Supplementary Material for

Lipid perturbations in the saliva, plasma, and feces of patients with non-small cell lung cancer

Bo Young Hwang1, Jae Won Seo1, Can Muftuoglu2,3, Ufuk Mert3,4, Filiz Guldaval5, Milad Asadi2,3, Haydar Soydaner Karakus6, Tuncay Goksel3,6, Ali Veral7, Ayse Caner2,3.8\*, Myeong Hee Moon1\*

1Department of Chemistry, Yonsei University, Seodaemun-gu, Seoul, 03722, Korea

2 Institute of Health Sciences, Department of Basic Oncology, Ege University, Izmir, Turkey

3 Translational Pulmonary Research Center, Ege University (EgeSAM), Izmir, Turkey

4Ataturk Health Care Vocational School, Ege University, Izmir, Turkey

5Chest Disease Department, Izmir Dr. Suat Seren Chest Disease and Surgery Training and Research Hospital, Izmir, Turkey

6Department of Pulmonary Medicine, Faculty of Medicine, Ege University, Izmir, Turkey

7Department of Pathology, Ege University, Faculty of Medicine, Izmir, Turkey

8Department of Parasitology, Faculty of Medicine, Ege University, Izmir, Turkey

**Table of Contents**

Lipid analysis with *nUHPLC-ESI-MS/MS* ………...…...….……S-2

Figure S1 .…….………….………….………….………...………….……S-3

Figure S2 .…….………….………….………….………...………….……S-3

Table S1 .…….………….………….………….………...………….……S-4

Table S2 .…….………….………….………….………...………….……S-5

Table S3 .…….………….………….………….………...………….……S-6

Table S4 .…….………….………….………….………...………….……S-8

Table S5 .…….………….………….………….………...………….……S-10

Table S6 .…….………….………….………….………...………….……S-24

**ESI +**

**ESI -**

**Feces**

**Saliva**



**Plasma**



Figure S1. Base peak chromatograms of lipid extracts from saliva, plasma, and feces of patients with NSCLC at positive (ESI+) and negative (ESI-) ion modes of nUHPLC-ESI-MS/MS.

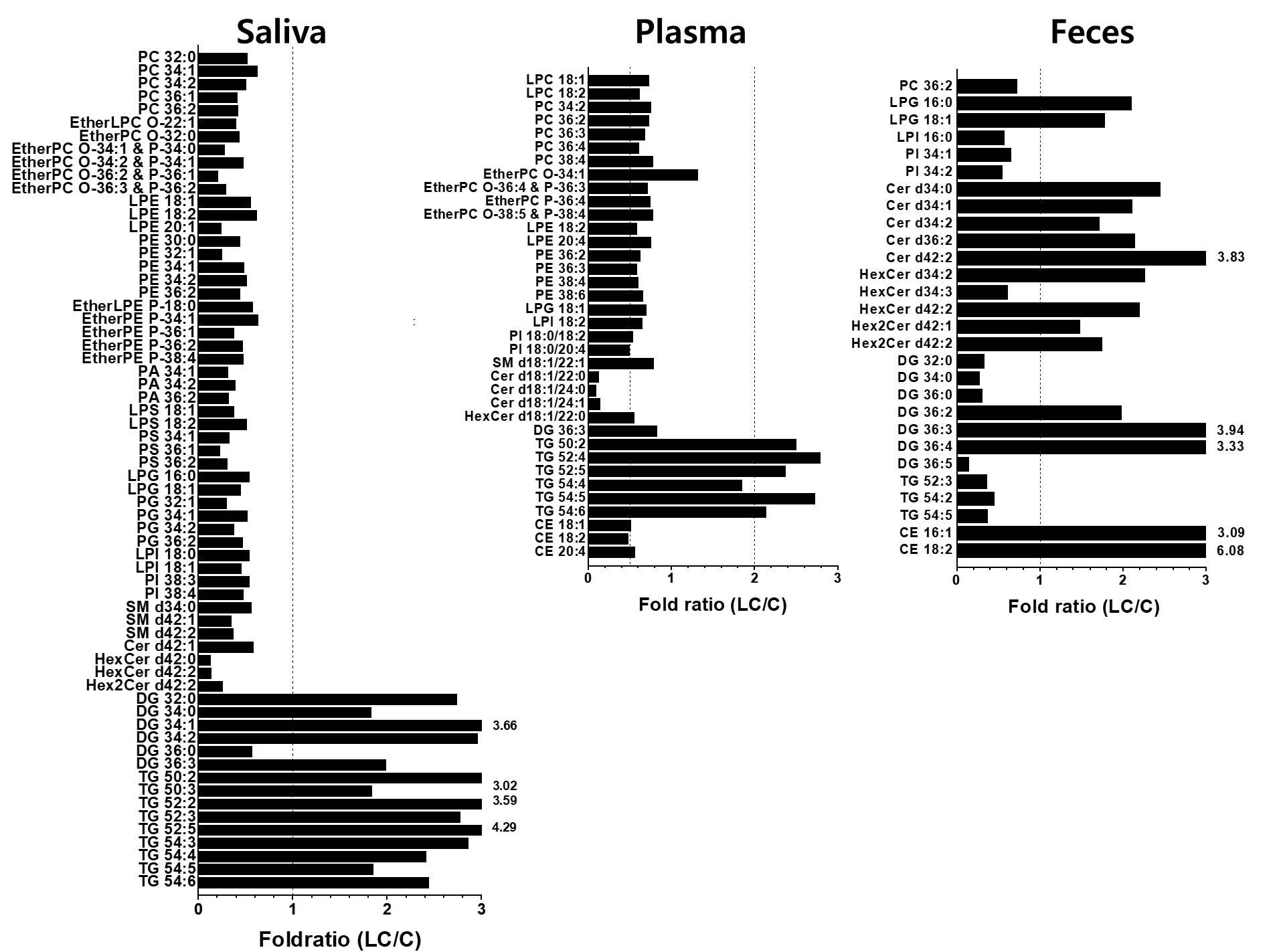


Figure S2. Bar graphs showing fold ratio (LC/C) of each lipid species with statistical significance (*p* < 0.05) in fecal, saliva, and plasma samples with LC compared to controls.

Table S1: List of lipid standards used for this study. Lipids marked with \* were used to prepare an internal standard lipid mixture.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| No. | Class | Acyl Chains | No. | Class | Acyl Chains |
| 1 | LPC | 16:0 | 25 | LPG | 17:1 |
| 2 | LPC | 17:1 | 26 | LPG | 13:0\* |
| 3 | LPC | 18:1-D7\* | 27 | PG | 17:0/17:0 |
| 4 | PC | 15:0/18:1-D7\* | 28 | PG | 15:0/18:1-D7\* |
| 5 | PC | 16:0/16:0 | 29 | LPI | 17:1 |
| 6 | PC | 17:0/17:0 | 30 | LPI | 13:0\* |
| 7 | PC | 18:1/18:0 | 31 | PI | 16:0-D31/18:1 |
| 8 | EtherPC | P-18:0/18:1-D9 | 32 | PI | 15:0/18:1-D7\* |
| 9 | LPE | 14:0 | 33 | SM | d18:1/17:0 |
| 10 | LPE | 17:1 | 34 | SM | d18:1/18:1-D9\* |
| 11 | LPE | 18:1-D7\* | 35 | Cer | d18:1/17:0 |
| 12 | PE | 12:0/12:0 | 36 | Cer | d18:1-D7/24:1 |
| 13 | PE | 16:0/16:0 | 37 | Cer | d18:1-D7/24:0\* |
| 14 | PE | 15:0/18:1-D7\* | 38 | HexCer | d18:1/17:0 |
| 15 | PE | 17:0/17:0 | 39 | HexCer | d18:1-D7/15:0\* |
| 16 | EtherPE | P-18:0/18:1-D9 | 40 | Hex2Cer | d18:1/16:0 |
| 17 | LPA | 17:0\* | 41 | Hex2Cer | d18:1/17:0 |
| 18 | LPA | 17:1 | 42 | Hex2Cer | d18:1-D7/15:0\* |
| 19 | PA | 15:0/18:1-D7\* | 43 | DG | 15:0/18:1-D7\* |
| 20 | PA | 17:0/17:0 | 44 | DG | 1,3-18:0-D5 |
| 21 | LPS | 17:1 | 45 | TG | 15:0/18:1-D7/15:0\* |
| 22 | LPS | 13:0\* | 46 | TG | 17:0/17:1/17:0-D5 |
| 23 | PS | 17:0/17:0 | 47 | CE | 17:0 |
| 24 | PS | 15:0/18:1-D7\* | 48 | CE | 18:1-D7\* |

Table S2: Type of precursor and quantifier ions of each lipid class and collision energy for SRM quantification

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| No. | Class | Type of precursor /quantifier ions | Acyl chain | | Collision  energy (V) |
| External standard | Internal  standard |
| 1 | LPC | [M+H]+/[Pcho+H]+ | 17:1 | 18:1-D7 | 40 |
| 2 | PC | [M+H]+/[Pcho+H]+ | 17:0/17:0 | 15:0/18:1-D7 | 40 |
| 3 | EtherPC | [M+H]+/[Pcho+H]+ | P-18:0/18:1-D9 | PC 15:0/18:1-D7 | 40 |
| 4 | LPE | [M+H]+/[M+H-141]+ | 17:1 | 18:1-D7 | 20 |
| 5 | PE | [M+H]+/[M+H-141]+ | 17:0/17:0 | 15:0/18:1-D7 | 20 |
| 6 | EtherPE | [M+H]+/ [M+H-RCOOCH2CHCH2OH]+ | P-18:0/18:1-D9 | PE 15:0/18:1-D7 | 30 |
| 7 | LPA | [M-H]-/[M-H-RCOOH]- | 17:0 | 17:1 | 35 |
| 8 | LPG | [M-H]-/[RCOO]- | 17:1 | 13:0 | 35 |
| 9 | PG | [M-H]-/[RCOO]- | 17:0/17:0 | 15:0/18:1-D7 | 35 |
| 10 | LPI | [M-H]-/[RCOO]- | 17:1 | 13:0 | 35 |
| 11 | PI | [M-H]-/[RCOO]- | 16:0-D31/18:1 | 15:0/18:1-D7 | 35 |
| 12 | SM | [M+H]+/[Pcho+H]+ | d18:1/17:0 | d18:1/18:1-D9 | 40 |
| 13 | Cer | [M+H]+/[d18:1]+ | d18:1-D7/24:1 | d18:1-D7/24:0 | 30 |
| 14 | Hex Cer | [M+H]+/[d18:1]+ | d18:1/17:0 | d18:1-D7/15:0 | 30 |
| 15 | Hex2Cer | [M+H]+/[d18:1]+ | d18:1/17:0 | d18:1-D7/13:0 | 50 |
| 16 | DG | [M+NH4]+/[M+H-RCOOH]+ | 1,3-18:0-D5 | 15:0/18:1-D7 | 35 |
| 17 | TG | [M+NH4]+/[M+H-RCOOH]+ | 17:0/17:1/17:0-D5 | 15:0/18:1-D7/15:0 | 35 |
| 18 | CE | [M+NH4]+/[Chole]+ | 17:0 | 18:1-D7 | 30 |
| ※ 141 Da : ethanolamine, Pcho : phosphocholine, Chole : Cholesterol | | | | | |

Table S3: Slopes and intercepts of the calibration curve of each lipid class

|  |  |  |  |
| --- | --- | --- | --- |
| Saliva | | | |
| class | slope | y-intercept | R2 |
| LPC | 1.9913 | 0.0585 | 0.998 |
| PC | 4.2368 | (0.1765) | 0.997 |
| EtherPC | 1.2347 | 0.1388 | 0.992 |
| LPE | 1.9064 | 0.0464 | 0.993 |
| PE | 14.2269 | (0.3364) | 0.992 |
| EtherPE | 1.8008 | 0.2004 | 0.992 |
| LPA | 2.0119 | 0.0064 | 0.994 |
| PA | 0.4716 | 0.0057 | 0.993 |
| LPS | 0.9314 | 0.3693 | 0.995 |
| PS | 0.8169 | 0.2198 | 0.995 |
| LPG | 7.7986 | (0.0219) | 0.995 |
| PG | 1.9112 | (0.0670) | 0.996 |
| LPI | 0.0792 | 0.0192 | 0.999 |
| PI | 0.7823 | 0.0037 | 0.996 |
| SM | 0.8927 | 0.8497 | 0.994 |
| Cer | 4.2431 | 0.1077 | 0.999 |
| HexCer | 2.3422 | 0.0072 | 0.990 |
| Hex2Cer | 0.2956 | 0.0586 | 0.996 |
| DG | 0.4466 | 0.0054 | 1.000 |
| TG | 0.7076 | 0.0323 | 0.999 |
| CE | 0.5914 | 0.0630 | 0.997 |
| Plasma | | | |
| class | slope | y-intercept | R2 |
| LPC | 2.6673 | 0.2034 | 0.997 |
| PC | 4.4555 | (0.0463) | 0.995 |
| EtherPC | 2.2140 | (0.0049) | 0.999 |
| LPE | 2.2037 | (0.0832) | 0.996 |
| PE | 0.9412 | 0.0139 | 0.988 |
| EtherPE | 0.9986 | (0.0192) | 0.984 |
| LPG | 0.1864 | (0.0106) | 0.994 |
| PG | 0.5927 | (0.0356) | 0.992 |
| LPI | 0.1218 | (0.0012) | 0.991 |
| PI | 0.4714 | 0.0371 | 0.997 |
| SM | 1.2610 | 0.0211 | 0.989 |
| Cer | 1.5294 | (0.0330) | 0.996 |
| HexCer | 1.1734 | 0.0299 | 0.993 |
| DG | 1.5608 | 0.1109 | 0.996 |
| TG | 0.8722 | (0.0344) | 0.997 |
| CE | 2.4883 | (0.0957) | 0.984 |
| Feces | | | |
| class | slope | y-intercept | R2 |
| LPC | 1.1421 | 0.0046 | 0.998 |
| PC | 0.8265 | 0.0039 | 0.992 |
| LPE | 0.5383 | (0.0032) | 0.996 |
| PE | 9.8917 | (0.0147) | 0.999 |
| LPG | 2.0193 | 0.0210 | 0.998 |
| PG | 2.9598 | (0.3508) | 0.992 |
| LPI | 0.3030 | (0.0007) | 0.997 |
| PI | 0.1579 | (0.0018) | 0.995 |
| LPS | 0.1130 | 0.0001 | 0.993 |
| PS | 1.1268 | 0.0003 | 0.995 |
| SM | 0.7525 | 0.0031 | 0.998 |
| Cer | 2.8732 | (0.0056) | 0.991 |
| HexCer | 0.5467 | 0.0033 | 0.993 |
| Hex2Cer | 0.5150 | 0.0076 | 0.999 |
| DG | 0.4466 | (0.0000) | 0.997 |
| TG | 0.7076 | 0.0007 | 0.992 |
| CE | 0.5914 | (0.0020) | 1.000 |

Table S4. Limit of detection (LOD) and limit of quantitation (LOQ) values of external lipid standards based on calibration curves and the type of internal standards spiked to lipid extracts by nUHPLC-ESI-MS/MS.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Saliva | | | | |
| class | external standard | internal standard | LOD (pmol) | LOQ (pmol) |
| LPC | 17:1 | 18:1-D7 | 0.05 | 0.17 |
| PC | 17:0/17:0 | 15:0/18:1-D7 | 0.09 | 0.29 |
| EtherPC | P-18:0/18:1-D9 | PC 15:0/18:1-D7 | 0.07 | 0.24 |
| LPE | 17:1 | 18:1-D7 | 0.04 | 0.12 |
| PE | 17:0/17:0 | 15:0/18:1-D7 | 0.13 | 0.42 |
| EtherPE | P-18:0/18:1-D9 | PE 15:0/18:1-D7 | 0.08 | 0.26 |
| LPA | 17:0 | 17:1 | 0.02 | 0.06 |
| PA | 17:0/17:0 | 15:0/18:1-D7 | 0.08 | 0.27 |
| LPS | 17:1 | 13:0 | 0.21 | 0.71 |
| PS | 17:0/17:0 | 15:0/18:1-D7 | 0.10 | 0.35 |
| LPG | 17:1 | 13:0 | 0.06 | 0.20 |
| PG | 17:0/17:0 | 15:0/18:1-D7 | 0.11 | 0.36 |
| LPI | 17:1 | 13:0 | 0.09 | 0.30 |
| PI | 16:0-D31/18:1 | 15:0/18:1-D7 | 0.00 | 0.01 |
| SM | d18:1/17:0 | d18:1/18:1-D9 | 0.12 | 0.40 |
| Cer | d18:1-D7/24:1 | d18:1-D7/24:0 | 0.03 | 0.10 |
| HexCer | d18:1/17:0 | d18:1-D7/15:0 | 0.07 | 0.25 |
| Hex2Cer | d18:1/17:0 | d18:1-D7/15:0 | 0.01 | 0.03 |
| DG | 1,3-18:0-D5 | 15:0/18:1-D7 | 0.01 | 0.04 |
| TG | 17:0/17:1/17:0-D5 | 15:0/18:1-D7/15:0 | 0.02 | 0.05 |
| CE | 17:0 | 18:1-D7 | 0.07 | 0.25 |
| Plasma | | | | |
| class | external standard | internal standard | LOD (pmol) | LOQ (pmol) |
| LPC | 17:1 | 18:1-D7 | 0.09 | 0.29 |
| PC | 17:0/17:0 | 15:0/18:1-D7 | 0.04 | 0.14 |
| EtherPC | P-18:0/18:1-D9 | PC 15:0/18:1-D7 | 0.06 | 0.21 |
| LPE | 17:1 | 18:1-D7 | 0.06 | 0.19 |
| PE | 17:0/17:0 | 15:0/18:1-D7 | 0.05 | 0.18 |
| EtherPE | P-18:0/18:1-D9 | PE 15:0/18:1-D7 | 0.04 | 0.14 |
| LPG | 17:1 | 13:0 | 0.02 | 0.06 |
| PG | 17:0/17:0 | 15:0/18:1-D7 | 0.10 | 0.34 |
| LPI | 17:1 | 13:0 | 0.08 | 0.27 |
| PI | 16:0-D31/18:1 | 15:0/18:1-D7 | 0.08 | 0.25 |
| SM | d18:1/17:0 | d18:1/18:1-D9 | 0.13 | 0.43 |
| Cer | d18:1-D7/24:1 | d18:1-D7/24:0 | 0.05 | 0.18 |
| HexCer | d18:1/17:0 | d18:1-D7/15:0 | 0.05 | 0.18 |
| DG | 1,3-18:0-D5 | 15:0/18:1-D7 | 0.10 | 0.33 |
| TG | 17:0/17:1/17:0-D5 | 15:0/18:1-D7/15:0 | 0.03 | 0.08 |
| CE | 17:0 | 18:1-D7 | 0.07 | 0.25 |
| Feces | | | | |
| class | calibration standard | internal standard | LOD (pmol) | LOQ (pmol) |
| LPC | 17:1 | 18:1-D7 | 0.00 | 0.02 |
| PC | 17:0/17:0 | 15:0/18:1-D7 | 0.04 | 0.12 |
| LPE | 17:1 | 18:1-D7 | 0.00 | 0.01 |
| PE | 17:0/17:0 | 15:0/18:1-D7 | 0.01 | 0.03 |
| LPG | 17:1 | 13:0 | 0.01 | 0.04 |
| PG | 17:0/17:0 | 15:0/18:1-D7 | 0.04 | 0.15 |
| LPI | 17:1 | 13:0 | 0.01 | 0.03 |
| PI | 16:0-D31/18:1 | 15:0/18:1-D7 | 0.05 | 0.17 |
| LPS | 17:1 | 13:0 | 0.01 | 0.05 |
| PS | 17:0/17:0 | 15:0/18:1-D7 | 0.05 | 0.17 |
| SM | d18:1/17:0 | d18:1/18:1-D9 | 0.01 | 0.03 |
| Cer | d18:1-D7/24:1 | d18:1-D7/24:0 | 0.01 | 0.04 |
| HexCer | d18:1/17:0 | d18:1-D7/15:0 | 0.02 | 0.05 |
| Hex2Cer | d18:1/17:0 | d18:1-D7/15:0 | 0.01 | 0.04 |
| DG | 1,3-18:0-D5 | 15:0/18:1-D7 | 0.02 | 0.05 |
| TG | 17:0/17:1/17:0-D5 | 15:0/18:1-D7/15:0 | 0.02 | 0.05 |
| CE | 17:0 | 18:1-D7 | 0.01 | 0.03 |
| ※ Limit of detection = 3 × standard deviation of y-intercept / slope,  Limit of qunatitation = 10 × standard deviation of y-intercept / slope | | | | |
|

Table S5. Concentration of lipid species (nmol/mL) in saliva, plasma, and fecal samples from both the control and the lung cancer groups. Lipid concentration was calculated from a calibration curve of each lipid class. Species marked with underline for high abundance species in each lipid class. Numbers in the parenthesis represent the quantified/identified numbers of lipids. N.D. represents for “not detectable” as below LOD (S/N = 3). Concentration values marked with grey represent for the calculated concentration below LOQ (S/N=10). Lipid concentration was calculated from a calibration curve of each lipid class. Species marked with underline for high abundance species in each lipid class. Numbers in the parenthesis represent the quantified/identified numbers of lipids. N.D. represents for “not detectable” as below LOD (S/N = 3). Concentration values marked with grey represent for the calculated concentration below LOQ (S/N=10).

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Saliva | | | | | | |
| Class | Molecular  species | *m/z* | Concentration (nmol/mL) | | abund. (%) | Fold ratio |
| C | LC | LC/C |
| LPC | 14:0 | 468.309 | 0.03 ± 0.03 | 0.04 ± 0.00 | 1.2 | 1.16 ± 1.08 |
| (9) | 16:1 | 494.324 | 0.08 ± 0.01 | 0.12 ± 0.01 | 3.1 | 1.48 ± 0.25 |
|  | 16:0 | 496.340 | 0.42 ± 0.14 | 0.45 ± 0.01 | 17.5 | 1.00 ± 0.30 |
|  | 18:2 | 520.340 | 0.55 ± 0.08 | 0.51 ± 0.02 | 21.3 | 0.78 ± 0.11 |
|  | 18:1 | 522.355 | 1.02 ± 0.07 | 0.99 ± 0.02 | 40.0 | 0.75 ± 0.06 |
|  | 18:0 | 524.371 | 0.20 ± 0.05 | 0.20 ± 0.01 | 8.2 | 0.93 ± 0.22 |
|  | 20:4 | 544.340 | 0.15 ± 0.05 | 0.11 ± 0.01 | 6.2 | 0.53 ± 0.18\*\* |
|  | 20:3 | 546.355 | 0.06 ± 0.02 | 0.04 ± 0.00 | 2.5 | **0.49 ± 0.13\*\*** |
|  | 22:5 | 570.355 | N.D. | N.D. | - | - |
| PC | 30:0 | 706.538 | 0.06 ± 0.01 | 0.05 ± 0.08 | 0.8 | 0.91 ± 0.61 |
| (21) | 32:1 | 732.554 | 0.29 ± 0.02 | 0.19 ± 0.09 | 3.9 | 0.66 ± 0.15 |
|  | 32:0 | 734.569 | 0.63 ± 0.05 | 0.32 ± 0.16 | 8.3 | 0.52 ± 0.13\*\* |
|  | 34:2 | 758.569 | 1.14 ± 0.06 | 0.57 ± 0.13 | 15.1 | **0.50 ± 0.06\*\*** |
|  | 34:1 | 760.585 | 1.27 ± 0.11 | 0.79 ± 0.17 | 16.9 | 0.62 ± 0.08\*\* |
|  | 34:0 | 762.601 | 0.28 ± 0.04 | 0.05 ± 0.02 | 3.7 | **0.17 ± 0.04\*\*** |
|  | 36:4 | 782.569 | 0.38 ± 0.03 | 0.07 ± 0.01 | 5.0 | **0.18 ± 0.02\*\*** |
|  | 36:3 | 784.585 | 0.65 ± 0.01 | 0.33 ± 0.02 | 8.7 | 0.51 ± 0.02\*\* |
|  | 36:2 | 786.601 | 1.29 ± 0.08 | 0.54 ± 0.08 | 17.2 | **0.42 ± 0.04\*\*** |
|  | 36:1 | 788.616 | 0.96 ± 0.17 | 0.40 ± 0.06 | 12.8 | **0.41 ± 0.08\*\*** |
|  | 36:0 | 790.632 | N.D. | N.D. | - | - |
|  | 38:6 | 806.569 | 0.07 ± 0.00 | N.D. | 0.9 | - |
|  | 38:5 | 808.585 | 0.12 ± 0.01 | 0.04 ± 0.00 | 1.6 | **0.36 ± 0.02\*\*** |
|  | 38:4 | 810.601 | 0.11 ± 0.01 | 0.04 ± 0.01 | 1.4 | **0.41 ± 0.04\*\*** |
|  | 38:3 | 812.616 | 0.12 ± 0.01 | N.D. | 1.6 | **-** |
|  | 38:2 | 814.632 | 0.12 ± 0.02 | N.D. | 1.5 | **-** |
|  | 38:1 | 816.648 | 0.04 ± 0.01 | N.D. | 0.5 | - |
|  | 40:6 | 834.601 | N.D. | N.D. | - | - |
|  | 40:2 | 842.663 | N.D. | N.D. | - | - |
|  | 42:0 | 874.726 | N.D. | N.D. | - | - |
|  | 44:1 | 900.742 | N.D. | N.D. | - | - |
| EtherLPC | O-16:1 and P-16:0 | 482.361 | 0.04 ± 0.00 | N.D. | 5.5 | - |
| (6) | O-16:0 | 480.345 | 0.09 ± 0.00 | 0.03 ± 0.00 | 14.3 | **0.27 ± 0.04\*\*** |
|  | O-18:1 and P-18:0 | 508.376 | 0.05 ± 0.00 | N.D. | 7.1 | **-** |
|  | O-22:1 | 564.439 | 0.11 ± 0.00 | 0.04 ± 0.00 | 17.1 | **0.39 ± 0.05\*\*** |
|  | P-24:1 | 592.470 | 0.10 ± 0.00 | N.D. | 15.5 | **-** |
|  | O-24:1 | 590.455 | 0.27 ± 0.01 | 0.15 ± 0.02 | 40.5 | 0.55 ± 0.09 |
| EtherPC | O-32:2 and P-32:1 | 716.559 | 0.20 ± 0.02 | 0.14 ± 0.00 | 1.2 | 0.71 ± 0.32 |
| (19) | O-32:1 and P-32:0 | 718.575 | 0.79 ± 0.01 | 0.43 ± 0.02 | 4.8 | 0.55 ± 0.06\*\* |
|  | O-32:0 | 720.590 | 1.78 ± 0.02 | 0.76 ± 0.05 | 10.8 | **0.43 ± 0.05\*\*** |
|  | O-34:3 and P-34:2 | 742.575 | 0.49 ± 0.01 | 0.24 ± 0.01 | 3.0 | **0.49 ± 0.04\*\*** |
|  | O-34:2 and P-34:1 | 744.590 | 2.05 ± 0.04 | 0.97 ± 0.05 | 12.4 | **0.47 ± 0.06\*\*** |
|  | O-34:1 and P-34:0 | 746.606 | 2.96 ± 0.05 | 0.82 ± 0.05 | 18.0 | **0.28 ± 0.03\*\*** |
|  | O-36:4 | 768.590 | 0.50 ± 0.00 | 0.18 ± 0.01 | 3.0 | **0.36 ± 0.03\*\*** |
|  | O-36:3 and P-36:2 | 770.606 | 0.90 ± 0.02 | 0.26 ± 0.01 | 5.5 | **0.29 ± 0.03\*\*** |
|  | O-36:2 and P-36:1 | 772.622 | 2.01 ± 0.05 | 0.41 ± 0.01 | 12.2 | **0.20 ± 0.03\*\*** |
|  | O-36:0 | 776.653 | 0.14 ± 0.00 | N.D. | 0.8 | **-** |
|  | O-38:5 and P-38:4 | 794.606 | 0.57 ± 0.01 | 0.16 ± 0.01 | 3.4 | **0.29 ± 0.03\*\*** |
|  | O-38:4 | 796.622 | 0.65 ± 0.01 | 0.16 ± 0.01 | 4.0 | **0.24 ± 0.03\*\*** |
|  | O-38:3 | 798.637 | 0.53 ± 0.01 | 0.11 ± 0.01 | 3.2 | **0.20 ± 0.03\*\*** |
|  | O-38:2 | 800.653 | 0.66 ± 0.02 | 0.10 ± 0.00 | 4.0 | **0.15 ± 0.02\*\*** |
|  | O-38:1 | 802.668 | 0.38 ± 0.01 | 0.04 ± 0.00 | 2.3 | **0.12 ± 0.02\*\*** |
|  | O-38:0 | 804.684 | 0.05 ± 0.00 | N.D. | 0.3 | - |
|  | O-40:3 | 826.668 | 0.54 ± 0.02 | 0.12 ± 0.01 | 3.3 | **0.21 ± 0.03\*\*** |
|  | O-40:2 and P-40:1 | 828.684 | 0.50 ± 0.02 | 0.06 ± 0.00 | 3.0 | **0.12 ± 0.02\*\*** |
|  | O-42:3 and P-42:2 | 854.700 | 0.79 ± 0.02 | 0.11 ± 0.01 | 4.8 | **0.14 ± 0.02\*\*** |
| LPE | 14:0 | 426.262 | 0.06 ± 0.01 | 0.04 ± 0.01 | 2.1 | 0.52 ± 0.23\* |
| (13) | 16:1 | 452.277 | 0.21 ± 0.00 | 0.15 ± 0.01 | 6.1 | 0.73 ± 0.10 |
|  | 16:0 | 454.293 | 0.47 ± 0.00 | 0.32 ± 0.01 | 13.2 | 0.74 ± 0.04 |
|  | 18:2 | 478.293 | 0.57 ± 0.01 | 0.35 ± 0.01 | 16.3 | 0.57 ± 0.08\*\* |
|  | 18:1 | 480.309 | 1.05 ± 0.04 | 0.57 ± 0.01 | 29.6 | 0.54 ± 0.10\*\* |
|  | 18:0 | 482.324 | 0.21 ± 0.01 | 0.21 ± 0.02 | 5.9 | 1.33 ± 0.33 |
|  | 20:4 | 502.293 | 0.46 ± 0.02 | 0.28 ± 0.01 | 12.6 | 0.68 ± 0.15 |
|  | 20:3 | 504.309 | 0.04 ± 0.00 | 0.04 ± 0.01 | 1.0 | 1.16 ± 0.47 |
|  | 20:2 | 506.324 | 0.02 ± 0.00 | N.D. | 0.6 | - |
|  | 20:1 | 508.340 | 0.57 ± 0.01 | 0.14 ± 0.01 | 7.9 | **0.32 ± 0.06\*\*** |
|  | 22:6 | 526.2928 | 0.07 ± 0.00 | 0.06 ± 0.00 | 2.0 | 1.11 ± 0.11 |
|  | 22:4 | 530.324 | 0.09 ± 0.00 | 0.04 ± 0.00 | 2.2 | **0.42 ± 0.07\*\*** |
|  | 24:0 | 566.418 | 0.03 ± 0.00 | 0.02 ± 0.01 | 0.5 | 1.09 ± 1.04 |
| PE | 30:1 | 662.476 | 0.09 ± 0.00 | N.D. | 3.6 | - |
| (14) | 30:0 | 664.491 | 0.22 ± 0.00 | 0.09 ± 0.06 | 9.1 | **0.44 ± 0.05\*\*** |
|  | 32:2 | 688.491 | 0.12 ± 0.00 | N.D. | 5.2 | - |
|  | 32:1 | 690.507 | 0.25 ± 0.00 | 0.06 ± 0.06 | 10.7 | **0.25 ± 0.03\*\*** |
|  | 32:0 | 692.523 | N.D. | N.D. | - | - |
|  | 34:3 | 714.507 | 0.05 ± 0.00 | N.D. | 2.0 | - |
|  | 34:2 | 716.523 | 0.31 ± 0.00 | 0.16 ± 0.07 | 13.3 | 0.51 ± 0.04\*\* |
|  | 34:1 | 718.538 | 0.21 ± 0.01 | 0.10 ± 0.06 | 8.8 | **0.48 ± 0.09\*\*** |
|  | 36:4 | 740.523 | 0.05 ± 0.00 | N.D. | 1.9 | - |
|  | 36:3 | 742.538 | 0.14 ± 0.00 | N.D. | 5.9 | - |
|  | 36:2 | 744.554 | 0.25 ± 0.00 | 0.11 ± 0.04 | 10.8 | **0.44 ± 0.03\*\*** |
|  | 36:1 | 746.569 | 0.31 ± 0.00 | 0.34 ± 0.19 | 13.0 | 1.10 ± 0.11 |
|  | 38:5 | 766.538 | N.D. | N.D. | - | - |
|  | 38:2 | 772.585 | 0.37 ± 0.01 | 0.28 ± 0.13 | 15.5 | 0.76 ± 0.09 |
| EtherLPE | P-16:0 | 438.298 | 0.29 ± 0.00 | 0.24 ± 0.01 | 35.3 | 0.83 ± 0.07 |
| (4) | P-18:1 | 464.314 | 0.10 ± 0.00 | 0.08 ± 0.00 | 11.9 | 0.76 ± 0.07 |
|  | P-18:0 | 466.329 | 0.37 ± 0.01 | 0.21 ± 0.01 | 44.1 | 0.57 ± 0.07\* |
|  | P-20:0 | 494.361 | 0.07 ± 0.00 | 0.04 ± 0.00 | 8.7 | 0.52 ± 0.06\* |
| EtherPE | P-32:1 | 674.512 | 0.44 ± 0.01 | 0.43 ± 0.02 | 2.4 | 0.98 ± 0.11 |
| (15) | P-34:2 | 700.528 | 0.84 ± 0.05 | 0.52 ± 0.05 | 4.6 | 0.62 ± 0.17\* |
|  | P-34:1 | 702.543 | 4.46 ± 0.05 | 2.80 ± 0.21 | 24.1 | 0.63 ± 0.06\* |
|  | P-34:0 | 704.559 | 0.56 ± 0.03 | 0.43 ± 0.04 | 3.0 | 0.77 ± 0.19 |
|  | P-36:5 | 730.575 | 1.15 ± 0.01 | 0.59 ± 0.04 | 6.2 | 0.52 ± 0.05\* |
|  | P-36:2 | 728.559 | 2.18 ± 0.03 | 1.02 ± 0.06 | 11.7 | **0.47 ± 0.04\*\*** |
|  | P-36:1 | 748.528 | 2.09 ± 0.04 | 0.77 ± 0.03 | 11.3 | **0.37 ± 0.04\*\*** |
|  | P-38:6 | 750.543 | 0.46 ± 0.01 | 0.36 ± 0.02 | 2.5 | 0.77 ± 0.08 |
|  | P-38:4 | 752.559 | 2.33 ± 0.03 | 1.10 ± 0.05 | 12.6 | **0.47 ± 0.04\*\*** |
|  | O-38:4 and P-38:3 | 754.575 | 0.80 ± 0.01 | 0.34 ± 0.02 | 4.3 | **0.43 ± 0.04\*\*** |
|  | P-38:2 | 756.590 | 0.38 ± 0.01 | 0.16 ± 0.01 | 2.0 | **0.44 ± 0.05\*\*** |
|  | P-38:1 | 758.606 | 0.66 ± 0.02 | 0.34 ± 0.02 | 3.6 | 0.51 ± 0.08\* |
|  | P-38:0 | 760.622 | 0.94 ± 0.02 | 0.35 ± 0.03 | 5.1 | **0.37 ± 0.05\*\*** |
|  | P-40:5 | 778.575 | 0.46 ± 0.00 | 0.18 ± 0.01 | 2.5 | **0.40 ± 0.03\*\*** |
|  | P-40:4 | 780.590 | 0.78 ± 0.01 | 0.17 ± 0.02 | 4.2 | **0.22 ± 0.03\*\*** |
| LPA | 16:1 | 407.220 | N.D. | N.D. | - | - |
| (8) | 16:0 | 409.236 | 0.09 ± 0.01 | 0.07 ± 0.02 | 16.9 | 0.53 ± 0.23\* |
|  | 18:3 | 431.220 | N.D. | N.D. | - | - |
|  | 18:2 | 433.236 | 0.06 ± 0.00 | 0.05 ± 0.01 | 11.0 | 0.63 ± 0.17 |
|  | 18:1 | 432.252 | N.D. | N.D. | - | - |
|  | 18:0 | 437.267 | 0.47 ± 0.03 | 0.13 ± 0.03 | 69.4 | **0.30 ± 0.12** |
|  | 20:4 | 457.236 | 0.02 ± 0.00 | N.D. | 2.8 | **-** |
|  | 20:3 | 459.252 | N.D. | N.D. | - | - |
| PA | 30:0 | 619.434 | 0.04 ± 0.00 | N.D. | 1.5 | - |
| (6) | 34:2 | 671.466 | 0.45 ± 0.01 | 0.17 ± 0.00 | 17.1 | **0.39 ± 0.03\*\*** |
|  | 34:1 | 673.481 | 0.82 ± 0.01 | 0.25 ± 0.00 | 31.0 | **0.31 ± 0.02\*\*** |
|  | 36:3 | 697.481 | 0.31 ± 0.00 | 0.09 ± 0.00 | 11.6 | **0.31 ± 0.02\*\*** |
|  | 36:2 | 699.497 | 0.84 ± 0.01 | 0.27 ± 0.00 | 31.8 | **0.32 ± 0.03\*\*** |
|  | 38:4 | 723.497 | 0.19 ± 0.01 | 0.08 ± 0.00 | 7.1 | **0.42 ± 0.09\*\*** |
| LPS | 16:1 | 494.253 | 0.24 ± 0.01 | 0.16 ± 0.01 | 3.6 | 0.65 ± 0.17 |
| (10) | 16:0 | 496.268 | N.D. | N.D. | - | - |
|  | 18:2 | 520.268 | 1.03 ± 0.03 | 0.52 ± 0.06 | 15.5 | 0.51 ± 0.14\*\* |
|  | 18:1 | 522.284 | 4.05 ± 0.15 | 1.52 ± 0.14 | 61.2 | **0.38 ± 0.10\*\*** |
|  | 18:0 | 524.299 | 0.18 ± 0.01 | 0.10 ± 0.03 | 2.6 | 0.57 ± 0.36 |
|  | 20:4 | 544.268 | 0.65 ± 0.02 | 0.27 ± 0.03 | 9.8 | **0.42 ± 0.10\*\*** |
|  | 20:3 | 546.284 | 0.25 ± 0.01 | 0.14 ± 0.02 | 3.8 | 0.54 ± 0.17\* |
|  | 22:6 | 568.268 | 0.14 ± 0.01 | 0.10 ± 0.02 | 2.1 | 0.70 ± 0.34 |
|  | 22:5 | 570.284 | N.D. | N.D. | - | - |
|  | 22:0 | 580.362 | 0.08 ± 0.01 | N.D. | 1.2 | - |
| PS | 30:0 | 706.467 | 0.05 ± 0.01 | N.D. | 0.3 | - |
| (18) | 32:2 | 730.467 | 0.10 ± 0.01 | 0.04 ± 0.00 | 0.6 | **0.38 ± 0.22\*** |
|  | 32:1 | 732.482 | 0.16 ± 0.01 | 0.05 ± 0.01 | 0.9 | **0.28 ± 0.15\*\*** |
|  | 34:2 | 758.498 | 0.50 ± 0.02 | 0.11 ± 0.00 | 2.7 | **0.23 ± 0.05\*\*** |
|  | 34:1 | 760.513 | 1.23 ± 0.06 | 0.39 ± 0.01 | 6.6 | **0.32 ± 0.08\*\*** |
|  | 36:3 | 784.513 | 0.17 ± 0.01 | N.D. | 0.9 | - |
|  | 36:2 | 786.529 | 2.45 ± 0.08 | 0.74 ± 0.02 | 13.1 | **0.30 ± 0.05\*\*** |
|  | 36:1 | 788.545 | 12.02 ± 0.20 | 2.72 ± 0.10 | 64.4 | **0.23 ± 0.03\*\*** |
|  | 38:4 | 810.529 | 0.51 ± 0.03 | 0.09 ± 0.00 | 2.7 | **0.17 ± 0.06\*\*** |
|  | 38:3 | 812.545 | 0.38 ± 0.01 | 0.14 ± 0.00 | 2.1 | **0.35 ± 0.05\*\*** |
|  | 38:2 | 814.560 | 0.27 ± 0.00 | 0.07 ± 0.00 | 1.5 | **0.26 ± 0.03\*\*** |
|  | 38:1 | 816.576 | 0.06 ± 0.01 | 0.08 ± 0.00 | 0.3 | 1.36 ± 0.99 |
|  | 40:6 | 834.529 | 0.17 ± 0.00 | 0.10 ± 0.01 | 0.9 | 0.57 ± 0.10\* |
|  | 40:2 | 842.592 | 0.14 ± 0.00 | 0.04 ± 0.00 | 0.8 | 0.27 ± 0.04\* |
|  | 40:1 | 844.607 | 0.13 ± 0.01 | 0.06 ± 0.00 | 0.7 | **0.45 ± 0.11\*\*** |
|  | 42:3 | 868.607 | N.D. | N.D. | - | - |
|  | 42:2 | 870.623 | 0.08 ± 0.00 | N.D. | 0.4 | - |
|  | 42:1 | 872.639 | 0.23 ± 0.02 | 0.04 ± 0.00 | 1.2 | **0.16 ± 0.05\*\*** |
| LPG | 14:1 | 453.226 | N.D. | N.D. | - | - |
| (9) | 14:0 | 455.242 | N.D. | N.D. | - | - |
|  | 16:1 | 481.257 | N.D. | N.D. | - | - |
|  | 16:0 | 483.273 | 0.10 ± 0.00 | 0.05 ± 0.03 | 33.1 | 0.54 ± 0.14\* |
|  | 18:2 | 507.273 | 0.03 ± 0.00 | 0.02 ± 0.01 | 9.4 | 0.56 ± 0.25\* |
|  | 18:1 | 509.289 | 0.13 ± 0.02 | 0.06 ± 0.03 | 44.2 | **0.44 ± 0.25\*** |
|  | 18:0 | 511.304 | 0.04 ± 0.01 | 0.02 ± 0.02 | 13.2 | 0.53 ± 0.58\* |
|  | 20:3 | 533.289 | N.D. | N.D. | - | - |
|  | 20:1 | 537.320 | N.D. | N.D. | - | - |
| PG | 30:1 | 691.456 | N.D. | N.D. | - | - |
| (19) | 30:0 | 693.471 | 0.08 ± 0.03 | 0.05 ± 0.00 | 3.4 | 0.66 ± 0.98 |
|  | 32:1 | 719.487 | 0.22 ± 0.23 | 0.07 ± 0.00 | 9.4 | **0.30 ± 1.49\*\*** |
|  | 32:0 | 721.503 | 0.14 ± 0.08 | 0.13 ± 0.01 | 5.9 | 0.96 ± 2.56 |
|  | 34:3 | 743.487 | 0.04 ± 0.08 | N.D. | 1.5 | - |
|  | 34:2 | 745.503 | 0.25 ± 0.07 | 0.09 ± 0.01 | 10.7 | **0.37 ± 0.52\*\*** |
|  | 34:1 | 747.518 | 0.60 ± 0.23 | 0.31 ± 0.03 | 25.7 | 0.52 ± 0.95\* |
|  | 34:0 | 749.534 | 0.15 ± 0.14 | 0.03 ± 0.00 | 6.5 | **0.20 ± 0.82\*\*** |
|  | 36:4 | 769.503 | 0.09 ± 0.14 | 0.04 ± 0.00 | 4.0 | **0.38 ± 2.73\*\*** |
|  | 36:3 | 771.518 | 0.20 ± 0.08 | 0.08 ± 0.01 | 8.6 | **0.38 ± 0.74\*\*** |
|  | 36:2 | 773.534 | 0.46 ± 0.16 | 0.21 ± 0.04 | 19.7 | **0.46 ± 0.77\*\*** |
|  | 36:1 | 775.550 | 0.11 ± 0.02 | 0.08 ± 0.02 | 4.6 | 0.75 ± 0.81 |
|  | 36:0 | 777.565 | N.D. | N.D. | - | - |
|  | 38:5 | 795.518 | N.D. | N.D. | - | - |
|  | 38:4 | 797.534 | N.D. | N.D. | - | - |
|  | 38:3 | 799.550 | N.D. | N.D. | - | - |
|  | 38:2 | 801.565 | N.D. | N.D. | - | - |
|  | 40:7 | 819.518 | N.D. | N.D. | - | - |
|  | 40:6 | 821.534 | N.D. | N.D. | - | - |
| LPI | 16:1 | 569.273 | 0.54 ± 0.03 | 0.75 ± 0.00 | 3.4 | 1.40 ± 0.34 |
| (8) | 16:0 | 571.289 | 2.63 ± 0.47 | 1.87 ± 0.01 | 16.6 | 0.71 ± 0.60 |
|  | 18:2 | 595.289 | 1.48 ± 0.10 | 1.36 ± 0.00 | 9.4 | 0.92 ± 0.31 |
|  | 18:1 | 597.305 | 3.78 ± 0.42 | 1.71 ± 0.01 | 23.9 | 0.45 ± 0.24\* |
|  | 18:0 | 599.320 | 6.00 ± 0.31 | 3.24 ± 0.01 | 37.9 | 0.54 ± 0.14\*\* |
|  | 20:4 | 619.289 | 0.98 ± 0.08 | 0.57 ± 0.00 | 6.2 | 0.59 ± 0.23 |
|  | 20:3 | 621.305 | 0.42 ± 0.01 | 0.21 ± 0.00 | 2.7 | 0.51 ± 0.12\* |
|  | 22:5 | 645.305 | N.D. | N.D. | - | - |
| PI | 28:0 | 753.456 | 0.01 ± 0.00 | 0.00 ± 0.00 | 0.1 | 0.56 ± 0.43 |
| (22) | 30:0 | 781.487 | 0.03 ± 0.01 | 0.02 ± 0.00 | 0.4 | 0.72 ± 0.67 |
|  | 32:2 | 805.487 | 0.06 ± 0.00 | 0.04 ± 0.00 | 0.7 | 0.56 ± 0.08\*\* |
|  | 32:1 | 807.503 | 0.27 ± 0.01 | 0.21 ± 0.00 | 2.9 | 0.77 ± 0.13 |
|  | 32:0 | 809.519 | 0.18 ± 0.05 | 0.10 ± 0.00 | 1.9 | 0.56 ± 0.75\* |
|  | 34:3 | 831.503 | 0.08 ± 0.00 | 0.06 ± 0.00 | 0.8 | 0.79 ± 0.08 |
|  | 34:2 | 833.519 | 0.61 ± 0.01 | 0.65 ± 0.01 | 6.5 | 1.06 ± 0.12 |
|  | 34:1 | 835.534 | 1.25 ± 0.04 | 0.96 ± 0.03 | 13.3 | 0.77 ± 0.13 |
|  | 34:0 | 837.550 | 0.37 ± 0.03 | 0.13 ± 0.01 | 3.9 | **0.35 ± 0.12\*\*** |
|  | 36:4 | 857.519 | 0.15 ± 0.00 | 0.13 ± 0.00 | 1.6 | 0.86 ± 0.10 |
|  | 36:3 | 859.534 | 0.42 ± 0.00 | 0.26 ± 0.00 | 4.5 | 0.63 ± 0.04 |
|  | 36:2 | 861.550 | 1.55 ± 0.06 | 1.09 ± 0.07 | 16.5 | 0.70 ± 0.16 |
|  | 36:1 | 863.566 | 0.99 ± 0.04 | 0.53 ± 0.02 | 10.5 | 0.54 ± 0.11 |
|  | 36:0 | 865.581 | 0.02 ± 0.00 | 0.01 ± 0.00 | 0.2 | **0.28 ± 0.26\*\*** |
|  | 38:6 | 881.519 | 0.02 ± 0.00 | 0.01 ± 0.00 | 0.2 | 0.76 ± 0.22 |
|  | 38:5 | 883.534 | 0.12 ± 0.00 | 0.06 ± 0.00 | 1.3 | 0.49 ± 0.05\* |
|  | 38:4 | 885.550 | 2.09 ± 0.07 | 0.99 ± 0.03 | 22.3 | **0.47 ± 0.08\*\*** |
|  | 38:3 | 887.566 | 0.95 ± 0.03 | 0.51 ± 0.03 | 10.1 | 0.54 ± 0.11\* |
|  | 38:2 | 889.581 | 0.07 ± 0.00 | 0.07 ± 0.00 | 0.8 | 0.94 ± 0.31 |
|  | 38:1 | 891.597 | 0.01 ± 0.00 | 0.01 ± 0.00 | 0.1 | 0.68 ± 0.39 |
|  | 40:5 | 911.566 | 0.05 ± 0.00 | 0.03 ± 0.00 | 0.5 | 0.64 ± 0.09 |
|  | 40:4 | 913.581 | 0.07 ± 0.00 | 0.06 ± 0.00 | 0.8 | 0.83 ± 0.16 |
| SM | d32:1 | 675.544 | 1.55 ± 0.03 | 0.87 ± 0.03 | 4.5 | 0.56 ± 0.06\*\* |
| (16) | d32:0 | 677.559 | 0.27 ± 0.01 | 0.23 ± 0.01 | 0.8 | 0.84 ± 0.09 |
|  | d34:2 | 701.559 | 1.02 ± 0.02 | 0.57 ± 0.02 | 3.0 | 0.55 ± 0.07\*\* |
|  | d34:1 | 703.575 | 8.86 ± 0.12 | 8.09 ± 0.24 | 25.7 | 0.91 ± 0.08 |
|  | d34:0 | 705.591 | 6.83 ± 0.16 | 3.82 ± 0.17 | 19.8 | 0.56 ± 0.08\*\* |
|  | d36:2 | 729.591 | 0.28 ± 0.01 | 0.10 ± 0.01 | 0.8 | **0.37 ± 0.06\*\*** |
|  | d36:1 | 731.606 | 1.00 ± 0.02 | 0.46 ± 0.02 | 2.9 | **0.46 ± 0.06\*\*** |
|  | d36:0 | 733.622 | 1.30 ± 0.03 | 0.63 ± 0.02 | 3.8 | **0.49 ± 0.06\*\*** |
|  | d38:2 | 757.622 | 0.10 ± 0.00 | N.D. | 0.3 | - |
|  | d38:1 | 759.637 | 0.75 ± 0.04 | 0.36 ± 0.01 | 2.2 | **0.48 ± 0.11\*\*** |
|  | d40:2 | 785.653 | 0.57 ± 0.02 | 0.18 ± 0.01 | 1.6 | **0.32 ± 0.06\*\*** |
|  | d40:1 | 787.669 | 1.67 ± 0.10 | 0.63 ± 0.02 | 4.8 | **0.38 ± 0.11\*\*** |
|  | d40:0 | 789.684 | 1.20 ± 0.06 | 0.33 ± 0.01 | 3.5 | **0.28 ± 0.07\*\*** |
|  | d42:2 | 813.684 | 5.36 ± 0.23 | 1.98 ± 0.06 | 15.5 | **0.37 ± 0.08\*\*** |
|  | d42:1 | 815.700 | 2.54 ± 0.14 | 0.87 ± 0.04 | 7.3 | **0.34 ± 0.09\*\*** |
|  | d42:0 | 817.716 | 1.21 ± 0.07 | 0.34 ± 0.02 | 3.5 | **0.28 ± 0.08\*\*** |
| Cer | d34:2 | 536.504 | 0.11 ± 0.01 | 0.56 ± 0.10 | 2.3 | **5.17 ± 1.29\*\*** |
| (15) | d34:1 | 538.519 | 0.59 ± 0.04 | 1.09 ± 0.42 | 12.9 | 1.83 ± 0.71\* |
|  | d34:0 | 540.535 | 0.54 ± 0.02 | 1.00 ± 0.55 | 11.7 | 1.85 ± 0.62\* |
|  | d36:2 | 564.535 | 0.04 ± 0.00 | 0.08 ± 0.04 | 0.9 | 1.90 ± 0.46\* |
|  | d36:1 | 566.551 | 0.24 ± 0.01 | 0.37 ± 0.09 | 5.2 | 1.56 ± 0.29 |
|  | d36:0 | 568.566 | 0.34 ± 0.01 | 0.28 ± 0.11 | 7.3 | 0.84 ± 0.19 |
|  | d38:1 | 594.582 | 0.20 ± 0.01 | 0.19 ± 0.08 | 4.3 | 0.97 ± 0.22 |
|  | d38:0 | 596.598 | 0.29 ± 0.00 | 0.08 ± 0.05 | 6.3 | **0.27 ± 0.08\*\*** |
|  | d40:1 | 622.613 | 0.21 ± 0.00 | 0.22 ± 0.05 | 4.6 | 1.03 ± 0.12 |
|  | d40:0 | 624.629 | 0.19 ± 0.00 | 0.14 ± 0.06 | 4.1 | 0.76 ± 0.16 |
|  | d42:2 | 648.629 | 0.48 ± 0.01 | 0.48 ± 0.08 | 10.3 | 1.01 ± 0.10 |
|  | d42:1 | 650.645 | 0.49 ± 0.01 | 0.28 ± 0.04 | 10.7 | 0.58 ± 0.05\* |
|  | d42:0 | 652.660 | 0.31 ± 0.01 | 0.46 ± 0.16 | 6.8 | 1.46 ± 0.35 |
|  | d44:1 | 678.676 | 0.27 ± 0.01 | 0.27 ± 0.13 | 5.8 | 1.02 ± 0.24 |
|  | d44:0 | 680.692 | 0.30 ± 0.00 | 0.21 ± 0.04 | 6.6 | 0.69 ± 0.07 |
| HexCer | d34:1 | 862.625 | 0.36 ± 0.04 | 0.05 ± 0.01 | 20.8 | **0.14 ± 0.07\*\*** |
| (4) | d40:0 | 946.719 | 0.33 ± 0.01 | 0.04 ± 0.01 | 19.3 | **0.13 ± 0.03\*\*** |
|  | d42:2 | 972.735 | 0.48 ± 0.02 | 0.06 ± 0.02 | 28.0 | **0.13 ± 0.03\*\*** |
|  | d42:0 | 974.750 | 0.55 ± 0.02 | 0.07 ± 0.01 | 31.9 | **0.12 ± 0.03\*\*** |
| Hex2Cer | d34:1 | 862.625 | 1.31 ± 0.02 | 0.76 ± 0.06 | 32.0 | 0.58 ± 0.06 |
| (4) | d40:1 | 946.719 | 0.32 ± 0.01 | 0.05 ± 0.01 | 7.8 | **0.14 ± 0.03\*\*** |
|  | d42:2 | 972.735 | 1.96 ± 0.09 | 0.49 ± 0.06 | 47.6 | **0.25 ± 0.06\*\*** |
|  | d42:1 | 974.750 | 0.52 ± 0.02 | 0.11 ± 0.02 | 12.7 | **0.22 ± 0.05\*\*** |
| DG | 30:0 | 558.509 | 0.76 ± 0.02 | 2.67 ± 0.12 | 1.4 | **3.52 ± 0.84\*\*** |
| (14) | 32:2 | 582.509 | 0.30 ± 0.01 | 1.73 ± 0.05 | 0.6 | **5.71 ± 1.29\*\*** |
|  | 32:1 | 584.525 | 1.61 ± 0.02 | 5.74 ± 0.19 | 3.0 | **3.57 ± 0.56\*\*** |
|  | 32:0 | 586.541 | 5.19 ± 0.06 | 14.19 ± 0.41 | 9.7 | **2.73 ± 0.38\*\*** |
|  | 34:2 | 610.541 | 4.94 ± 0.06 | 14.60 ± 0.46 | 9.2 | **2.95 ± 0.45\*\*** |
|  | 34:1 | 612.556 | 7.05 ± 0.08 | 25.83 ± 0.78 | 13.1 | **3.67 ± 0.53\*\*** |
|  | 34:0 | 614.572 | 5.63 ± 0.11 | 10.28 ± 0.52 | 10.5 | 1.82 ± 0.44\*\* |
|  | 36:4 | 634.541 | 1.94 ± 0.04 | 10.01 ± 0.34 | 3.6 | **5.16 ± 0.93\*\*** |
|  | 36:3 | 636.556 | 4.46 ± 0.04 | 8.84 ± 0.22 | 8.3 | 1.98 ± 0.23\*\* |
|  | 36:2 | 638.572 | 8.89 ± 0.12 | 16.84 ± 0.58 | 16.6 | 1.89 ± 0.31\* |
|  | 36:1 | 640.588 | 2.70 ± 0.05 | 4.38 ± 0.28 | 5.0 | 1.62 ± 0.48\* |
|  | 36:0 | 642.603 | 4.91 ± 0.09 | 2.77 ± 0.09 | 9.1 | 0.57 ± 0.10\*\* |
|  | 38:4 | 662.572 | 3.38 ± 0.07 | 1.78 ± 0.08 | 6.3 | 0.52 ± 0.12\*\* |
|  | 38:3 | 664.588 | 1.88 ± 0.03 | 1.25 ± 0.04 | 3.5 | 0.66 ± 0.10 |
| TG | 38:0 | 684.614 | 1.07 ± 0.18 | 13.47 ± 5.61 | 1.2 | **12.62 ± 17.76\*\*** |
| (43) | 40:0 | 712.645 | 0.55 ± 0.03 | 5.41 ± 0.81 | 0.6 | **9.75 ± 4.92\*\*** |
|  | 42:2 | 736.645 | 0.37 ± 0.01 | 2.25 ± 0.57 | 0.4 | **6.08 ± 4.46** |
|  | 42:1 | 738.661 | 0.72 ± 0.02 | 2.11 ± 0.33 | 0.8 | **2.91 ± 1.36** |
|  | 42:0 | 740.676 | 0.77 ± 0.02 | 3.14 ± 0.38 | 0.8 | **4.07 ± 1.47\*\*** |
|  | 44:3 | 762.661 | 0.29 ± 0.01 | 0.80 ± 0.23 | 0.3 | **2.78 ± 2.27** |
|  | 44:2 | 764.676 | 0.90 ± 0.01 | 1.94 ± 0.13 | 1.0 | **2.16 ± 0.45\*** |
|  | 44:1 | 766.692 | 1.00 ± 0.04 | 4.47 ± 0.99 | 1.1 | **4.49 ± 2.90\*\*** |
|  | 44:0 | 768.708 | 0.43 ± 0.01 | 2.49 ± 0.23 | 0.5 | **5.79 ± 1.70\*\*** |
|  | 46:3 | 790.692 | 0.61 ± 0.01 | 1.06 ± 0.21 | 0.7 | 1.75 ± 1.00 |
|  | 46:2 | 792.708 | 1.46 ± 0.03 | 3.33 ± 0.32 | 1.6 | **2.27 ± 0.67\*** |
|  | 46:1 | 794.723 | 1.28 ± 0.03 | 4.34 ± 0.36 | 1.4 | **3.39 ± 0.88\*\*** |
|  | 46:0 | 796.739 | 0.59 ± 0.02 | 1.67 ± 0.25 | 0.6 | **2.80 ± 1.26\*\*** |
|  | 48:3 | 818.723 | 1.28 ± 0.03 | 1.12 ± 0.18 | 1.4 | 0.87 ± 0.41 |
|  | 48:2 | 820.739 | 2.07 ± 0.03 | 3.77 ± 0.29 | 2.2 | 1.82 ± 0.41\* |
|  | 48:1 | 822.755 | 1.81 ± 0.01 | 6.07 ± 0.87 | 2.0 | **3.35 ± 1.35\*\*** |
|  | 48:0 | 824.770 | 0.59 ± 0.01 | 1.66 ± 0.27 | 0.6 | **2.83 ± 1.32\*\*** |
|  | 50:3 | 846.755 | 3.98 ± 0.04 | 7.30 ± 0.32 | 4.3 | 1.83 ± 0.24\*\* |
|  | 50:2 | 848.770 | 4.63 ± 0.05 | 14.01 ± 1.49 | 5.0 | **3.02 ± 0.92\*\*** |
|  | 50:1 | 850.786 | 1.82 ± 0.06 | 6.21 ± 2.09 | 2.0 | **3.41 ± 3.27\*\*** |
|  | 50:0 | 852.802 | 0.32 ± 0.01 | 0.37 ± 0.11 | 0.3 | 1.16 ± 0.96 |
|  | 52:6 | 868.739 | 0.54 ± 0.02 | 0.72 ± 0.03 | 0.6 | 1.32 ± 0.25 |
|  | 52:5 | 870.755 | 2.78 ± 0.05 | 9.98 ± 1.27 | 3.0 | **3.59 ± 1.32\*\*** |
|  | 52:4 | 872.770 | 8.52 ± 0.11 | 19.45 ± 0.76 | 9.2 | **2.28 ± 0.29\*** |
|  | 52:3 | 874.786 | 8.52 ± 0.13 | 23.60 ± 2.00 | 9.2 | **2.77 ± 0.69\*\*** |
|  | 52:2 | 876.802 | 5.04 ± 0.18 | 21.61 ± 3.16 | 5.5 | **4.29 ± 1.90\*\*** |
|  | 52:1 | 878.817 | 0.98 ± 0.06 | 2.62 ± 0.76 | 1.1 | **2.68 ± 2.32\*\*** |
|  | 54:8 | 892.739 | 0.11 ± 0.01 | 0.01 ± 0.01 | 0.1 | **0.08 ± 0.28\*** |
|  | 54:7 | 894.755 | 0.98 ± 0.05 | 1.56 ± 0.09 | 1.1 | 1.59 ± 0.44 |
|  | 54:6 | 896.770 | 6.83 ± 0.23 | 16.67 ± 0.80 | 7.4 | **2.44 ± 0.51\*** |
|  | 54:5 | 898.786 | 9.58 ± 0.16 | 17.72 ± 0.78 | 10.4 | 1.85 ± 0.27\* |
|  | 54:4 | 900.802 | 8.61 ± 0.17 | 20.75 ± 1.01 | 9.3 | **2.41 ± 0.40\*\*** |
|  | 54:3 | 902.817 | 5.25 ± 0.28 | 14.97 ± 1.32 | 5.7 | **2.85 ± 1.00\*\*** |
|  | 54:2 | 904.833 | 1.25 ± 0.10 | 2.87 ± 0.63 | 1.4 | **2.30 ± 1.65\*\*** |
|  | 54:0 | 906.849 | 0.22 ± 0.01 | 0.32 ± 0.17 | 0.2 | 1.44 ± 2.25 |
|  | 56:8 | 920.770 | 0.70 ± 0.01 | 0.31 ± 0.15 | 0.8 | 0.43 ± 0.58\* |
|  | 56:7 | 922.786 | 1.50 ± 0.03 | 1.01 ± 0.26 | 1.6 | 0.68 ± 0.49 |
|  | 56:6 | 924.802 | 1.70 ± 0.02 | 0.21 ± 0.04 | 1.8 | **0.12 ± 0.07\*\*** |
|  | 56:5 | 926.817 | 1.12 ± 0.04 | 0.68 ± 0.05 | 1.2 | 0.61 ± 0.15\* |
|  | 56:4 | 928.833 | 0.56 ± 0.04 | 0.40 ± 0.03 | 0.6 | 0.71 ± 0.25 |
|  | 56:3 | 930.849 | 0.27 ± 0.02 | 0.17 ± 0.02 | 0.3 | 0.64 ± 0.30 |
|  | 56:2 | 932.864 | 0.11 ± 0.01 | 0.09 ± 0.02 | 0.1 | 0.87 ± 0.57 |
|  | 58:8 | 948.801 | 0.43 ± 0.01 | 0.08 ± 0.01 | 0.5 | **0.19 ± 0.08\*\*** |
| Plasma | | | | | | |
| Class | Molecular  species | *m/z* | Concentration (nmol/mL) | | abund. (%) | Fold ratio |
| C | LC | LC/C |
| LPC | 14:0 | 468.5 | 3.13 ± 0.56 | 3.05 ± 0.40 | 1.9 | 0.98 ± 0.22 |
| (14) | 16:1 | 494.5 | 3.89 ± 0.66 | 3.74 ± 0.65 | 2.4 | 0.96 ± 0.23 |
|  | 16:0 | 496.5 | 63.93 ± 8.77 | 58.49 ± 7.09 | 39.0 | 0.91 ± 0.17 |
|  | 18:2 | 520.5 | 49.70 ± 6.79 | 30.31 ± 5.00 | 30.3 | 0.61 ± 0.13\*\* |
|  | 18:1 | 522.5 | 16.13 ± 1.99 | 11.69 ± 0.93 | 9.8 | 0.72 ± 0.11\*\* |
|  | 18:0 | 524.5 | 9.78 ± 2.21 | 8.02 ± 1.11 | 6.0 | 0.82 ± 0.22\* |
|  | 20:4 | 544.5 | 10.68 ± 1.70 | 8.35 ± 1.52 | 6.5 | 0.78 ± 0.19\*\* |
|  | 20:3 | 546.5 | 3.12 ± 0.42 | 2.40 ± 0.37 | 1.9 | 0.77 ± 0.16\*\* |
|  | 20:2 | 548.5 | 0.42 ± 0.10 | 0.34 ± 0.07 | 0.3 | 0.81 ± 0.26\*\* |
|  | 20:1 | 550.5 | N.D. | N.D. | - | - |
|  | 20:0 | 552.5 | 0.28 ± 0.08 | 0.23 ± 0.05 | 0.2 | 0.82 ± 0.29 |
|  | 22:6 | 568.5 | 1.99 ± 0.36 | 1.35 ± 0.26 | 1.2 | 0.68 ± 0.18\*\* |
|  | 22:5 | 570.5 | 0.46 ± 0.09 | 0.33 ± 0.07 | 0.3 | 0.72 ± 0.20\*\* |
|  | 22:4 | 572.5 | 0.28 ± 0.08 | N.D. | 0.2 | - |
| EtherLPC | O-16:0 | 480.5 | 1.10 ± 0.24 | 1.09 ± 0.21 | 57.6 | 0.99 ± 0.29 |
| (3) | O-16:1 and P-16:0 | 482.5 | N.D. | N.D. | - | - |
|  | O-18:0 | 510.5 | 0.81 ± 0.22 | 0.93 ± 0.18 | 42.4 | 1.15 ± 0.38 |
| PC | 30:0 | 706.5 | 1.34 ± 0.27 | 1.18 ± 0.29 | 0.3 | 0.87 ± 0.28 |
| (25) | 32:2 | 730.5 | 3.14 ± 0.61 | 2.00 ± 0.37 | 0.7 | 0.64 ± 0.17\*\* |
|  | 32:1 | 732.5 | 5.38 ± 1.14 | 5.17 ± 0.76 | 1.2 | 0.96 ± 0.25 |
|  | 32:0 | 734.5 | 2.83 ± 0.67 | 2.95 ± 0.48 | 0.6 | 1.04 ± 0.30 |
|  | 34:4 | 754.5 | 1.28 ± 0.26 | 0.89 ± 0.17 | 0.3 | 0.70 ± 0.19\*\* |
|  | 34:3 | 756.5 | 5.66 ± 0.78 | 3.44 ± 0.55 | 1.3 | 0.61 ± 0.13\*\* |
|  | 34:2 | 758.5 | 114.82 ± 16.89 | 85.66 ± 7.79 | 25.8 | 0.75 ± 0.13\*\* |
|  | 34:1 | 760.5 | 50.63 ± 8.12 | 50.21 ± 7.65 | 11.4 | 0.99 ± 0.22 |
|  | 34:0 | 762.5 | 5.23 ± 0.86 | 5.64 ± 0.82 | 1.2 | 1.08 ± 0.24 |
|  | 36:6 | 778.5 | 0.27 ± 0.11 | 0.17 ± 0.07 | 0.1 | 0.64 ± 0.36\* |
|  | 36:4 | 782.5 | 53.28 ± 7.90 | 32.14 ± 5.07 | 12.0 | 0.60 ± 0.13\*\* |
|  | 36:3 | 784.5 | 39.88 ± 4.45 | 26.92 ± 3.93 | 9.0 | 0.67 ± 0.12\*\* |
|  | 36:2 | 786.5 | 59.58 ± 9.46 | 43.05 ± 7.16 | 13.4 | 0.72 ± 0.17\*\* |
|  | 36:1 | 788.5 | 18.04 ± 3.20 | 15.99 ± 3.07 | 4.0 | 0.89 ± 0.23 |
|  | 36:0 | 790.5 | 1.98 ± 0.47 | 1.74 ± 0.36 | 0.4 | 0.88 ± 0.28 |
|  | 38:7 | 804.5 | 0.64 ± 0.17 | 0.52 ± 0.11 | 0.1 | 0.82 ± 0.28 |
|  | 38:6 | 806.5 | 17.15 ± 2.35 | 10.09 ± 1.75 | 3.8 | 0.59 ± 0.13\*\* |
|  | 38:5 | 808.5 | 12.09 ± 1.60 | 7.61 ± 1.58 | 2.7 | 0.63 ± 0.15\*\* |
|  | 38:4 | 810.5 | 20.98 ± 3.81 | 16.23 ± 2.45 | 4.7 | 0.77 ± 0.18\*\* |
|  | 38:3 | 812.5 | 14.87 ± 3.13 | 13.97 ± 2.58 | 3.3 | 0.94 ± 0.26 |
|  | 38:2 | 814.5 | 8.74 ± 1.77 | 9.78 ± 2.16 | 2.0 | 1.12 ± 0.34 |
|  | 40:8 | 830.5 | 0.77 ± 0.18 | 0.60 ± 0.17 | 0.2 | 0.79 ± 0.29\*\* |
|  | 40:7 | 832.5 | 1.26 ± 0.23 | 0.71 ± 0.21 | 0.3 | 0.57 ± 0.19\*\* |
|  | 40:6 | 834.5 | 3.85 ± 0.68 | 2.77 ± 0.33 | 0.9 | 0.72 ± 0.15\*\* |
|  | 40:5 | 836.5 | 1.90 ± 0.34 | 1.66 ± 0.35 | 0.4 | 0.87 ± 0.24 |
| EtherPC | P-32:0 | 718.5 | 1.58 ± 0.27 | 1.66 ± 0.35 | 2.1 | 1.06 ± 0.28 |
| (19) | O-32:0 | 720.5 | 1.77 ± 0.32 | 2.24 ± 0.46 | 2.3 | 1.26 ± 0.34\*\* |
|  | O-34:3 | 742.5 | 3.70 ± 0.67 | 2.79 ± 0.55 | 4.9 | 0.75 ± 0.20\*\* |
|  | O-34:2 and P-34:1 | 744.5 | 6.27 ± 1.09 | 5.76 ± 1.01 | 8.3 | 0.92 ± 0.23 |
|  | O-34:1 | 746.5 | 4.67 ± 1.04 | 6.13 ± 1.28 | 6.1 | 1.31 ± 0.40\*\* |
|  | O-34:0 | 748.5 | 1.15 ± 0.32 | 1.54 ± 0.33 | 1.5 | 1.33 ± 0.46\*\* |
|  | P-36:4 | 766.5 | 5.73 ± 0.95 | 4.24 ± 0.84 | 7.5 | 0.74 ± 0.19\*\* |
|  | O-36:4 and P-36:3 | 768.5 | 9.87 ± 1.37 | 7.03 ± 1.32 | 13.0 | 0.71 ± 0.17\*\* |
|  | O-36:3 and P-36:2 | 770.5 | 4.91 ± 0.91 | 4.55 ± 0.84 | 6.5 | 0.93 ± 0.24 |
|  | O-36:2 and P-36:1 | 772.5 | 7.65 ± 1.30 | 7.92 ± 1.21 | 10.1 | 1.03 ± 0.24 |
|  | P-38:5 | 792.5 | 3.10 ± 0.52 | 2.38 ± 0.61 | 4.1 | 0.77 ± 0.23\*\* |
|  | O-38:5 and P-38:4 | 794.5 | 9.08 ± 1.04 | 7.00 ± 1.57 | 12.0 | 0.77 ± 0.19\*\* |
|  | O-38:4 | 796.5 | 7.97 ± 1.18 | 7.73 ± 1.26 | 10.5 | 0.97 ± 0.21 |
|  | O-38:3 | 798.5 | 2.71 ± 0.38 | 4.91 ± 0.94 | 3.6 | 1.81 ± 0.43\*\* |
|  | O-40:6 and P-40:5 | 820.5 | 1.84 ± 0.34 | 1.82 ± 0.39 | 2.4 | 0.99 ± 0.28 |
|  | O-40:5 and P-40:4 | 822.5 | 1.61 ± 0.26 | 2.01 ± 0.54 | 2.1 | 1.25 ± 0.39\*\* |
|  | O-40:4 | 824.5 | 1.18 ± 0.29 | 1.77 ± 0.54 | 1.6 | 1.50 ± 0.59\*\* |
|  | O-42:6 | 848.5 | 0.56 ± 0.14 | 0.54 ± 0.19 | 0.7 | 0.97 ± 0.41 |
|  | O-42:5 | 850.5 | 0.54 ± 0.16 | 0.94 ± 0.25 | 0.7 | 1.75 ± 0.71\*\* |
| LPE | 14:0 | 426.5 | N.D. | N.D. | - | - |
| (9) | 16:1 | 452.5 | N.D. | N.D. | - | - |
|  | 16:0 | 454.5 | 0.48 ± 0.21 | 0.44 ± 0.22 | 4.9 | 0.91 ± 0.60 |
|  | 18:2 | 478.5 | 4.29 ± 1.45 | 2.49 ± 1.06 | 43.6 | 0.58 ± 0.31\*\* |
|  | 18:1 | 480.5 | 0.80 ± 0.34 | 0.49 ± 0.23 | 8.1 | 0.62 ± 0.39\*\* |
|  | 18:0 | 482.5 | 0.55 ± 0.30 | 0.48 ± 0.30 | 5.6 | 0.87 ± 0.72 |
|  | 20:4 | 502.5 | 2.39 ± 0.61 | 1.79 ± 0.66 | 24.3 | 0.75 ± 0.33\*\* |
|  | 22:6 | 526.5 | 1.13 ± 0.44 | 0.80 ± 0.42 | 11.5 | 0.71 ± 0.46\* |
|  | 22:5 | 528.5 | 0.20 ± 0.10 | N.D. | 2.1 | - |
| PE | 34:2 | 716.5 | 2.67 ± 0.55 | 2.65 ± 1.06 | 7.2 | 0.99 ± 0.45 |
| (13) | 34:1 | 718.5 | 1.17 ± 0.40 | 1.13 ± 0.50 | 3.2 | 0.97 ± 0.54 |
|  | 36:4 | 740.5 | 3.59 ± 0.67 | 3.01 ± 1.34 | 9.7 | 0.84 ± 0.40 |
|  | 36:3 | 742.5 | 3.16 ± 0.78 | 1.84 ± 0.85 | 8.6 | 0.58 ± 0.30\*\* |
|  | 36:2 | 744.5 | 5.83 ± 1.45 | 3.63 ± 1.00 | 15.8 | 0.62 ± 0.23\*\* |
|  | 36:1 | 746.5 | 1.67 ± 0.60 | 1.45 ± 0.62 | 4.5 | 0.86 ± 0.48 |
|  | 38:6 | 764.5 | 4.23 ± 1.67 | 2.74 ± 0.96 | 11.4 | 0.65 ± 0.34\*\* |
|  | 38:5 | 766.5 | 2.80 ± 0.71 | 1.95 ± 0.93 | 7.6 | 0.70 ± 0.37\*\* |
|  | 38:4 | 768.5 | 7.23 ± 1.95 | 4.28 ± 1.85 | 19.6 | 0.59 ± 0.30\*\* |
|  | 38:3 | 770.5 | 1.55 ± 0.52 | 0.96 ± 0.37 | 4.2 | 0.62 ± 0.32\*\* |
|  | 40:7 | 790.5 | 0.53 ± 0.24 | 0.30 ± 0.17 | 1.4 | 0.55 ± 0.40\*\* |
|  | 40:6 | 792.5 | 1.72 ± 0.69 | 1.09 ± 0.49 | 4.7 | 0.63 ± 0.38\*\* |
|  | 40:5 | 794.5 | 0.77 ± 0.29 | 0.42 ± 0.19 | 2.1 | 0.54 ± 0.33\*\* |
| EtherPE | O-36:4 and P-36:3 | 726.5 | 0.54 ± 0.23 | 0.41 ± 0.27 | 12.8 | 0.76 ± 0.60 |
| (7) | P-36:2 | 728.5 | 1.41 ± 0.42 | 1.45 ± 0.56 | 33.4 | 1.03 ± 0.51 |
|  | O-36:2 and P-36:1 | 730.5 | 0.28 ± 0.13 | 0.30 ± 0.15 | 6.7 | 1.06 ± 0.75 |
|  | O-38:5 | 752.5 | 0.94 ± 0.28 | 0.81 ± 0.45 | 22.4 | 0.86 ± 0.54 |
|  | O-38:4 and P-38:3 | 754.5 | 0.77 ± 0.34 | 0.62 ± 0.22 | 18.4 | 0.81 ± 0.46 |
|  | P-38:1 | 758.5 | 0.27 ± 0.10 | 0.16 ± 0.08 | 6.3 | 0.61 ± 0.38\*\* |
|  | P-40:7 | 774.5 | N.D. | N.D. | - | - |
| LPG | 14:0 | 455.5 | N.D. | N.D. | - | - |
| (6) | 16:1 | 481.5 | N.D. | N.D. | - | - |
|  | 16:0 | 483.5 | N.D. | N.D. | - | - |
|  | 18:2 | 507.5 | 0.18 ± 0.03 | 0.17 ± 0.04 | 42.0 | 0.95 ± 0.27 |
|  | 18:1 | 509.5 | 0.24 ± 0.06 | 0.17 ± 0.05 | 58.0 | 0.69 ± 0.26\*\* |
|  | 18:0 | 511.5 | N.D. | N.D. | - | - |
| PG | 16:0/16:0 | 721.5 | 0.34 ± 0.02 | N.D. | 100 | - |
| (7) | 16:0/18:1 | 747.5 | N.D. | N.D. | - | - |
|  | 18:0/16:1 | 747.5 | N.D. | N.D. | - | - |
|  | 18:1/18:2 | 771.5 | N.D. | N.D. | - | - |
|  | 18:0/18:2 | 773.5 | N.D. | N.D. | - | - |
|  | 18:1/18:1 | 773.5 | N.D. | N.D. | - | - |
|  | 18:0/18:1 | 775.5 | N.D. | N.D. | - | - |
|  | 16:0/22:5 | 795.5 | N.D. | N.D. | - | - |
| LPI | 18:2 | 595.5 | 2.75 ± 0.81 | 1.77 ± 0.61 | 35.8 | 0.64 ± 0.29\*\* |
| (5) | 18:1 | 597.5 | 0.87 ± 0.13 | 0.66 ± 0.15 | 11.3 | 0.76 ± 0.21\*\* |
|  | 18:0 | 599.5 | 0.49 ± 0.18 | 0.35 ± 0.11 | 6.4 | 0.71 ± 0.35\* |
|  | 20:4 | 619.5 | 2.95 ± 0.22 | 2.71 ± 0.66 | 38.5 | 0.92 ± 0.23 |
|  | 20:3 | 621.5 | 0.61 ± 0.16 | 0.53 ± 0.15 | 8.0 | 0.86 ± 0.34 |
| PI | 16:0/16:0 | 809.5 | N.D. | N.D. | - | - |
| (13) | 16:1/18:1 | 833.5 | N.D. | N.D. | - | - |
|  | 18:1/16:0 | 835.5 | 4.22 ± 1.31 | 4.79 ± 2.33 | 4.7 | 1.13 ± 0.65 |
|  | 16:0/20:5 | 855.5 | 0.33 ± 0.10 | 0.31 ± 0.19 | 0.4 | 0.94 ± 0.65 |
|  | 18:1/18:2 | 859.5 | 2.22 ± 1.18 | 0.69 ± 0.18 | 2.5 | **0.31 ± 0.18\*\*** |
|  | 18:0/18:2 | 861.5 | 14.60 ± 2.60 | 7.80 ± 2.42 | 16.3 | 0.53 ± 0.19\*\* |
|  | 18:1/18:1 | 861.5 | 6.08 ± 2.14 | 3.19 ± 1.20 | 6.8 | 0.52 ± 0.27\*\* |
|  | 18:1/18:0 | 863.5 | 5.02 ± 1.28 | 2.78 ± 0.81 | 5.6 | 0.55 ± 0.22\*\* |
|  | 22:6/16:0 | 881.5 | N.D. | N.D. | - | - |
|  | 18:0/20:4 | 885.5 | 47.32 ± 6.60 | 23.13 ± 3.76 | 53.0 | **0.49 ± 0.10\*\*** |
|  | 18:0/20:3 | 887.5 | 8.88 ± 1.48 | 6.01 ± 1.04 | 9.9 | 0.68 ± 0.16\*\* |
|  | 18:0/20:2 | 889.5 | 0.69 ± 0.36 | 0.25 ± 0.05 | 0.8 | **0.36 ± 0.20\*\*** |
|  | 18:1/22:6 | 907.5 | N.D. | N.D. | - | - |
| SM | d18:2/14:0 | 673.5 | 1.17 ± 0.36 | 0.72 ± 0.32 | 0.4 | 0.62 ± 0.33\*\* |
| (8) | d18:1/16:0 | 703.5 | 86.13 ± 12.41 | 84.28 ± 12.77 | 29.6 | 0.98 ± 0.20 |
|  | d18:2/18:0 | 729.5 | 7.55 ± 1.17 | 7.67 ± 1.30 | 2.6 | 1.02 ± 0.23 |
|  | d18:1/18:0 | 731.5 | 17.41 ± 3.02 | 19.88 ± 4.75 | 6.0 | 1.14 ± 0.34 |
|  | d18:0/20:2 | 757.5 | 12.68 ± 2.25 | 9.85 ± 2.31 | 4.4 | 0.78 ± 0.23\*\* |
|  | d18:1/22:1 | 785.5 | 80.94 ± 13.97 | 63.29 ± 13.99 | 27.9 | 0.78 ± 0.22\*\* |
|  | d18:1/24:1 | 813.5 | 60.33 ± 12.49 | 67.31 ± 15.72 | 20.8 | 1.12 ± 0.35 |
|  | d18:1/24:0 | 815.5 | 24.38 ± 5.74 | 24.69 ± 6.95 | 8.4 | 1.01 ± 0.37 |
| Cer | d16:1/24:0 | 622.5 | 1.17 ± 0.49 | 0.05 ± 0.01 | 2.5 | **0.05 ± 0.02\*\*** |
| (8) | d18:1/22:0 | 622.5 | 7.68 ± 0.95 | 0.91 ± 0.14 | 16.4 | **0.12 ± 0.02\*\*** |
|  | d18:0/22:0 | 624.5 | 0.38 ± 0.20 | N.D. | 0.8 | - |
|  | d18:1/24:1 | 648.5 | 8.20 ± 2.79 | 1.11 ± 0.11 | 17.5 | **0.14 ± 0.05\*\*** |
|  | d18:2/24:0 | 648.5 | 4.69 ± 0.78 | 0.35 ± 0.13 | 10.0 | **0.07 ± 0.03\*\*** |
|  | d18:1/24:0 | 650.5 | 24.36 ± 5.85 | 2.14 ± 0.74 | 52.0 | **0.09 ± 0.04\*\*** |
|  | d18:1/26:0 | 678.5 | 0.21 ± 0.15 | N.D. | 0.5 | - |
|  | d20:1/24:0 | 678.5 | 0.20 ± 0.16 | N.D. | 0.4 | - |
| HexCer | d18:1/22:0 | 784.5 | 3.86 ± 1.92 | 2.10 ± 0.68 | 33.3 | 0.55 ± 0.32\*\* |
| (3) | d18:1/24:1 | 810.5 | 3.32 ± 1.68 | 2.52 ± 1.02 | 28.7 | 0.76 ± 0.49 |
|  | d18:1/24:0 | 812.5 | 4.39 ± 2.50 | 3.20 ± 2.09 | 37.9 | 0.73 ± 0.63 |
| DG | 32:1 | 584.5 | 0.86 ± 0.63 | 0.48 ± 0.32 | 2.7 | 0.56 ± 0.55\* |
| (10) | 32:0 | 586.5 | 2.66 ± 2.57 | 1.62 ± 0.80 | 8.5 | 0.61 ± 0.66 |
|  | 34:2 | 610.5 | 2.75 ± 1.50 | 2.26 ± 1.06 | 8.8 | 0.82 ± 0.59 |
|  | 34:1 | 612.5 | 4.50 ± 2.33 | 4.83 ± 2.10 | 14.4 | 1.07 ± 0.72 |
|  | 34:0 | 614.5 | 1.22 ± 0.73 | 1.04 ± 0.58 | 3.9 | 0.85 ± 0.70 |
|  | 36:4 | 634.5 | 0.30 ± 0.19 | N.D. | 1.0 | - |
|  | 36:3 | 636.5 | 5.99 ± 2.27 | 4.92 ± 2.35 | 19.2 | 0.82 ± 0.50\* |
|  | 36:2 | 638.5 | 11.75 ± 3.47 | 12.18 ± 6.29 | 37.6 | 1.04 ± 0.62 |
|  | 36:1 | 640.5 | 0.89 ± 0.25 | 1.19 ± 0.65 | 2.9 | 1.33 ± 0.82 |
|  | 36:0 | 642.5 | 0.33 ± 0.03 | 0.31 ± 0.11 | 1.1 | 0.96 ± 0.35 |
| TG | 40:1 | 710.5 | 0.09 ± 0.04 | 0.21 ± 0.10 | 0.0 | **2.26 ± 1.41\*** |
| (42) | 40:0 | 712.5 | 0.16 ± 0.11 | 0.79 ± 0.29 | 0.1 | **5.09 ± 3.98\*\*** |
|  | 42:2 | 736.5 | N.D. | 0.42 ± 0.15 | - | - |
|  | 42:1 | 738.5 | 0.10 ± 0.06 | 0.68 ± 0.22 | 0.1 | **6.53 ± 4.55\*\*** |
|  | 42:0 | 740.5 | 0.47 ± 0.26 | 1.28 ± 0.34 | 0.3 | **2.73 ± 1.69\*\*** |
|  | 44:2 | 764.5 | 0.11 ± 0.02 | 0.48 ± 0.24 | 0.1 | **4.22 ± 2.17\*** |
|  | 44:1 | 766.5 | 0.66 ± 0.45 | 0.98 ± 0.33 | 0.4 | 1.48 ± 1.13 |
|  | 44:0 | 768.5 | 1.28 ± 0.60 | 1.40 ± 0.74 | 0.7 | 1.10 ± 0.78 |
|  | 46:3 | 790.5 | 0.30 ± 0.06 | 0.87 ± 0.44 | 0.2 | **2.93 ± 1.58\*\*** |
|  | 46:2 | 792.5 | 1.09 ± 0.69 | 1.41 ± 1.01 | 0.6 | 1.29 ± 1.23 |
|  | 46:1 | 794.5 | 2.46 ± 1.46 | 3.59 ± 0.66 | 1.3 | 1.46 ± 0.91 |
|  | 46:0 | 796.5 | 2.30 ± 1.33 | 2.19 ± 1.08 | 1.2 | 0.95 ± 0.72 |
|  | 48:4 | 816.5 | 0.11 ± 0.03 | 0.15 ± 0.09 | 0.1 | 1.39 ± 0.92 |
|  | 48:3 | 818.5 | 1.50 ± 0.32 | 3.17 ± 0.73 | 0.8 | **2.11 ± 0.67\*\*** |
|  | 48:2 | 820.5 | 2.78 ± 1.56 | 4.03 ± 1.84 | 1.5 | 1.45 ± 1.05 |
|  | 48:1 | 822.5 | 4.95 ± 1.50 | 8.10 ± 4.50 | 2.7 | 1.64 ± 1.04 |
|  | 48:0 | 824.5 | 3.93 ± 2.35 | 10.08 ± 8.06 | 2.1 | **2.56 ± 2.55\*** |
|  | 50:5 | 842.5 | 0.18 ± 0.10 | 0.27 ± 0.10 | 0.1 | 1.53 ± 1.06 |
|  | 50:4 | 844.5 | 0.67 ± 0.20 | 0.78 ± 0.28 | 0.4 | 1.15 ± 0.54 |
|  | 50:3 | 846.5 | 10.07 ± 5.11 | 12.02 ± 5.94 | 5.4 | 1.19 ± 0.85 |
|  | 50:2 | 848.5 | 11.31 ± 2.66 | 28.22 ± 7.01 | 6.1 | **2.50 ± 0.85\*\*** |
|  | 50:1 | 850.5 | 1.20 ± 0.70 | 2.09 ± 0.43 | 0.6 | 1.75 ± 1.07 |
|  | 50:0 | 852.5 | 3.09 ± 1.08 | 4.86 ± 2.51 | 1.7 | 1.57 ± 0.98 |
|  | 52:6 | 868.5 | 0.28 ± 0.18 | 0.90 ± 0.49 | 0.1 | **3.23 ± 2.76\*\*** |
|  | 52:5 | 870.5 | 5.15 ± 0.93 | 12.18 ± 4.96 | 2.8 | **2.37 ± 1.05\*\*** |
|  | 52:4 | 872.5 | 7.41 ± 0.35 | 20.65 ± 8.27 | 4.0 | **2.79 ± 1.12\*\*** |
|  | 52:3 | 874.5 | 48.81 ± 13.30 | 59.75 ± 20.62 | 26.2 | 1.22 ± 0.54 |
|  | 52:2 | 876.5 | 3.59 ± 0.43 | 5.21 ± 2.40 | 1.9 | 1.45 ± 0.69 |
|  | 52:1 | 878.5 | 3.99 ± 1.36 | 5.12 ± 2.12 | 2.1 | 1.28 ± 0.69 |
|  | 52:0 | 880.5 | 0.29 ± 0.11 | 1.12 ± 0.60 | 0.2 | **3.84 ± 2.49** |
|  | 54:7 | 894.5 | 0.65 ± 0.26 | 2.59 ± 1.48 | 0.4 | **3.97 ± 2.78\*\*** |
|  | 54:6 | 896.5 | 5.50 ± 2.07 | 11.73 ± 5.21 | 3.0 | **2.13 ± 1.24\*\*** |
|  | 54:5 | 898.5 | 11.98 ± 4.16 | 32.61 ± 15.39 | 6.4 | **2.72 ± 1.59\*\*** |
|  | 54:4 | 900.5 | 18.56 ± 7.69 | 34.15 ± 8.54 | 10.0 | 1.84 ± 0.89\*\* |
|  | 54:3 | 902.5 | 23.18 ± 13.45 | 33.10 ± 10.91 | 12.5 | 1.43 ± 0.95 |
|  | 54:2 | 904.5 | 5.23 ± 1.40 | 8.67 ± 0.66 | 2.8 | 1.66 ± 0.46 |
|  | 54:1 | 906.5 | 0.41 ± 0.19 | 0.79 ± 0.18 | 0.2 | 1.95 ± 1.02\*\* |
|  | 54:0 | 908.5 | 0.12 ± 0.05 | 0.26 ± 0.20 | 0.1 | **2.23 ± 1.98** |
|  | 56:8 | 920.5 | 0.40 ± 0.13 | 1.15 ± 0.48 | 0.2 | **2.87 ± 1.54\*\*** |
|  | 56:7 | 922.5 | 0.53 ± 0.19 | 0.93 ± 0.29 | 0.3 | 1.73 ± 0.82\*\* |
|  | 56:6 | 924.5 | 0.67 ± 0.15 | 1.44 ± 0.30 | 0.4 | **2.17 ± 0.66\*\*** |
|  | 56:5 | 926.5 | 0.50 ± 0.12 | 0.99 ± 0.35 | 0.3 | 1.96 ± 0.83\*\* |
| CE | 16:1 | 640.5 | 4.54 ± 1.45 | 3.28 ± 0.43 | 1.1 | 0.72 ± 0.25\* |
| (9) | 16:0 | 642.5 | 3.21 ± 0.30 | 1.96 ± 0.67 | 0.8 | 0.61 ± 0.22\*\* |
|  | 18:3 | 664.5 | 18.65 ± 2.28 | 9.09 ± 0.74 | 4.5 | **0.49 ± 0.07\*\*** |
|  | 18:2 | 666.5 | 250.34 ± 84.49 | 118.15 ± 40.00 | 60.5 | **0.47 ± 0.23\*\*** |
|  | 18:1 | 668.5 | 55.74 ± 15.51 | 28.44 ± 8.21 | 13.5 | 0.51 ± 0.20\*\* |
|  | 20:5 | 688.5 | 6.92 ± 3.13 | 3.45 ± 0.59 | 1.7 | **0.50 ± 0.24\*** |
|  | 20:4 | 690.5 | 49.64 ± 15.05 | 27.52 ± 8.07 | 12.0 | 0.55 ± 0.23\*\* |
|  | 20:3 | 692.5 | 9.63 ± 2.31 | 5.05 ± 1.79 | 2.3 | 0.52 ± 0.22\*\* |
|  | 22:6 | 714.5 | 15.13 ± 2.82 | 6.01 ± 1.91 | 3.7 | **0.40 ± 0.15\*\*** |
| Feces | | | | | | |
| Class | Molecular  species | *m/z* | Concentration (nmol/mg) | | abund. (%) | Fold ratio |
| C | LC | LC/C |
| LPC | 16:0 | 496.5 | 0.19 ± 0.03 | 0.15 ± 0.05 | 35.7 | 0.79 ± 0.29 |
| (5) | 18:2 | 520.5 | 0.05 ± 0.02 | 0.02 ± 0.00 | 9.9 | **0.37 ± 0.17\*\*** |
|  | 18:1 | 522.5 | 0.09 ± 0.01 | 0.05 ± 0.01 | 16.2 | 0.53 ± 0.13\*\* |
|  | 18:0 | 524.5 | 0.19 ± 0.03 | 0.15 ± 0.07 | 35.0 | 0.80 ± 0.41 |
|  | 20:0 | 552.5 | 0.02 ± 0.01 | 0.01 ± 0.01 | 3.1 | 0.76 ± 0.47 |
| PC | 30:0 | 706.5 | 0.03 ± 0.01 | 0.26 ± 0.03 | 15.8 | **9.67 ± 2.27\*\*** |
| (9) | 32:1 | 732.5 | N.D. | 0.05 ± 0.01 | - | - |
|  | 32:0 | 734.5 | 0.02 ± 0.00 | 0.06 ± 0.01 | 10.7 | **3.23 ± 0.56\*\*** |
|  | 34:3 | 756.5 | N.D. | N.D. | - | - |
|  | 34:2 | 758.5 | 0.03 ± 0.01 | 0.02 ± 0.00 | 20.3 | 0.63 ± 0.17 |
|  | 34:1 | 760.5 | 0.04 ± 0.00 | 0.05 ± 0.01 | 26.5 | 1.17 ± 0.15 |
|  | 36:4 | 782.5 | 0.02 ± 0.00 | N.D. | 9.7 | - |
|  | 36:3 | 784.5 | N.D. | 0.02 ± 0.01 | - | - |
|  | 36:2 | 786.5 | 0.03 ± 0.00 | 0.02 ± 0.00 | 17.0 | 0.72 ± 0.18\*\* |
| LPE | 14:0 | 426.5 | 0.03 ± 0.01 | 0.02 ± 0.00 | 2.2 | 0.64 ± 0.33 |
| (5) | 16:0 | 454.5 | 1.03 ± 0.19 | 1.06 ± 0.25 | 74.2 | 1.02 ± 0.30 |
|  | 18:2 | 478.5 | 0.05 ± 0.02 | 0.03 ± 0.01 | 3.3 | 0.58 ± 0.34\*\* |
|  | 18:1 | 480.5 | 0.13 ± 0.05 | 0.15 ± 0.07 | 9.6 | 1.16 ± 0.66 |
|  | 18:0 | 482.5 | 0.15 ± 0.06 | 0.13 ± 0.06 | 10.6 | 0.85 ± 0.52 |
| LPG | 14:0 | 455.5 | 0.02 ± 0.01 | 0.02 ± 0.01 | 7.3 | 0.91 ± 0.57 |
| (6) | 16:0 | 483.5 | 0.09 ± 0.04 | 0.19 ± 0.09 | 32.8 | **2.10 ± 1.37\*\*** |
|  | 18:2 | 507.5 | 0.02 ± 0.01 | 0.01 ± 0.01 | 8.2 | 0.61 ± 0.40\* |
|  | 18:1 | 509.5 | 0.11 ± 0.05 | 0.20 ± 0.07 | 41.0 | 1.77 ± 1.04\*\* |
|  | 18:0 | 511.5 | 0.03 ± 0.01 | 0.09 ± 0.04 | 10.8 | **2.87 ± 1.88\*\*** |
|  | 20:2 | 535.5 | N.D. | N.D. | - | - |
| PG | 12:0/14:0 | 637.5 | N.D. | N.D. | - | - |
| (14) | 12:0/16:0 | 665.5 | N.D. | N.D. | - | - |
|  | 14:0/14:0 | 665.5 | N.D. | N.D. | - | - |
|  | 14:0/16:0 | 693.5 | N.D. | N.D. | - | - |
|  | 14:0/18:1 | 719.5 | N.D. | N.D. | - | - |
|  | 16:1/16:0 | 719.5 | N.D. | N.D. | - | - |
|  | 16:0/16:0 | 721.5 | 0.02 ± 0.01 | 0.04 ± 0.02 | 7.9 | **2.66 ± 1.76\*\*** |
|  | 16:0/18:2 | 745.5 | 0.08 ± 0.04 | 0.04 ± 0.01 | 43.8 | 0.53 ± 0.31 |
|  | 18:1/16:0 | 747.5 | 0.04 ± 0.02 | 0.08 ± 0.03 | 18.8 | **2.18 ± 1.37\*\*** |
|  | 18:0/16:0 | 749.5 | 0.03 ± 0.02 | 0.10 ± 0.04 | 17.8 | **2.92 ± 1.79\*\*** |
|  | 18:1/18:2 | 771.5 | N.D. | 0.02 ± 0.01 | - | - |
|  | 18:1/18:1 | 773.5 | N.D. | N.D. | - | - |
|  | 18:0/18:1 | 775.5 | N.D. | 0.03 ± 0.01 | - | - |
|  | 20:1/16:0 | 775.5 | 0.02 ± 0.01 | 0.03 ± 0.01 | 11.8 | 1.31 ± 0.87 |
| LPI | 16:0 | 571.5 | 0.38 ± 0.19 | 0.22 ± 0.09 | 88.8 | 0.57 ± 0.37\* |
| (2) | 18:0 | 599.5 | 0.05 ± 0.02 | 0.03 ± 0.01 | 11.2 | 0.52 ± 0.30\*\* |
| PI | 16:0/18:2 | 833.5 | 0.23 ± 0.11 | 0.12 ± 0.06 | 37.6 | 0.55 ± 0.37\* |
| (4) | 16:0/18:1 | 835.5 | 0.19 ± 0.09 | 0.12 ± 0.05 | 31.0 | 0.65 ± 0.40\* |
|  | 18:0/18:2 | 861.5 | 0.11 ± 0.05 | 0.07 ± 0.03 | 18.8 | 0.58 ± 0.38\* |
|  | 18:1/18:0 | 863.5 | 0.08 ± 0.03 | 0.65 ± 0.30 | 12.5 | **8.64 ± 5.54\*\*** |
| SM | d18:1/16:0 | 703.5 | N.D. | N.D. | - | - |
| Cer | d16:1/16:1 | 508.5 | 0.03 ± 0.01 | 0.02 ± 0.01 | 2.6 | 0.97 ± 0.41 |
| (28) | d16:1/16:0 | 510.5 | N.D. | 0.01 ± 0.00 | - | - |
|  | d18:1/14:0 | 510.5 | N.D. | N.D. | - | - |
|  | d18:2/16:1 | 534.5 | 0.03 ± 0.01 | 0.04 ± 0.02 | 3.2 | 1.33 ± 0.84 |
|  | d18:1/16:1 | 536.5 | 0.01 ± 0.00 | 0.02 ± 0.01 | 1.1 | **2.12 ± 1.34\*\*** |
|  | d18:2/16:0 | 536.5 | N.D. | 0.01 ± 0.00 | - | - |
|  | d16:1/18:0 | 538.5 | 0.13 ± 0.02 | 0.22 ± 0.08 | 13.1 | 1.71 ± 0.73\* |
|  | d18:1/16:0 | 538.5 | 0.20 ± 0.07 | 0.41 ± 0.19 | 20.4 | **2.11 ± 1.21\*\*** |
|  | d18:0/16:0 | 540.5 | 0.11 ± 0.01 | 0.26 ± 0.13 | 11.0 | **2.44 ± 1.24\*\*** |
|  | d18:1/18:2 | 562.5 | 0.03 ± 0.01 | 0.68 ± 0.14 | 2.7 | **25.99 ± 10.06\*\*** |
|  | d18:1/18:1 | 564.5 | 0.06 ± 0.01 | 0.13 ± 0.06 | 6.3 | **2.13 ± 1.12\*** |
|  | d18:1/18:0 | 566.5 | 0.03 ± 0.01 | 0.35 ± 0.07 | 3.6 | **10.05 ± 3.22\*\*** |
|  | d18:0/18:0 | 568.5 | 0.03 ± 0.01 | 0.36 ± 0.15 | 3.6 | **10.26 ± 4.91\*\*** |
|  | d18:1/20:1 | 592.5 | N.D. | N.D. | - | - |
|  | d20:1/18:1 | 592.5 | N.D. | N.D. | - | - |
|  | d18:0/20:0 | 596.5 | N.D. | 0.02 ± 0.00 | - | - |
|  | d16:1/24:1 | 618.5 | N.D. | 0.02 ± 0.01 | - | - |
|  | d18:1/22:2 | 618.5 | 0.02 ± 0.01 | 0.02 ± 0.01 | 1.9 | 0.88 ± 0.56 |
|  | d18:2/22:1 | 618.5 | 0.05 ± 0.01 | 0.25 ± 0.06 | 5.4 | **4.71 ± 1.42\*\*** |
|  | d18:1/22:1 | 620.5 | 0.04 ± 0.01 | 0.13 ± 0.01 | 4.4 | **3.18 ± 0.97\*\*** |
|  | d16:1/24:0 | 622.5 | N.D. | N.D. | - | - |
|  | d18:1/22:0 | 622.5 | 0.02 ± 0.00 | 0.10 ± 0.03 | 2.1 | **4.69 ± 1.67\*\*** |
|  | d18:2/24:1 | 646.5 | 0.03 ± 0.01 | 0.04 ± 0.02 | 3.1 | 1.37 ± 0.65 |
|  | d18:1/24:1 | 648.5 | 0.09 ± 0.02 | 0.36 ± 0.08 | 9.8 | **3.83 ± 1.02\*\*** |
|  | d18:1/24:0 | 650.5 | 0.03 ± 0.01 | 0.18 ± 0.06 | 2.9 | **6.30 ± 2.47\*\*** |
|  | d18:0/24:0 | 652.5 | N.D. | 0.02 ± 0.00 | - | - |
|  | d20:1/24:1 | 676.5 | 0.03 ± 0.01 | 0.06 ± 0.00 | 2.7 | **2.34 ± 0.57\*** |
|  | d20:1/24:0 | 678.5 | N.D. | N.D. | - | - |
| HexCer | d18:2/16:1 | 696.5 | 0.32 ± 0.06 | 0.20 ± 0.05 | 33.7 | 0.61 ± 0.18\*\* |
| (7) | d18:1/16:1 | 698.5 | 0.17 ± 0.03 | 0.39 ± 0.04 | 18.3 | **2.26 ± 0.44\*\*** |
|  | d18:1/16:0 | 700.5 | 0.03 ± 0.01 | 0.08 ± 0.02 | 3.5 | **2.36 ± 1.17\*\*** |
|  | d18:1/18:0 | 728.5 | 0.02 ± 0.01 | 0.06 ± 0.01 | 2.4 | **2.55 ± 1.24\*\*** |
|  | d18:1/22:0 | 784.5 | 0.03 ± 0.02 | 0.06 ± 0.03 | 3.4 | 1.89 ± 1.29\*\* |
|  | d18:1/24:1 | 810.5 | 0.32 ± 0.07 | 0.69 ± 0.20 | 33.1 | **2.19 ± 0.78\*\*** |
|  | d18:1/24:0 | 812.5 | 0.05 ± 0.02 | 0.11 ± 0.05 | 5.6 | **2.01 ± 1.28\*\*** |
| Hex2Cer | d18:1/16:0 | 862.5 | 0.04 ± 0.02 | 0.07 ± 0.03 | 14.7 | 1.58 ± 1.06 |
| (4) | d18:1/22:0 | 946.5 | 0.04 ± 0.02 | 0.02 ± 0.01 | 13.2 | **0.48 ± 0.25\*\*** |
|  | d18:1/24:1 | 972.5 | 0.15 ± 0.07 | 0.25 ± 0.11 | 51.3 | 1.74 ± 1.11\*\* |
|  | d18:1/24:0 | 974.5 | 0.06 ± 0.03 | 0.09 ± 0.03 | 20.7 | 1.48 ± 0.86\* |
| DG | 14:0\_14:0 | 530.5 | 0.15 ± 0.07 | 0.18 ± 0.08 | 0.4 | 1.18 ± 0.78 |
| (28) | 16:1\_14:0 | 556.5 | 1.13 ± 0.52 | 1.25 ± 0.49 | 2.7 | 1.11 ± 0.67 |
|  | 16:0\_14:0 | 558.5 | 0.45 ± 0.17 | 0.71 ± 0.33 | 1.1 | 1.59 ± 0.95\* |
|  | 16:1\_16:1 | 582.5 | 0.34 ± 0.16 | 0.20 ± 0.10 | 0.8 | 0.59 ± 0.40\* |
|  | 16:1\_16:0 | 584.5 | 0.08 ± 0.04 | 0.07 ± 0.03 | 0.2 | 0.80 ± 0.55 |
|  | 18:1\_14:0 | 584.5 | 0.35 ± 0.12 | 0.47 ± 0.22 | 0.8 | 1.33 ± 0.76 |
|  | 16:0\_16:0 | 586.5 | 4.79 ± 2.07 | 1.57 ± 0.62 | 11.3 | **0.33 ± 0.19\*\*** |
|  | 18:2\_16:0 | 610.5 | 1.48 ± 0.66 | 5.83 ± 2.69 | 3.5 | **3.94 ± 2.54\*\*** |
|  | 18:1\_16:0 | 612.5 | 2.04 ± 1.01 | 2.93 ± 1.39 | 4.8 | 1.44 ± 0.99 |
|  | 18:0\_16:0 | 614.5 | 3.80 ± 1.82 | 1.03 ± 0.44 | 9.0 | **0.27 ± 0.17\*\*** |
|  | 18:3\_18:2 | 632.5 | 5.32 ± 0.41 | 0.72 ± 0.33 | 12.6 | **0.14 ± 0.06\*\*** |
|  | 18:2\_18:2 | 634.5 | 8.06 ± 3.82 | 26.87 ± 12.38 | 19.1 | **3.33 ± 2.20\*\*** |
|  | 18:2\_18:1 | 636.5 | 2.48 ± 1.14 | 9.78 ± 0.94 | 5.9 | **3.95 ± 1.86\*\*** |
|  | 18:1\_18:1 | 638.5 | 6.60 ± 2.42 | 13.05 ± 6.22 | 15.6 | 1.98 ± 1.19\* |
|  | 18:1\_18:0 | 640.5 | 1.71 ± 0.80 | 2.31 ± 1.09 | 4.1 | 1.35 ± 0.89 |
|  | 18:0\_18:0 | 642.5 | 2.01 ± 0.82 | 0.61 ± 0.29 | 4.8 | **0.30 ± 0.19\*\*** |
|  | 20:4\_18:1 | 660.5 | 0.10 ± 0.05 | 0.04 ± 0.02 | 0.2 | **0.38 ± 0.26\*\*** |
|  | 20:3\_18:1 | 662.5 | 0.03 ± 0.01 | 0.03 ± 0.01 | 0.1 | 0.88 ± 0.59 |
|  | 20:2\_18:2 | 662.5 | 0.03 ± 0.02 | 0.03 ± 0.02 | 0.1 | 0.86 ± 0.67 |
|  | 20:2\_18:1 | 664.5 | 0.04 ± 0.02 | 0.06 ± 0.03 | 0.1 | 1.48 ± 0.95 |
|  | 20:1\_18:2 | 664.5 | 0.03 ± 0.02 | 0.06 ± 0.03 | 0.1 | 1.80 ± 1.23\* |
|  | 20:1\_18:1 | 666.5 | 0.05 ± 0.02 | 0.09 ± 0.04 | 0.1 | 1.80 ± 1.07\*\* |
|  | 20:0\_18:2 | 666.5 | 0.28 ± 0.11 | 0.11 ± 0.05 | 0.7 | **0.39 ± 0.24\*\*** |
|  | 20:0\_18:1 | 668.5 | 0.33 ± 0.13 | 0.19 ± 0.09 | 0.8 | 0.59 ± 0.36\*\* |
|  | 22:0\_18:2 | 694.5 | 0.12 ± 0.04 | 0.08 ± 0.04 | 0.3 | 0.67 ± 0.41 |
|  | 22:0\_18:1 | 696.5 | 0.25 ± 0.12 | 0.17 ± 0.09 | 0.6 | 0.67 ± 0.47 |
|  | 24:0\_18:2 | 722.5 | 0.10 ± 0.04 | 0.03 ± 0.02 | 0.2 | **0.34 ± 0.22\*\*** |
|  | 24:0\_18:1 | 724.5 | 0.09 ± 0.04 | 0.07 ± 0.02 | 0.2 | 0.70 ± 0.42 |
| TG | 36:0 | 656.5 | N.D. | N.D. | - | - |
| (46) | 38:0 | 684.5 | N.D. | N.D. | - | - |
|  | 40:0 | 712.5 | N.D. | N.D. | - | - |
|  | 42:2 | 736.5 | N.D. | N.D. | - | - |
|  | 42:1 | 738.5 | N.D. | N.D. | - | - |
|  | 42:0 | 740.5 | N.D. | N.D. | - | - |
|  | 44:2 | 764.5 | N.D. | N.D. | - | - |
|  | 44:1 | 766.5 | 0.02 ± 0.01 | N.D. | 0.1 | - |
|  | 44:0 | 768.5 | N.D. | N.D. | - | - |
|  | 46:3 | 790.5 | N.D. | N.D. | - | - |
|  | 46:2 | 792.5 | N.D. | 0.12 ± 0.00 | - | - |
|  | 46:1 | 794.5 | N.D. | 0.15 ± 0.02 | - | - |
|  | 46:0 | 796.5 | 0.02 ± 0.01 | 0.02 ± 0.01 | 0.1 | 0.92 ± 0.54 |
|  | 48:3 | 818.5 | N.D. | 1.18 ± 0.28 | - | - |
|  | 48:2 | 820.5 | 0.02 ± 0.01 | 0.03 ± 0.01 | 0.1 | 1.36 ± 0.89 |
|  | 48:1 | 822.5 | 0.02 ± 0.01 | 0.06 ± 0.03 | 0.1 | **2.37 ± 1.53\*\*** |
|  | 48:0 | 824.5 | 0.43 ± 0.20 | 0.89 ± 0.42 | 2.2 | **2.08 ± 1.38\*** |
|  | 50:4 | 844.5 | N.D. | N.D. | - | - |
|  | 50:3 | 846.5 | 0.02 ± 0.01 | 0.06 ± 0.03 | 0.1 | **3.27 ± 2.15\*\*** |
|  | 50:2 | 848.5 | 0.02 ± 0.01 | 0.04 ± 0.02 | 0.1 | **2.08 ± 1.36\*\*** |
|  | 50:1 | 850.5 | 0.34 ± 0.15 | 0.21 ± 0.10 | 1.7 | 0.62 ± 0.41\* |
|  | 50:0 | 852.5 | 0.09 ± 0.04 | 0.14 ± 0.06 | 0.4 | 1.65 ± 1.07\* |
|  | 52:6 | 868.5 | N.D. | N.D. | - | - |
|  | 52:5 | 870.5 | 0.02 ± 0.01 | 0.05 ± 0.02 | 0.1 | **2.35 ± 1.58\*\*** |
|  | 52:4 | 872.5 | 1.74 ± 0.48 | 1.81 ± 0.89 | 9.0 | 1.04 ± 0.59 |
|  | 52:3 | 874.5 | 1.14 ± 0.51 | 0.41 ± 0.18 | 5.9 | **0.36 ± 0.22\*\*** |
|  | 52:2 | 876.5 | 1.01 ± 0.39 | 0.71 ± 0.36 | 5.2 | 0.70 ± 0.44 |
|  | 52:1 | 878.5 | 0.16 ± 0.08 | 0.12 ± 0.06 | 0.8 | 0.74 ± 0.51 |
|  | 52:0 | 880.5 | 0.06 ± 0.03 | 0.07 ± 0.04 | 0.3 | 1.18 ± 0.80 |
|  | 54:9 | 890.5 | N.D. | N.D. | - | - |
|  | 54:8 | 892.5 | 0.08 ± 0.01 | N.D. | 0.4 | - |
|  | 54:7 | 894.5 | 0.49 ± 0.01 | 0.06 ± 0.02 | 2.5 | **0.11 ± 0.05\*\*** |
|  | 54:6 | 896.5 | 0.44 ± 0.18 | 3.21 ± 1.57 | 2.3 | **7.32 ± 4.69\*\*** |
|  | 54:5 | 898.5 | 5.49 ± 1.77 | 1.99 ± 0.85 | 28.5 | **0.36 ± 0.19\*\*** |
|  | 54:4 | 900.5 | 3.02 ± 1.42 | 2.38 ± 0.26 | 15.7 | 0.79 ± 0.38 |
|  | 54:3 | 902.5 | 3.68 ± 0.36 | 4.34 ± 2.08 | 19.1 | 1.18 ± 0.58 |
|  | 54:2 | 904.5 | 0.73 ± 0.08 | 0.33 ± 0.16 | 3.8 | **0.45 ± 0.23\*\*** |
|  | 54:1 | 906.5 | 0.10 ± 0.03 | 0.05 ± 0.02 | 0.5 | **0.47 ± 0.25\*\*** |
|  | 54:0 | 908.5 | 0.02 ± 0.01 | 0.02 ± 0.01 | 0.1 | 0.96 ± 0.59 |
|  | 56:6 | 924.5 | N.D. | N.D. | - | - |
|  | 56:5 | 926.5 | 0.02 ± 0.01 | 0.01 ± 0.00 | 0.1 | **0.40 ± 0.22\*** |
|  | 56:4 | 928.5 | 0.03 ± 0.01 | 0.02 ± 0.01 | 0.2 | 0.53 ± 0.30\*\* |
|  | 56:3 | 930.5 | 0.03 ± 0.01 | 0.07 ± 0.03 | 0.1 | **2.50 ± 1.41\*\*** |
|  | 56:2 | 932.5 | 0.03 ± 0.01 | 0.01 ± 0.01 | 0.1 | 0.56 ± 0.33 |
|  | 56:1 | 934.5 | N.D. | N.D. | - | - |
|  | 56:0 | 936.5 | N.D. | N.D. | - | - |
| CE | 16:1 | 640.5 | 0.96 ± 0.34 | 2.96 ± 1.24 | 25.5 | **3.09 ± 1.71\*\*** |
| (7) | 16:0 | 642.5 | 0.09 ± 0.04 | 1.43 ± 0.61 | 2.4 | **15.75 ± 9.61\*\*** |
|  | 18:3 | 664.5 | 0.56 ± 0.26 | 0.30 ± 0.14 | 14.9 | 0.54 ± 0.36 |
|  | 18:2 | 666.5 | 1.53 ± 0.74 | 9.29 ± 3.19 | 40.7 | **6.08 ± 3.62\*\*** |
|  | 18:1 | 668.5 | 0.46 ± 0.08 | 1.85 ± 0.83 | 12.2 | **4.05 ± 1.95\*\*** |
|  | 20:4 | 690.5 | 0.06 ± 0.02 | 0.36 ± 0.13 | 1.5 | **6.47 ± 3.46\*\*** |
|  | 20:3 | 692.5 | 0.10 ± 0.05 | 3.20 ± 0.27 | 2.7 | **31.20 ± 15.23\*\*** |

Table S6. Isomeric structure of PC, PE, and TG identified from CID spectra.

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Saliva | | | | | | | |
| Class | Molecular  species | Acyl chains | *m/z* | Class | Molecular  species | Acyl chains | *m/z* |
| PC | 32:1 | 16:0/16:1 | 732.554 |  | 48:3 | 16:1\_16:1\_16:1 | 818.723 |
|  |  | 14:0/18:1 | 732.554 |  |  | 18:1\_16:1\_14:1 | 818.723 |
|  | 34:1 | 16:0/18:1 | 760.585 |  |  | 18:2\_16:0\_14:1 | 818.723 |
|  |  | 18:0/16:1 | 760.585 |  |  | 18:2\_16:1\_14:0 | 818.723 |
|  | 36:3 | 18:1/18:2 | 784.585 |  |  | 18:2\_18:1\_12:0 | 818.723 |
|  |  | 20:3/16:0 | 784.585 |  | 48:2 | 16:1\_16:1\_16:0 | 820.739 |
|  | 36:2 | 18:0/18:2 | 786.601 |  |  | 18:0\_16:1\_14:1 | 820.739 |
|  |  | 18:1/18:1 | 786.601 |  |  | 18:1\_16:0\_14:1 | 820.739 |
|  | 38:4 | 18:0/20:4 | 810.601 |  |  | 18:1\_16:1\_14:0 | 820.739 |
|  |  | 16:0/22:4 | 810.601 |  |  | 18:1\_18:1\_12:0 | 820.739 |
|  | 38:2 | 20:0/18:2 | 814.632 |  |  | 18:2\_16:0\_14:0 | 820.739 |
|  |  | 16:0/22:2 | 814.632 |  |  | 18:2\_18:0\_12:0 | 820.739 |
|  |  | 18:0/20:2 | 814.632 |  | 48:1 | 16:1\_16:0\_16:0 | 822.755 |
|  | 42:0 | 24:0/18:0 | 874.726 |  |  | 18:0\_16:1\_14:0 | 822.755 |
|  |  | 26:0/16:0 | 874.726 |  |  | 18:1\_16:0\_14:0 | 822.755 |
|  | 44:1 | 24:0/18:1 | 900.742 |  | 48:0 | 16:0\_16:0\_16:0 | 824.770 |
|  |  | 18:0/24:1 | 900.742 |  |  | 18:0\_16:0\_14:0 | 824.770 |
| PE | 30:1 | 14:0/16:1 | 662.476 |  | 50:3 | 18:1\_16:1\_16:1 | 846.755 |
|  |  | 16:0/14:1 | 662.476 |  |  | 18:2\_16:1\_16:0 | 846.755 |
|  |  | 18:1/12:0 | 662.476 |  |  | 18:2\_18:1\_14:0 | 846.755 |
|  | 30:0 | 16:0/14:0 | 664.491 |  | 50:2 | 18:0\_16:1\_16:1 | 848.770 |
|  |  | 18:0/12:0 | 664.491 |  |  | 18:1\_16:1\_16:0 | 848.770 |
|  | 32:2 | 16:1/16:1 | 688.491 |  |  | 18:1\_18:1\_14:0 | 848.770 |
|  |  | 14:0/18:2 | 688.491 |  |  | 18:2\_16:0\_16:0 | 848.770 |
|  |  | 18:1/14:1 | 688.491 |  |  | 18:2\_18:0\_14:0 | 848.770 |
|  | 32:1 | 16:0/16:1 | 690.507 |  | 50:1 | 18:1\_16:0\_16:0 | 850.786 |
|  |  | 14:0/18:1 | 690.507 |  |  | 18:1\_18:0\_14:0 | 850.786 |
|  | 34:3 | 16:1/18:2 | 714.507 |  | 50:0 | 18:0\_16:0\_16:0 | 852.802 |
|  |  | 16:0/18:3 | 714.507 |  |  | 18:0\_18:0\_14:0 | 852.802 |
|  |  | 20:3/14:0 | 714.507 |  | 52:6 | 18:3\_18:2\_16:1 | 868.739 |
|  | 34:2 | 16:0/18:2 | 716.523 |  |  | 18:3\_18:3\_16:0 | 868.739 |
|  |  | 16:1/18:1 | 716.523 |  | 52:5 | 18:2\_18:2\_16:1 | 870.755 |
|  | 34:1 | 16:0/18:1 | 718.538 |  |  | 18:3\_18:1\_16:1 | 870.755 |
|  |  | 18:0/16:1 | 718.538 |  |  | 18:3\_18:2\_16:0 | 870.755 |
|  | 36:3 | 18:1/18:2 | 742.538 |  | 52:4 | 18:2\_18:1\_16:1 | 872.770 |
|  |  | 16:0/20:3 | 742.538 |  |  | 18:2\_18:2\_16:0 | 872.770 |
|  |  | 18:3/18:0 | 742.538 |  | 52:3 | 18:1\_18:1\_16:1 | 874.786 |
|  | 36:2 | 18:0/18:2 | 744.554 |  |  | 18:2\_18:0\_16:1 | 874.786 |
|  |  | 18:1/18:1 | 744.554 |  |  | 18:2\_18:1\_16:0 | 874.786 |
|  |  | 16:0/20:2 | 744.554 |  | 52:2 | 18:1\_18:0\_16:1 | 876.802 |
|  | 36:1 | 18:0/18:1 | 746.569 |  |  | 18:1\_18:1\_16:0 | 876.802 |
|  |  | 20:1/16:0 | 746.569 |  |  | 18:2\_18:0\_16:0 | 876.802 |
|  | 38:5 | 16:0/22:5 | 766.538 |  | 52:1 | 18:1\_18:0\_16:0 | 878.817 |
|  |  | 18:1/20:4 | 766.538 |  |  | 18:0\_18:0\_16:0 | 880.833 |
|  |  | 20:3/18:2 | 766.538 |  | 54:7 | 18:3\_18:2\_18:2 | 894.755 |
|  | 38:2 | 20:0/18:2 | 772.585 |  |  | 18:3\_18:3\_18:1 | 894.755 |
|  |  | 20:1/18:1 | 772.585 |  |  | 20:4\_18:2\_16:1 | 894.755 |
|  |  | 18:0/20:2 | 772.585 |  | 54:6 | 18:2\_18:2\_18:2 | 896.770 |
|  |  | 22:2/16:0 | 772.585 |  |  | 18:3\_18:2\_18:1 | 896.770 |
| TG | 40:0 | 14:0\_14:0\_12:0 | 712.645 |  | 54:5 | 18:2\_18:2\_18:1 | 898.786 |
|  |  | 16:0\_12:0\_12:0 | 712.645 |  |  | 18:3\_18:1\_18:1 | 898.786 |
|  | 42:1 | 14:1\_14:0\_14:0 | 738.661 |  | 54:4 | 18:2\_18:1\_18:1 | 900.802 |
|  |  | 16:0\_14:1\_12:0 | 738.661 |  |  | 18:2\_18:2\_18:0 | 900.802 |
|  |  | 16:1\_14:0\_12:0 | 738.661 |  |  | 18:3\_18:1\_18:0 | 900.802 |
|  |  | 18:1\_12:0\_12:0 | 738.661 |  |  | 20:3\_18:1\_16:0 | 900.802 |
|  | 42:0 | 14:0\_14:0\_14:0 | 740.676 |  | 54:3 | 18:1\_18:1\_18:1 | 902.817 |
|  |  | 16:0\_14:0\_12:0 | 740.676 |  |  | 18:2\_18:1\_18:0 | 902.817 |
|  |  | 18:0\_12:0\_12:0 | 740.676 |  | 54:0 | 18:1\_18:0\_18:0 | 906.849 |
|  | 44:3 | 16:1\_14:1\_14:1 | 762.661 |  |  | 20:0\_18:0\_16:0 | 906.849 |
|  |  | 18:2\_14:1\_12:0 | 762.661 |  | 56:8 | 20:4\_18:2\_18:2 | 920.770 |
|  | 44:2 | 16:0\_14:1\_14:1 | 764.676 |  |  | 20:4\_20:4\_16:0 | 920.770 |
|  |  | 18:1\_14:1\_12:0 | 764.676 |  | 56:7 | 20:3\_18:2\_18:2 | 922.786 |
|  |  | 18:2\_14:0\_12:0 | 764.676 |  |  | 20:3\_18:3\_18:1 | 922.786 |
|  | 44:1 | 16:0\_14:1\_14:0 | 766.692 |  |  | 20:3\_20:3\_16:1 | 922.786 |
|  |  | 16:1\_14:0\_14:0 | 766.692 |  |  | 20:4\_18:2\_18:1 | 922.786 |
|  |  | 18:0\_14:1\_12:0 | 766.692 |  | 56:5 | 20:1\_18:3\_18:1 | 926.817 |
|  |  | 18:1\_14:0\_12:0 | 766.692 |  |  | 20:2\_18:2\_18:1 | 926.817 |
|  | 44:0 | 16:0\_14:0\_14:0 | 768.708 |  |  | 20:2\_18:3\_18:0 | 926.817 |
|  |  | 16:0\_16:0\_12:0 | 768.708 |  |  | 20:3\_18:1\_18:1 | 926.817 |
|  |  | 18:0\_14:0\_12:0 | 768.708 |  |  | 20:3\_18:2\_18:0 | 926.817 |
|  | 46:3 | 16:1\_16:1\_14:1 | 790.692 |  |  | 20:3\_20:2\_16:0 | 926.817 |
|  |  | 18:1\_14:1\_14:1 | 790.692 |  | 56:4 | 20:0\_18:2\_18:2 | 928.833 |
|  |  | 18:2\_14:1\_14:0 | 790.692 |  |  | 20:1\_18:2\_18:1 | 928.833 |
|  |  | 18:2\_16:1\_12:0 | 790.692 |  |  | 20:2\_18:1\_18:1 | 928.833 |
|  | 46:2 | 16:1\_16:0\_14:1 | 792.708 |  | 56:3 | 20:0\_18:2\_18:1 | 930.849 |
|  |  | 16:1\_16:1\_14:0 | 792.708 |  |  | 20:1\_18:1\_18:1 | 930.849 |
|  |  | 18:1\_14:1\_14:0 | 792.708 |  | 56:2 | 20:0\_18:1\_18:1 | 932.864 |
|  |  | 18:1\_16:1\_12:0 | 792.708 |  |  | 20:1\_18:1\_18:0 | 932.864 |
|  |  | 18:2\_14:0\_14:0 | 792.708 |  |  | 20:1\_20:0\_16:1 | 932.864 |
|  |  | 18:2\_16:0\_12:0 | 792.708 |  |  | 20:1\_20:1\_16:0 | 932.864 |
|  | 46:1 | 16:1\_16:0\_14:0 | 794.723 |  |  | 22:0\_18:1\_16:1 | 932.864 |
|  |  | 18:0\_16:1\_12:0 | 794.723 |  |  | 22:0\_18:2\_16:0 | 932.864 |
|  |  | 18:1\_14:0\_14:0 | 794.723 |  |  | 24:0\_16:1\_16:1 | 932.864 |
|  |  | 18:1\_16:0\_12:0 | 794.723 |  | 58:8 | 20:4\_20:4\_18:0 | 948.801 |
|  | 46:0 | 16:0\_16:0\_14:0 | 796.739 |  |  | 22:5\_18:2\_18:1 | 948.801 |
|  |  | 18:0\_14:0\_14:0 | 796.739 |  |  | 22:6\_18:1\_18:1 | 948.801 |
|  |  | 18:0\_16:0\_12:0 | 796.739 |  |  |  |  |
| Plasma | | | | | | | |
| Class | Molecular  species | Acyl chains | *m/z* | Class | Molecular  species | Acyl chains | *m/z* |
| PC | 32:2 | 14:0/18:2 | 730.538 |  |  | 18:2\_14:1\_14:0 | 790.692 |
|  |  | 16:1/16:1 | 730.538 |  |  | 18:2\_16:1\_12:0 | 790.692 |
|  | 32:1 | 14:0/18:1 | 732.554 |  | 46:2 | 16:1\_16:0\_14:1 | 792.708 |
|  |  | 16:0/16:1 | 732.554 |  |  | 16:1\_16:1\_14:0 | 792.708 |
|  | 34:4 | 14:0/20:4 | 754.538 |  |  | 18:1\_14:1\_14:0 | 792.708 |
|  |  | 16:2/18:2 | 754.538 |  |  | 18:1\_16:1\_12:0 | 792.708 |
|  | 34:3 | 14:0/20:3 | 756.554 |  |  | 18:2\_14:0\_14:0 | 792.708 |
|  |  | 16:0/18:3 | 756.554 |  |  | 18:2\_16:0\_12:0 | 792.708 |
|  |  | 16:1/18:2 | 756.554 |  | 46:1 | 16:0\_16:0\_14:1 | 794.723 |
|  | 36:4 | 16:0/20:4 | 782.569 |  |  | 16:1\_16:0\_14:0 | 794.723 |
|  |  | 18:2/18:2 | 782.569 |  |  | 18:1\_14:0\_14:0 | 794.723 |
|  | 36:3 | 16:0/20:3 | 784.585 |  |  | 18:1\_16:0\_12:0 | 794.723 |
|  |  | 18:1/18:2 | 784.585 |  | 48:4 | 18:2\_16:1\_14:1 | 816.708 |
|  | 36:2 | 16:0/20:2 | 786.601 |  |  | 18:2\_18:2\_12:0 | 816.708 |
|  |  | 18:0/18:2 | 786.601 |  |  | 18:3\_18:1\_12:0 | 816.708 |
|  |  | 18:1/18:1 | 786.601 |  | 48:3 | 16:1\_16:1\_16:1 | 818.723 |
|  | 36:1 | 16:0/20:1 | 788.616 |  |  | 18:1\_16:1\_14:1 | 818.723 |
|  |  | 18:0/18:1 | 788.616 |  |  | 18:2\_16:0\_14:1 | 818.723 |
|  | 38:7 | 16:1/22:6 | 804.554 |  |  | 18:2\_16:1\_14:0 | 818.723 |
|  |  | 18:2/20:5 | 804.554 |  |  | 18:2\_18:1\_12:0 | 818.723 |
|  | 38:6 | 16:0/22:6 | 806.569 |  | 48:2 | 16:1\_16:1\_16:0 | 820.739 |
|  |  | 18:1/20:5 | 806.569 |  |  | 18:1\_16:0\_14:1 | 820.739 |
|  |  | 18:2/20:4 | 806.569 |  |  | 18:1\_16:1\_14:0 | 820.739 |
|  | 38:5 | 16:0/22:5 | 808.585 |  |  | 18:1\_18:1\_12:0 | 820.739 |
|  |  | 18:0/20:5 | 808.585 |  |  | 18:2\_16:0\_14:0 | 820.739 |
|  |  | 18:1/20:4 | 808.585 |  | 48:1 | 16:1\_16:0\_16:0 | 822.755 |
|  | 38:4 | 16:0/22:4 | 810.601 |  |  | 18:0\_16:1\_14:0 | 822.755 |
|  |  | 18:0/20:4 | 810.601 |  |  | 18:1\_16:0\_14:0 | 822.755 |
|  |  | 18:1/20:3 | 810.601 |  | 48:0 | 16:0\_16:0\_16:0 | 824.770 |
|  | 38:2 | 18:0/20:2 | 814.632 |  |  | 18:0\_16:0\_14:0 | 824.770 |
|  |  | 20:0/18:2 | 814.632 |  | 50:5 | 18:2\_18:2\_14:1 | 842.723 |
|  |  | 20:1/18:1 | 814.632 |  |  | 18:3\_16:1\_16:1 | 842.723 |
|  | 40:8 | 20:4/20:4 | 830.569 |  |  | 18:3\_18:2\_14:0 | 842.723 |
|  |  | 22:6/18:2 | 830.569 |  | 50:4 | 18:1\_16:2\_16:1 | 844.739 |
|  | 40:7 | 18:1/22:6 | 832.585 |  |  | 18:2\_16:1\_16:1 | 844.739 |
|  |  | 20:3/20:4 | 832.585 |  |  | 18:2\_18:1\_14:1 | 844.739 |
|  |  | 22:5/18:2 | 832.585 |  |  | 18:2\_18:2\_14:0 | 844.739 |
|  | 40:6 | 18:0/22:6 | 834.601 |  |  | 18:3\_16:1\_16:0 | 844.739 |
|  |  | 18:1/22:5 | 834.601 |  |  | 18:3\_18:1\_14:0 | 844.739 |
|  |  | 20:2/20:4 | 834.601 |  | 50:3 | 18:1\_16:1\_16:1 | 846.755 |
|  |  | 20:3/20:3 | 834.601 |  |  | 18:1\_18:1\_14:1 | 846.755 |
| PE | 36:5 | 16:0/20:5 | 738.507 |  |  | 18:2\_18:1\_14:0 | 846.755 |
|  |  | 16:1/20:4 | 738.507 |  | 50:2 | 18:1\_16:1\_16:0 | 848.770 |
|  | 36:4 | 16:0/20:4 | 740.522 |  |  | 18:1\_18:1\_14:0 | 848.770 |
|  |  | 18:2/18:2 | 740.522 |  |  | 18:2\_16:0\_16:0 | 848.770 |
|  |  | 18:1/18:3 | 740.523 |  | 50:1 | 18:0\_16:1\_16:0 | 850.786 |
|  | 36:3 | 16:0/20:3 | 742.538 |  |  | 18:1\_16:0\_16:0 | 850.786 |
|  |  | 18:1/18:2 | 742.538 |  | 52:6 | 18:2\_18:2\_16:2 | 868.739 |
|  | 36:1 | 16:0/20:1 | 746.569 |  |  | 18:3\_18:2\_16:1 | 868.739 |
|  |  | 18:0/18:1 | 746.569 |  |  | 20:4\_16:1\_16:1 | 868.739 |
|  | 38:6 | 18:2/20:4 | 764.522 |  | 52:5 | 18:2\_18:2\_16:1 | 870.755 |
|  |  | 22:6/16:0 | 764.522 |  |  | 18:3\_18:1\_16:1 | 870.755 |
|  |  | 18:1/20:5 | 764.523 |  |  | 18:3\_18:2\_16:0 | 870.755 |
|  | 38:5 | 16:0/22:5 | 766.538 |  | 52:4 | 18:2\_18:1\_16:1 | 872.770 |
|  |  | 18:0/20:5 | 766.538 |  |  | 18:2\_18:2\_16:0 | 872.770 |
|  |  | 18:1/20:4 | 766.538 |  |  | 18:3\_18:1\_16:0 | 872.770 |
|  | 38:4 | 18:0/20:4 | 768.554 |  | 52:3 | 18:1\_18:1\_16:1 | 874.786 |
|  |  | 18:1/20:3 | 768.554 |  |  | 18:2\_18:1\_16:0 | 874.786 |
|  | 40:6 | 18:0/22:6 | 792.554 |  | 52:2 | 18:1\_18:0\_16:1 | 876.802 |
|  |  | 18:1/22:5 | 792.554 |  |  | 18:1\_18:1\_16:0 | 876.802 |
|  | 40:5 | 18:0/22:5 | 794.569 |  |  | 18:2\_18:0:16:0 | 876.802 |
|  |  | 20:1/20:4 | 794.569 |  | 52:1 | 18:0\_18:0\_16:1 | 878.817 |
| TG | 40:1 | 14:1\_14:0\_12:0 | 710.629 |  |  | 18:1\_18:0\_16:0 | 878.817 |
|  |  | 16:1\_12:0\_12:0 | 710.629 |  | 54:7 | 18:3\_18:2\_18:2 | 894.755 |
|  | 40:0 | 14:0\_14:0\_12:0 | 712.645 |  |  | 20:4\_18:2\_16:1 | 894.755 |
|  |  | 16:0\_12:0\_12:0 | 712.645 |  | 54:6 | 18:2\_18:2\_18:2 | 896.770 |
|  | 42:2 | 16:1\_14:1\_12:0 | 736.645 |  |  | 18:3\_18:2\_18:1 | 896.770 |
|  |  | 16:1\_14:1\_12:0 | 736.645 |  |  | 20:4\_18:1\_16:1 | 896.770 |
|  |  | 18:2\_12:0\_12:0 | 736.645 |  | 54:5 | 18:2\_18:2\_18:1 | 898.786 |
|  | 42:1 | 14:1\_14:0\_14:0 | 738.661 |  |  | 18:3\_18:1\_18:1 | 898.786 |
|  |  | 16:0\_14:1\_12:0 | 738.661 |  |  | 20:3\_18:2\_16:0 | 898.786 |
|  |  | 16:1\_14:0\_12:0 | 738.661 |  | 54:4 | 18:2\_18:1\_18:1 | 900.802 |
|  |  | 18:1\_12:0\_12:0 | 738.661 |  |  | 18:2\_18:2\_18:0 | 900.802 |
|  | 42:0 | 14:0\_14:0\_14:0 | 740.676 |  |  | 20:3\_18:1\_16:0 | 900.802 |
|  |  | 16:0\_14:0\_12:0 | 740.676 |  | 54:3 | 18:1\_18:1\_18:1 | 902.817 |
|  | 44:2 | 16:0\_14:1\_14:1 | 764.676 |  |  | 18:2\_18:1\_18:0 | 902.817 |
|  |  | 16:1\_14:1\_14:0 | 764.676 |  |  | 20:2\_18:1\_16:0 | 902.817 |
|  |  | 16:1\_16:1\_12:0 | 764.676 |  | 54:2 | 18:1\_18:1\_18:0 | 904.833 |
|  |  | 18:1\_14:1\_12:0 | 764.676 |  |  | 20:1\_18:1\_16:0 | 904.833 |
|  |  | 18:2\_14:0\_12:0 | 764.676 |  | 54:0 | 18:0\_18:0\_18:0 | 908.864 |
|  | 44:1 | 16:0\_14:1\_14:0 | 766.692 |  |  | 24:0\_16:0\_14:0 | 908.864 |
|  |  | 16:1\_14:0\_14:0 | 766.692 |  | 56:8 | 20:4\_18:2\_18:2 | 920.770 |
|  |  | 16:1\_16:0\_12:0 | 766.692 |  |  | 22:6\_18:2\_16:0 | 920.770 |
|  |  | 18:1\_14:0\_12:0 | 766.692 |  | 56:7 | 20:4\_18:2\_18:1 | 922.786 |
|  | 44:0 | 16:0\_14:0\_14:0 | 768.708 |  |  | 20:5\_18:1\_18:1 | 922.786 |
|  |  | 16:0\_16:0\_12:0 | 768.708 |  |  | 22:5\_18:2\_16:0 | 922.786 |
|  |  | 18:0\_14:0\_12:0 | 768.708 |  | 56:6 | 20:4\_18:1\_18:1 | 924.802 |
|  | 46:3 | 16:1\_16:1\_14:1 | 790.692 |  |  | 22:4\_18:2\_16:0 | 924.802 |
|  |  | 18:1\_14:1\_14:1 | 790.692 |  |  | 22:5\_18:1\_16:0 | 924.802 |
| Feces | | | | | | | |
| Class | Molecular  species | Acyl chains | *m/z* | Class | Molecular  species | Acyl chains | *m/z* |
| TG | 40:0 | 14:0\_14:0\_12:0 | 712.645 |  | 48:3 | 16:1\_16:1\_16:1 | 818.723 |
|  |  | 16:0\_12:0\_12:0 | 712.645 |  |  | 18:1\_16:1\_14:1 | 818.723 |
|  | 42:2 | 16:1\_14:1\_12:0 | 736.645 |  |  | 18:2\_16:1\_14:0 | 818.723 |
|  |  | 18:2\_12:0\_12:0 | 736.645 |  | 48:2 | 16:1\_16:1\_16:0 | 820.739 |
|  | 42:1 | 14:1\_14:0\_14:0 | 738.661 |  |  | 18:1\_16:1\_14:0 | 820.739 |
|  |  | 16:0\_14:1\_12:0 | 738.661 |  | 48:1 | 16:1\_16:0\_16:0 | 822.755 |
|  |  | 16:1\_14:0\_12:0 | 738.661 |  |  | 18:1\_16:0\_14:0 | 822.755 |
|  |  | 18:1\_12:0\_12:0 | 738.661 |  | 50:4 | 18:2\_16:1\_16:1 | 844.739 |
|  | 42:0 | 14:0\_14:0\_14:0 | 740.676 |  |  | 18:2\_18:2\_14:0 | 844.739 |
|  |  | 16:0\_14:0\_12:0 | 740.676 |  | 50:3 | 18:1\_16:1\_16:1 | 846.755 |
|  |  | 18:0\_12:0\_12:0 | 740.676 |  |  | 18:2\_16:1\_16:0 | 846.755 |
|  | 44:2 | 16:0\_14:1\_14:1 | 764.676 |  |  | 18:2\_18:1\_14:0 | 846.755 |
|  |  | 16:1\_14:1\_14:0 | 764.676 |  | 50:2 | 18:0\_16:1\_16:1 | 848.770 |
|  |  | 16:1\_16:1\_12:0 | 764.676 |  |  | 18:1\_16:1:\_16:0 | 848.770 |
|  |  | 18:1\_14:1\_12:0 | 764.676 |  | 52:5 | 18:2\_18:2\_16:1 | 870.755 |
|  | 44:1 | 16:0\_14:1\_14:0 | 766.692 |  |  | 18:3\_18:2\_16:0 | 870.755 |
|  |  | 16:1\_14:0\_14:0 | 766.692 |  | 54:4 | 18:2\_18:1\_18:1 | 900.802 |
|  |  | 16:1\_16:0\_12:0 | 766.692 |  |  | 18:2\_18:2\_18:0 | 900.802 |
|  |  | 18:1\_14:0\_12:0 | 766.692 |  | 54:3 | 18:1\_18:1\_18:1 | 902.817 |
|  | 44:0 | 16:0\_14:0\_14:0 | 768.708 |  |  | 18:2\_18:1\_18:0 | 902.817 |
|  |  | 16:0\_16:0\_12:0 | 768.708 |  | 54:1 | 18:1\_18:0\_18:0 | 906.849 |
|  |  | 18:0\_14:0\_12:0 | 768.708 |  |  | 20:0\_18:0\_16:1 | 906.849 |
|  | 46:2 | 16:1\_16:0\_14:1 | 792.708 |  |  | 20:0\_18:1\_16:0 | 906.849 |
|  |  | 16:1\_16:1\_14:0 | 792.708 |  | 56:4 | 20:0\_18:2\_18:2 | 928.833 |
|  |  | 18:1\_16:1\_12:0 | 792.708 |  |  | 20:1\_18:2\_18:1 | 928.833 |
|  | 46:1 | 16:1\_16:0\_14:0 | 794.723 |  | 56:3 | 20:0\_18:2\_18:1 | 930.849 |
|  |  | 18:1\_14:0\_14:0 | 794.723 |  |  | 20:1\_18:1\_18:1 | 930.849 |
|  |  | 18:1\_16:0\_12:0 | 794.723 |  | 56:2 | 20:0\_18:1\_18:1 | 932.864 |
|  | 46:0 | 16:0\_16:0\_14:0 | 796.739 |  |  | 22:0\_18:1\_16:1 | 932.864 |
|  |  | 18:0\_14:0\_14:0 | 796.739 |  |  |  |  |