	1.196	1.008	0.992	1.225	0.870	0.981	0.730	5.65.E+00	5.25.E+00	5.73.E+00	5.85.E+00	5.47.E+00	5.26.E+00	5.57.E+00	5.70.E+00	5.68.E+00	1.035	1.043	0.918	0.987	1.087	0.992	0.804
PC 15:0-20:5	LC/MS_Lipid	9.68.E-02	2.78.E-01	1.59.E-01	1.04.E-01	2.85.E-01	1.49.E-01	9.94.E-02	2.48.E-01	1.57.E-01	1.079	1.025	0.938	1.027	0.891	0.987	0.536	2.63.E-01	2.89.E-01	2.55.E-01	2.84.E-01	2.56.E-01	2.61.E-01	2.61.E-01	2.90.E-01	2.68.E-01	1.078	0.886	1.024	0.990	1.005	1.053	0.898
PC 16:0e-20:5	LC/MS_Lipid	7.64.E+00	7.66.E+00	8.16.E+00	7.40.E+00	8.34.E+00	9.09.E+00	7.47.E+00	8.62.E+00	7.85.E+00	0.969	1.088	1.114	0.978	1.125	0.962	0.577	7.93.E+00	6.76.E+00	7.76.E+00	7.59.E+00	7.67.E+00	7.37.E+00	7.45.E+00	7.01.E+00	8.06.E+00	0.957	1.135	0.949	0.939	1.038	1.038	0.987
PC 16:0p-20:4	LC/MS_Lipid	7.64.E+00	7.66.E+00	8.16.E+00	7.40.E+00	8.34.E+00	9.09.E+00	7.47.E+00	8.62.E+00	7.85.E+00	0.969	1.088	1.114	0.978	1.125	0.962	0.577	7.93.E+00	6.76.E+00	7.76.E+00	7.59.E+00	7.67.E+00	7.37.E+00	7.45.E+00	7.01.E+00	8.06.E+00	0.957	1.135	0.949	0.939	1.038	1.038	0.987
PC 15:0-20:4	LC/MS_Lipid	5.89.E-01	1.05.E+00	6.88.E-01	7.35.E-01	1.04.E+00	6.10.E-01	6.84.E-01	9.62.E-01	6.89.E-01	1.248	0.992	0.886	1.161	0.919	1.001	0.933	9.41.E-01	9.70.E-01	1.00.E+00	1.05.E+00	9.25.E-01	8.60.E-01	9.85.E-01	1.04.E+00	9.16.E-01	1.116	0.953	0.859	1.046	1.075	0.915	0.831
PC 16:1e-20:3	LC/MS_Lipid	1.09.E+01	1.43.E+01	1.20.E+01	1.28.E+01	1.40.E+01	1.22.E+01	1.32.E+01	1.28.E+01	1.18.E+01	1.181	0.981	1.016	1.214	0.899	0.989	0.744	1.15.E+01	1.05.E+01	1.18.E+01	1.14.E+01	1.13.E+01	1.06.E+01	1.15.E+01	1.13.E+01	1.17.E+01	0.994	1.075	0.900	0.999	1.077	0.989	0.693
PC 17:1-18:2	LC/MS_Lipid	1.45.E+00	1.61.E+00	1.52.E+00	1.75.E+00	1.61.E+00	1.48.E+00	1.79.E+00	1.52.E+00	1.49.E+00	1.210	0.997	0.970	1.238	0.940	0.977	0.706	1.33.E+00	1.30.E+00	1.34.E+00	1.44.E+00	1.29.E+00	1.18.E+00	1.45.E+00	1.41.E+00	1.36.E+00	1.081	0.996	0.876	1.089	1.087	1.012	0.274
PC 18:1e-18:2	LC/MS_Lipid	2.98.E+00	2.56.E+00	2.84.E+00	3.43.E+00	2.58.E+00	2.93.E+00	3.48.E+00	2.40.E+00	2.84.E+00	1.149	1.007	1.033	1.166	0.936	1.002	0.492	2.21.E+00	2.00.E+00	2.21.E+00	2.17.E+00	2.09.E+00	2.07.E+00	2.15.E+00	2.08.E+00	2.17.E+00	0.984	1.044	0.938	0.974	1.038	0.983	0.847
PC 18:2e-18:1	LC/MS_Lipid	3.29.E+00	3.23.E+00	3.91.E+00	3.82.E+00	3.19.E+00	3.94.E+00	3.90.E+00	2.95.E+00	3.83.E+00	1.161	0.989	1.006	1.185	0.912	0.980	0.700	2.70.E+00	2.42.E+00	2.29.E+00	2.51.E+00	2.13.E+00	2.22.E+00	2.43.E+00	2.59.E+00	2.41.E+00	0.927	0.882	0.966	0.899	1.072	1.052	0.321
PC 17:1-18:1/17:0-18:2	LC/MS_Lipid	8.04.E+00	7.14.E+00	5.13.E+00	9.30.E+00	7.14.E+00	5.31.E+00	9.63.E+00	6.65.E+00	5.18.E+00	1.157	1.001	1.035	1.198	0.932	1.010	0.568	6.61.E+00	6.27.E+00	6.78.E+00	6.93.E+00	6.65.E+00	6.40.E+00	6.56.E+00	6.58.E+00	6.87.E+00	1.048	1.061	0.944	0.994	1.051	1.013	0.823
PC 18:0p-18:1/18:1e-18:1	LC/MS_Lipid	4.86.E+00	3.92.E+00	4.55.E+00	5.50.E+00	3.88.E+00	4.65.E+00	5.54.E+00	3.60.E+00	4.35.E+00	1.132	0.988	1.022	1.140	0.918	0.958	0.610	3.32.E+00	3.00.E+00	3.28.E+00	3.35.E+00	3.28.E+00	3.10.E+00	3.24.E+00	3.13.E+00	3.45.E+00	1.009	1.093	0.947	0.976	1.045	1.053	0.841
PC 16:0e-20:2	LC/MS_Lipid	1.00.E+00	6.69.E-01	1.07.E+00	1.05.E+00	7.87.E-01	1.12.E+00	1.07.E+00	7.47.E-01	1.06.E+00	1.050	1.176	1.049	1.063	1.116	0.990	0.089	6.60.E-01	6.13.E-01	6.44.E-01	6.50.E-01	6.29.E-01	5.99.E-01	6.40.E-01	6.22.E-01	6.77.E-01	0.985	1.025	0.930	0.971	1.015	1.052	0.643
PC 17:0-18:1/17:1-18:0/16:0-19:1	LC/MS_Lipid	2.91.E+00	4.02.E+00	3.12.E+00	3.24.E+00	4.09.E+00	3.14.E+00	3.36.E+00	3.89.E+00	2.89.E+00	1.113	1.016	1.007	1.156	0.968	0.924	0.661	3.73.E+00	3.49.E+00	3.82.E+00	3.83.E+00	3.62.E+00	3.50.E+00	3.59.E+00	3.77.E+00	3.79.E+00	1.025	1.037	0.916	0.962	1.082	0.992	0.888
PC 16:1-20:5	LC/MS_Lipid	9.51.E-02	2.24.E-01	4.51.E-01	1.06.E-01	5.53.E-01	4.70.E-01	9.17.E-02	2.88.E-01	4.50.E-01	1.118	2.468	1.040	0.965	1.287	0.997	0.357	3.07.E-01	2.80.E-01	2.80.E-01	2.99.E-01	2.81.E-01	2.74.E-01	2.56.E-01	2.68.E-01	3.01.E-01	0.973	1.002	0.979	0.835	0.954	1.072	0.696
PC 14:0-22:6	LC/MS_Lipid	5.47.E-01	1.14.E+00	1.15.E+00	5.57.E-01	1.21.E+00	1.20.E+00	5.80.E-01	1.20.E+00	1.16.E+00	1.017	1.061	1.045	1.061	1.053	1.012	0.113	1.19.E+00	1.22.E+00	1.19.E+00	1.23.E+00	1.16.E+00	1.16.E+00	1.15.E+00	1.20.E+00	1.19.E+00	1.034	0.955	0.971	0.961	0.983	1.001	0.765
PC 18:2-18:3	LC/MS_Lipid	2.35.E+00	3.35.E+00	5.76.E+00	2.78.E+00	3.41.E+00	5.83.E+00	3.07.E+00	3.41.E+00	5.74.E+00	1.180	1.020	1.011	1.303	1.020	0.996	0.377	2.74.E+00	3.00.E+00	3.10.E+00	3.14.E+00	2.80.E+00	2.63.E+00	2.92.E+00	3.21.E+00	2.84.E+00	1.147	0.931	0.849	1.069	1.067	0.915	0.808
PC 14:0-22:5/16:1-20:4/16:0-20:5	LC/MS_Lipid	1.39.E+01	4.47.E+01	3.41.E+01	1.59.E+01	4.39.E+01	3.39.E+01	1.63.E+01	4.19.E+01	3.40.E+01	1.144	0.982	0.994	1.175	0.938	0.998	0.908	2.90.E+01	2.89.E+01	3.06.E+01	3.20.E+01	2.87.E+01	2.69.E+01	3.05.E+01	3.11.E+01	2.89.E+01	1.103	0.993	0.880	1.053	1.076	0.946	0.800
PC 18:2-18:2/18:1-18:3	LC/MS_Lipid	3.59.E+01	3.58.E+01	4.06.E+01	4.08.E+01	3.64.E+01	3.78.E+01	4.22.E+01	3.34.E+01	3.97.E+01	1.136	1.017	0.931	1.175	0.933	0.978	0.886	2.12.E+01	2.22.E+01	2.28.E+01	2.48.E+01	2.09.E+01	1.91.E+01	2.33.E+01	2.45.E+01	2.10.E+01	1.170	0.941	0.841	1.102	1.105	0.922	0.735
PC 16:0-20:4/16:1-20:3	LC/MS_Lipid	4.82.E+01	7.14.E+01	6.39.E+01	5.51.E+01	7.07.E+01	6.70.E+01	5.37.E+01	6.67.E+01	6.61.E+01	1.142	0.989	1.048	1.114	0.934	1.034	0.453	4.31.E+01	4.24.E+01	4.44.E+01	4.82.E+01	4.07.E+01	3.87.E+01	4.63.E+01	4.63.E+01	4.13.E+01	1.118	0.960	0.871	1.073	1.092	0.929	0.731
PC 18:1-18:2/16:0-20:3/18:0-18:3	LC/MS_Lipid	8.06.E+01	8.86.E+01	8.93.E+01	8.84.E+01	8.94.E+01	9.65.E+01	9.22.E+01	8.68.E+01	9.06.E+01	1.096	1.010	1.080	1.144	0.980	1.014	0.330	7.04.E+01	6.70.E+01	7.19.E+01	7.38.E+01	6.89.E+01	6.58.E+01	7.21.E+01	7.23.E+01	7.04.E+01	1.049	1.029	0.916	1.024	1.079	0.980	0.655
PC 18:1-18:1/18:0-18:2	LC/MS_Lipid	1.55.E+02	1.59.E+02	1.59.E+02	1.70.E+02	1.61.E+02	1.69.E+02	1.75.E+02	1.53.E+02	1.56.E+02	1.101	1.014	1.063	1.128	0.962	0.978	0.393	1.11.E+02	1.05.E+02	1.13.E+02	1.13.E+02	1.11.E+02	1.06.E+02	1.09.E+02	1.10.E+02	1.15.E+02	1.020	1.059	0.941	0.982	1.049	1.019	0.873
PC 18:0-18:1	LC/MS_Lipid	4.52.E+01	5.98.E+01	6.28.E+01	4.83.E+01	6.28.E+01	6.62.E+01	4.98.E+01	6.06.E+01	6.13.E+01	1.069	1.049	1.054	1.103	1.012	0.977	0.222	4.69.E+01	4.37.E+01	4.64.E+01	4.73.E+01	4.62.E+01	4.47.E+01	4.60.E+01	4.59.E+01	4.81.E+01	1.008	1.056	0.963	0.980	1.050	1.037	0.728
PC 16:0p-22:6	LC/MS_Lipid	1.32.E+00	2.05.E+00	1.76.E+00	1.43.E+00	2.11.E+00	2.03.E+00	1.53.E+00	2.09.E+00	1.85.E+00	1.081	1.028	1.153	1.156	1.016	1.056	0.180	1.58.E+00	1.55.E+00	1.66.E+00	1.72.E+00	1.57.E+00	1.50.E+00	1.64.E+00	1.63.E+00	1.61.E+00	1.090	1.009	0.908	1.039	1.047	0.975	0.862
PC 18:0-18:0	LC/MS_Lipid	1.60.E-01	3.70.E-01	1.35.E-01	1.40.E-01	3.44.E-01	2.85.E-01	1.34.E-01	4.89.E-01	2.08.E-01	0.876	0.928	2.108	0.836	1.319	1.541	0.644	4.08.E-01	3.72.E-01	3.96.E-01	3.74.E-01	3.83.E-01	3.78.E-01	3.71.E-01	3.93.E-01	3.96.E-01	0.916	1.031	0.954	0.910	1.057	1.001	0.608
PC 15:0-22:6	LC/MS_Lipid	4.38.E-01	5.82.E-01	3.51.E-01	4.81.E-01	6.18.E-01	3.87.E-01	4.60.E-01	5.73.E-01	3.59.E-01	1.098	1.062	1.105	1.049	0.985	1.025	0.009	4.10.E-01	4.46.E-01	4.79.E-01	4.86.E-01	4.17.E-01	3.81.E-01	4.53.E-01	4.55.E-01	4.33.E-01	1.185	0.935	0.796	1.104	1.021	0.903	0.854
PC 18:1e-20:5	LC/MS_Lipid	5.28.E-01	8.16.E-01	6.36.E-01	5.48.E-01	8.86.E-01	7.96.E-01	5.83.E-01	7.88.E-01	7.08.E-01	1.039	1.086	1.252	1.104	0.966	1.114	0.206	7.78.E-01	7.29.E-01	7.90.E-01	8.18.E-01	7.88.E-01	7.69.E-01	7.70.E-01	8.00.E-01	7.90.E-01	1.052	1.081	0.972	0.990	1.098	1.000	0.563
PC 16:0e-22:6	LC/MS_Lipid	4.35.E+00	5.56.E+00	4.83.E+00	4.70.E+00	5.69.E+00	5.24.E+00	4.92.E+00	5.73.E+00	4.79.E+00	1.079	1.024	1.085	1.130	1.032	0.992	0.269	4.25.E+00	3.95.E+00	4.23.E+00	4.34.E+00	4.18.E+00	3.99.E+00	4.20.E+00	4.16.E+00	4.25.E+00	1.022	1.059	0.941	0.989	1.054	1.004	0.876
PC 17:0-20:5/17:1-20:4	LC/MS_Lipid	6.42.E-01	1.15.E+00	7.97.E-01	7.27.E-01	1.18.E+00	8.51.E-01	7.23.E-01	1.16.E+00	8.04.E-01	1.132	1.026	1.068	1.126	1.011	1.008	0.085	7.82.E-01	8.07.E-01	8.33.E-01	8.57.E-01	7.77.E-01	7.33.E-01	8.57.E-01	8.62.E-01	7.85.E-01	1.096	0.963	0.879	1.097	1.068	0.942	0.556
PC 16:0e-22:5/18:0e-20:5	LC/MS_Lipid	8.02.E+00	7.56.E+00	7.86.E+00	8.78.E+00	8.01.E+00	8.71.E+00	9.27.E+00	7.80.E+00	7.73.E+00	1.095	1.059	1.108	1.156	1.031	0.983	0.251	5.77.E+00	5.31.E+00	5.71.E+00	5.77.E+00	5.64.E+00	5.33.E+00	5.62.E+00	5.48.E+00	5.84.E+00	0.999	1.063	0.933	0.973	1.032	1.023	0.931
PC 18:0p-20:4	LC/MS_Lipid	3.69.E+00	3.98.E+00	3.33.E+00	3.95.E+00	4.37.E+00	3.36.E+00	4.11.E+00	4.46.E+00	3.39.E+00	1.071	1.097	1.007	1.115	1.121	1.018	0.073	2.58.E+00	2.38.E+00	2.50.E+00	2.63.E+00	2.51.E+00	2.41.E+00	2.46.E+00	2.52.E+00	2.60.E+00	1.019	1.053	0.964	0.953	1.059	1.041	0.888
PC 17:0-20:4	LC/MS_Lipid	1.93.E+00	2.35.E+00	1.46.E+00	2.04.E+00	2.42.E+00	1.62.E+00	2.14.E+00	2.42.E+00	1.43.E+00	1.055	1.032	1.114	1.106	1.032	0.985	0.278	1.30.E+00	1.20.E+00	1.28.E+00	1.34.E+00	1.25.E+00	1.27.E+00	1.27.E+00	1.27.E+00	1.33.E+00	1.034	1.046	0.992	0.978	1.059	1.039	0.573
PC 18:1e-20:3	LC/MS_Lipid	1.89.E+00	1.78.E+00	1.83.E+00	1.90.E+00	1.98.E+00	2.03.E+00	2.17.E+00	2.03.E+00	1.74.E+00	1.004	1.113	1.105	1.144	1.143	0.951	0.473	7.20.E-01	6.17.E-01	6.62.E-01	6.81.E-01	6.83.E-01	6.36.E-01	6.82.E-01	6.67.E-01	7.03.E-01	0.946	1.107	0.961	0.947	1.081	1.061	0.797
PC 18:0e-20:4	LC/MS_Lipid	9.12.E+00	7.43.E+00	5.50.E+00	9.30.E+00	7.87.E+00	6.20.E+00	9.56.E+00	7.87.E+00	5.56.E+00	1.019	1.060	1.126	1.049	1.060	1.011	0.174	6.69.E+00	6.03.E+00	6.63.E+00	6.58.E+00	6.57.E+00	6.17.E+00	6.43.E+00	6.43.E+00	6.80.E+00	0.984	1.091	0.930	0.961	1.067	1.025	0.889
PC 17:0-20:3/19:1-18:2	LC/MS_Lipid	9.24.E-01	8.55.E-01	5.96.E-01	9.55.E-01	8.95.E-01	6.78.E-01	1.01.E+00	8.97.E-01	5.97.E-01	1.033	1.047	1.137	1.094	1.050	1.002	0.270	4.80.E-01	4.56.E-01	4.81.E-01	4.76.E-01	4.84.E-01	4.57.E-01	4.64.E-01	4.68.E-01	4.95.E-01	0.992	1.063	0.951	0.967	1.028	1.029	0.964
PC 19:1-18:1/19:0-18:2	LC/MS_Lipid	1.68.E+00	1.63.E+00	1.58.E+00	1.68.E+00	1.77.E+00	1.77.E+00	1.76.E+00	1.72.E+00	1.55.E+00	0.999	1.084	1.124	1.051	1.055	0.986	0.335	1.32.E+00	1.25.E+00	1.44.E+00	1.43.E+00	1.30.E+00	1.20.E+00	1.46.E+00	1.28.E+00	1.35.E+00	1.086	1.047	0.835	1.104	1.026	0.940	0.824
PC 19:0-18:1/18:0-19:1	LC/MS_Lipid	7.12.E-01	7.38.E-01	6.69.E-01	6.52.E-01	8.69.E-01	7.99.E-01	6.70.E-01	8.77.E-01	6.56.E-01	0.916	1.176	1.194	0.940	1.187	0.980	0.556	6.34.E-01	6.19.E-01	5.49.E-01	6.56.E-01	6.09.E-01	5.56.E-01	5.39.E-01	5.99.E-01	6.88.E-01	1.034	0.984	1.014	0.849	0.969	1.253	0.989
PC 18:2-20:5/16:1-22:6	LC/MS_Lipid	1.73.E+00	4.08.E+00	3.79.E+00	1.89.E+00	4.08.E+00	4.01.E+00	1.98.E+00	4.06.E+00	3.85.E+00	1.093	1.001	1.058	1.144	0.995	1.017	0.288	2.16.E+00	2.31.E+00	2.29.E+00	2.36.E+00	2.14.E+00	2.03.E+00	2.18.E+00	2.35.E+00	2.12.E+00	1.095	0.927	0.888	1.012	1.014	0.928	0.815
PC 18:2-20:4/16:0-22:6	LC/MS_Lipid	5.84.E+01	7.68.E+01	6.42.E+01	6.34.E+01	7.87.E+01	6.87.E+01	6.47.E+01	7.76.E+01	6.59.E+01	1.087	1.025	1.071	1.109	1.011	1.026	0.092	5.14.E+01	5.08.E+01	5.41.E+01	5.64.E+01	5.01.E+01	4.53.E+01	5.47.E+01	5.59.E+01	4.96.E+01	1.098	0.987	0.837	1.064	1.101	0.916	0.701
PC 18:1-20:4	LC/MS_Lipid	1.18.E+01	1.48.E+01	1.25.E+01	1.26.E+01	1.51.E+01	1.45.E+01	1.26.E+01	1.53.E+01	1.33.E+01	1.069	1.023	1.160	1.072	1.036	1.066	0.113	1.19.E+01	1.17.E+01	1.19.E+01	1.26.E+01	1.16.E+01	1.12.E+01	1.21.E+01	1.21.E+01	1.17.E+01	1.060	0.990	0.943	1.017	1.038	0.983	0.852
PC 18:0-20:5	LC/MS_Lipid	8.20.E+00	1.47.E+01	1.31.E+01	8.17.E+00	1.52.E+01	1.45.E+01	9.26.E+00	1.50.E+01	1.29.E+01	0.996	1.031	1.110	1.128	1.022	0.988	0.568	8.83.E+00	8.51.E+00	9.00.E+00	9.37.E+00	8.85.E+00	8.41.E+00	9.07.E+00	9.36.E+00	8.92.E+00	1.061	1.040	0.934	1.027	1.100	0.991	0.565
PC 18:1-20:3	LC/MS_Lipid	4.54.E+00	4.70.E+00	4.95.E+00	4.76.E+00	4.51.E+00	5.57.E+00	5.09.E+00	4.83.E+00	5.07.E+00	1.049	0.960	1.125	1.122	1.027	1.024	0.511	3.28.E+00	3.09.E+00	3.36.E+00	3.41.E+00	3.35.E+00	3.11.E+00	3.34.E+00	3.38.E+00	3.33.E+00	1.042	1.082	0.926	1.018	1.094	0.991	0.677
PC 18:0-20:4	LC/MS_Lipid	3.24.E+01	4.36.E+01	3.73.E+01	3.40.E+01	4.55.E+01	4.20.E+01	3.51.E+01	4.53.E+01	3.69.E+01	1.050	1.045	1.124	1.083	1.041	0.988	0.235	3.02.E+01	2.84.E+01	3.06.E+01	3.01.E+01	3.03.E+01	2.81.E+01	2.93.E+01	2.97.E+01	3.06.E+01	0.998	1.066	0.918	0.969	1.045	1.000	0.943
PC 18:1-20:2/18:0-20:3	LC/MS_Lipid	2.77.E+01	3.09.E+01	2.86.E+01	2.89.E+01	3.26.E+01	3.11.E+01	3.00.E+01	3.26.E+01	2.84.E+01	1.043	1.054	1.091	1.084	1.055	0.996	0.189	2.37.E+01	2.19.E+01	2.33.E+01	2.39.E+01	2.25.E+01	2.22.E+01	2.29.E+01	2.31.E+01	2.36.E+01	1.010	1.025	0.953	0.969	1.055	1.016	0.810
PC 16:0-22:2	LC/MS_Lipid	2.98.E+00	3.35.E+00	3.00.E+00	3.06.E+00	3.52.E+00	3.34.E+00	3.28.E+00	3.57.E+00	3.02.E+00	1.026	1.052	1.114	1.100	1.068	1.006	0.268	2.53.E+00	2.34.E+00	2.48.E+00	2.66.E+00	2.56.E+00	2.30.E+00	2.32.E+00	2.55.E+00	2.42.E+00	1.050	1.092	0.926	0.918	1.089	0.973	0.836
PC 18:0-20:2	LC/MS_Lipid	5.71.E+00	5.98.E+00	6.91.E+00	5.64.E+00	6.34.E+00	7.57.E+00	5.93.E+00	6.62.E+00	6.72.E+00	0.988	1.060	1.096	1.038	1.108	0.973	0.567	5.13.E+00	4.73.E+00	5.03.E+00	5.04.E+00	4.79.E+00	4.78.E+00	4.86.E+00	4.91.E+00	5.15.E+00	0.984	1.012	0.951	0.947	1.038	1.026	0.720
PC 20:0-18:1	LC/MS_Lipid	1.21.E+01	9.92.E+00	1.15.E+01	1.04.E+01	1.12.E+01	1.54.E+01	1.16.E+01	1.34.E+01	1.14.E+01	0.856	1.131	1.335	0.958	1.347	0.991	0.766	1.10.E+01	9.69.E+00	1.09.E+01	1.03.E+01	1.07.E+01	9.95.E+00	9.99.E+00	1.02.E+01	1.10.E+01	0.939	1.103	0.916	0.911	1.055	1.013	0.932
PC 18:1e-22:6	LC/MS_Lipid	1.64.E+00	1.65.E+00	1.61.E+00	1.67.E+00	1.73.E+00	1.84.E+00	1.77.E+00	1.81.E+00	1.56.E+00	1.023	1.048	1.143	1.083	1.094	0.971	0.462	1.23.E+00	1.28.E+00	1.28.E+00	1.27.E+00	1.30.E+00	1.25.E+00	1.21.E+00	1.26.E+00	1.27.E+00	1.036	1.018	0.978	0.984	0.991	0.996	0.499
PC 17:0-22:6	LC/MS_Lipid	8.90.E-01	1.02.E+00	6.71.E-01	9.56.E-01	1.02.E+00	6.69.E-01	1.00.E+00	1.05.E+00	6.70.E-01	1.074	1.005	0.997	1.127	1.030	0.998	0.263	6.46.E-01	6.03.E-01	6.48.E-01	6.80.E-01	6.28.E-01	6.10.E-01	6.38.E-01	6.69.E-01	6.44.E-01	1.054	1.041	0.941	0.988	1.108	0.993	0.780
PC 18:1e-22:5	LC/MS_Lipid	4.75.E-01	4.48.E-01	3.79.E-01	4.50.E-01	6.33.E-01	6.63.E-01	5.30.E-01	3.98.E-01	4.98.E-01	0.948	1.411	1.748	1.115	0.889	1.313	0.282	3.94.E-01	3.87.E-01	4.00.E-01	4.20.E-01	3.73.E-01	3.70.E-01	3.69.E-01	4.14.E-01	3.79.E-01	1.064	0.965	0.925	0.936	1.070	0.948	0.940
PC 18:0p-22:5	LC/MS_Lipid	2.18.E+00	2.05.E+00	1.45.E+00	2.49.E+00	2.23.E+00	1.62.E+00	2.32.E+00	2.29.E+00	1.47.E+00	1.140	1.092	1.115	1.062	1.121	1.012	0.057	1.66.E+00	1.53.E+00	1.65.E+00	1.64.E+00	1.63.E+00	1.52.E+00	1.61.E+00	1.57.E+00	1.68.E+00	0.985	1.067	0.926	0.966	1.030	1.021	0.921
PC 19:0-20:3	LC/MS_Lipid	4.32.E-01	3.30.E-01	3.00.E-01	3.69.E-01	3.18.E-01	3.84.E-01	3.87.E-01	3.63.E-01	3.14.E-01	0.854	0.966	1.278	0.897	1.103	1.047	0.996	2.77.E-01	2.76.E-01	3.14.E-01	2.59.E-01	2.58.E-01	2.23.E-01	2.63.E-01	2.81.E-01	2.80.E-01	0.935	0.933	0.712	0.948	1.018	0.893	0.164
PC 20:4-20:4	LC/MS_Lipid	9.26.E-01	1.51.E+00	1.41.E+00	1.06.E+00	1.55.E+00	1.42.E+00	1.05.E+00	1.46.E+00	1.42.E+00	1.148	1.027	1.007	1.134	0.968	1.006	0.385	7.58.E-01	8.27.E-01	7.78.E-01	9.03.E-01	7.61.E-01	6.46.E-01	8.66.E-01	9.12.E-01	7.20.E-01	1.190	0.920	0.829	1.142	1.102	0.925	0.643
PC 20:3-20:4	LC/MS_Lipid	4.41.E-01	5.29.E-01	4.67.E-01	5.06.E-01	5.36.E-01	4.81.E-01	5.23.E-01	5.16.E-01	4.77.E-01	1.146	1.013	1.030	1.185	0.975	1.023	0.388	3.43.E-01	3.43.E-01	3.51.E-01	3.81.E-01	3.27.E-01	3.06.E-01	3.67.E-01	3.82.E-01	3.32.E-01	1.112	0.952	0.873	1.071	1.114	0.946	0.591
PC 18:1-22:6	LC/MS_Lipid	1.22.E+00	1.43.E+00	1.59.E+00	1.26.E+00	1.49.E+00	1.76.E+00	1.26.E+00	1.47.E+00	1.62.E+00	1.039	1.041	1.108	1.038	1.024	1.019	0.121	8.30.E-01	8.18.E-01	8.48.E-01	8.87.E-01	7.80.E-01	7.71.E-01	8.79.E-01	8.88.E-01	8.09.E-01	1.068	0.954	0.910	1.058	1.085	0.954	0.499
PC 20:2-20:4/18:1-22:5	LC/MS_Lipid	8.92.E-01	1.05.E+00	1.14.E+00	9.31.E-01	1.10.E+00	1.30.E+00	9.81.E-01	1.07.E+00	1.10.E+00	1.043	1.043	1.141	1.100	1.015	0.964	0.377	6.39.E-01	6.28.E-01	6.32.E-01	6.86.E-01	6.84.E-01	6.04.E-01	6.46.E-01	6.86.E-01	6.65.E-01	1.075	1.088	0.957	1.011	1.092	1.052	0.446
PC 18:0-22:6	LC/MS_Lipid	1.00.E+01	1.39.E+01	1.20.E+01	1.08.E+01	1.42.E+01	1.34.E+01	1.14.E+01	1.43.E+01	1.20.E+01	1.079	1.025	1.120	1.140	1.029	1.000	0.279	1.28.E+01	1.25.E+01	1.30.E+01	1.32.E+01	1.27.E+01	1.22.E+01	1.30.E+01	1.29.E+01	1.26.E+01	1.030	1.015	0.938	1.015	1.039	0.969	0.842
PC 18:0-22:5	LC/MS_Lipid	4.32.E+00	5.71.E+00	5.15.E+00	4.62.E+00	5.94.E+00	5.67.E+00	4.80.E+00	5.73.E+00	5.17.E+00	1.069	1.039	1.101	1.113	1.003	1.003	0.199	3.54.E+00	3.38.E+00	3.50.E+00	3.60.E+00	3.41.E+00	3.29.E+00	3.48.E+00	3.57.E+00	3.49.E+00	1.019	1.008	0.938	0.983	1.056	0.997	0.697

PC 20:1-20:3/18:0-22:4	LC/MS_Lipid	1.90.E+00	2.28.E+00	2.03.E+00	1.91.E+00	2.34.E+00	2.21.E+00	1.97.E+00	2.39.E+00	1.84.E+00	1.004	1.026	1.087	1.040	1.050	0.908	0.687	1.20.E+00	1.03.E+00	1.11.E+00	1.10.E+00	1.08.E+00	1.08.E+00	1.06.E+00	1.10.E+00	1.11.E+00	0.914	1.053	0.973	0.880	1.064	0.993	0.797
PC 18:1-22:0	LC/MS_Lipid	4.54.E-02	5.46.E-02	4.28.E-02	5.59.E-02	5.25.E-02	4.03.E-02	5.27.E-02	4.54.E-02	4.85.E-02	1.231	0.963	0.942	1.160	0.833	1.135	0.914	3.13.E-02	3.14.E-02	2.69.E-02	3.03.E-02	2.43.E-02	1.95.E-02	3.49.E-02	3.63.E-02	2.02.E-02	0.969	0.775	0.725	1.115	1.158	0.751	0.240
PC 19:0-22:6	LC/MS_Lipid	8.63.E-02	1.13.E-01	1.01.E-01	5.96.E-02	1.30.E-01	1.32.E-01	9.46.E-02	1.17.E-01	1.02.E-01	0.691	1.148	1.302	1.095	1.037	1.006	0.902	7.70.E-02	9.39.E-02	9.85.E-02	1.01.E-01	7.29.E-02	9.34.E-02	7.79.E-02	1.08.E-01	9.17.E-02	1.316	0.777	0.949	1.012	1.147	0.931	0.966
LPE 16:0 (sn-1)	LC/MS_Lipid	5.24.E-02	4.96.E-02	8.49.E-02	6.17.E-02	4.09.E-02	8.22.E-02	5.57.E-02	4.42.E-02	8.26.E-02	1.178	0.825	0.968	1.064	0.890	0.972	0.925	3.89.E-02	4.54.E-02	3.39.E-02	3.67.E-02	3.96.E-02	3.80.E-02	3.26.E-02	3.86.E-02	3.82.E-02	0.944	0.872	1.121	0.837	0.850	1.128	0.613
LPE 16:0 (sn-2)	LC/MS_Lipid	7.96.E-02	7.33.E-02	1.08.E-01	8.64.E-02	7.09.E-02	1.16.E-01	8.34.E-02	7.56.E-02	1.10.E-01	1.086	0.966	1.074	1.048	1.031	1.020	0.380	6.33.E-02	6.48.E-02	5.79.E-02	5.62.E-02	5.72.E-02	6.24.E-02	5.20.E-02	5.51.E-02	6.48.E-02	0.888	0.883	1.076	0.822	0.850	1.118	0.558
LPE 18:2 (sn-1)	LC/MS_Lipid	1.01.E-01	1.12.E-01	1.63.E-01	1.40.E-01	9.78.E-02	1.63.E-01	1.34.E-01	8.83.E-02	1.65.E-01	1.382	0.873	1.000	1.321	0.788	1.015	0.834	7.77.E-02	7.99.E-02	6.87.E-02	7.33.E-02	6.79.E-02	6.95.E-02	7.10.E-02	6.73.E-02	7.23.E-02	0.944	0.850	1.012	0.914	0.842	1.053	0.346
LPE 18:2 (sn-2)	LC/MS_Lipid	1.43.E-01	1.28.E-01	1.91.E-01	1.69.E-01	1.22.E-01	1.86.E-01	1.69.E-01	1.10.E-01	1.90.E-01	1.183	0.959	0.972	1.180	0.860	0.996	0.874	9.67.E-02	9.96.E-02	9.09.E-02	8.90.E-02	9.37.E-02	9.21.E-02	9.80.E-02	9.35.E-02	9.85.E-02	0.921	0.940	1.013	1.014	0.939	1.084	0.338
LPE 18:1 (sn-1)	LC/MS_Lipid	5.16.E-02	5.12.E-02	1.07.E-01	7.31.E-02	4.92.E-02	9.80.E-02	6.63.E-02	4.21.E-02	1.04.E-01	1.417	0.962	0.918	1.285	0.824	0.972	0.877	4.37.E-02	4.82.E-02	4.41.E-02	3.80.E-02	4.03.E-02	3.94.E-02	4.21.E-02	4.34.E-02	4.10.E-02	0.870	0.835	0.894	0.963	0.899	0.929	0.006
LPE 18:1 (sn-2)	LC/MS_Lipid	9.99.E-02	1.06.E-01	2.12.E-01	1.34.E-01	1.07.E-01	2.10.E-01	1.35.E-01	9.06.E-02	2.13.E-01	1.346	1.016	0.990	1.350	0.857	1.004	0.641	7.32.E-02	7.81.E-02	6.40.E-02	6.33.E-02	7.09.E-02	6.42.E-02	7.08.E-02	7.52.E-02	7.04.E-02	0.865	0.909	1.002	0.967	0.963	1.099	0.128
LPE 18:0 (sn-1)	LC/MS_Lipid	1.01.E-01	1.13.E-01	1.70.E-01	1.51.E-01	1.09.E-01	1.48.E-01	1.32.E-01	8.63.E-02	1.61.E-01	1.497	0.966	0.872	1.308	0.763	0.948	0.839	4.12.E-02	6.40.E-02	4.28.E-02	4.90.E-02	4.15.E-02	4.49.E-02	4.93.E-02	5.32.E-02	4.62.E-02	1.189	0.647	1.051	1.196	0.831	1.080	0.768
LPE 18:0 (sn-2)	LC/MS_Lipid	1.57.E-01	1.76.E-01	2.27.E-01	2.14.E-01	1.71.E-01	2.06.E-01	1.96.E-01	1.44.E-01	2.24.E-01	1.363	0.971	0.909	1.248	0.818	0.987	0.855	7.31.E-02	9.62.E-02	7.33.E-02	7.78.E-02	7.73.E-02	7.47.E-02	8.30.E-02	8.20.E-02	7.85.E-02	1.065	0.803	1.019	1.135	0.853	1.071	0.722
LPE 20:4 (sn-1)	LC/MS_Lipid	4.35.E-02	5.94.E-02	7.48.E-02	6.76.E-02	4.92.E-02	6.05.E-02	6.25.E-02	3.92.E-02	8.09.E-02	1.554	0.827	0.808	1.436	0.659	1.082	0.985	4.61.E-02	4.71.E-02	3.93.E-02	2.95.E-02	3.61.E-02	3.25.E-02	3.32.E-02	3.98.E-02	4.09.E-02	0.641	0.766	0.828	0.720	0.845	1.041	0.050
LPE 20:4 (sn-2)	LC/MS_Lipid	4.77.E-02	5.98.E-02	7.55.E-02	6.70.E-02	5.05.E-02	6.15.E-02	6.08.E-02	4.53.E-02	6.43.E-02	1.405	0.846	0.814	1.275	0.758	0.852	0.871	4.04.E-02	4.60.E-02	4.15.E-02	3.92.E-02	3.66.E-02	3.81.E-02	4.41.E-02	3.94.E-02	4.30.E-02	0.971	0.796	0.917	1.093	0.858	1.036	0.203
LPE 22:6 (sn-1)	LC/MS_Lipid	4.15.E-02	6.60.E-02	8.71.E-02	5.41.E-02	5.62.E-02	7.89.E-02	5.88.E-02	4.20.E-02	8.40.E-02	1.304	0.852	0.906	1.417	0.636	0.965	0.935	4.81.E-02	4.08.E-02	4.46.E-02	3.92.E-02	3.60.E-02	4.42.E-02	3.93.E-02	3.72.E-02	4.31.E-02	0.815	0.883	0.991	0.818	0.913	0.967	0.116
LPE 22:6 (sn-2)	LC/MS_Lipid	3.21.E-02	5.01.E-02	6.72.E-02	5.11.E-02	5.30.E-02	5.66.E-02	4.88.E-02	4.08.E-02	6.92.E-02	1.588	1.057	0.843	1.518	0.814	1.030	0.879	3.42.E-02	3.56.E-02	3.56.E-02	3.39.E-02	3.54.E-02	3.66.E-02	3.17.E-02	3.46.E-02	3.98.E-02	0.992	0.994	1.029	0.927	0.970	1.117	0.989
PE 16:0-16:1/14:0-18:1	LC/MS_Lipid	1.69.E-02	1.86.E-02	3.07.E-02	1.67.E-02	1.92.E-02	2.83.E-02	1.75.E-02	1.87.E-02	2.59.E-02	0.988	1.036	0.920	1.032	1.007	0.842	0.583	2.20.E-02	2.69.E-02	2.60.E-02	2.38.E-02	2.09.E-02	1.94.E-02	2.63.E-02	2.22.E-02	2.55.E-02	1.081	0.776	0.748	1.194	0.823	0.982	0.332
PE 16:0p-18:1	LC/MS_Lipid	1.16.E-02	9.87.E-03	1.20.E-02	1.06.E-02	9.98.E-03	1.34.E-02	1.08.E-02	1.02.E-02	1.29.E-02	0.914	1.011	1.113	0.928	1.029	1.074	0.951	1.23.E-02	1.39.E-02	1.10.E-02	9.97.E-03	1.00.E-02	1.07.E-02	1.28.E-02	1.12.E-02	1.19.E-02	0.810	0.724	0.969	1.036	0.809	1.082	0.153
PE 16:0e-18:1	LC/MS_Lipid	3.79.E-02	3.47.E-02	6.03.E-02	3.94.E-02	3.77.E-02	7.31.E-02	4.16.E-02	3.67.E-02	4.88.E-02	1.041	1.088	1.213	1.097	1.058	0.811	0.467	2.15.E-02	2.42.E-02	2.15.E-02	2.53.E-02	2.54.E-02	2.36.E-02	2.17.E-02	2.48.E-02	2.42.E-02	1.173	1.050	1.098	1.010	1.022	1.130	0.158
PE 16:0-18:3	LC/MS_Lipid	2.27.E-02	2.51.E-02	3.41.E-02	3.03.E-02	2.35.E-02	3.24.E-02	2.11.E-02	3.07.E-02	3.19.E-02	1.335	0.936	0.950	0.930	1.225	0.934	0.924	1.65.E-02	1.66.E-02	1.94.E-02	1.84.E-02	1.59.E-02	1.58.E-02	1.49.E-02	1.53.E-02	1.98.E-02	1.114	0.958	0.816	0.901	0.924	1.021	0.846
PE 16:1-18:1/16:0-18:2	LC/MS_Lipid	1.02.E-01	6.37.E-02	7.03.E-02	1.02.E-01	7.02.E-02	9.15.E-02	1.09.E-01	8.55.E-02	6.72.E-02	1.006	1.101	1.301	1.072	1.341	0.956	0.547	1.19.E-01	1.01.E-01	1.08.E-01	1.05.E-01	1.07.E-01	1.13.E-01	1.02.E-01	9.69.E-02	1.21.E-01	0.881	1.061	1.053	0.856	0.958	1.125	0.930
PE 16:0-18:1	LC/MS_Lipid	7.20.E-02	5.81.E-02	5.56.E-02	7.74.E-02	5.24.E-02	7.42.E-02	7.86.E-02	5.46.E-02	5.89.E-02	1.074	0.903	1.336	1.090	0.940	1.060	0.572	8.04.E-02	8.90.E-02	8.07.E-02	7.66.E-02	8.60.E-02	7.77.E-02	7.55.E-02	7.99.E-02	8.70.E-02	0.952	0.966	0.963	0.938	0.898	1.078	0.677
PE 16:0p-20:4	LC/MS_Lipid	3.37.E-02	4.71.E-02	4.28.E-02	3.05.E-02	4.25.E-02	4.69.E-02	3.37.E-02	5.10.E-02	3.51.E-02	0.905	0.903	1.094	1.001	1.083	0.820	0.947	3.80.E-02	3.35.E-02	3.70.E-02	3.70.E-02	3.65.E-02	4.04.E-02	3.63.E-02	3.40.E-02	3.56.E-02	0.972	1.089	1.091	0.953	1.016	0.960	0.175
PE 16:0p-20:3/16:0e-20:4	LC/MS_Lipid	5.14.E-02	6.66.E-02	7.15.E-02	5.87.E-02	6.96.E-02	9.29.E-02	5.42.E-02	6.97.E-02	6.75.E-02	1.142	1.045	1.300	1.054	1.047	0.944	0.233	5.81.E-02	5.42.E-02	5.27.E-02	5.46.E-02	5.42.E-02	5.10.E-02	5.00.E-02	5.82.E-02	5.93.E-02	0.939	1.001	0.968	0.861	1.075	1.126	0.763
PE 18:1p-18:1/18:0p-18:2/18:0e-18:3	LC/MS_Lipid	9.32.E-02	5.96.E-02	6.01.E-02	9.26.E-02	7.23.E-02	6.40.E-02	8.64.E-02	6.22.E-02	5.49.E-02	0.994	1.214	1.066	0.927	1.044	0.915	0.097	3.90.E-02	4.55.E-02	3.15.E-02	4.30.E-02	4.02.E-02	3.91.E-02	4.32.E-02	4.12.E-02	3.95.E-02	1.102	0.883	1.241	1.108	0.906	1.256	0.684
PE 17:0-18:2	LC/MS_Lipid	7.32.E-03	4.03.E-03	1.37.E-03	9.37.E-03	2.78.E-03	2.51.E-03	1.09.E-02	3.91.E-03	3.60.E-03	1.280	0.689	1.829	1.484	0.969	2.622	0.192	4.69.E-03	4.66.E-03	5.30.E-03	5.19.E-03	3.71.E-03	3.83.E-03	3.86.E-03	5.55.E-03	5.38.E-03	1.106	0.797	0.722	0.823	1.192	1.014	0.616
PE 18:0e-18:2	LC/MS_Lipid	5.36.E-02	4.96.E-02	5.24.E-02	4.24.E-02	5.20.E-02	5.95.E-02	4.73.E-02	5.85.E-02	5.53.E-02	0.791	1.048	1.136	0.882	1.180	1.056	0.861	1.70.E-02	1.56.E-02	1.38.E-02	1.27.E-02	1.22.E-02	1.40.E-02	1.41.E-02	1.03.E-02	1.75.E-02	0.745	0.784	1.015	0.830	0.659	1.270	0.506
PE 18:0p-18:1	LC/MS_Lipid	4.12.E-02	3.70.E-02	4.12.E-02	4.27.E-02	4.23.E-02	4.64.E-02	4.35.E-02	3.99.E-02	3.75.E-02	1.036	1.143	1.127	1.056	1.078	0.909	0.250	2.18.E-02	2.78.E-02	2.46.E-02	2.74.E-02	2.28.E-02	2.28.E-02	3.05.E-02	2.96.E-02	2.38.E-02	1.259	0.820	0.926	1.400	1.064	0.968	0.405
PE 18:0e-18:1	LC/MS_Lipid	2.22.E-02	3.10.E-02	2.24.E-02	2.72.E-02	3.13.E-02	2.91.E-02	2.70.E-02	2.49.E-02	2.07.E-02	1.227	1.011	1.298	1.217	0.803	0.923	0.232	1.21.E-02	1.34.E-02	1.11.E-02	1.46.E-02	9.79.E-03	1.02.E-02	1.55.E-02	1.18.E-02	1.09.E-02	1.211	0.728	0.924	1.289	0.876	0.983	0.710
PE 18:2-18:3	LC/MS_Lipid	6.06.E-03	6.67.E-03	2.00.E-02	5.72.E-03	6.49.E-03	2.20.E-02	8.88.E-03	6.98.E-03	2.15.E-02	0.945	0.973	1.101	1.466	1.047	1.072	0.317	3.79.E-03	7.56.E-03	3.24.E-03	6.73.E-03	6.25.E-03	5.16.E-03	6.72.E-03	8.95.E-03	5.46.E-03	1.774	0.827	1.592	1.773	1.183	1.684	0.176
PE 16:0-20:5	LC/MS_Lipid	2.41.E-02	5.58.E-02	4.81.E-02	3.12.E-02	5.01.E-02	5.29.E-02	3.09.E-02	5.36.E-02	4.51.E-02	1.292	0.899	1.099	1.278	0.961	0.936	0.832	4.09.E-02	3.86.E-02	3.54.E-02	4.15.E-02	3.41.E-02	4.10.E-02	4.66.E-02	3.97.E-02	3.56.E-02	1.014	0.884	1.160	1.139	1.030	1.008	0.707
PE 18:2-18:2	LC/MS_Lipid	5.82.E-02	5.48.E-02	9.65.E-02	6.38.E-02	6.08.E-02	9.65.E-02	8.61.E-02	5.09.E-02	9.39.E-02	1.097	1.110	0.999	1.480	0.929	0.973	0.712	2.46.E-02	1.97.E-02	2.30.E-02	1.76.E-02	2.35.E-02	2.21.E-02	2.25.E-02	1.82.E-02	2.63.E-02	0.714	1.193	0.962	0.912	0.926	1.146	0.866
PE 16:0-20:4	LC/MS_Lipid	7.99.E-02	6.95.E-02	5.41.E-02	8.03.E-02	6.81.E-02	8.38.E-02	9.14.E-02	7.27.E-02	6.99.E-02	1.005	0.980	1.548	1.144	1.046	1.291	0.405	9.19.E-02	7.67.E-02	8.40.E-02	7.24.E-02	8.79.E-02	9.03.E-02	7.57.E-02	7.11.E-02	8.78.E-02	0.788	1.146	1.075	0.824	0.927	1.045	0.689
PE 18:1-18:2	LC/MS_Lipid	1.71.E-01	9.56.E-02	1.29.E-01	1.41.E-01	9.82.E-02	1.66.E-01	1.82.E-01	1.00.E-01	1.26.E-01	0.822	1.027	1.283	1.064	1.049	0.978	0.970	9.74.E-02	1.11.E-01	1.21.E-01	1.12.E-01	1.06.E-01	9.00.E-02	1.13.E-01	9.21.E-02	1.19.E-01	1.151	0.961	0.747	1.165	0.832	0.986	0.847
PE 18:1-18:1/18:0-18:2	LC/MS_Lipid	5.69.E-01	3.77.E-01	3.48.E-01	5.16.E-01	3.97.E-01	4.86.E-01	5.40.E-01	4.01.E-01	3.62.E-01	0.907	1.054	1.399	0.949	1.065	1.043	0.688	3.83.E-01	4.01.E-01	3.98.E-01	3.98.E-01	3.75.E-01	3.37.E-01	3.96.E-01	3.95.E-01	3.69.E-01	1.040	0.935	0.848	1.036	0.986	0.926	0.386
PE 16:0-20:1/18:0-18:1	LC/MS_Lipid	2.23.E-01	2.04.E-01	1.96.E-01	2.34.E-01	2.14.E-01	2.40.E-01	2.48.E-01	2.23.E-01	2.06.E-01	1.048	1.051	1.222	1.111	1.095	1.047	0.235	1.43.E-01	1.56.E-01	1.54.E-01	1.56.E-01	1.41.E-01	1.32.E-01	1.64.E-01	1.65.E-01	1.42.E-01	1.092	0.906	0.854	1.146	1.061	0.921	0.375
PE 16:0p-22:6	LC/MS_Lipid	1.88.E-02	2.85.E-02	2.32.E-02	1.84.E-02	3.04.E-02	2.26.E-02	2.19.E-02	2.44.E-02	2.44.E-02	0.979	1.067	0.972	1.168	0.857	1.052	0.991	1.57.E-02	1.88.E-02	1.39.E-02	1.83.E-02	1.67.E-02	1.19.E-02	2.10.E-02	1.59.E-02	1.35.E-02	1.164	0.887	0.857	1.336	0.843	0.970	0.821
PE 18:0p-20:5/18:1p-20:4/16:0e-22:6	LC/MS_Lipid	9.11.E-02	1.25.E-01	1.40.E-01	9.88.E-02	1.43.E-01	1.63.E-01	9.91.E-02	1.24.E-01	1.29.E-01	1.084	1.140	1.163	1.088	0.986	0.918	0.119	1.09.E-01	1.04.E-01	1.08.E-01	1.18.E-01	1.07.E-01	1.17.E-01	1.08.E-01	1.05.E-01	1.11.E-01	1.079	1.028	1.087	0.990	1.010	1.027	0.040
PE 18:1p-20:3/16:0p-22:4	LC/MS_Lipid	3.60.E-02	5.05.E-02	5.57.E-02	3.91.E-02	4.68.E-02	6.19.E-02	4.23.E-02	4.47.E-02	4.42.E-02	1.087	0.927	1.112	1.174	0.886	0.794	0.577	4.42.E-02	5.13.E-02	4.59.E-02	4.92.E-02	5.73.E-02	5.01.E-02	4.61.E-02	4.84.E-02	5.01.E-02	1.115	1.118	1.091	1.043	0.943	1.092	0.123
PE 18:0p-20:4	LC/MS_Lipid	1.32.E-01	2.31.E-01	1.74.E-01	1.54.E-01	2.51.E-01	1.92.E-01	1.41.E-01	2.24.E-01	1.71.E-01	1.169	1.085	1.101	1.071	0.970	0.980	0.009	1.17.E-01	1.26.E-01	1.09.E-01	1.24.E-01	1.20.E-01	1.14.E-01	1.34.E-01	1.23.E-01	1.12.E-01	1.067	0.959	1.041	1.150	0.978	1.024	0.513
PE 18:1e-20:3	LC/MS_Lipid	1.20.E-01	2.17.E-01	1.58.E-01	1.29.E-01	2.37.E-01	1.90.E-01	1.30.E-01	2.16.E-01	1.50.E-01	1.078	1.091	1.203	1.087	0.994	0.949	0.119	7.02.E-02	6.92.E-02	7.39.E-02	6.99.E-02	7.79.E-02	7.00.E-02	6.65.E-02	7.06.E-02	7.54.E-02	0.995	1.127	0.947	0.948	1.020	1.021	0.849
PE 16:1-22:6/18:2-20:5	LC/MS_Lipid	7.94.E-03	1.45.E-02	1.48.E-02	1.18.E-02	1.44.E-02	1.94.E-02	1.14.E-02	1.43.E-02	1.90.E-02	1.482	0.993	1.313	1.438	0.985	1.280	0.133	9.14.E-03	9.00.E-03	1.06.E-02	9.12.E-03	8.51.E-03	4.91.E-03	8.69.E-03	8.28.E-03	7.04.E-03	0.997	0.946	0.463	0.951	0.920	0.663	0.344
PE 18:2-20:4/18:1-20:5	LC/MS_Lipid	3.39.E-01	2.99.E-01	2.71.E-01	3.86.E-01	2.74.E-01	2.67.E-01	3.87.E-01	2.61.E-01	2.46.E-01	1.140	0.916	0.986	1.141	0.871	0.908	0.858	2.01.E-01	1.93.E-01	1.95.E-01	1.80.E-01	1.99.E-01	1.90.E-01	1.95.E-01	1.90.E-01	2.00.E-01	0.895	1.034	0.973	0.970	0.983	1.026	0.618
PE 16:0-22:6/16:1-22:5/20:2-18:4	LC/MS_Lipid	3.39.E-01	2.99.E-01	2.71.E-01	3.86.E-01	2.74.E-01	2.67.E-01	3.87.E-01	2.61.E-01	2.46.E-01	1.140	0.916	0.985	1.141	0.871	0.908	0.858	2.01.E-01	1.93.E-01	1.95.E-01	1.80.E-01	1.99.E-01	1.90.E-01	1.95.E-01	1.90.E-01	2.00.E-01	0.895	1.034	0.973	0.970	0.983	1.026	0.618
PE 18:1-20:4	LC/MS_Lipid	9.19.E-02	6.33.E-02	6.56.E-02	8.46.E-02	6.79.E-02	1.01.E-01	9.47.E-02	8.24.E-02	7.47.E-02	0.920	1.073	1.539	1.030	1.302	1.139	0.573	8.94.E-02	9.13.E-02	8.48.E-02	8.47.E-02	1.00.E-01	9.23.E-02	8.91.E-02	9.19.E-02	9.12.E-02	0.947	1.099	1.088	0.997	1.007	1.076	0.578
PE 18:0-20:5	LC/MS_Lipid	4.11.E-02	5.41.E-02	4.58.E-02	4.10.E-02	4.98.E-02	5.96.E-02	5.44.E-02	5.66.E-02	4.55.E-02	0.998	0.920	1.301	1.324	1.047	0.992	0.725	5.01.E-02	4.64.E-02	4.24.E-02	4.86.E-02	4.73.E-02	4.48.E-02	4.99.E-02	4.21.E-02	5.25.E-02	0.969	1.018	1.057	0.994	0.907	1.238	0.858
PE 18:0-20:4	LC/MS_Lipid	3.15.E-01	2.85.E-01	2.22.E-01	3.14.E-01	2.85.E-01	2.75.E-01	3.38.E-01	3.09.E-01	2.10.E-01	0.996	1.000	1.238	1.074	1.084	0.947	0.728	2.21.E-01	2.37.E-01	2.40.E-01	2.14.E-01	2.38.E-01	2.16.E-01	2.26.E-01	2.27.E-01	2.18.E-01	0.968	1.005	0.902	1.024	0.956	0.909	0.415
PE 20:1-18:2	LC/MS_Lipid	2.56.E-02	2.03.E-02	2.31.E-02	2.64.E-02	2.42.E-02	2.90.E-02	3.29.E-02	3.32.E-02	2.05.E-02	1.030	1.193	1.253	1.286	1.640	0.888	0.443	2.58.E-02	1.90.E-02	2.26.E-02	2.05.E-02	1.84.E-02	1.64.E-02	2.16.E-02	2.34.E-02	2.14.E-02	0.797	0.968	0.725	0.839	1.230	0.949	0.178
PE 18:0-20:3	LC/MS_Lipid	8.53.E-02	8.04.E-02	6.63.E-02	1.00.E-01	7.73.E-02	6.99.E-02	9.43.E-02	7.41.E-02	5.79.E-02	1.175	0.962	1.054	1.105	0.922	0.873	0.379	4.38.E-02	4.72.E-02	4.32.E-02	4.69.E-02	4.37.E-02	4.93.E-02	4.86.E-02	4.89.E-02	4.32.E-02	1.071	0.926	1.142	1.108	1.037	1.001	0.692
PE 18:1-20:1	LC/MS_Lipid	1.04.E-02	5.36.E-03	4.59.E-03	1.11.E-02	5.68.E-03	4.96.E-03	1.13.E-02	5.23.E-03	6.35.E-03	1.068	1.059	1.082	1.085	0.974	1.384	0.289	2.92.E-03	3.89.E-03	3.01.E-03	3.60.E-03	4.39.E-03	2.79.E-03	4.43.E-03	4.46.E-03	4.40.E-03	1.234	1.129	0.927	1.516	1.147	1.460	0.063
PE 20:0-18:2	LC/MS_Lipid	2.50.E-02	3.67.E-02	3.24.E-02	2.69.E-02	3.51.E-02	3.84.E-02	2.93.E-02	3.35.E-02	3.33.E-02	1.075	0.957	1.184	1.172	0.915	1.026	0.648	1.95.E-02	2.04.E-02	1.63.E-02	1.59.E-02	1.67.E-02	1.98.E-02	1.89.E-02	1.87.E-02	1.61.E-02	0.815	0.816	1.212	0.969	0.915	0.987	0.786
PE 18:0-20:1	LC/MS_Lipid	1.21.E-02	2.11.E-02	1.34.E-02	1.32.E-02	1.88.E-02	1.80.E-02	1.66.E-02	1.66.E-02	1.45.E-02	1.089	0.888	1.342	1.369	0.787	1.077	0.886	8.91.E-03	1.10.E-02	1.02.E-02	9.24.E-03	5.92.E-03	8.56.E-03	1.40.E-02	1.29.E-02	7.31.E-03	1.037	0.538	0.842	1.573	1.172	0.719	0.358
PE 18:0p-22:6/18:1p-22:5	LC/MS_Lipid	5.59.E-02	9.35.E-02	6.48.E-02	6.11.E-02	9.63.E-02	7.65.E-02	5.89.E-02	8.15.E-02	6.55.E-02	1.093	1.029	1.181	1.053	0.871	1.011	0.147	4.86.E-02	5.72.E-02	4.68.E-02	5.38.E-02	4.95.E-02	5.04.E-02	5.67.E-02	6.56.E-02	4.44.E-02	1.107	0.866	1.076	1.167	1.146	0.948	0.600
PE 17:0-22:6	LC/MS_Lipid	6.29.E-03	4.31.E-03	2.03.E-03	5.21.E-03	2.64.E-03	3.08.E-03	5.03.E-03	2.60.E-03	2.00.E-03	0.829	0.613	1.521	0.800	0.605	0.986	0.339	3.77.E-03	4.78.E-03	4.56.E-03	4.15.E-03	3.00.E-03	2.53.E-03	4.13.E-03	2.65.E-03	3.09.E-03	1.102	0.627	0.554	1.095	0.554	0.677	0.245
PE 18:0p-22:5/18:1p-22:4	LC/MS_Lipid	8.39.E-02	1.20.E-01	9.01.E-02	6.85.E-02	1.35.E-01	1.08.E-01	7.92.E-02	1.40.E-01	7.33.E-02	0.816	1.127	1.201	0.944	1.163	0.813	0.838	8.66.E-02	9.44.E-02	8.68.E-02	9.51.E-02	8.70.E-02	9.25.E-02	9.00.E-02	9.88.E-02	7.99.E-02	1.098	0.922	1.066	1.039	1.047	0.921	0.904
PE 18:1-22:6	LC/MS_Lipid	2.03.E-02	1.71.E-02	2.19.E-02	1.76.E-02	1.74.E-02	3.45.E-02	2.04.E-02	1.82.E-02	2.18.E-02	0.863	1.015	1.576	1.001	1.066	0.994	0.670	1.92.E-02	1.81.E-02	2.10.E-02	2.43.E-02	2.17.E-02	2.39.E-02	2.16.E-02	1.90.E-02	2.20.E-02	1.267	1.201	1.142	1.128	1.053	1.047	0.003
PE 18:0-22:6	LC/MS_Lipid	9.16.E-02	9.84.E-02	7.39.E-02	9.12.E-02	1.02.E-01	8.92.E-02	9.35.E-02	9.72.E-02	6.19.E-02	0.995	1.032	1.206	1.021	0.987	0.838	0.387	1.00.E-01	9.74.E-02	1.18.E-01	9.98.E-02	9.93.E-02	9.43.E-02	9.36.E-02	9.66.E-02	1.03.E-01	0.996	1.019	0.801	0.935	0.991	0.877	0.430
PE 18:0-22:5	LC/MS_Lipid	5.68.E-02	5.17.E-02	3.90.E-02	5.05.E-02	5.16.E-02	5.03.E-02	5.01.E-02	5.60.E-02	4.14.E-02	0.889	0.999	1.288	0.881	1.083	1.060	0.904	4.02.E-02	3.94.E-02	4.38.E-02	4.44.E-02	4.10.E-02	4.08.E-02	4.10.E-02	4.70.E-02	4.10.E-02	1.105	1.040	0.930	1.021	1.193	0.935	0.794
FA 12:0_Lauric acid	LC/MS_Lipid	5.43.E-02	3.09.E-02	4.17.E-02	5.06.E-02	4.01.E-02	4.34.E-02	6.10.E-02	5.86.E-02	5.58.E-02	0.931	1.299	1.042	1.122	1.896	1.338	0.041	1.54.E-01	8.71.E-02	8.80.E-02	1.12.E-01	1.09.E-01	9.55.E-02	8.71.E-02	8.93.E-02	8.29.E-02	0.727	1.257	1.085	0.567	1.026	0.942	0.428
FA 14:1 (n-5)_Myristoleic acid	LC/MS_Lipid	2.35.E-02	1.97.E-02	3.98.E-02	3.09.E-02	1.88.E-02	3.11.E-02	2.80.E-02	1.66.E-02	4.11.E-02	1.315	0.951	0.781	1.191	0.839	1.032	0.916	5.07.E-02	2.94.E-02	2.94.E-02	4.21.E-02	3.93.E-02	3.34.E-02	2.71.E-02	3.10.E-02	3.21.E-02	0.831	1.337	1.139	0.535	1.053	1.093	0.460
FA 14:0_Myristic acid	LC/MS_Lipid	9.24.E-02	9.23.E-02	1.36.E-01	1.38.E-01	8.73.E-02	1.16.E-01	1.31.E-01	7.29.E-02	1.48.E-01	1.492	0.946	0.850	1.421	0.790	1.085	0.836	2.99.E-01	2.10.E-01	2.01.E-01	2.43.E-01	2.34.E-01	2.12.E-01	2.44.E-01	1.93.E-01	2.29.E-01	0.812	1.115	1.053	0.817	0.920	1.135	0.810
FA 16:1 (n-7)_Palmitoleic acid	LC/MS_Lipid	5.65.E-01	2.73.E-01	9.88.E-01	6.64.E-01	2.94.E-01	8.40.E-01	6.78.E-01	2.44.E-01	9.93.E-01	1.176	1.077	0.849	1.200	0.895	1.004	0.805	9.15.E-01	6.11.E-01	6.86.E-01	7.78.E-01	7.07.E-01	6.89.E-01	5.90.E-01	6.80.E-01	7.26.E-01	0.851	1.156	1.004	0.645	1.114	1.059	0.725
FA 16:0_Palmitic acid	LC/MS_Lipid	3.37.E+00	2.90.E+00	3.72.E+00	3.53.E+00	2.81.E+00	3.57.E+00	3.91.E+00	2.92.E+00	3.89.E+00	1.048	0.969	0.961	1.162	1.006	1.046	0.143	1.11.E+01	7.65.E+00	8.48.E+00	8.48.E+00	9.66.E+00	8.00.E+00	7.78.E+00	7.32.E+00	8.85.E+00	0.767	1.264	0.943	0.703	0.957	1.043	0.654
FA 17:1 (n-7)_cis-10-Heptadecanoic acid	LC/MS_Lipid	4.82.E-02	3.92.E-02	5.61.E-02	6.23.E-02	3.71.E-02	5.78.E-02	6.16.E-02	3.44.E-02	5.69.E-02	1.291	0.945	1.031	1.278	0.877	1.014	0.589	1.22.E-01	8.64.E-02	9.56.E-02	9.65.E-02	9.72.E-02	8.92.E-02	8.74.E-02	8.68.E-02	1.08.E-01	0.794	1.124	0.933	0.719	1.004	1.132	0.793
FA 18:4 (n-3)_Stearidonic acid	LC/MS_Lipid	4.94.E-03	5.54.E-03	1.29.E-02	7.71.E-03	6.99.E-03	1.27.E-02	6.06.E-03	6.98.E-03	1.58.E-02	1.560	1.263	0.984	1.226	1.260	1.223	0.278	1.52.E-02	1.01.E-02	9.91.E-03	1.22.E-02	1.08.E-02	1.35.E-02	1.08.E-02	1.20.E-02	1.19.E-02	0.805	1.065	1.359	0.714	1.181	1.202	0.940
FA 18:3 (n-3)_Alpha-linolenic acid_(n-6)_gamma-Linolenic acid	LC/MS_Lipid	1.95.E-01	1.70.E-01	4.50.E-01	2.55.E-01	1.73.E-01	3.94.E-01	2.73.E-01	1.47.E-01	4.34.E-01	1.304	1.018	0.875	1.397	0.862	0.965	0.899	2.51.E-01	1.90.E-01	2.03.E-01	2.22.E-01	2.06.E-01	2.07.E-01	1.82.E-01	2.12.E-01	1.97.E-01	0.885	1.084	1.015	0.725	1.115	0.970	0.644
FA 18:2 (n-6)_Linoleic acid	LC/MS_Lipid	1.45.E+00	1.16.E+00	1.94.E+00	1.79.E+00	1.14.E+00	1.62.E+00	1.91.E+00	1.01.E+00	1.94.E+00	1.238	0.978	0.834	1.315	0.872	0.997	0.800	2.40.E+00	1.99.E+00	2.01.E+00	2.36.E+00	2.06.E+00	2.06.E+00	1.83.E+00	2.13.E+00	1.94.E+00	0.986	1.037	1.027	0.763	1.070	0.968	0.487
FA 18:1 (n-9)_cis-Oleic acid_(n-7)_cis-Vaccenic acid	LC/MS_Lipid	4.24.E+00	2.79.E+00	5.87.E+00	4.86.E+00	2.83.E+00	5.25.E+00	5.31.E+00	2.58.E+00	5.93.E+00	1.148	1.012	0.895	1.253	0.923	1.011	0.640	8.75.E+00	6.36.E+00	7.18.E+00	7.91.E+00	7.51.E+00	7.49.E+00	5.96.E+00	7.02.E+00	6.94.E+00	0.905	1.181	1.044	0.681	1.104	0.968	0.438
FA 18:0_Stearic acid	LC/MS_Lipid	2.89.E+00	2.92.E+00	2.03.E+00	3.01.E+00	2.40.E+00	2.03.E+00	3.09.E+00	2.55.E+00	2.14.E+00	1.043	0.824	1.000	1.070	0.875	1.053	0.678	5.23.E+00	3.87.E+00	4.40.E+00	4.55.E+00	4.56.E+00	4.25.E+00	3.77.E+00	4.29.E+00	4.36.E+00	0.869	1.178	0.965	0.721	1.110	0.990	0.686
FA 20:5 (n-3)_Eicosapentaenoic acid	LC/MS_Lipid	1.55.E-02	3.91.E-02	2.81.E-02	1.90.E-02	3.68.E-02	2.63.E-02	2.22.E-02	3.33.E-02	2.53.E-02	1.229	0.939	0.936	1.429	0.850	0.899	0.967	3.53.E-02	2.62.E-02	2.51.E-02	3.33.E-02	2.83.E-02	2.89.E-02	2.68.E-02	2.89.E-02	2.81.E-02	0.944	1.080	1.153	0.758	1.102	1.122	0.727
FA 20:4 (n-6)_Arachidonic acid	LC/MS_Lipid	2.62.E-01	3.86.E-01	3.04.E-01	2.94.E-01	3.91.E-01	2.75.E-01	3.00.E-01	3.47.E-01	2.99.E-01	1.123	1.013	0.905	1.145	0.897	0.982	0.967	3.68.E-01	2.76.E-01	3.04.E-01	3.42.E-01	3.19.E-01	3.03.E-01	2.70.E-01	3.17.E-01	2.81.E-01	0.929	1.157	0.998	0.733	1.150	0.925	0.542
FA 20:3 (n-6)_Dihomo-gamma-linolenic acid_(n-9)_Mead acid	LC/MS_Lipid	4.80.E-02	4.81.E-02	5.83.E-02	4.48.E-02	5.00.E-02	5.04.E-02	5.11.E-02	4.35.E-02	5.02.E-02	0.934	1.039	0.865	1.066	0.904	0.861	0.593	7.30.E-02	5.68.E-02	5.53.E-02	6.85.E-02	6.14.E-02	6.11.E-02	5.41.E-02	6.12.E-02	5.73.E-02	0.938	1.082	1.106	0.741	1.078	1.035	0.545
FA 20:2 (n-6)_cis-11-14-Eicosadienoic acid	LC/MS_Lipid	6.09.E-02	7.23.E-02	8.46.E-02	6.77.E-02	6.62.E-02	6.94.E-02	8.26.E-02	5.48.E-02	8.22.E-02	1.111	0.916	0.820	1.356	0.759	0.971	0.810	1.29.E-01	9.57.E-02	9.93.E-02	1.23.E-01	1.05.E-01	9.67.E-02	9.04.E-02	1.14.E-01	1.00.E-01	0.948	1.096	0.974	0.698	1.191	1.012	0.845
FA 20:1 (n-9)_cis-11-Eicosenoic acid	LC/MS_Lipid	1.41.E-01	1.11.E-01	2.24.E-01	1.67.E-01	1.11.E-01	1.97.E-01	1.78.E-01	1.06.E-01	2.36.E-01	1.179	1.003	0.878	1.258	0.956	1.055	0.503	3.13.E-01	2.33.E-01	2.60.E-01	2.76.E-01	2.96.E-01	2.40.E-01	2.15.E-01	2.40.E-01	2.73.E-01	0.882	1.268	0.921	0.687	1.027	1.050	0.659
FA 22:6 (n-3)_Docosahexaenoic acid	LC/MS_Lipid	8.65.E-02	1.72.E-01	1.37.E-01	1.01.E-01	1.55.E-01	1.13.E-01	1.02.E-01	1.39.E-01	1.29.E-01	1.164	0.904	0.828	1.178	0.811	0.941	0.722	2.10.E-01	1.82.E-01	1.78.E-01	2.11.E-01	1.81.E-01	1.74.E-01	1.68.E-01	1.93.E-01	1.63.E-01	1.006	0.998	0.976	0.798	1.063	0.913	0.478
FA 22:5 (n-6)_Docosapentaenoic acid	LC/MS_Lipid	7.25.E-02	1.04.E-01	1.01.E-01	7.75.E-02	1.00.E-01	9.40.E-02	8.92.E-02	9.27.E-02	1.01.E-01	1.069	0.965	0.934	1.230	0.894	1.007	0.822	1.36.E-01	9.73.E-02	1.07.E-01	1.17.E-01	1.06.E-01	9.89.E-02	1.02.E-01	1.14.E-01	9.47.E-02	0.860	1.086	0.925	0.751	1.176	0.885	0.672
FA 22:4 (n-6)_Docosatetraenoic acid	LC/MS_Lipid	2.76.E-02	4.29.E-02	3.97.E-02	3.78.E-02	4.11.E-02	3.40.E-02	3.99.E-02	3.61.E-02	4.08.E-02	1.371	0.959	0.858	1.445	0.841	1.030	0.896	7.10.E-02	5.57.E-02	5.91.E-02	7.31.E-02	5.85.E-02	5.80.E-02	5.53.E-02	6.23.E-02	5.17.E-02	1.028	1.050	0.982	0.779	1.118	0.874	0.462
FA 23:0_Tricosanoic acid	LC/MS_Lipid	6.97.E-02	8.95.E-02	1.00.E-01	9.35.E-02	8.62.E-02	8.51.E-02	9.37.E-02	7.22.E-02	1.01.E-01	1.341	0.964	0.847	1.344	0.807	1.009	0.972	9.05.E-02	9.35.E-02	8.99.E-02	1.08.E-01	9.61.E-02	8.44.E-02	8.90.E-02	9.86.E-02	9.25.E-02	1.193	1.027	0.939	0.984	1.054	1.029	0.754
FA 24:1 (n-9)_Nervonic acid	LC/MS_Lipid	1.20.E-01	1.46.E-01	1.47.E-01	1.36.E-01	1.49.E-01	1.56.E-01	1.49.E-01	1.35.E-01	1.57.E-01	1.140	1.016	1.066	1.242	0.920	1.069	0.502	1.71.E-01	1.55.E-01	1.60.E-01	1.69.E-01	1.74.E-01	1.47.E-01	1.70.E-01	1.69.E-01	1.74.E-01	0.984	1.119	0.920	0.989	1.093	1.090	0.549
FA 25:0_Pentacosanoic acid	LC/MS_Lipid	1.98.E-01	2.31.E-01	2.17.E-01	2.64.E-01	2.31.E-01	2.01.E-01	2.18.E-01	2.22.E-01	2.35.E-01	1.338	1.001	0.923	1.101	0.963	1.080	0.736	1.07.E-01	5.56.E-02	5.54.E-02	6.29.E-02	5.48.E-02	5.98.E-02	7.48.E-02	3.75.E-02	7.69.E-02	0.586	0.987	1.080	0.697	0.675	1.389	0.653
AC 2:0	LC/MS_Lipid	4.03.E+00	3.45.E+00	3.37.E+00	3.69.E+00	3.67.E+00	4.13.E+00	4.00.E+00	3.92.E+00	3.55.E+00	0.915	1.063	1.224	0.993	1.135	1.054	0.680	5.51.E+00	4.65.E+00	5.24.E+00	5.50.E+00	5.33.E+00	5.26.E+00	4.70.E+00	4.65.E+00	5.55.E+00	0.999	1.146	1.004	0.852	1.000	1.060	0.495
AC 4:0	LC/MS_Lipid	2.02.E-02	1.28.E-02	4.62.E-02	1.82.E-02	1.68.E-02	6.37.E-02	2.43.E-02	1.80.E-02	4.61.E-02	0.898	1.317	1.378	1.203	1.410	0.998	0.542	2.13.E-02	1.86.E-02	1.98.E-02	2.16.E-02	1.90.E-02	1.79.E-02	1.56.E-02	1.50.E-02	1.82.E-02	1.015	1.021	0.905	0.735	0.807	0.918	0.094
AC 6:0	LC/MS_Lipid	8.28.E-03	4.23.E-03	6.99.E-03	7.34.E-03	5.66.E-03	1.09.E-02	8.63.E-03	8.23.E-03	7.22.E-03	0.886	1.336	1.559	1.042	1.945	1.033	0.579	5.71.E-03	4.09.E-03	3.94.E-03	4.83.E-03	4.39.E-03	4.12.E-03	3.13.E-03	4.52.E-03	4.42.E-03	0.847	1.072	1.044	0.549	1.103	1.121	0.740
AC 8:0	LC/MS_Lipid	3.72.E-02	4.91.E-02	4.90.E-02	4.19.E-02	4.97.E-02	5.18.E-02	4.41.E-02	4.47.E-02	5.73.E-02	1.125	1.011	1.058	1.184	0.910	1.171	0.521	3.65.E-02	3.21.E-02	3.90.E-02	4.20.E-02	3.57.E-02	2.84.E-02	3.71.E-02	3.52.E-02	3.62.E-02	1.150	1.113	0.729	1.018	1.097	0.927	0.978
AC 10:0	LC/MS_Lipid	8.51.E-02	9.25.E-02	1.10.E-01	7.89.E-02	1.01.E-01	1.36.E-01	8.49.E-02	1.14.E-01	1.13.E-01	0.927	1.088	1.230	0.998	1.230	1.028	0.588	1.17.E-01	9.04.E-02	1.04.E-01	9.04.E-02	9.54.E-02	9.77.E-02	9.45.E-02	8.65.E-02	1.14.E-01	0.776	1.056	0.936	0.811	0.957	1.094	0.600
AC 12:0	LC/MS_Lipid	2.04.E-02	2.63.E-02	2.67.E-02	1.59.E-02	2.54.E-02	3.56.E-02	1.94.E-02	2.99.E-02	2.93.E-02	0.782	0.965	1.332	0.955	1.137	1.094	0.859	3.71.E-02	2.96.E-02	3.86.E-02	3.61.E-02	3.80.E-02	3.70.E-02	3.45.E-02	3.35.E-02	3.74.E-02	0.974	1.285	0.960	0.930	1.132	0.970	0.660
AC 14:0	LC/MS_Lipid	4.92.E-03	9.51.E-03	8.27.E-03	6.96.E-03	7.23.E-03	8.73.E-03	7.31.E-03	8.58.E-03	8.25.E-03	1.413	0.760	1.057	1.484	0.902	0.998	0.873	1.57.E-02	1.13.E-02	1.16.E-02	1.08.E-02	1.32.E-02	1.14.E-02	1.19.E-02	1.16.E-02	1.33.E-02	0.687	1.169	0.985	0.755	1.032	1.141	0.813
AC 14:1	LC/MS_Lipid	2.69.E-02	2.84.E-02	5.25.E-02	2.54.E-02	3.18.E-02	6.21.E-02	2.87.E-02	3.38.E-02	5.22.E-02	0.944	1.119	1.184	1.063	1.188	0.994	0.540	4.21.E-02	3.15.E-02	3.50.E-02	3.71.E-02	3.18.E-02	3.36.E-02	3.40.E-02	2.83.E-02	3.51.E-02	0.880	1.009	0.960	0.808	0.899	1.002	0.251
AC 16:0	LC/MS_Lipid	3.84.E-02	4.11.E-02	3.76.E-02	3.54.E-02	4.44.E-02	4.20.E-02	3.86.E-02	4.07.E-02	4.09.E-02	0.922	1.080	1.117	1.003	0.990	1.088	0.724	5.90.E-02	4.86.E-02	5.70.E-02	6.03.E-02	5.35.E-02	5.18.E-02	4.82.E-02	5.48.E-02	5.76.E-02	1.022	1.102	0.909	0.816	1.128	1.010	0.927
AC 16:1	LC/MS_Lipid	8.74.E-03	7.34.E-03	1.34.E-02	1.36.E-02	1.07.E-02	1.47.E-02	1.13.E-02	9.58.E-03	1.43.E-02	1.553	1.463	1.101	1.293	1.305	1.073	0.028	1.46.E-02	1.33.E-02	1.21.E-02	1.33.E-02	1.27.E-02	1.66.E-02	9.64.E-03	1.44.E-02	1.37.E-02	0.911	0.958	1.378	0.661	1.082	1.139	0.708
AC 18:0	LC/MS_Lipid	1.98.E-02	1.44.E-02	1.25.E-02	2.01.E-02	1.66.E-02	1.76.E-02	2.46.E-02	1.93.E-02	1.15.E-02	1.016	1.155	1.411	1.243	1.339	0.924	0.467	2.45.E-02	1.84.E-02	2.01.E-02	1.94.E-02	2.16.E-02	2.44.E-02	2.11.E-02	1.65.E-02	2.35.E-02	0.791	1.176	1.212	0.862	0.899	1.166	0.842
AC 18:1	LC/MS_Lipid	6.49.E-02	3.70.E-02	7.19.E-02	6.16.E-02	4.80.E-02	9.75.E-02	7.33.E-02	5.64.E-02	9.04.E-02	0.949	1.298	1.357	1.129	1.525	1.258	0.143	6.04.E-02	4.64.E-02	5.13.E-02	5.78.E-02	5.53.E-02	5.51.E-02	4.95.E-02	4.69.E-02	6.72.E-02	0.957	1.191	1.076	0.819	1.009	1.310	0.869
AC 18:2	LC/MS_Lipid	2.80.E-02	2.56.E-02	3.33.E-02	3.19.E-02	2.89.E-02	3.82.E-02	3.52.E-02	2.98.E-02	4.49.E-02	1.142	1.131	1.147	1.258	1.168	1.348	0.021	1.68.E-02	1.57.E-02	1.93.E-02	1.84.E-02	1.83.E-02	1.38.E-02	1.78.E-02	1.69.E-02	1.84.E-02	1.094	1.171	0.719	1.058	1.080	0.954	0.906

Derivatized metabolites in GC/MS analysis are labeled with 'TMS' (trimethylsilylation) and/or 'meto' (methoximation).

Ether-linked lipid species are labeled with 'e' (plasmanyl) or 'p' (plasmenyl).

Four types of methods, which targeted hydrophilic metabolites (GC/MS), cationic metabolites (LC/MS_Cation), anionic metabolites (LC/MS_Anion) and lipids (LC/MS_Lipid), were employed, and they were shown in the column of 'Method'.

P-values were calculated using the one-way repeated measures ANOVA.

N.D. indicates that the metabolite peak was not detected.

N.A. indicates that statistical test is not available due to insufficiency of the metabolite data.

Abbreviations: LPC, lysophosphatidylcholine; PC, phosphatidylcholine; LPE, lysophosphatidylethanolamine; PE, phosphatidylethanolamine; FA, fatty acid; AC, acylcarnitine

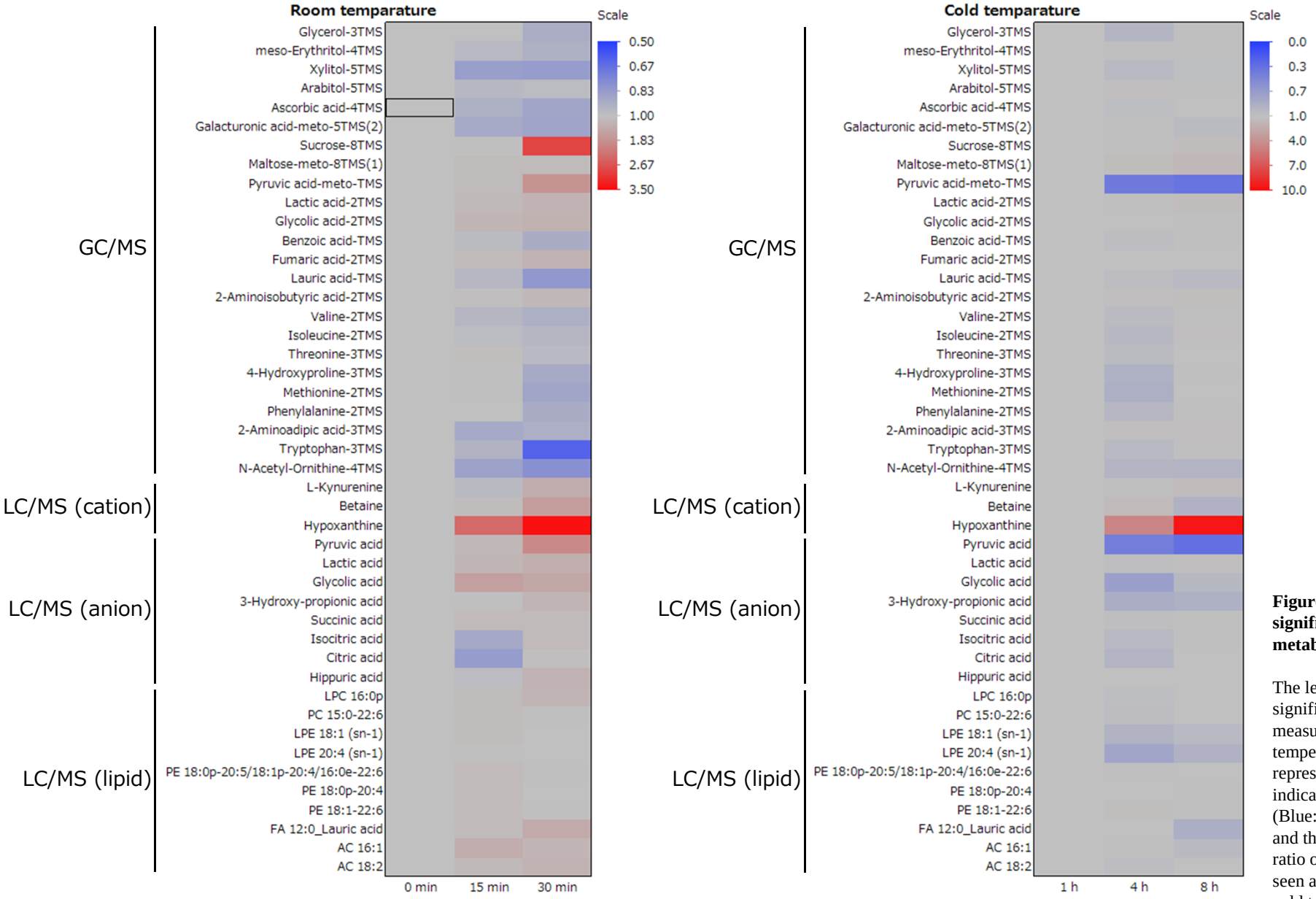


Figure S1. Heat map visualization of the significant changes in the plasma levels of metabolites caused by the storage conditions

The levels, of which the metabolites were significantly altered (one-way repeated measures ANOVA, $p < 0.05$) by storage at room temperature or cold temperature, are represented with the heat maps. Color key indicates the relative value of each metabolite (Blue: lowest, Red: highest; See the color scale), and the relative value is the geometric mean ratio of the plasma metabolite level to the level seen at 0 min at room temperature or at 1 h at cold temperature.