

Supplementary materials

The Lipid Asset is Unbalanced in Peripheral Nerve Sheath Tumors

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† Contributed equally

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Figure S1. Principal component analysis for the (A) untargeted lipidomics and (B) targeted sphingolipidomics. Multivariate analysis was performed by the free available software MetaboAnalyst 5.0. Data were checked for integrity, filtered by interquartile range, generalized log-transformed, and auto-scaled prior to the multivariate analysis.

Table S1. List of all the single lipid species identified using an untargeted lipidomics approach across each histotype. Each lipid was identified with monoisotopic molecular adducts in positive electrospray ionization (m/z), name, and mass intensities scaled for protein content in each group.

Table S2. List of all the single lipid species identified using an untargeted lipidomics approach across each histotype. Each lipid was identified with monoisotopic molecular adducts in negative electrospray ionization (m/z), name, and mass intensities scaled for protein content in each group.

Table S3. List of all the sphingolipids species identified using a targeted approach across each histotype. Each sphingolipid was identified with multiple reaction monitoring mass transition (MRM) in positive electrospray ionization, name, and concentration (pmol/mg protein) in each group.

Figure S1. Principal component analysis for the **(A)** untargeted lipidomics and **(B)** targeted sphingolipidomics. Multivariate analysis was performed by the free available software MetaboAnalyst 5.0 (ver. 5.0, McGill Data Center and Compute Canada, Montréal, Canada, <https://www.metaboanalyst.ca>, accessed on 18 December 2021). Data were checked for integrity, filtered by interquartile range, generalized log-transformed, and auto-scaled prior to the multivariate analysis.

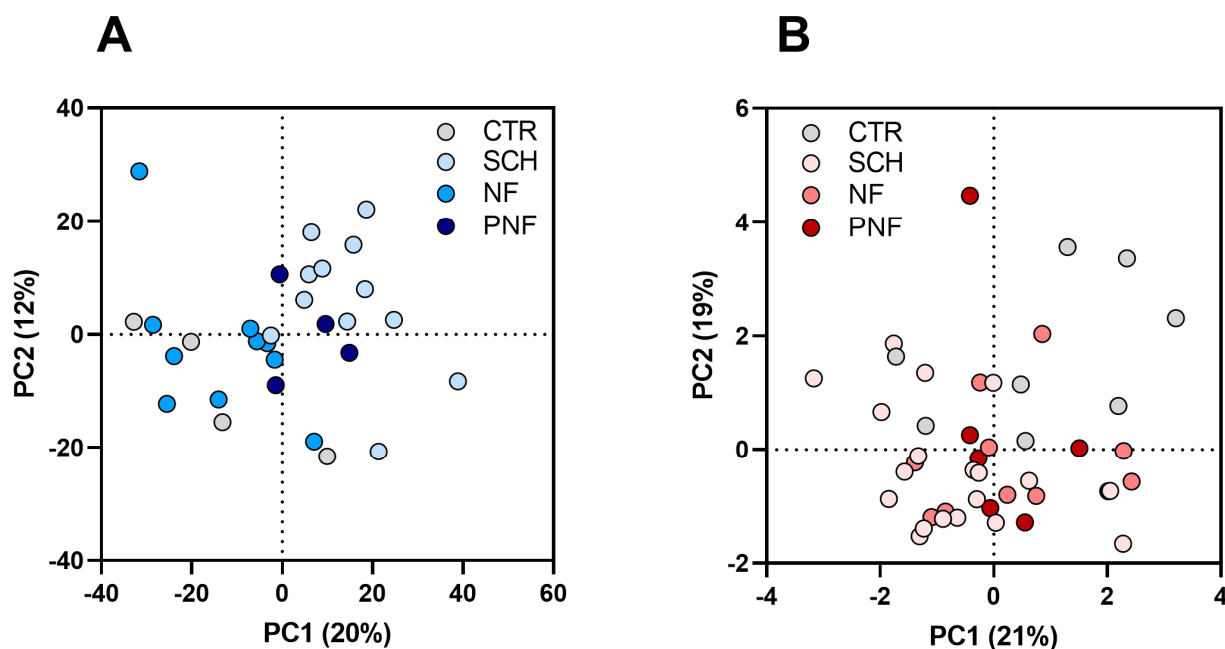


Table S1. List of all the single lipid species identified using an untargeted lipidomics approach across each histotype. Each lipid was identified with monoisotopic molecular adducts in positive electrospray ionization (m/z), name, and mass intensities scaled for protein content in each group.

| Mass m/z | Metabolite name | CTR | | SCH | | NF | | PNF | |
|---------------|-----------------|---------|---------|---------|---------|---------|---------|---------|--------|
| | | mean | dev | mean | dev | mean | dev | mean | dev |
| 372.3103 9 | CAR 14:0 | 3580.64 | 2116.52 | 2330.05 | 1275.36 | 4827.49 | 4045.71 | 1453.51 | 643.71 |
| 396.3142 4 | CAR 16:2 | 50.90 | 40.83 | 80.76 | 105.40 | 138.28 | 108.77 | 75.86 | 81.21 |
| 394.2941 6 | CAR 16:3 | 211.08 | 222.76 | 131.09 | 163.10 | 314.89 | 285.73 | 39.50 | 18.27 |
| 414.3572 1 | CAR 17:0 | 1497.17 | 650.51 | 694.22 | 357.49 | 1028.75 | 1302.43 | 1135.00 | 356.97 |
| 426.3591 9 | CAR 18:1 | 94.25 | 101.06 | 55.76 | 44.38 | 180.46 | 201.85 | 28.35 | 15.54 |
| 442.3923 3 | CAR 19:0 | 139.82 | 55.89 | 93.18 | 53.94 | 171.70 | 251.86 | 98.19 | 37.86 |
| 432.3181 8 | CAR 19:5 | 193.62 | 245.18 | 59.31 | 33.25 | 73.68 | 67.73 | 61.57 | 11.75 |
| 456.4045 1 | CAR 20:0 | 612.80 | 936.78 | 168.66 | 122.21 | 979.63 | 1764.55 | 122.48 | 104.02 |
| 446.3248 3 | CAR 20:5 | 52.07 | 28.16 | 34.31 | 33.92 | 63.39 | 40.16 | 14.01 | 3.47 |
| 484.4334 4 | CAR 22:0 | 80.63 | 101.25 | 33.17 | 22.83 | 166.24 | 262.50 | 25.70 | 18.47 |
| 482.4207 5 | CAR 22:1 | 482.70 | 811.88 | 139.18 | 96.89 | 338.44 | 206.84 | 83.28 | 67.05 |
| 478.3888 5 | CAR 22:3 | 66.79 | 80.65 | 41.75 | 42.80 | 86.71 | 51.92 | 15.27 | 7.73 |
| 512.4655 8 | CAR 24:0 | 165.65 | 161.24 | 90.42 | 89.63 | 206.84 | 184.60 | 48.38 | 26.55 |
| 510.4557 5 | CAR 24:1 | 178.35 | 199.72 | 107.29 | 95.69 | 218.12 | 190.15 | 58.59 | 49.49 |
| 508.4403 1 | CAR 24:2 | 48.60 | 62.21 | 27.18 | 18.51 | 57.63 | 38.16 | 11.94 | 7.61 |
| 504.4057 3 | CAR 24:4 | 88.89 | 108.95 | 70.32 | 40.26 | 168.88 | 137.57 | 32.56 | 16.46 |
| 540.5014 | CAR 26:0 | 121.75 | 74.46 | 85.20 | 64.27 | 261.96 | 228.90 | 49.27 | 15.65 |
| 538.4868 8 | CAR 26:1 | 112.75 | 89.70 | 69.96 | 58.32 | 105.09 | 90.72 | 32.34 | 18.95 |
| 668.6345 2 | CE 18:1 | 16.22 | 24.56 | 41.24 | 48.63 | 46.15 | 94.65 | 23.24 | 16.93 |
| 666.6165 8 | CE 18:2 | 461.94 | 782.29 | 531.17 | 286.64 | 445.01 | 691.45 | 523.63 | 498.65 |
| 664.6018 1 | CE 18:3 | 20.74 | 36.86 | 48.37 | 38.68 | 23.87 | 48.66 | 22.58 | 20.86 |
| 694.6564 9 | CE 20:2 | 2.87 | 5.27 | 22.87 | 44.23 | 15.96 | 46.17 | 1.44 | 0.88 |
| 692.6356 2 | CE 20:3 | 40.59 | 79.46 | 227.74 | 451.47 | 126.32 | 367.62 | 26.07 | 24.29 |
| 688.6059 | CE 20:5 | 64.45 | 124.49 | 218.02 | 317.54 | 70.35 | 187.64 | 130.37 | 201.66 |

| Mass <i>m/z</i> | Metabolite name | CTR | | SCH | | NF | | PNF | |
|--------------------|------------------------------------|--------------|--------------|-------------|--------------|--------------|--------------|-------------|------------|
| | | <i>mean</i> | <i>dev</i> | <i>mean</i> | <i>dev</i> | <i>mean</i> | <i>dev</i> | <i>mean</i> | <i>dev</i> |
| 722.6857 3 | CE 22:2 | 6.17 | 10.33 | 17.19 | 45.10 | 6.51 | 19.48 | 0.57 | 0.31 |
| 718.6547 9 | CE 22:4 | 37.05 | 72.62 | 325.82 | 703.74 | 126.45 | 389.09 | 5.31 | 6.00 |
| 714.6078 5 | CE 22:6 | 3.46 | 3.52 | 30.20 | 62.54 | 4.20 | 8.07 | 14.86 | 23.09 |
| 748.7003 2 | CE 24:3 | 2.68 | 4.87 | 5.38 | 7.42 | 4.43 | 13.03 | 0.49 | 0.46 |
| 744.6672 4 | CE 24:5 | 34.77 | 68.56 | 29.15 | 46.41 | 13.66 | 39.36 | 1.47 | 1.42 |
| 772.6950 7 | CE 26:5 | 54.72 | 107.31 | 9.63 | 10.53 | 4.35 | 11.53 | 1.03 | 1.08 |
| 388.3064 9 | Cer 21:1;4O | 122.76 | 99.11 | 111.18 | 82.92 | 254.75 | 205.34 | 50.86 | 27.94 |
| 368.3138 4 | Cer 22:1;3O Cer 14:1;2O/8:0;O | 432.98 | 432.37 | 259.18 | 134.80 | 683.16 | 653.73 | 185.94 | 154.20 |
| 408.3066 1 | Cer 24:3;4O | 12982.2 4 | 13767.1 6 | 6333.14 | 3800.74 | 22649.6 1 | 23190.9 0 | 4747.00 | 3092.82 |
| 440.3734 4 | Cer 26:1;4O | 432.01 | 451.08 | 442.73 | 909.14 | 146.37 | 155.79 | 160.64 | 43.86 |
| 436.3375 9 | Cer 26:3;4O | 359.87 | 150.10 | 277.48 | 214.93 | 272.98 | 207.35 | 328.78 | 182.10 |
| 464.3739 9 | Cer 28:3;4O | 204.30 | 176.65 | 182.93 | 166.47 | 280.72 | 202.01 | 116.93 | 29.60 |
| 476.3762 5 | Cer 29:4;4O | 25.14 | 19.64 | 101.53 | 241.96 | 57.48 | 118.36 | 9.22 | 1.20 |
| 464.4475 1 | Cer 30:1;2O Cer 18:1;2O/12:0 | 30.76 | 21.22 | 3921.16 | 11588.3 5 | 117.52 | 113.33 | 25.02 | 8.06 |
| 478.4660 6 | Cer 31:1;2O Cer 17:1;2O/14:0 | 23.51 | 10.87 | 74.65 | 101.33 | 239.78 | 227.74 | 47.81 | 25.32 |
| 498.3502 2 | Cer 31:7;4O | 219.46 | 334.76 | 8.76 | 6.42 | 89.54 | 181.11 | 8.97 | 9.58 |
| 528.5006 1 | Cer 32:0;3O Cer 16:0;2O/16:0;O | 5.08 | 3.83 | 6.66 | 12.27 | 153.57 | 440.67 | 2.97 | 1.23 |
| 510.4912 1 | Cer 32:1;2O Cer 16:1;2O/16:0 | 102.79 | 66.84 | 110.87 | 88.96 | 900.33 | 1259.02 | 86.89 | 32.94 |
| 492.4722 9 | Cer 32:1;2O Cer 18:1;2O/14:0 | 200.26 | 150.13 | 219.44 | 172.10 | 1817.55 | 2602.98 | 153.81 | 62.31 |
| 508.4707 3 | Cer 32:1;3O Cer 18:1;2O/14:0;O | 8.13 | 5.39 | 8.65 | 11.47 | 174.79 | 455.32 | 7.98 | 2.32 |
| 508.4750 4 | Cer 32:1;3O Cer 19:0;2O/13:1;O | 3.64 | 2.77 | 5.09 | 10.67 | 87.98 | 246.82 | 2.03 | 0.52 |
| 490.4614 3 | Cer 32:2;2O Cer 18:2;2O/14:0 | 38.36 | 26.40 | 120.08 | 156.74 | 143.82 | 85.40 | 48.14 | 19.25 |
| 542.5183 7 | Cer 33:0;3O Cer 16:0;2O/17:0;O | 0.67 | 0.89 | 0.19 | 0.28 | 86.23 | 241.10 | 0.30 | 0.21 |
| 558.5118 4 | Cer 33:0;4O Cer 17:0;3O/16:0;(2OH) | 2.13 | 1.02 | 3.14 | 6.18 | 91.27 | 260.29 | 1.56 | 0.95 |
| 522.4901 1 | Cer 33:1;3O Cer 18:0;2O/15:1;O | 2.76 | 1.55 | 3.22 | 4.93 | 251.30 | 763.92 | 1.72 | 0.47 |

| Mass <i>m/z</i> | Metabolite name | CTR | | SCH | | NF | | PNF | |
|--------------------|------------------------------------|-------------|------------|-------------|------------|-------------|------------|-------------|------------|
| | | <i>mean</i> | <i>dev</i> | <i>mean</i> | <i>dev</i> | <i>mean</i> | <i>dev</i> | <i>mean</i> | <i>dev</i> |
| 536.4711 3 | Cer 33:2;4O | 236.25 | 275.49 | 7.60 | 5.51 | 94.86 | 103.45 | 17.96 | 26.11 |
| 518.4516 6 | Cer 33:3;3O Cer 18:2;2O/15:1;O | 27.00 | 10.89 | 41.92 | 58.20 | 92.46 | 64.99 | 33.18 | 11.32 |
| 540.5321 7 | Cer 34:0;2O Cer 18:0;2O/16:0 | 2.78 | 1.46 | 77.35 | 177.10 | 10.19 | 13.15 | 2.50 | 2.81 |
| 520.5070 8 | Cer 34:1;2O Cer 18:1;2O/16:0 | 290.27 | 306.19 | 46.30 | 39.67 | 198.13 | 178.56 | 65.39 | 17.95 |
| 554.5131 8 | Cer 34:1;3O Cer 18:1;2O/16:0;O | 14.35 | 10.59 | 22.45 | 36.83 | 133.44 | 228.30 | 28.15 | 22.19 |
| 536.5037 2 | Cer 34:1;3O Cer 19:0;2O/15:1;O | 30.43 | 28.42 | 31.40 | 39.50 | 1892.13 | 5680.23 | 25.36 | 12.94 |
| 552.4977 4 | Cer 34:1;4O Cer 18:1;3O/16:0;(2OH) | 4.63 | 3.05 | 7.19 | 13.01 | 207.96 | 617.69 | 2.39 | 0.71 |
| 518.4933 5 | Cer 34:2;2O Cer 18:2;2O/16:0 | 31.88 | 26.14 | 238.35 | 406.52 | 48.99 | 41.53 | 15.68 | 12.88 |
| 534.4852 9 | Cer 34:2;3O Cer 18:2;2O/16:0;O | 2.05 | 1.42 | 1.89 | 2.97 | 55.03 | 155.31 | 1.25 | 0.33 |
| 568.4923 1 | Cer 34:2;4O Cer 19:1;3O/15:1;(2OH) | 1.94 | 1.21 | 1.23 | 1.37 | 55.89 | 161.50 | 1.50 | 0.94 |
| 560.4241 9 | Cer 34:6;4O | 156.93 | 136.40 | 163.07 | 273.59 | 81.44 | 73.89 | 78.58 | 16.29 |
| 566.5150 1 | Cer 35:2;3O Cer 19:0;2O/16:2;O | 4.58 | 2.63 | 5.62 | 9.85 | 130.06 | 382.26 | 3.42 | 1.89 |
| 552.4088 1 | Cer 35:8;4O | 877.82 | 897.77 | 229.56 | 151.88 | 261.41 | 287.54 | 325.50 | 94.08 |
| 566.5593 9 | Cer 36:0;3O Cer 18:0;2O/18:0;O | 17.51 | 5.92 | 37.59 | 68.10 | 38.91 | 37.53 | 5.32 | 2.75 |
| 548.5360 7 | Cer 36:1;2O Cer 18:1;2O/18:0 | 36.00 | 53.97 | 72.81 | 93.86 | 58.93 | 65.83 | 31.24 | 21.36 |
| 546.5232 5 | Cer 36:2;2O Cer 18:2;2O/18:0 | 22.49 | 28.57 | 55.63 | 95.42 | 18.35 | 12.63 | 13.76 | 9.25 |
| 562.5317 4 | Cer 36:2;3O Cer 16:1;2O/20:1;O | 0.90 | 1.27 | 4.61 | 14.21 | 1.49 | 1.63 | 58.56 | 116.15 |
| 562.5177 6 | Cer 36:2;3O Cer 18:2;2O/18:0;O | 1.95 | 0.49 | 18.14 | 37.80 | 12.21 | 12.83 | 2.35 | 1.04 |
| 576.4958 5 | Cer 36:3;4O | 71.90 | 34.28 | 82.71 | 56.42 | 601.38 | 975.60 | 202.88 | 144.31 |
| 574.4840 7 | Cer 36:4;4O | 5.50 | 3.98 | 4.36 | 3.34 | 46.55 | 117.31 | 4.30 | 1.61 |
| 570.4550 8 | Cer 36:6;4O | 174.91 | 126.53 | 168.73 | 302.37 | 1877.63 | 3105.12 | 71.31 | 28.86 |
| 568.4465 3 | Cer 36:7;4O | 164.18 | 124.38 | 51.20 | 25.45 | 73.50 | 72.94 | 65.29 | 7.23 |
| 568.4279 2 | Cer 36:8;3O Cer 12:2;2O/24:6;O | 4.93 | 2.84 | 93.95 | 122.43 | 144.90 | 191.36 | 58.79 | 74.46 |
| 562.5587 2 | Cer 37:1;2O Cer 16:1;2O/21:0 | 8.73 | 1.52 | 36.30 | 36.46 | 91.53 | 80.82 | 13.11 | 6.61 |
| 600.4644 2 | Cer 37:7;4O | 68.15 | 54.59 | 51.24 | 64.44 | 404.45 | 482.98 | 27.13 | 7.85 |

| Mass m/z | Metabolite name | CTR | | SCH | | NF | | PNF | |
|---------------|------------------------------------|--------|---------|--------|---------|---------|---------|--------|--------|
| | | mean | dev | mean | dev | mean | dev | mean | dev |
| 578.5867 9 | Cer 38:0;2O Cer 18:0;2O/20:0 | 894.90 | 731.01 | 144.83 | 208.57 | 343.42 | 272.09 | 185.76 | 312.85 |
| 576.5723 9 | Cer 38:1;2O Cer 16:1;2O/22:0 | 502.97 | 466.49 | 493.97 | 342.73 | 2395.58 | 2356.23 | 266.27 | 247.01 |
| 572.5326 5 | Cer 38:3;2O Cer 19:0;2O/19:3 | 1.68 | 1.41 | 1.62 | 1.96 | 110.62 | 329.02 | 0.89 | 0.33 |
| 598.4937 7 | Cer 38:6;4O | 137.45 | 227.22 | 48.35 | 107.72 | 85.55 | 104.01 | 23.01 | 31.41 |
| 614.4708 3 | Cer 38:7;4O | 216.07 | 245.79 | 536.44 | 1344.05 | 118.75 | 97.12 | 110.26 | 22.96 |
| 640.5926 5 | Cer 39:1;4O Cer 18:0;3O/21:1;(2OH) | 395.49 | 267.03 | 78.05 | 48.38 | 536.07 | 967.80 | 180.60 | 202.09 |
| 622.5905 8 | Cer 39:2;3O Cer 18:1;2O/21:1;O | 112.79 | 52.32 | 85.65 | 70.54 | 154.20 | 167.86 | 43.55 | 19.13 |
| 616.5338 7 | Cer 39:4;4O | 45.16 | 26.77 | 35.95 | 24.79 | 44.09 | 51.94 | 33.76 | 15.95 |
| 636.5913 7 | Cer 40:2;3O Cer 18:1;2O/22:1;O | 262.25 | 129.07 | 52.49 | 24.73 | 387.62 | 525.53 | 105.33 | 65.52 |
| 616.5659 8 | Cer 40:3;3O Cer 18:3;2O/22:0;O | 28.85 | 14.75 | 23.61 | 15.73 | 112.76 | 57.15 | 26.13 | 30.60 |
| 634.6134 | Cer 41:1;3O Cer 18:1;2O/23:0;O | 747.41 | 1025.90 | 134.55 | 156.21 | 336.05 | 527.71 | 191.58 | 200.35 |
| 650.6079 7 | Cer 41:2;3O Cer 18:2;2O/23:0;O | 11.62 | 8.94 | 12.89 | 16.85 | 121.39 | 338.34 | 11.22 | 7.43 |
| 630.5878 9 | Cer 41:3;3O Cer 17:0;2O/24:3;O | 104.84 | 58.93 | 89.80 | 42.67 | 113.23 | 99.29 | 52.05 | 27.46 |
| 684.6529 5 | Cer 42:0;4O Cer 18:0;3O/24:0;(2OH) | 6.58 | 2.46 | 5.82 | 2.16 | 553.88 | 1724.02 | 11.10 | 9.41 |
| 648.6285 4 | Cer 42:1;3O Cer 18:1;2O/24:0;O | 23.76 | 34.01 | 6.27 | 7.71 | 5.37 | 6.75 | 17.80 | 23.35 |
| 630.6189 6 | Cer 42:2;2O Cer 18:1;2O/24:1 | 3.90 | 1.07 | 33.09 | 51.36 | 2.99 | 2.31 | 10.17 | 11.60 |
| 626.5859 4 | Cer 42:4;2O Cer 18:2;2O/24:2 | 104.75 | 77.31 | 160.64 | 154.02 | 227.91 | 144.85 | 52.00 | 29.63 |
| 622.5524 9 | Cer 42:6;2O Cer 18:1;2O/24:5 | 94.49 | 60.11 | 22.06 | 15.05 | 153.74 | 292.43 | 54.93 | 63.40 |
| 698.6689 5 | Cer 43:0;4O | 10.42 | 3.93 | 7.46 | 6.79 | 497.02 | 1556.26 | 4.16 | 2.19 |
| 646.6491 1 | Cer 43:1;2O Cer 18:1;2O/25:0 | 34.18 | 18.90 | 187.43 | 156.83 | 142.63 | 283.70 | 35.49 | 22.08 |
| 662.6480 1 | Cer 43:1;3O Cer 20:0;2O/23:1;O | 8.79 | 10.73 | 5.44 | 2.45 | 454.77 | 1402.38 | 10.46 | 8.15 |
| 696.6882 9 | Cer 44:0;3O Cer 19:0;2O/25:0;O | 9.34 | 3.75 | 9.61 | 4.34 | 1402.88 | 4401.29 | 6.80 | 2.16 |
| 676.6616 8 | Cer 44:1;3O Cer 18:1;2O/26:0;O | 17.55 | 16.24 | 18.30 | 16.08 | 172.24 | 503.43 | 17.39 | 15.62 |
| 658.6470 9 | Cer 44:2;2O Cer 18:1;2O/26:1 | 19.92 | 16.62 | 89.42 | 119.67 | 30.14 | 33.28 | 10.39 | 7.66 |
| 688.6377 | Cer 44:3;4O | 11.46 | 11.10 | 33.46 | 49.38 | 16.09 | 12.30 | 10.13 | 5.67 |
| 654.6171 9 | Cer 44:4;2O Cer 18:2;2O/26:2 | 52.54 | 25.56 | 82.87 | 124.37 | 35.83 | 23.04 | 54.47 | 88.62 |

| Mass <i>m/z</i> | Metabolite name | CTR | | SCH | | NF | | PNF | |
|--------------------|------------------------------------|--------------|--------------|--------------|--------------|-------------|------------|-------------|------------|
| | | <i>mean</i> | <i>dev</i> | <i>mean</i> | <i>dev</i> | <i>mean</i> | <i>dev</i> | <i>mean</i> | <i>dev</i> |
| 684.5769 7 | Cer 44:5;4O Cer 18:0;3O/26:5;(2OH) | 69.91 | 79.68 | 8.77 | 8.40 | 26.30 | 26.93 | 44.42 | 62.17 |
| 666.5810 5 | Cer 44:6;3O Cer 18:1;2O/26:5;O | 465.75 | 519.47 | 47.40 | 48.87 | 80.07 | 55.14 | 49.12 | 29.32 |
| 680.5795 3 | Cer 45:6;3O Cer 19:0;2O/26:6;O | 47.98 | 43.41 | 148.52 | 257.13 | 39.70 | 34.14 | 15.04 | 13.94 |
| 710.6078 5 | Cer 46:6;4O Cer 18:1;2O/28:5;2O | 284.31 | 385.86 | 562.12 | 810.06 | 392.64 | 419.01 | 217.21 | 149.09 |
| 778.6380 6 | Cer 50:9;4O Cer 18:2;2O/32:7;2O | 27.05 | 38.44 | 19.71 | 35.84 | 25.64 | 27.97 | 9.57 | 8.99 |
| 814.7484 1 | Cer 53:3;4O | 81.48 | 99.59 | 45.53 | 96.44 | 120.03 | 222.93 | 64.49 | 86.17 |
| 924.7915 | Cer 62:11;4O Cer 18:2;2O/44:9;2O | 776.64 | 915.59 | 35.39 | 41.47 | 200.78 | 404.54 | 277.98 | 532.70 |
| 863.6922 6 | CoQ10 | 517.15 | 642.19 | 2776.64 | 3608.78 | 356.20 | 295.69 | 335.95 | 464.30 |
| 395.2769 2 | DG 18:0 | 139.80 | 60.59 | 41.42 | 52.67 | 142.47 | 120.26 | 65.35 | 96.49 |
| 409.2785 6 | DG 19:0 | 112.19 | 62.63 | 49.02 | 40.09 | 293.53 | 288.87 | 48.43 | 37.32 |
| 437.3195 5 | DG 21:0 | 44.67 | 37.80 | 157.15 | 411.53 | 29.78 | 18.83 | 22.44 | 3.90 |
| 435.3089 6 | DG 21:1 | 113.23 | 90.74 | 51.49 | 35.42 | 67.30 | 45.82 | 57.29 | 13.15 |
| 465.3455 8 | DG 23:0 | 302.28 | 146.21 | 114.54 | 75.67 | 1220.12 | 1307.25 | 156.76 | 169.81 |
| 463.3204 3 | DG 23:1 | 54.13 | 37.22 | 10.61 | 11.05 | 52.76 | 115.33 | 165.23 | 316.80 |
| 461.3241 3 | DG 23:2 | 370.55 | 467.39 | 31.90 | 31.39 | 671.49 | 1853.26 | 214.04 | 401.96 |
| 459.3031 9 | DG 23:3 | 44.25 | 36.45 | 94.74 | 214.04 | 35.60 | 21.57 | 23.06 | 7.85 |
| 457.2866 5 | DG 23:4 | 2191.77 | 2321.82 | 583.53 | 294.68 | 912.14 | 1053.69 | 931.32 | 243.65 |
| 479.3754 3 | DG 24:0 | 260.82 | 239.71 | 78.33 | 102.98 | 101.43 | 72.14 | 67.38 | 34.40 |
| 475.3461 | DG 24:2 | 144.90 | 157.58 | 42.68 | 25.36 | 48.01 | 40.38 | 39.84 | 7.66 |
| 473.3187 6 | DG 24:3 | 12534.8 2 | 12594.3 7 | 29072.1 4 | 69859.8 4 | 4910.56 | 5777.60 | 5318.55 | 1264.45 |
| 471.2939 5 | DG 24:4 | 141.09 | 138.24 | 37.10 | 15.25 | 44.31 | 26.87 | 49.09 | 10.10 |
| 491.3691 7 | DG 25:1 | 50.65 | 21.40 | 39.97 | 28.66 | 114.98 | 77.11 | 85.03 | 65.24 |
| 487.3344 1 | DG 25:3 | 1104.86 | 1113.03 | 7697.61 | 20630.1 4 | 460.12 | 441.32 | 450.85 | 108.61 |
| 485.3192 1 | DG 25:4 | 1005.53 | 1034.21 | 346.01 | 284.74 | 376.50 | 453.70 | 420.53 | 117.71 |
| 503.3704 5 | DG 26:2 | 420.82 | 324.15 | 30.50 | 25.77 | 65.37 | 51.10 | 469.64 | 898.30 |
| 501.3550 1 | DG 26:3 | 6715.14 | 12216.4 4 | 95.76 | 110.69 | 731.89 | 1556.55 | 886.77 | 1009.04 |

| Mass <i>m/z</i> | Metabolite name | CTR | | SCH | | NF | | PNF | |
|--------------------|----------------------|---------------|---------------|---------------|---------------|---------------|---------------|---------------|---------------|
| | | <i>mean</i> | <i>dev</i> | <i>mean</i> | <i>dev</i> | <i>mean</i> | <i>dev</i> | <i>mean</i> | <i>dev</i> |
| 499.3413 7 | DG 26:4 | 1421.55 | 1234.31 | 482.51 | 436.42 | 462.92 | 574.32 | 577.18 | 155.70 |
| 497.3237 | DG 26:5 | 447.20 | 721.31 | 26.36 | 32.23 | 100.43 | 170.64 | 137.27 | 109.90 |
| 521.4036 9 | DG 27:0 | 92.68 | 90.28 | 156.84 | 349.16 | 167.06 | 241.90 | 13.72 | 5.90 |
| 519.4043 6 | DG 27:1 | 23.88 | 9.85 | 23.70 | 15.84 | 89.61 | 70.09 | 59.83 | 57.15 |
| 517.3943 5 | DG 27:2 | 163.90 | 151.20 | 41.73 | 36.05 | 111.59 | 115.35 | 88.64 | 60.32 |
| 512.4309 7 | DG 27:2 DG 12:0_15:2 | 752.12 | 932.28 | 46.79 | 37.56 | 1139.20 | 3085.78 | 383.50 | 714.33 |
| 515.3662 1 | DG 27:3 | 356.93 | 364.64 | 4797.90 | 13645.3 7 | 146.67 | 169.61 | 163.24 | 31.70 |
| 513.3479 6 | DG 27:4 | 683.22 | 697.52 | 491.16 | 869.33 | 247.90 | 281.91 | 271.47 | 36.04 |
| 511.3435 4 | DG 27:5 | 234.45 | 267.51 | 64.63 | 62.92 | 85.59 | 72.23 | 62.39 | 20.04 |
| 535.4273 1 | DG 28:0 | 693.23 | 709.00 | 152.44 | 98.57 | 229.98 | 284.05 | 247.98 | 162.86 |
| 533.4163 8 | DG 28:1 | 34857.8 8 | 36411.1 3 | 9124.66 | 5648.94 | 13122.5 1 | 17012.5 0 | 14428.4 3 | 8553.22 |
| 531.4090 6 | DG 28:2 | 656026. 44 | 682950. 38 | 162590. 10 | 101980. 07 | 266593. 82 | 344977. 69 | 290423. 34 | 164801. 14 |
| 529.3898 9 | DG 28:3 | 162.63 | 181.41 | 37.47 | 26.44 | 70.93 | 64.20 | 71.88 | 55.26 |
| 527.3657 2 | DG 28:4 | 37.75 | 34.79 | 328.46 | 982.65 | 17.37 | 14.45 | 15.43 | 2.14 |
| 525.3568 7 | DG 28:5 | 136.41 | 118.20 | 40.30 | 19.72 | 52.47 | 50.88 | 55.35 | 13.80 |
| 547.4160 8 | DG 29:1 | 106.23 | 86.84 | 44.90 | 32.31 | 54.80 | 46.37 | 52.30 | 9.97 |
| 543.3983 8 | DG 29:3 | 1377.52 | 1581.21 | 7442.94 | 18112.0 0 | 633.17 | 746.24 | 800.24 | 219.82 |
| 541.3873 9 | DG 29:4 | 6626.12 | 11563.4 4 | 211.55 | 226.10 | 919.54 | 1813.20 | 1575.69 | 1464.94 |
| 563.4599 6 | DG 30:0 | 18.78 | 13.33 | 90.55 | 245.80 | 23.18 | 15.17 | 13.38 | 4.52 |
| 554.4814 5 | DG 30:2 DG 14:1_16:1 | 54.47 | 43.16 | 0.60 | 0.64 | 57.66 | 161.92 | 205.68 | 410.31 |
| 555.3915 4 | DG 30:4 | 1271.46 | 692.74 | 602.09 | 293.80 | 732.39 | 704.63 | 710.74 | 230.75 |
| 553.3895 3 | DG 30:5 | 23513.4 1 | 10461.0 5 | 11589.1 4 | 5743.55 | 12541.3 6 | 13742.0 9 | 13961.4 8 | 5594.18 |
| 551.3748 2 | DG 30:6 | 886.98 | 725.70 | 144.39 | 176.98 | 377.99 | 743.94 | 388.83 | 358.54 |
| 549.3580 3 | DG 30:7 | 50.16 | 32.66 | 19.41 | 27.37 | 20.98 | 25.88 | 37.47 | 20.50 |
| 577.4845 | DG 31:0 | 18.03 | 9.35 | 29.85 | 22.76 | 130.10 | 161.34 | 54.59 | 20.94 |
| 569.4266 4 | DG 31:4 | 16.43 | 9.75 | 91.20 | 175.10 | 34.04 | 21.99 | 12.99 | 8.68 |

| Mass m/z | Metabolite name | CTR | | SCH | | NF | | PNF | |
|---------------|----------------------|---------|---------|---------|--------------|--------------|--------------|--------------|--------------|
| | | mean | dev | mean | dev | mean | dev | mean | dev |
| 567.4162 6 | DG 31:5 | 21.37 | 11.59 | 53.75 | 90.62 | 34.91 | 15.53 | 14.13 | 4.81 |
| 565.3772 | DG 31:6 | 853.08 | 984.61 | 204.66 | 288.69 | 42333.4 3 | 70305.7 3 | 1207.87 | 1564.99 |
| 563.3924 6 | DG 31:7 | 37.07 | 14.93 | 49.37 | 63.32 | 65.46 | 34.44 | 27.61 | 15.93 |
| 591.4973 8 | DG 32:0 | 24.64 | 20.02 | 2.96 | 1.94 | 11.35 | 18.55 | 348.55 | 693.89 |
| 589.4636 2 | DG 32:1 | 159.38 | 108.91 | 69.26 | 38.80 | 83.46 | 63.83 | 78.30 | 28.21 |
| 584.5268 6 | DG 32:1 DG 16:0_16:1 | 4196.81 | 3986.35 | 92.55 | 64.65 | 3559.75 | 9448.67 | 10806.4 8 | 21454.3 1 |
| 582.5073 2 | DG 32:2 DG 16:1_16:1 | 85.13 | 66.79 | 8.14 | 5.05 | 193.50 | 535.60 | 752.24 | 1494.62 |
| 583.4281 | DG 32:4 | 140.12 | 57.31 | 5916.38 | 14587.3 3 | 85.30 | 108.97 | 121.82 | 41.71 |
| 577.3837 9 | DG 32:7 | 101.11 | 90.80 | 1509.02 | 4329.55 | 51.89 | 45.17 | 46.72 | 10.57 |
| 605.5036 6 | DG 33:0 | 1057.42 | 654.87 | 429.05 | 204.82 | 577.01 | 636.03 | 581.26 | 186.09 |
| 598.5389 4 | DG 33:1 DG 15:0_18:1 | 68.41 | 36.56 | 29.19 | 16.07 | 178.02 | 232.71 | 173.99 | 280.17 |
| 601.4976 2 | DG 33:2 | 85.32 | 42.40 | 42.62 | 30.00 | 80.12 | 39.76 | 36.49 | 8.42 |
| 591.3989 3 | DG 33:7 | 68.47 | 54.60 | 624.56 | 1597.01 | 37.59 | 28.77 | 41.13 | 5.65 |
| 589.3884 3 | DG 33:8 | 62.51 | 37.13 | 28.22 | 15.00 | 95.53 | 69.60 | 29.85 | 9.37 |
| 619.5290 5 | DG 34:0 | 24.63 | 20.53 | 1.41 | 1.21 | 9.04 | 19.04 | 292.53 | 584.07 |
| 617.5169 7 | DG 34:1 | 283.17 | 158.23 | 208.46 | 230.80 | 733.79 | 797.02 | 246.84 | 178.71 |
| 613.4881 6 | DG 34:3 | 6.09 | 4.71 | 49.01 | 112.10 | 5.68 | 3.51 | 3.62 | 1.07 |
| 608.5269 8 | DG 34:3 DG 16:0_18:3 | 30.39 | 15.99 | 8.71 | 5.76 | 126.83 | 318.41 | 65.50 | 118.07 |
| 609.4439 7 | DG 34:5 | 3.34 | 2.30 | 266.02 | 773.90 | 6.74 | 5.84 | 1.64 | 0.29 |
| 601.4043 6 | DG 34:9 | 72.84 | 56.51 | 866.52 | 2451.13 | 41.22 | 43.99 | 41.02 | 7.83 |
| 624.5557 3 | DG 35:2 DG 17:0_18:2 | 62.49 | 42.93 | 16.09 | 7.40 | 112.88 | 161.83 | 80.26 | 118.26 |
| 627.4899 3 | DG 35:3 | 48.18 | 25.03 | 665.68 | 1558.06 | 45.86 | 51.81 | 56.84 | 20.25 |
| 625.4929 2 | DG 35:4 | 330.07 | 174.64 | 165.67 | 136.97 | 420.55 | 343.31 | 125.95 | 80.87 |
| 623.4489 1 | DG 35:5 | 119.26 | 70.60 | 46.58 | 56.20 | 119.44 | 87.68 | 38.70 | 31.02 |
| 619.4434 8 | DG 35:7 | 10.90 | 6.50 | 57.63 | 118.26 | 12.02 | 7.05 | 5.01 | 2.32 |

| Mass <i>m/z</i> | Metabolite name | CTR | | SCH | | NF | | PNF | |
|--------------------|------------------------|-------------|------------|-------------|------------|--------------|--------------|-------------|------------|
| | | <i>mean</i> | <i>dev</i> | <i>mean</i> | <i>dev</i> | <i>mean</i> | <i>dev</i> | <i>mean</i> | <i>dev</i> |
| 645.5433 3 | DG 36:1 | 267.21 | 229.88 | 229.78 | 261.90 | 279.94 | 136.31 | 129.17 | 117.10 |
| 638.5667 7 | DG 36:2 DG 18:1_18:1 | 7872.16 | 5528.99 | 2119.12 | 1730.98 | 12879.2 6 | 20238.3 1 | 5592.89 | 7338.26 |
| 634.5361 3 | DG 36:4 DG 16:0_20:4 | 3025.48 | 2137.81 | 1262.26 | 1206.92 | 6268.87 | 7383.30 | 1977.52 | 1712.86 |
| 641.4027 1 | DG 37:10 | 75.35 | 33.17 | 36.90 | 13.18 | 198.10 | 171.20 | 51.48 | 19.96 |
| 652.5871 | DG 37:2 DG 18:1_19:1 | 25.93 | 18.95 | 10.69 | 6.19 | 36.27 | 39.21 | 16.20 | 6.29 |
| 653.5061 6 | DG 37:4 | 9.28 | 6.19 | 39.75 | 90.41 | 22.57 | 17.82 | 7.47 | 2.94 |
| 648.5517 6 | DG 37:4 DG 17:0_20:4 | 92.57 | 66.35 | 53.76 | 41.36 | 167.76 | 144.91 | 45.54 | 17.89 |
| 647.4614 9 | DG 37:7 | 19.21 | 9.15 | 416.48 | 1056.42 | 7.42 | 11.68 | 10.63 | 2.21 |
| 645.4646 6 | DG 37:8 | 109.72 | 54.48 | 51.56 | 67.23 | 111.97 | 72.93 | 38.26 | 32.02 |
| 675.5793 5 | DG 38:0 | 2929.66 | 3235.76 | 1831.45 | 2592.01 | 1253.65 | 805.36 | 1073.63 | 689.17 |
| 673.5966 8 | DG 38:1 | 77.25 | 145.34 | 156.61 | 160.67 | 77.37 | 91.04 | 92.00 | 73.19 |
| 671.5712 9 | DG 38:2 | 187.37 | 369.39 | 344.18 | 174.22 | 87.46 | 88.89 | 322.12 | 265.71 |
| 667.5211 8 | DG 38:4 | 29.98 | 14.42 | 126.26 | 286.89 | 72.64 | 56.23 | 21.80 | 7.46 |
| 665.5136 7 | DG 38:5 | 59.71 | 14.95 | 26.74 | 28.52 | 185.40 | 184.21 | 48.32 | 39.64 |
| 663.4854 7 | DG 38:6 | 112.62 | 96.24 | 299.99 | 815.99 | 53.51 | 66.19 | 53.64 | 17.05 |
| 661.4923 1 | DG 38:7 | 12.56 | 13.53 | 171.99 | 517.66 | 21.24 | 17.80 | 90.25 | 173.43 |
| 659.4644 2 | DG 38:8 | 67.98 | 61.99 | 1095.81 | 2743.48 | 51.75 | 82.27 | 38.96 | 11.06 |
| 685.5715 3 | DG 39:2 | 85.27 | 49.86 | 44.45 | 19.98 | 230.78 | 225.71 | 63.67 | 23.47 |
| 679.5208 7 | DG 39:5 | 38.41 | 40.20 | 55.86 | 94.91 | 36.40 | 27.98 | 8.21 | 2.29 |
| 681.4592 3 | DG 40:11 | 90.48 | 67.74 | 33.00 | 23.63 | 37.00 | 35.20 | 32.36 | 2.53 |
| 695.5604 2 | DG 40:4 | 10.51 | 7.99 | 23.98 | 41.06 | 13.90 | 8.08 | 5.76 | 3.74 |
| 693.5412 6 | DG 40:5 | 23.82 | 21.51 | 11.09 | 9.99 | 13.33 | 7.41 | 5.56 | 4.06 |
| 691.5281 4 | DG 40:6 | 14.24 | 11.22 | 35.49 | 76.83 | 9.23 | 5.92 | 3.43 | 1.96 |
| 686.5667 7 | DG 40:6 DG 16:0_24:6 | 0.84 | 0.54 | 9.86 | 22.55 | 2.97 | 2.40 | 0.56 | 0.12 |
| 686.5745 2 | DG 40:6 DG 18:1_22:5 | 124.85 | 71.26 | 39.99 | 27.44 | 164.51 | 135.58 | 49.66 | 24.54 |
| 689.4902 3 | DG 40:7 | 97.94 | 57.69 | 43.34 | 58.49 | 88.55 | 54.02 | 35.72 | 34.49 |

| Mass <i>m/z</i> | Metabolite name | CTR | | SCH | | NF | | PNF | |
|--------------------|----------------------|-------------|------------|-------------|------------|-------------|------------|-------------|------------|
| | | <i>mean</i> | <i>dev</i> | <i>mean</i> | <i>dev</i> | <i>mean</i> | <i>dev</i> | <i>mean</i> | <i>dev</i> |
| 685.4675 3 | DG 40:9 | 69.74 | 61.92 | 268.25 | 778.43 | 54.50 | 31.70 | 44.92 | 33.93 |
| 695.4644 8 | DG 41:11 | 12.62 | 8.10 | 42.07 | 80.71 | 19.84 | 17.30 | 8.03 | 2.85 |
| 711.5921 6 | DG 41:3 | 141.77 | 184.13 | 252.29 | 340.77 | 215.08 | 212.99 | 105.99 | 61.76 |
| 709.5728 1 | DG 41:4 | 370.32 | 204.57 | 187.22 | 114.85 | 679.61 | 546.51 | 278.57 | 169.66 |
| 705.5299 7 | DG 41:6 | 183.55 | 147.17 | 105.17 | 63.29 | 203.00 | 130.33 | 119.11 | 56.72 |
| 703.5053 7 | DG 41:7 | 176.29 | 148.15 | 89.70 | 141.70 | 180.05 | 164.70 | 58.23 | 50.85 |
| 701.5177 6 | DG 41:8 | 1.98 | 1.56 | 21.87 | 40.02 | 8.14 | 14.70 | 3.46 | 2.63 |
| 699.4979 9 | DG 41:9 | 7.46 | 4.47 | 13.76 | 15.43 | 11.97 | 10.56 | 6.50 | 3.22 |
| 722.6710 8 | DG 42:2 DG 18:1_24:1 | 16.32 | 10.21 | 17.10 | 8.46 | 13.27 | 9.25 | 19.76 | 24.23 |
| 719.5499 3 | DG 42:6 | 90.82 | 56.39 | 46.58 | 24.99 | 205.11 | 173.64 | 59.04 | 23.58 |
| 715.5191 7 | DG 42:8 | 29.23 | 26.62 | 37.59 | 58.39 | 35.17 | 24.78 | 76.49 | 82.49 |
| 713.5006 7 | DG 42:9 | 1087.99 | 1018.16 | 607.68 | 501.80 | 1086.42 | 727.63 | 567.28 | 317.47 |
| 745.6652 8 | DG 43:0 | 48.08 | 44.52 | 68.04 | 154.06 | 193.46 | 246.68 | 18.82 | 7.02 |
| 725.5180 7 | DG 43:10 | 168.64 | 147.20 | 81.26 | 130.29 | 116.12 | 84.44 | 49.40 | 45.21 |
| 735.5674 4 | DG 43:5 | 28.75 | 31.09 | 19.58 | 26.63 | 1177.28 | 3592.89 | 17.08 | 6.15 |
| 731.5408 9 | DG 43:7 | 2154.44 | 1595.39 | 4864.80 | 4760.96 | 7003.08 | 5559.20 | 2543.38 | 1271.20 |
| 727.5238 | DG 43:9 | 53.59 | 43.90 | 123.32 | 156.71 | 176.05 | 182.17 | 43.55 | 30.87 |
| 757.6607 7 | DG 44:1 | 110.37 | 75.81 | 153.81 | 329.27 | 183.47 | 197.87 | 42.91 | 25.06 |
| 739.5204 5 | DG 44:10 | 1056.87 | 1144.94 | 626.67 | 670.52 | 658.09 | 288.29 | 468.93 | 280.35 |
| 737.5132 4 | DG 44:11 | 50.54 | 25.85 | 193.74 | 225.61 | 285.73 | 300.12 | 134.71 | 121.34 |
| 735.4918 8 | DG 44:12 | 3.58 | 3.11 | 88.44 | 283.67 | 2.72 | 2.31 | 1.31 | 0.55 |
| 753.6348 3 | DG 44:3 | 15.39 | 12.35 | 461.95 | 1212.80 | 7.45 | 9.84 | 8.94 | 5.83 |
| 747.5899 | DG 44:6 | 31.91 | 39.26 | 111.86 | 273.47 | 37.37 | 30.71 | 6.67 | 1.47 |
| 743.5497 4 | DG 44:8 | 24.04 | 7.96 | 54.42 | 47.59 | 186.04 | 261.68 | 27.67 | 10.26 |
| 741.5502 3 | DG 44:9 | 692.84 | 913.44 | 290.66 | 348.07 | 1331.06 | 2009.89 | 464.73 | 338.70 |
| 753.5343 | DG 45:10 | 106.93 | 70.76 | 165.77 | 140.36 | 269.83 | 339.24 | 109.40 | 70.75 |
| 749.5122 7 | DG 45:12 | 16.34 | 8.53 | 35.52 | 46.28 | 22.02 | 18.92 | 13.87 | 7.08 |

| Mass <i>m/z</i> | Metabolite name | CTR | | SCH | | NF | | PNF | |
|--------------------|---|-------------|------------|-------------|------------|--------------|--------------|-------------|------------|
| | | <i>mean</i> | <i>dev</i> | <i>mean</i> | <i>dev</i> | <i>mean</i> | <i>dev</i> | <i>mean</i> | <i>dev</i> |
| 757.5640 9 | DG 45:8 | 8645.78 | 5408.90 | 9328.74 | 7183.15 | 18136.3 2 | 10046.3 8 | 8803.69 | 4377.69 |
| 755.5621 3 | DG 45:9 | 15.08 | 11.85 | 26.75 | 28.68 | 51.31 | 88.75 | 10.89 | 4.38 |
| 767.5426 | DG 46:10 | 63.32 | 23.68 | 52.53 | 58.02 | 226.30 | 264.68 | 25.32 | 5.84 |
| 765.5380 2 | DG 46:11 | 248.10 | 131.35 | 135.33 | 87.38 | 421.98 | 276.61 | 113.10 | 44.11 |
| 763.5145 3 | DG 46:12 | 124.59 | 59.65 | 136.46 | 100.49 | 270.51 | 180.80 | 116.75 | 81.98 |
| 771.5763 5 | DG 46:8 | 175.74 | 77.43 | 248.22 | 227.19 | 1121.67 | 1457.61 | 215.43 | 78.18 |
| 769.5847 2 | DG 46:9 | 52.92 | 50.77 | 35.72 | 37.35 | 146.26 | 250.78 | 37.38 | 19.67 |
| 781.5639 | DG 47:10 | 34.43 | 19.37 | 60.88 | 54.13 | 62.44 | 60.04 | 23.48 | 10.54 |
| 779.5567 6 | DG 47:11 | 141.15 | 106.30 | 93.41 | 79.09 | 165.50 | 97.32 | 60.57 | 23.31 |
| 775.547 | DG 47:13 | 32.46 | 13.99 | 29.95 | 26.56 | 70.73 | 53.13 | 26.34 | 15.20 |
| 791.5304 6 | DG 48:12 | 225.63 | 199.25 | 116.37 | 84.22 | 220.06 | 94.11 | 105.24 | 57.95 |
| 803.5448 | DG 49:13 | 35.99 | 32.45 | 48.45 | 72.70 | 54.13 | 43.27 | 24.97 | 8.38 |
| 823.6059 | DG 50:10 | 81.63 | 18.34 | 53.18 | 36.76 | 312.99 | 350.89 | 66.90 | 16.19 |
| 857.7981 6 | DG 51:0 | 4.89 | 4.31 | 7.14 | 11.79 | 93.14 | 272.88 | 403.20 | 464.16 |
| 833.5826 4 | DG 51:12 | 544.80 | 244.65 | 419.79 | 324.94 | 1112.23 | 559.82 | 233.63 | 100.23 |
| 841.6675 4 | DG 51:8 | 60.86 | 52.09 | 37.36 | 27.84 | 554.39 | 986.13 | 54.82 | 19.85 |
| 845.6259 8 | DG 52:13 | 101.57 | 71.12 | 36.04 | 15.40 | 115.09 | 71.78 | 41.22 | 14.25 |
| 642.5396 7 | DG O-38:7 DG O-16:1_22:6 | 71.20 | 80.59 | 85.04 | 55.72 | 110.36 | 79.30 | 38.28 | 38.24 |
| 834.6013 8 | Hex2Cer 32:1;2O Hex2Cer 18:1;2O/14:0 | 56.02 | 52.58 | 65.74 | 153.07 | 46.81 | 35.44 | 15.07 | 2.60 |
| 848.6142 | Hex2Cer 33:1;2O Hex2Cer 17:1;2O/16:0 | 123.09 | 111.42 | 67.77 | 89.71 | 163.25 | 126.56 | 37.00 | 19.80 |
| 862.6289 1 | Hex2Cer 34:1;2O Hex2Cer 18:1;2O/16:0 | 1559.06 | 2282.33 | 273.98 | 287.00 | 635.45 | 324.96 | 140.25 | 56.68 |
| 1024.679 93 | Hex3Cer 34:1;2O Hex3Cer 18:1;2O/16:0 | 1080.90 | 1843.59 | 48.32 | 64.63 | 191.44 | 155.38 | 86.37 | 92.90 |
| 644.5094 6 | HexCer 30:1;2O HexCer 18:1;2O/12:0 | 14.12 | 10.72 | 721.24 | 2233.13 | 16.70 | 12.23 | 6.79 | 2.52 |
| 674.5532 8 | HexCer 32:0;2O | 12.75 | 7.57 | 28.00 | 49.44 | 14.56 | 8.13 | 16.73 | 12.88 |
| 672.5426 6 | HexCer 32:1;2O HexCer 18:1;2O/14:0 | 15.98 | 10.54 | 52.77 | 97.27 | 19.29 | 12.49 | 8.11 | 2.37 |
| 686.5594 5 | HexCer 33:1;2O HexCer 17:1;2O/16:0 | 23.72 | 14.56 | 54.18 | 75.77 | 38.06 | 21.98 | 18.99 | 9.21 |
| 702.5850 8 | HexCer 34:0;2O HexCer 18:0;2O/16:0 | 219.06 | 139.30 | 624.45 | 1111.75 | 428.79 | 430.78 | 107.10 | 48.92 |

| Mass m/z | Metabolite name | CTR | | SCH | | NF | | PNF | |
|---------------|---|---------|---------|---------|--------------|---------|---------|---------|---------|
| | | mean | dev | mean | dev | mean | dev | mean | dev |
| 700.5700 1 | HexCer 34:1;2O HexCer 18:1;2O/16:0 | 145.24 | 87.76 | 1183.51 | 2378.21 | 247.41 | 207.81 | 75.06 | 37.41 |
| 716.5764 8 | HexCer 34:1;3O HexCer 16:1;2O/18:0;O | 83.85 | 52.64 | 74.97 | 40.39 | 249.00 | 210.47 | 66.51 | 22.62 |
| 716.5676 3 | HexCer 34:1;3O HexCer 18:1;2O/16:0;O | 28.04 | 23.47 | 75.42 | 148.96 | 32.60 | 19.25 | 14.34 | 4.35 |
| 698.5559 1 | HexCer 34:2;2O HexCer 18:2;2O/16:0 | 287.36 | 316.77 | 4647.78 | 8477.75 | 299.70 | 300.36 | 119.75 | 120.33 |
| 696.5352 2 | HexCer 34:2;3O HexCer 17:1;2O/17:1;O | 10.64 | 8.04 | 25.97 | 53.20 | 15.92 | 12.23 | 16.56 | 11.87 |
| 714.5806 9 | HexCer 35:1;2O HexCer 17:1;2O/18:0 | 59.24 | 84.96 | 100.26 | 160.70 | 50.42 | 40.52 | 45.09 | 28.75 |
| 726.5650 6 | HexCer 35:3;3O HexCer 18:2;2O/17:1;O | 36.87 | 53.70 | 111.10 | 184.13 | 25.52 | 16.45 | 26.66 | 20.41 |
| 728.6058 3 | HexCer 36:1;2O HexCer 18:1;2O/18:0 | 274.77 | 429.47 | 572.50 | 816.25 | 338.29 | 345.47 | 235.90 | 163.50 |
| 726.5856 3 | HexCer 36:2;2O HexCer 18:2;2O/18:0 | 211.03 | 341.57 | 1342.59 | 2764.15 | 123.22 | 104.09 | 112.14 | 82.25 |
| 736.5829 5 | HexCer 37:3;3O HexCer 18:2;2O/19:1;O | 142.16 | 93.60 | 93.61 | 44.20 | 363.56 | 269.86 | 113.38 | 53.27 |
| 732.5455 9 | HexCer 37:5;3O | 406.20 | 259.07 | 913.00 | 903.32 | 1433.79 | 1146.59 | 505.47 | 224.86 |
| 756.6328 7 | HexCer 38:1;2O HexCer 18:1;2O/20:0 | 189.91 | 236.31 | 192.76 | 328.63 | 450.44 | 645.77 | 301.39 | 370.97 |
| 746.5627 4 | HexCer 38:5;3O | 47.54 | 33.61 | 67.25 | 87.04 | 84.15 | 67.83 | 56.26 | 23.13 |
| 760.5571 3 | HexCer 39:5;3O | 212.50 | 252.87 | 87.15 | 51.34 | 262.34 | 117.28 | 115.29 | 43.94 |
| 796.651 | HexCer 41:1;3O HexCer 18:1;2O/23:0;O | 655.39 | 420.52 | 353.52 | 260.84 | 1601.08 | 1529.05 | 367.71 | 89.21 |
| 269.0879 8 | Inosine | 122.90 | 174.74 | 137.13 | 214.44 | 248.87 | 293.63 | 82.35 | 41.61 |
| 468.3094 5 | LPC 14:0 | 355.24 | 346.74 | 344.12 | 263.13 | 224.11 | 160.37 | 180.38 | 80.22 |
| 482.3227 5 | LPC 15:0 | 150.49 | 140.58 | 135.22 | 67.82 | 217.78 | 332.03 | 63.60 | 27.87 |
| 482.3162 2 | LPC 15:0/0:0 | 290.76 | 295.33 | 153.87 | 277.00 | 71.64 | 38.24 | 44.09 | 27.23 |
| 480.3139 6 | LPC 15:1/0:0 | 50.51 | 35.05 | 636.22 | 1722.05 | 63.75 | 41.53 | 48.83 | 54.49 |
| 476.2704 2 | LPC 15:3 | 5800.06 | 4367.32 | 2194.88 | 3305.91 | 3585.59 | 8154.12 | 5554.47 | 4630.84 |
| 496.3411 9 | LPC 16:0/0:0 | 45.30 | 46.69 | 628.92 | 1507.47 | 42.04 | 34.36 | 14.32 | 2.34 |
| 494.3183 3 | LPC 16:1 | 3232.47 | 4361.05 | 2026.68 | 1160.60 | 2001.77 | 3469.00 | 987.13 | 471.26 |
| 494.3276 4 | LPC 16:1/0:0 | 38.68 | 59.70 | 9535.45 | 29294.7 9 | 26.16 | 25.31 | 6.24 | 1.88 |
| 488.2765 5 | LPC 16:4/0:0 | 12.51 | 4.35 | 998.28 | 2545.97 | 33.54 | 26.05 | 8.78 | 4.79 |

| Mass m/z | Metabolite name | CTR | | SCH | | NF | | PNF | |
|---------------|-----------------|--------------|--------------|--------------|---------|---------|---------|---------|---------|
| | | mean | dev | mean | dev | mean | dev | mean | dev |
| 510.3522 6 | LPC 17:0 | 61.67 | 55.09 | 96.37 | 140.27 | 82.71 | 74.70 | 26.29 | 11.74 |
| 510.3522 9 | LPC 17:0/0:0 | 742.41 | 1096.15 | 151.14 | 134.91 | 503.93 | 1039.58 | 136.20 | 60.54 |
| 508.3434 1 | LPC 17:1 | 54.66 | 46.31 | 90.32 | 65.57 | 209.97 | 436.35 | 25.49 | 10.29 |
| 508.3367 6 | LPC 17:1/0:0 | 148.92 | 142.91 | 116.32 | 59.75 | 208.95 | 276.38 | 65.90 | 35.66 |
| 524.3725 6 | LPC 18:0 | 10679.4 4 | 11020.1 6 | 5891.67 | 5542.29 | 8860.81 | 9040.81 | 6262.94 | 4141.87 |
| 524.3672 5 | LPC 18:0/0:0 | 9.79 | 6.65 | 1650.11 | 3874.51 | 28.52 | 20.40 | 9.48 | 2.69 |
| 522.3533 3 | LPC 18:1 | 103.14 | 126.21 | 85.75 | 83.64 | 132.87 | 172.04 | 31.97 | 16.11 |
| 522.3591 3 | LPC 18:1/0:0 | 91.36 | 103.46 | 251.51 | 396.67 | 86.34 | 65.03 | 46.79 | 29.10 |
| 520.3314 8 | LPC 18:2 | 404.77 | 274.86 | 75.67 | 74.32 | 643.14 | 727.49 | 3219.58 | 6339.83 |
| 518.3228 1 | LPC 18:3 | 691.77 | 674.19 | 1087.94 | 883.02 | 582.18 | 492.56 | 267.91 | 176.95 |
| 516.3116 5 | LPC 18:4/0:0 | 158.70 | 197.48 | 80.40 | 35.96 | 92.71 | 79.46 | 37.37 | 11.94 |
| 538.3905 6 | LPC 19:0 | 114.34 | 126.27 | 42.15 | 24.48 | 93.84 | 68.49 | 39.44 | 19.27 |
| 538.3877 | LPC 19:0/0:0 | 414.33 | 450.93 | 175.20 | 124.01 | 287.10 | 257.80 | 171.34 | 104.24 |
| 528.3151 9 | LPC 19:5 | 62.08 | 37.06 | 57.19 | 43.30 | 41.62 | 14.31 | 20.28 | 7.81 |
| 552.4003 3 | LPC 20:0 | 760.27 | 725.92 | 246.27 | 232.68 | 926.39 | 1247.94 | 428.21 | 358.94 |
| 550.3825 1 | LPC 20:1 | 2814.59 | 3348.47 | 664.03 | 516.96 | 981.17 | 839.03 | 832.78 | 867.68 |
| 550.3856 8 | LPC 20:1/0:0 | 6500.63 | 8034.41 | 1562.43 | 1377.58 | 2934.85 | 2948.69 | 2219.46 | 2160.58 |
| 548.3682 3 | LPC 20:2 | 3122.08 | 5155.00 | 611.98 | 543.42 | 762.98 | 723.76 | 497.38 | 465.59 |
| 546.3544 9 | LPC 20:3/0:0 | 409.25 | 388.70 | 756.19 | 586.35 | 589.15 | 406.97 | 282.80 | 172.95 |
| 544.3424 1 | LPC 20:4 | 8219.33 | 10355.1 8 | 10467.7 8 | 9475.95 | 7152.04 | 5515.83 | 4570.11 | 2583.25 |
| 542.3208 6 | LPC 20:5 | 58.96 | 64.26 | 77.75 | 83.42 | 70.44 | 46.77 | 44.47 | 41.63 |
| 560.3702 4 | LPC 21:3 | 89.85 | 107.62 | 42.44 | 42.40 | 54.35 | 41.68 | 24.88 | 10.13 |
| 580.4349 4 | LPC 22:0/0:0 | 126.09 | 113.24 | 68.50 | 60.48 | 245.06 | 302.66 | 89.83 | 47.10 |
| 578.4177 2 | LPC 22:1 | 294.19 | 272.89 | 98.92 | 71.32 | 221.79 | 159.50 | 164.31 | 135.24 |
| 576.4068 | LPC 22:2 | 122.93 | 125.00 | 60.04 | 43.52 | 69.72 | 43.32 | 51.64 | 35.36 |
| 574.3858 6 | LPC 22:3 | 122.50 | 153.19 | 46.32 | 29.50 | 52.74 | 21.80 | 29.56 | 13.45 |

| Mass <i>m/z</i> | Metabolite name | CTR | | SCH | | NF | | PNF | |
|--------------------|-----------------|-------------|------------|-------------|--------------|-------------|------------|-------------|------------|
| | | <i>mean</i> | <i>dev</i> | <i>mean</i> | <i>dev</i> | <i>mean</i> | <i>dev</i> | <i>mean</i> | <i>dev</i> |
| 572.3737 2 | LPC 22:4 | 272.25 | 350.62 | 156.41 | 116.76 | 105.99 | 68.05 | 58.74 | 41.89 |
| 570.3541 9 | LPC 22:5 | 139.53 | 164.92 | 189.99 | 184.71 | 112.91 | 91.29 | 61.29 | 62.40 |
| 570.3576 | LPC 22:5/0:0 | 165.43 | 209.84 | 201.64 | 197.47 | 103.66 | 72.33 | 62.52 | 65.95 |
| 568.3408 8 | LPC 22:6 | 1000.26 | 1319.87 | 1228.37 | 968.80 | 876.56 | 737.58 | 466.20 | 294.54 |
| 608.4663 7 | LPC 24:0/0:0 | 346.73 | 325.44 | 219.39 | 203.86 | 838.06 | 1457.97 | 230.89 | 133.33 |
| 606.4516 6 | LPC 24:1 | 260.94 | 293.97 | 121.17 | 102.81 | 307.66 | 329.11 | 189.91 | 126.76 |
| 604.4426 9 | LPC 24:2 | 30.01 | 25.77 | 24.24 | 14.68 | 30.14 | 17.88 | 25.23 | 15.07 |
| 600.4013 1 | LPC 24:4/0:0 | 94.91 | 85.97 | 34.38 | 20.12 | 127.69 | 147.27 | 44.45 | 30.10 |
| 622.4821 2 | LPC 25:0/0:0 | 70.60 | 95.13 | 24.33 | 18.19 | 75.32 | 108.33 | 23.04 | 14.58 |
| 636.4953 6 | LPC 26:0 | 46.28 | 35.97 | 24.03 | 17.65 | 66.48 | 63.93 | 25.66 | 14.87 |
| 636.4968 3 | LPC 26:0/0:0 | 222.29 | 287.26 | 93.38 | 134.35 | 329.02 | 489.15 | 100.44 | 66.69 |
| 634.4785 8 | LPC 26:1/0:0 | 245.03 | 325.48 | 121.60 | 97.08 | 184.81 | 184.91 | 137.82 | 87.36 |
| 632.4711 3 | LPC 26:2 | 33.01 | 19.35 | 35.37 | 31.37 | 35.18 | 25.12 | 27.90 | 18.88 |
| 624.3870 8 | LPC 26:6 | 92.73 | 49.32 | 21.32 | 27.27 | 68.59 | 63.23 | 22.79 | 21.94 |
| 622.4026 5 | LPC 26:7 | 644.50 | 740.49 | 73.73 | 46.13 | 214.77 | 226.69 | 154.92 | 90.12 |
| 664.5300 3 | LPC 28:0 | 643.62 | 719.19 | 143.78 | 98.23 | 1142.86 | 2182.14 | 327.73 | 294.14 |
| 662.5117 8 | LPC 28:1 | 119.71 | 125.01 | 64.68 | 46.94 | 201.55 | 168.32 | 91.44 | 83.88 |
| 652.4413 5 | LPC 28:6 | 192.53 | 128.37 | 51.33 | 34.05 | 99.67 | 89.27 | 69.55 | 13.23 |
| 650.4005 7 | LPC 28:7 | 256.54 | 345.53 | 29.47 | 16.55 | 80.43 | 53.03 | 55.79 | 20.18 |
| 454.3296 8 | LPC O-14:0 | 47.11 | 31.99 | 2974.86 | 7341.56 | 36.43 | 31.03 | 18.68 | 5.35 |
| 496.3756 7 | LPC O-17:0 | 140.27 | 117.31 | 6546.08 | 17170.6 8 | 124.04 | 76.25 | 50.32 | 34.38 |
| 494.3509 5 | LPC O-17:1 | 258.80 | 416.95 | 5872.73 | 15207.3 7 | 101.00 | 81.42 | 32.42 | 17.40 |
| 504.3444 8 | LPC O-18:3 | 119.09 | 168.66 | 4609.65 | 10711.3 1 | 81.33 | 64.70 | 25.34 | 8.56 |
| 502.3223 3 | LPC O-18:4 | 321.84 | 432.83 | 407.92 | 780.62 | 216.70 | 165.08 | 69.03 | 34.97 |
| 538.4260 9 | LPC O-20:0 | 105.65 | 80.55 | 3924.49 | 10968.1 6 | 138.43 | 97.10 | 61.62 | 31.22 |
| 534.3901 4 | LPC O-20:2 | 73.43 | 85.01 | 3161.36 | 9236.98 | 78.36 | 46.19 | 35.42 | 16.05 |

| Mass m/z | Metabolite name | CTR | | SCH | | NF | | PNF | |
|---------------|-----------------|--------------|--------------|--------------|--------------|---------|---------|---------|--------|
| | | mean | dev | mean | dev | mean | dev | mean | dev |
| 564.44 | LPC O-22:1 | 58.26 | 58.23 | 253.50 | 672.00 | 40.70 | 26.91 | 24.84 | 6.48 |
| 588.4418 3 | LPC O-24:3 | 27.08 | 16.73 | 972.47 | 2891.54 | 89.48 | 133.26 | 20.02 | 14.67 |
| 614.4585 6 | LPC O-26:4 | 7.68 | 3.81 | 320.07 | 738.92 | 7.51 | 4.62 | 3.97 | 1.14 |
| 454.2928 2 | LPE 16:0 | 557.95 | 712.50 | 117.69 | 76.99 | 172.87 | 107.77 | 110.84 | 102.24 |
| 480.3166 2 | LPE 18:1 | 15559.3 7 | 17413.7 9 | 2226.16 | 2532.61 | 1804.51 | 1679.95 | 1238.24 | 857.78 |
| 478.2920 2 | LPE 18:2 | 184.26 | 173.38 | 96.90 | 94.64 | 231.04 | 271.90 | 70.87 | 34.02 |
| 510.3577 | LPE 20:0 | 426.70 | 570.94 | 16.73 | 12.44 | 74.40 | 108.47 | 41.08 | 36.86 |
| 508.3411 6 | LPE 20:1 | 1620.52 | 1823.09 | 98.64 | 84.34 | 188.20 | 130.72 | 287.42 | 330.45 |
| 502.2941 | LPE 20:4 | 2342.98 | 1769.75 | 1871.76 | 2576.17 | 1978.04 | 2396.23 | 967.08 | 723.02 |
| 538.3888 5 | LPE 22:0 | 185.46 | 293.20 | 6.05 | 4.11 | 35.78 | 89.32 | 10.73 | 10.58 |
| 536.3701 2 | LPE 22:1 | 253.45 | 278.29 | 17.05 | 9.60 | 44.73 | 33.49 | 39.18 | 41.12 |
| 530.3275 1 | LPE 22:4 | 180.02 | 118.37 | 188.43 | 273.66 | 170.31 | 161.77 | 70.41 | 24.44 |
| 528.3099 4 | LPE 22:5 | 96.57 | 57.19 | 85.56 | 77.03 | 83.72 | 48.52 | 31.62 | 15.39 |
| 526.2920 5 | LPE 22:6 | 984.05 | 824.07 | 511.53 | 706.70 | 707.69 | 958.96 | 248.54 | 255.13 |
| 564.3999 | LPE 24:1 | 224.64 | 250.63 | 18.53 | 16.69 | 41.54 | 47.14 | 23.38 | 18.92 |
| 558.3543 7 | LPE 24:4 | 73.50 | 114.88 | 18.04 | 20.95 | 40.83 | 36.46 | 30.99 | 30.82 |
| 424.2832 3 | LPE O-15:1 | 48.82 | 39.86 | 1111.10 | 2789.98 | 37.99 | 29.25 | 12.33 | 6.16 |
| 440.3105 5 | LPE O-16:0 | 917.71 | 951.37 | 4492.83 | 10811.8 8 | 232.62 | 172.82 | 113.96 | 103.65 |
| 438.2981 3 | LPE O-16:1 | 24.46 | 26.76 | 172.66 | 503.61 | 19.84 | 13.34 | 8.18 | 3.09 |
| 436.2810 4 | LPE O-16:2 | 42.58 | 29.99 | 3071.51 | 7367.66 | 76.18 | 74.99 | 18.95 | 4.01 |
| 452.3132 3 | LPE O-17:1 | 443.73 | 498.94 | 15499.0 0 | 41887.1 1 | 413.67 | 454.58 | 61.55 | 26.92 |
| 450.2949 5 | LPE O-17:2 | 77.36 | 46.78 | 633.49 | 1421.62 | 139.10 | 145.06 | 38.33 | 14.43 |
| 468.3394 8 | LPE O-18:0 | 417.52 | 477.16 | 2374.84 | 5698.31 | 108.98 | 82.74 | 41.78 | 35.42 |
| 466.3302 3 | LPE O-18:1 | 22.18 | 23.44 | 233.11 | 707.52 | 16.35 | 11.38 | 5.67 | 1.96 |
| 464.3158 3 | LPE O-18:2 | 531.94 | 828.89 | 651.96 | 1820.39 | 170.31 | 150.27 | 35.65 | 5.61 |
| 462.2962 | LPE O-18:3 | 84.27 | 83.70 | 1787.99 | 4211.05 | 41.78 | 20.86 | 22.88 | 6.23 |
| 480.3445 1 | LPE O-19:1 | 40.94 | 47.56 | 1307.97 | 4105.29 | 23.95 | 16.77 | 8.69 | 3.11 |

| Mass <i>m/z</i> | Metabolite name | CTR | | SCH | | NF | | PNF | |
|--------------------|-----------------|-------------|------------|-------------|--------------|-------------|------------|-------------|------------|
| | | <i>mean</i> | <i>dev</i> | <i>mean</i> | <i>dev</i> | <i>mean</i> | <i>dev</i> | <i>mean</i> | <i>dev</i> |
| 494.3629 2 | LPE O-20:1 | 86.52 | 104.74 | 5101.76 | 14994.1 6 | 98.25 | 96.42 | 16.79 | 7.22 |
| 492.3475 6 | LPE O-20:2 | 247.81 | 362.94 | 6734.66 | 16616.9 6 | 86.11 | 66.59 | 28.78 | 19.32 |
| 506.3585 5 | LPE O-21:2 | 27.10 | 27.64 | 203.21 | 484.47 | 16.87 | 9.87 | 7.27 | 1.30 |
| 522.3924 6 | LPE O-22:1 | 22.81 | 23.93 | 1187.68 | 3588.55 | 24.53 | 21.93 | 5.79 | 0.99 |
| 520.3769 5 | LPE O-22:2 | 39.89 | 46.71 | 5403.50 | 13955.3 8 | 37.00 | 28.22 | 10.40 | 2.88 |
| 518.3612 1 | LPE O-22:3 | 25.03 | 20.87 | 1107.74 | 3201.90 | 14.94 | 8.75 | 9.79 | 2.05 |
| 516.3427 1 | LPE O-22:4 | 14.94 | 11.87 | 202.49 | 571.23 | 17.75 | 11.70 | 7.12 | 2.90 |
| 550.4127 8 | LPE O-24:1 | 10.63 | 7.96 | 178.63 | 454.17 | 9.64 | 6.05 | 3.70 | 0.87 |
| 548.4080 8 | LPE O-24:2 | 61.02 | 63.52 | 4616.45 | 11808.0 5 | 52.43 | 36.87 | 16.83 | 3.16 |
| 546.3997 2 | LPE O-24:3 | 2182.90 | 2243.46 | 3446.53 | 7528.28 | 878.80 | 1010.09 | 906.84 | 222.65 |
| 544.3726 2 | LPE O-24:4 | 19.09 | 18.20 | 460.78 | 1122.18 | 20.90 | 15.81 | 7.62 | 1.40 |
| 574.4256 | LPE O-26:3 | 62.23 | 68.12 | 55.02 | 123.41 | 27.07 | 18.76 | 20.94 | 3.93 |
| 572.4190 1 | LPE O-26:4 | 80.46 | 81.22 | 49.59 | 77.37 | 45.66 | 33.48 | 38.36 | 5.24 |
| 348.3123 8 | MG 16:0 | 68.26 | 51.24 | 52.33 | 44.15 | 264.95 | 269.62 | 57.71 | 41.38 |
| 342.285 | MG 16:3 | 153.03 | 150.72 | 79.06 | 83.11 | 113.88 | 65.79 | 55.07 | 31.52 |
| 376.3410 3 | MG 18:0 | 172.69 | 207.04 | 352.39 | 793.32 | 243.11 | 199.56 | 43.56 | 6.45 |
| 368.2804 3 | MG 18:4 | 138.93 | 61.71 | 118.29 | 108.82 | 488.84 | 672.91 | 69.52 | 42.34 |
| 404.3808 6 | MG 20:0 | 25.49 | 15.13 | 22.73 | 20.00 | 40.70 | 25.53 | 16.94 | 9.97 |
| 414.3585 5 | MG 21:2 | 129.89 | 101.33 | 11.81 | 5.92 | 101.85 | 185.58 | 36.09 | 56.93 |
| 472.4353 9 | MG 25:1 | 193.24 | 332.81 | 24.88 | 20.30 | 490.69 | 1115.36 | 12.89 | 2.55 |
| 480.4038 1 | MG 26:4 | 10.32 | 7.53 | 152.14 | 446.60 | 10.08 | 10.30 | 6.09 | 5.33 |
| 612.5028 7 | MG 36:8 | 110.33 | 178.09 | 36.04 | 65.13 | 77.18 | 81.25 | 20.06 | 32.37 |
| 258.2403 | NAE 13:0 | 111.99 | 147.70 | 20.74 | 12.39 | 49.32 | 34.49 | 33.17 | 18.45 |
| 256.2260 7 | NAE 13:1 | 121.82 | 119.23 | 82.87 | 47.58 | 207.95 | 202.78 | 47.95 | 34.73 |
| 270.2422 2 | NAE 14:1 | 550.77 | 547.80 | 401.71 | 285.30 | 819.97 | 761.67 | 205.00 | 174.79 |
| 286.2717 9 | NAE 15:0 | 50.96 | 48.43 | 35.38 | 46.65 | 112.62 | 113.26 | 18.91 | 4.07 |
| 278.2098 7 | NAE 15:4 | 49.49 | 47.22 | 64.87 | 112.40 | 32.62 | 25.68 | 23.15 | 11.01 |

| Mass <i>m/z</i> | Metabolite name | CTR | | SCH | | NF | | PNF | |
|--------------------|-----------------|-------------|------------|--------------|--------------|-------------|------------|-------------|------------|
| | | <i>mean</i> | <i>dev</i> | <i>mean</i> | <i>dev</i> | <i>mean</i> | <i>dev</i> | <i>mean</i> | <i>dev</i> |
| 300.2881 5 | NAE 16:0 | 127.94 | 107.13 | 109.04 | 131.61 | 653.30 | 536.42 | 79.71 | 50.83 |
| 298.2758 8 | NAE 16:1 | 128.52 | 103.50 | 74.18 | 52.13 | 156.52 | 93.11 | 50.71 | 13.65 |
| 314.3057 9 | NAE 17:0 | 14.88 | 13.80 | 813.01 | 1885.97 | 10.36 | 9.74 | 2.20 | 1.13 |
| 312.2908 6 | NAE 17:1 | 26.77 | 22.85 | 467.95 | 1344.87 | 16.78 | 16.11 | 5.55 | 1.77 |
| 328.3211 1 | NAE 18:0 | 492.88 | 468.47 | 271.38 | 339.04 | 1200.55 | 2427.17 | 142.17 | 76.14 |
| 326.3056 6 | NAE 18:1 | 172.53 | 100.63 | 274.59 | 279.62 | 1450.38 | 3563.91 | 74.77 | 41.99 |
| 324.2907 4 | NAE 18:2 | 106.46 | 140.81 | 108.75 | 170.87 | 44.54 | 21.46 | 18.85 | 11.92 |
| 322.2732 8 | NAE 18:3 | 1520.11 | 2067.95 | 882.22 | 848.94 | 610.18 | 353.49 | 212.62 | 128.87 |
| 320.2590 3 | NAE 18:4 | 25.32 | 24.23 | 28.13 | 40.42 | 39.81 | 28.75 | 9.87 | 5.69 |
| 342.3362 1 | NAE 19:0 | 455.18 | 444.31 | 216.70 | 175.63 | 390.22 | 439.59 | 241.55 | 149.68 |
| 340.3219 6 | NAE 19:1 | 10.34 | 6.67 | 188.98 | 476.31 | 12.47 | 9.29 | 3.81 | 0.88 |
| 338.3105 2 | NAE 19:2 | 32.55 | 35.81 | 1420.77 | 3524.94 | 31.96 | 26.46 | 8.59 | 2.91 |
| 334.2751 8 | NAE 19:4 | 13.04 | 16.17 | 94.37 | 166.82 | 15.41 | 17.70 | 2.34 | 0.55 |
| 332.2545 8 | NAE 19:5 | 189.01 | 299.66 | 17.89 | 11.42 | 72.37 | 51.84 | 21.71 | 19.40 |
| 354.3376 2 | NAE 20:1 | 164.12 | 105.72 | 129.88 | 87.57 | 3679.02 | 6010.64 | 113.33 | 31.56 |
| 352.3236 4 | NAE 20:2 | 61.74 | 53.53 | 39.33 | 16.08 | 91.91 | 59.68 | 32.29 | 17.76 |
| 350.3058 2 | NAE 20:3 | 390.29 | 485.51 | 989.39 | 2316.73 | 76.86 | 51.37 | 45.02 | 21.60 |
| 348.2893 7 | NAE 20:4 | 259.88 | 310.15 | 214.97 | 186.75 | 130.30 | 87.53 | 45.72 | 49.06 |
| 370.3679 8 | NAE 21:0 | 44.03 | 35.30 | 58.30 | 57.42 | 76.76 | 48.78 | 27.54 | 12.28 |
| 368.3517 5 | NAE 21:1 | 46.05 | 22.46 | 89.33 | 183.56 | 52.72 | 68.67 | 19.54 | 17.45 |
| 366.3384 4 | NAE 21:2 | 12.49 | 7.44 | 651.31 | 2045.70 | 20.56 | 20.60 | 4.16 | 1.21 |
| 364.3207 4 | NAE 21:3 | 83.89 | 82.04 | 4590.28 | 10541.8 4 | 21.07 | 9.81 | 8.32 | 5.32 |
| 362.3066 7 | NAE 21:4 | 72.51 | 90.65 | 6534.29 | 15507.4 6 | 20.38 | 14.71 | 5.66 | 2.38 |
| 360.2911 1 | NAE 21:5 | 175.97 | 217.74 | 22266.1 9 | 55913.0 8 | 74.65 | 53.81 | 21.14 | 11.09 |
| 384.3924 6 | NAE 22:0 | 64.64 | 39.71 | 149.46 | 215.30 | 37.26 | 25.72 | 44.79 | 51.30 |
| 380.3364 | NAE 22:2 | 178.54 | 104.78 | 101.68 | 155.95 | 575.92 | 439.57 | 920.08 | 1175.85 |

| Mass <i>m/z</i> | Metabolite name | CTR | | SCH | | NF | | PNF | |
|--------------------|-----------------|-------------|------------|-------------|--------------|-------------|--------------|-------------|------------|
| | | <i>mean</i> | <i>dev</i> | <i>mean</i> | <i>dev</i> | <i>mean</i> | <i>dev</i> | <i>mean</i> | <i>dev</i> |
| 374.3123 5 | NAE 22:5 | 2654.30 | 2884.20 | 1668.49 | 1586.81 | 1307.51 | 1522.04 | 775.57 | 552.57 |
| 398.3986 8 | NAE 23:0 | 264.99 | 174.28 | 111.34 | 70.60 | 196.84 | 199.84 | 91.97 | 13.83 |
| 396.3868 4 | NAE 23:1 | 16.09 | 17.27 | 33.84 | 80.56 | 12.04 | 5.73 | 9.66 | 14.86 |
| 412.4168 1 | NAE 24:0 | 96.04 | 82.43 | 25.19 | 27.25 | 260.77 | 416.18 | 98.43 | 122.72 |
| 404.3364 6 | NAE 24:4 | 1173.14 | 2229.41 | 35.67 | 30.75 | 429.51 | 1136.94 | 30.62 | 18.54 |
| 400.3123 5 | NAE 24:6 | 422.99 | 262.24 | 107.85 | 63.37 | 229.92 | 140.52 | 128.04 | 60.72 |
| 426.4292 | NAE 25:0 | 208.48 | 106.33 | 96.30 | 69.69 | 146.53 | 128.36 | 73.11 | 7.65 |
| 438.4279 5 | NAE 26:1 | 39.51 | 53.84 | 18.56 | 28.78 | 27.64 | 26.73 | 35.94 | 51.53 |
| 436.4113 8 | NAE 26:2 | 9.52 | 7.46 | 6.11 | 6.27 | 3352.43 | 10429.2 3 | 8.46 | 2.70 |
| 434.4013 7 | NAE 26:3 | 4.50 | 3.74 | 3.63 | 5.14 | 125.84 | 377.44 | 2.30 | 1.10 |
| 428.3537 9 | NAE 26:6 | 1594.83 | 2175.93 | 6366.46 | 17159.3 2 | 440.21 | 486.99 | 217.74 | 39.84 |
| 454.4530 6 | NAE 27:0 | 32.10 | 14.89 | 14.23 | 12.46 | 35.74 | 41.26 | 15.95 | 9.20 |
| 458.3819 9 | NAE 28:5 | 94.74 | 73.55 | 37.48 | 20.42 | 80.32 | 117.27 | 63.46 | 61.81 |
| 456.3666 7 | NAE 28:6 | 2112.34 | 2708.14 | 97.32 | 106.96 | 3727.96 | 10756.1 4 | 1257.96 | 2449.09 |
| 454.3735 4 | NAE 28:7 | 123.84 | 114.95 | 90.42 | 124.37 | 644.83 | 1139.87 | 39.27 | 12.92 |
| 379.2627 3 | NAOrn 16:4;O | 114.21 | 136.49 | 141.94 | 270.43 | 243.08 | 229.06 | 140.01 | 154.80 |
| 496.3057 9 | PC 15:0 | 79.38 | 88.12 | 388.51 | 1113.71 | 38.70 | 19.38 | 22.38 | 10.88 |
| 538.3486 9 | PC 18:0 | 73.17 | 93.83 | 382.97 | 952.66 | 80.27 | 112.36 | 18.62 | 14.74 |
| 552.3689 | PC 19:0 | 15.04 | 9.83 | 29.29 | 58.88 | 17.00 | 9.28 | 6.08 | 2.43 |
| 564.3655 4 | PC 20:1 | 49.62 | 37.14 | 173.10 | 358.02 | 75.01 | 46.14 | 30.38 | 16.28 |
| 580.4007 | PC 21:0 | 13.40 | 8.02 | 29.03 | 57.76 | 26.62 | 20.14 | 9.50 | 6.50 |
| 578.3810 4 | PC 21:1 | 190.44 | 296.69 | 16.76 | 7.82 | 37.08 | 29.24 | 64.27 | 59.34 |
| 574.3518 1 | PC 21:3 | 154.88 | 150.64 | 35.38 | 27.38 | 94.76 | 61.75 | 56.95 | 33.01 |
| 572.3329 5 | PC 21:4 | 297.12 | 412.80 | 43.01 | 32.19 | 33.81 | 25.16 | 63.72 | 36.14 |
| 594.4173 | PC 22:0 | 8.88 | 5.75 | 14.04 | 20.62 | 17.95 | 11.93 | 3.81 | 1.60 |
| 606.4116 8 | PC 23:1 | 25.68 | 24.61 | 35.07 | 80.76 | 20.79 | 12.43 | 10.34 | 5.13 |
| 600.3660 9 | PC 23:4 | 359.33 | 411.16 | 82.92 | 82.09 | 94.56 | 72.34 | 62.54 | 30.11 |

| Mass <i>m/z</i> | Metabolite name | CTR | | SCH | | NF | | PNF | |
|--------------------|----------------------|--------------|--------------|--------------|--------------|---------------|---------------|---------------|--------------|
| | | <i>mean</i> | <i>dev</i> | <i>mean</i> | <i>dev</i> | <i>mean</i> | <i>dev</i> | <i>mean</i> | <i>dev</i> |
| 622.4468 4 | PC 24:0 | 28.05 | 22.91 | 21.86 | 24.22 | 37.33 | 14.78 | 9.50 | 5.93 |
| 614.3833 6 | PC 24:4 | 529.79 | 572.91 | 77.67 | 56.75 | 277.11 | 150.73 | 74.29 | 36.93 |
| 636.4592 9 | PC 25:0 | 112.33 | 89.09 | 33.29 | 18.49 | 44.22 | 36.04 | 35.63 | 21.59 |
| 650.4772 3 | PC 26:0 | 62.83 | 88.98 | 26.09 | 23.28 | 60.97 | 48.81 | 54.69 | 48.32 |
| 650.4772 9 | PC 26:0 PC 10:0_16:0 | 68.69 | 59.80 | 55.42 | 60.96 | 124.76 | 86.12 | 46.84 | 21.13 |
| 648.4616 1 | PC 26:1 | 12.45 | 6.94 | 17.84 | 30.91 | 18.19 | 11.35 | 6.86 | 3.48 |
| 678.5093 4 | PC 28:0 | 20.20 | 13.12 | 7210.25 | 17378.2 7 | 21.45 | 14.63 | 15.79 | 13.67 |
| 678.5067 7 | PC 28:0 PC 14:0_14:0 | 6228.69 | 9407.41 | 3224.18 | 3379.89 | 4345.06 | 3600.14 | 5600.88 | 4720.62 |
| 676.4818 1 | PC 28:1 | 102.85 | 80.26 | 60.44 | 60.56 | 89.24 | 97.47 | 47.19 | 16.77 |
| 674.4667 4 | PC 28:2 | 57.81 | 55.06 | 226.36 | 419.19 | 112.50 | 156.24 | 45.98 | 37.80 |
| 670.4443 4 | PC 28:4 | 12.09 | 10.74 | 13.56 | 20.90 | 7.51 | 4.74 | 2.51 | 1.48 |
| 692.5230 7 | PC 29:0 PC 14:0_15:0 | 7624.68 | 9513.90 | 4512.16 | 3431.96 | 12324.1 4 | 12043.7 1 | 6478.10 | 4142.41 |
| 688.4910 9 | PC 29:2 | 10.63 | 5.10 | 332.89 | 1012.51 | 17.11 | 14.18 | 6.36 | 4.42 |
| 706.5401 6 | PC 30:0 PC 14:0_16:0 | 97510.6 0 | 69200.6 6 | 77405.8 1 | 48468.1 0 | 242286. 08 | 189757. 08 | 105195. 24 | 48727.8 8 |
| 706.5398 6 | PC 30:0 PC 15:0_15:0 | 114.62 | 110.57 | 92.25 | 63.17 | 885.25 | 2085.58 | 123.12 | 58.84 |
| 704.5304 | PC 30:1 | 477.33 | 381.32 | 277.96 | 178.22 | 530.89 | 351.10 | 318.25 | 174.45 |
| 704.5251 5 | PC 30:1 PC 14:0_16:1 | 2572.84 | 3336.72 | 3306.60 | 3438.04 | 3480.30 | 1926.63 | 5185.04 | 3404.63 |
| 702.5126 3 | PC 30:2 | 42.53 | 48.68 | 42.06 | 43.51 | 58.34 | 41.16 | 51.30 | 37.88 |
| 702.5083 | PC 30:2 PC 14:0_16:2 | 28.70 | 29.00 | 35.58 | 37.00 | 64.88 | 89.70 | 30.41 | 20.23 |
| 698.4590 5 | PC 30:4 PC 15:2_15:2 | 159.73 | 178.15 | 80.64 | 189.84 | 34.08 | 61.29 | 175.40 | 271.69 |
| 720.5666 5 | PC 31:0 | 174.65 | 244.63 | 59.50 | 83.63 | 799.60 | 1726.90 | 139.65 | 118.62 |
| 720.5687 9 | PC 31:0 PC 15:0_16:0 | 4348.02 | 3407.09 | 1101.12 | 1248.49 | 1918.82 | 2001.32 | 512.47 | 515.04 |
| 718.5456 5 | PC 31:1 | 233.35 | 156.17 | 106.58 | 59.30 | 460.67 | 354.56 | 135.01 | 39.36 |
| 718.5397 3 | PC 31:1 PC 15:0_16:1 | 2761.40 | 3166.10 | 2380.30 | 2041.60 | 10549.5 2 | 20713.7 4 | 3941.25 | 2221.48 |
| 716.5267 3 | PC 31:2 | 214.27 | 134.25 | 108.79 | 113.32 | 247.46 | 299.16 | 103.61 | 63.25 |
| 716.5238 | PC 31:2 PC 16:0_15:2 | 18.56 | 12.06 | 13.72 | 10.30 | 274.67 | 796.00 | 11.41 | 4.79 |
| 714.5018 3 | PC 31:3 | 222.13 | 232.58 | 208.16 | 222.93 | 315.45 | 390.27 | 183.87 | 162.58 |

| Mass m/z | Metabolite name | CTR | | SCH | | NF | | PNF | |
|---------------|----------------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|
| | | mean | dev | mean | dev | mean | dev | mean | dev |
| 734.5694 6 | PC 32:0 PC 16:0_16:0 | 125.02 | 102.34 | 66.84 | 53.60 | 265.93 | 346.57 | 162.98 | 162.52 |
| 730.5390 6 | PC 32:2 PC 16:0_16:2 | 6663.17 | 4834.63 | 14557.8 8 | 13822.6 6 | 24964.4 6 | 18525.1 7 | 8624.96 | 4581.95 |
| 730.5401 6 | PC 32:2 PC 16:1_16:1 | 15667.4 2 | 9767.57 | 20865.1 5 | 15842.9 7 | 41444.2 6 | 28016.4 0 | 17229.8 2 | 6159.24 |
| 728.5231 3 | PC 32:3 | 208.29 | 178.57 | 239.20 | 275.88 | 150.82 | 92.96 | 64.35 | 45.61 |
| 728.5235 | PC 32:3 PC 14:0_18:3 | 46.49 | 31.87 | 56.32 | 50.81 | 105.92 | 134.77 | 41.40 | 31.41 |
| 728.5250 9 | PC 32:3 PC 16:0_16:3 | 204.09 | 173.19 | 244.36 | 283.80 | 142.89 | 85.72 | 62.29 | 38.66 |
| 726.5124 5 | PC 32:4 | 59.30 | 64.23 | 91.12 | 106.64 | 68.13 | 37.13 | 68.67 | 69.55 |
| 726.4914 6 | PC 32:4 PC 16:2_16:2 | 50.88 | 55.77 | 27.15 | 49.80 | 27.45 | 44.86 | 66.26 | 98.82 |
| 746.5871 | PC 33:1 | 70.24 | 45.82 | 80.77 | 80.67 | 120.68 | 82.96 | 58.56 | 21.70 |
| 744.5568 8 | PC 33:2 | 242.25 | 189.40 | 323.82 | 246.62 | 973.69 | 1002.80 | 506.28 | 256.86 |
| 744.5515 7 | PC 33:2 PC 15:0_18:2 | 454.89 | 224.24 | 713.81 | 485.54 | 3952.94 | 4686.67 | 814.33 | 343.35 |
| 742.5399 8 | PC 33:3 | 35.43 | 16.76 | 109.99 | 166.04 | 114.61 | 96.52 | 38.19 | 13.76 |
| 738.5171 5 | PC 33:5 | 155.36 | 94.74 | 150.81 | 101.06 | 240.01 | 145.75 | 90.93 | 38.65 |
| 760.5910 6 | PC 34:1 PC 16:0_18:1 | 195.29 | 93.56 | 154.04 | 74.84 | 351.57 | 152.96 | 172.30 | 82.66 |
| 758.5589 | PC 34:2 | 1806.37 | 1042.08 | 2299.38 | 1647.92 | 4507.73 | 2045.98 | 2876.87 | 1335.26 |
| 756.5523 7 | PC 34:3 | 14.98 | 10.14 | 16.84 | 13.52 | 117.67 | 282.34 | 10.60 | 4.93 |
| 756.5571 9 | PC 34:3 PC 16:0_18:3 | 1160.48 | 406.74 | 1271.92 | 946.05 | 4333.23 | 3579.69 | 1567.36 | 1549.01 |
| 756.5502 9 | PC 34:3 PC 16:1_18:2 | 27053.3 9 | 16963.5 9 | 33578.7 0 | 25271.4 7 | 72891.5 3 | 34361.1 1 | 42297.7 2 | 20811.2 9 |
| 754.5459 6 | PC 34:4 | 58.62 | 38.84 | 98.86 | 81.21 | 119.33 | 79.88 | 65.82 | 56.33 |
| 754.5433 3 | PC 34:4 PC 14:0_20:4 | 5421.16 | 5391.45 | 4391.09 | 3690.61 | 3932.77 | 2189.05 | 2973.10 | 1432.54 |
| 754.5377 2 | PC 34:4 PC 16:2_18:2 | 35.91 | 22.67 | 151.26 | 207.98 | 223.51 | 335.59 | 45.30 | 18.71 |
| 752.5222 8 | PC 34:5 | 209.91 | 147.81 | 450.64 | 444.11 | 739.72 | 1071.54 | 259.35 | 170.23 |
| 752.5266 1 | PC 34:5 PC 16:0_18:5 | 252.59 | 181.53 | 466.64 | 429.85 | 735.39 | 1130.01 | 306.12 | 200.70 |
| 772.5777 | PC 35:2 PC 17:1_18:1 | 5377.71 | 2768.46 | 2287.82 | 1517.94 | 11871.0 7 | 11146.7 6 | 2580.70 | 946.41 |
| 770.5546 9 | PC 35:3 | 104.51 | 37.28 | 114.81 | 68.32 | 589.11 | 522.94 | 97.15 | 25.28 |
| 770.5651 2 | PC 35:3 PC 17:1_18:2 | 380.46 | 160.60 | 674.23 | 660.93 | 3041.11 | 4305.34 | 502.58 | 181.20 |
| 768.5584 7 | PC 35:4 | 44.31 | 24.12 | 35.06 | 28.67 | 111.18 | 219.50 | 23.64 | 10.51 |

| Mass m/z | Metabolite name | CTR | | SCH | | NF | | PNF | |
|---------------|----------------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|
| | | mean | dev | mean | dev | mean | dev | mean | dev |
| 768.5546 9 | PC 35:4 PC 15:0_20:4 | 2062.90 | 1588.64 | 1270.88 | 871.20 | 4220.43 | 2750.64 | 1461.58 | 467.50 |
| 766.5437 6 | PC 35:5 PC 16:0_19:5 | 231.84 | 192.00 | 57.51 | 34.87 | 153.15 | 100.46 | 59.54 | 27.19 |
| 766.5405 3 | PC 35:5 PC 18:1_17:4 | 120.56 | 67.23 | 81.78 | 44.80 | 265.96 | 185.29 | 80.32 | 41.95 |
| 788.6198 1 | PC 36:1 | 54.70 | 41.02 | 29.54 | 17.64 | 35.05 | 11.46 | 33.59 | 29.84 |
| 786.6020 5 | PC 36:2 | 60.31 | 38.39 | 37.54 | 24.45 | 50.14 | 23.18 | 48.70 | 42.69 |
| 782.5537 7 | PC 36:4 | 1762.55 | 1260.83 | 1705.74 | 1225.27 | 2649.54 | 1205.22 | 1473.15 | 1062.01 |
| 782.5693 4 | PC 36:4 PC 18:1_18:3 | 2313.91 | 926.09 | 2636.12 | 2106.71 | 8622.16 | 3931.41 | 2076.25 | 1379.16 |
| 782.5710 4 | PC 36:4 PC 18:2_18:2 | 11756.4 4 | 3503.44 | 22383.1 6 | 19653.4 3 | 60677.5 8 | 53893.8 1 | 18267.2 9 | 7221.14 |
| 780.5585 9 | PC 36:5 | 101.29 | 54.33 | 165.84 | 154.38 | 179.04 | 150.75 | 55.33 | 21.31 |
| 780.5477 3 | PC 36:5 PC 16:0_20:5 | 29512.8 3 | 24641.0 5 | 11325.1 5 | 7585.71 | 40798.3 7 | 26495.4 7 | 17435.1 3 | 16816.3 2 |
| 780.5555 4 | PC 36:5 PC 16:1_20:4 | 31304.5 4 | 24094.8 4 | 27132.4 0 | 19901.6 9 | 46339.1 4 | 23452.9 8 | 22461.4 7 | 14588.2 7 |
| 780.5562 1 | PC 36:5 PC 18:2_18:3 | 170.21 | 94.97 | 441.47 | 574.27 | 564.00 | 725.13 | 110.48 | 34.45 |
| 778.5399 2 | PC 36:6 | 422.52 | 213.43 | 565.56 | 424.25 | 1271.56 | 726.63 | 760.06 | 428.78 |
| 778.5391 2 | PC 36:6 PC 14:0_22:6 | 337.05 | 255.63 | 358.04 | 366.00 | 471.10 | 246.47 | 195.64 | 99.34 |
| 776.5225 8 | PC 36:7 | 88.91 | 85.72 | 117.04 | 103.82 | 123.00 | 97.54 | 56.85 | 28.32 |
| 798.5999 8 | PC 37:3 | 398.12 | 163.78 | 171.09 | 103.85 | 1047.26 | 1220.34 | 189.64 | 37.62 |
| 796.5864 9 | PC 37:4 PC 17:0_20:4 | 4601.06 | 2079.68 | 2193.29 | 1499.28 | 11093.3 4 | 12588.7 8 | 2366.01 | 410.44 |
| 794.5725 7 | PC 37:5 PC 17:1_20:4 | 367.98 | 179.92 | 255.79 | 169.48 | 813.20 | 583.84 | 229.72 | 62.22 |
| 792.5361 9 | PC 37:6 | 73.26 | 72.95 | 32.51 | 17.76 | 167.60 | 221.01 | 32.15 | 5.46 |
| 792.5561 5 | PC 37:6 PC 15:0_22:6 | 976.53 | 946.13 | 396.72 | 341.92 | 1182.14 | 776.29 | 486.65 | 399.19 |
| 790.5498 | PC 37:7 | 129.76 | 105.19 | 98.46 | 50.98 | 214.27 | 221.23 | 50.59 | 9.56 |
| 790.5477 3 | PC 37:7 PC 18:2_19:5 | 67.26 | 43.41 | 69.35 | 57.08 | 109.94 | 64.47 | 43.91 | 12.80 |
| 810.6046 1 | PC 38:4 | 18.67 | 16.68 | 7.38 | 7.52 | 54.38 | 143.96 | 6.15 | 4.76 |
| 808.5719 6 | PC 38:5 PC 16:0_22:5 | 12235.0 0 | 13488.2 3 | 3274.07 | 2899.36 | 3735.40 | 3236.84 | 5825.38 | 2380.23 |
| 808.5769 | PC 38:5 PC 20:1_18:4 | 252.69 | 239.60 | 78.52 | 33.90 | 96.56 | 93.30 | 111.20 | 52.04 |
| 806.5766 | PC 38:6 | 211.45 | 89.33 | 237.77 | 176.76 | 433.66 | 196.83 | 123.08 | 46.67 |
| 806.5553 6 | PC 38:6 PC 16:0_22:6 | 618.62 | 871.26 | 107.47 | 58.10 | 343.83 | 594.67 | 208.20 | 25.73 |

| Mass <i>m/z</i> | Metabolite name | CTR | | SCH | | NF | | PNF | |
|--------------------|-----------------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|
| | | <i>mean</i> | <i>dev</i> | <i>mean</i> | <i>dev</i> | <i>mean</i> | <i>dev</i> | <i>mean</i> | <i>dev</i> |
| 806.5696 4 | PC 38:6 PC 18:2_20:4 | 45329.3 0 | 23340.8 8 | 40689.7 0 | 27542.5 5 | 80704.8 3 | 38627.6 7 | 27950.5 6 | 13899.0 3 |
| 804.5576 8 | PC 38:7 | 504.24 | 322.08 | 605.33 | 608.56 | 936.08 | 695.22 | 246.07 | 126.31 |
| 804.5602 4 | PC 38:7 PC 16:1_22:6 | 725.34 | 472.47 | 524.76 | 363.69 | 937.20 | 534.46 | 290.31 | 138.21 |
| 804.5531 | PC 38:7 PC 18:2_20:5 | 176.70 | 89.40 | 444.84 | 694.42 | 367.63 | 212.53 | 144.12 | 143.36 |
| 822.6057 7 | PC 39:5 | 480.15 | 582.72 | 76.76 | 60.35 | 434.44 | 550.01 | 46.85 | 12.87 |
| 820.5905 2 | PC 39:6 | 112.09 | 129.79 | 21.50 | 9.28 | 74.42 | 58.37 | 22.79 | 4.88 |
| 818.5616 5 | PC 39:7 | 37.99 | 23.68 | 34.80 | 22.26 | 115.34 | 87.83 | 34.24 | 7.88 |
| 814.5358 3 | PC 39:9 PC 20:4_19:5 | 38.97 | 17.55 | 17.75 | 10.40 | 92.11 | 74.61 | 15.55 | 5.82 |
| 832.5766 | PC 40:7 | 100.47 | 121.09 | 29.98 | 21.13 | 91.46 | 126.44 | 49.41 | 12.54 |
| 832.5855 1 | PC 40:7 PC 18:2_22:5 | 215.96 | 101.80 | 199.91 | 166.06 | 459.64 | 283.89 | 144.35 | 71.04 |
| 832.5835 6 | PC 40:7 PC 20:3_20:4 | 1685.33 | 845.13 | 1376.02 | 1211.65 | 3223.12 | 1670.58 | 586.58 | 188.73 |
| 830.5574 3 | PC 40:8 | 1082.27 | 1520.77 | 162.83 | 88.64 | 281.87 | 185.99 | 174.08 | 73.98 |
| 830.5681 2 | PC 40:8 PC 18:2_22:6 | 6281.15 | 3887.12 | 6466.18 | 5568.49 | 12190.5 9 | 7519.45 | 4150.67 | 2189.21 |
| 830.5716 6 | PC 40:8 PC 20:4_20:4 | 15645.7 1 | 11595.0 1 | 13032.5 3 | 8786.01 | 22441.8 8 | 11167.3 5 | 7927.21 | 4027.34 |
| 830.5509 6 | PC 40:8 PC 22:3_18:5 | 416.25 | 619.36 | 44.69 | 27.23 | 88.09 | 89.81 | 75.89 | 24.80 |
| 828.5538 9 | PC 40:9 PC 20:4_20:5 | 80.02 | 72.85 | 100.87 | 150.24 | 107.86 | 59.63 | 32.91 | 8.61 |
| 850.6359 9 | PC 41:5 | 31.51 | 9.64 | 22.39 | 6.19 | 103.30 | 118.07 | 25.04 | 12.36 |
| 848.6287 2 | PC 41:6 PC 17:3_24:3 | 251.48 | 277.97 | 30.30 | 25.07 | 203.51 | 299.64 | 9.51 | 5.38 |
| 846.6070 6 | PC 41:7 | 109.53 | 115.66 | 30.81 | 24.48 | 119.93 | 116.76 | 18.27 | 2.38 |
| 852.5547 5 | PC 42:11 | 18.51 | 15.68 | 14.26 | 16.68 | 22.37 | 13.62 | 8.85 | 4.96 |
| 858.6176 1 | PC 42:8 | 190.45 | 239.43 | 37.13 | 24.96 | 105.24 | 56.72 | 48.00 | 26.61 |
| 858.5836 2 | PC 42:8 PC 21:4_21:4 | 251.12 | 336.54 | 41.26 | 29.61 | 103.49 | 62.60 | 66.20 | 24.28 |
| 856.5828 9 | PC 42:9 PC 20:4_22:5 | 257.33 | 130.41 | 111.71 | 130.28 | 288.20 | 209.61 | 85.23 | 42.93 |
| 870.6059 | PC 43:9 | 475.41 | 605.67 | 69.06 | 55.46 | 425.35 | 636.03 | 30.86 | 5.73 |
| 882.5976 6 | PC 44:10 PC 22:4_22:6 | 78.48 | 37.23 | 39.50 | 28.73 | 182.96 | 157.45 | 42.05 | 26.26 |
| 880.5855 1 | PC 44:11 PC 22:5_22:6 | 121.79 | 52.16 | 91.91 | 91.61 | 169.38 | 118.54 | 55.12 | 34.21 |
| 878.5749 5 | PC 44:12 PC 22:6_22:6 | 92.42 | 45.79 | 69.37 | 75.42 | 128.73 | 109.95 | 40.53 | 29.37 |

| Mass <i>m/z</i> | Metabolite name | CTR | | SCH | | NF | | PNF | |
|--------------------|-----------------|-------------|------------|-------------|------------|-------------|------------|-------------|------------|
| | | <i>mean</i> | <i>dev</i> | <i>mean</i> | <i>dev</i> | <i>mean</i> | <i>dev</i> | <i>mean</i> | <i>dev</i> |
| 884.6066 9 | PC 44:9 | 320.16 | 513.83 | 23.75 | 18.08 | 420.83 | 512.56 | 36.97 | 35.79 |
| 894.6070 6 | PC 45:11 | 132.61 | 197.22 | 21.36 | 19.66 | 58.64 | 72.68 | 6.75 | 2.79 |
| 924.7484 1 | PC 46:3 | 8.40 | 7.23 | 14.25 | 18.81 | 10.38 | 9.20 | 14.71 | 9.91 |
| 916.6827 4 | PC 46:7 | 5.85 | 2.69 | 6.72 | 4.84 | 22.06 | 28.34 | 9.14 | 9.99 |
| 678.5443 1 | PC O-29:0 | 80.51 | 90.88 | 27.95 | 13.45 | 148.11 | 127.65 | 60.38 | 55.32 |
| 676.5285 6 | PC O-29:1 | 60.25 | 37.82 | 24.90 | 18.27 | 74.37 | 61.90 | 29.53 | 18.46 |
| 692.5640 9 | PC O-30:0 | 248.71 | 226.81 | 253.07 | 317.97 | 412.51 | 297.97 | 134.13 | 71.59 |
| 690.5430 9 | PC O-30:1 | 135.72 | 162.81 | 51.59 | 27.67 | 220.41 | 337.41 | 108.94 | 70.64 |
| 688.5280 8 | PC O-30:2 | 115.60 | 109.51 | 86.54 | 97.24 | 150.69 | 120.85 | 123.01 | 100.01 |
| 686.5116 6 | PC O-30:3 | 36.21 | 23.65 | 19.05 | 10.28 | 77.60 | 104.73 | 35.30 | 31.47 |
| 678.4691 8 | PC O-30:7 | 438.52 | 281.20 | 162.03 | 138.58 | 233.21 | 208.41 | 171.75 | 75.51 |
| 702.5443 1 | PC O-31:2 | 34.81 | 33.93 | 48.12 | 67.92 | 65.73 | 61.99 | 30.76 | 23.17 |
| 694.4663 7 | PC O-31:6 | 72.70 | 56.65 | 34.72 | 32.04 | 38.56 | 26.54 | 29.89 | 10.88 |
| 690.4371 9 | PC O-31:8 | 168.83 | 223.96 | 25.84 | 11.83 | 53.16 | 33.86 | 38.65 | 10.40 |
| 718.5663 5 | PC O-32:1 | 3439.39 | 4829.68 | 845.54 | 714.59 | 5921.49 | 7034.76 | 2533.34 | 2947.54 |
| 714.5463 9 | PC O-32:3 | 75.91 | 43.65 | 75.28 | 61.30 | 239.74 | 185.45 | 198.84 | 247.39 |
| 712.5300 9 | PC O-32:4 | 73.69 | 74.28 | 23.67 | 22.68 | 273.71 | 676.22 | 18.68 | 7.06 |
| 710.5131 8 | PC O-32:5 | 13.14 | 21.46 | 7.64 | 6.00 | 88.73 | 250.54 | 4.16 | 0.92 |
| 708.4821 2 | PC O-32:6 | 163.24 | 137.17 | 59.42 | 87.32 | 375.57 | 638.60 | 45.26 | 39.18 |
| 706.4680 2 | PC O-32:7 | 118.35 | 136.80 | 54.84 | 79.55 | 269.59 | 448.33 | 34.76 | 31.10 |
| 704.4525 8 | PC O-32:8 | 74.86 | 47.00 | 21.39 | 25.42 | 65.39 | 73.22 | 17.49 | 15.47 |
| 734.6008 9 | PC O-33:0 | 61.21 | 11.13 | 66.90 | 43.95 | 288.85 | 291.81 | 65.31 | 19.25 |
| 730.5663 5 | PC O-33:2 | 3133.76 | 2245.46 | 1984.99 | 1700.60 | 4376.76 | 1983.43 | 1848.94 | 600.64 |
| 728.5617 1 | PC O-33:3 | 94.83 | 46.69 | 225.10 | 290.48 | 147.11 | 72.12 | 61.41 | 18.03 |
| 724.5322 9 | PC O-33:5 | 66.98 | 52.81 | 1023.00 | 2561.64 | 145.12 | 258.45 | 28.27 | 10.79 |

| Mass <i>m/z</i> | Metabolite name | CTR | | SCH | | NF | | PNF | |
|--------------------|-----------------|-------------|------------|-------------|------------|--------------|---------------|-------------|------------|
| | | <i>mean</i> | <i>dev</i> | <i>mean</i> | <i>dev</i> | <i>mean</i> | <i>dev</i> | <i>mean</i> | <i>dev</i> |
| 722.5327 1 | PC O-33:6 | 45.89 | 36.66 | 24.54 | 15.98 | 474.27 | 1306.45 | 47.94 | 17.71 |
| 720.4836 4 | PC O-33:7 | 57.67 | 34.40 | 15.34 | 16.41 | 56.62 | 60.82 | 17.93 | 13.12 |
| 744.5824 | PC O-34:2 | 1083.49 | 712.57 | 857.61 | 596.54 | 7251.05 | 9374.66 | 2142.33 | 2174.51 |
| 742.5650 6 | PC O-34:3 | 6214.95 | 3030.59 | 4645.95 | 3302.05 | 68882.9 5 | 118272. 62 | 8828.76 | 5950.93 |
| 740.5545 7 | PC O-34:4 | 178.24 | 94.47 | 111.28 | 64.95 | 628.24 | 781.37 | 153.25 | 110.49 |
| 738.5428 5 | PC O-34:5 | 110.39 | 136.68 | 24.61 | 26.67 | 88.76 | 93.32 | 8.62 | 6.54 |
| 736.5465 7 | PC O-34:6 | 161.21 | 141.06 | 380.28 | 1071.23 | 75.02 | 103.02 | 78.06 | 25.86 |
| 730.4678 3 | PC O-34:9 | 125.46 | 156.29 | 20.77 | 14.18 | 36.85 | 37.99 | 23.23 | 5.02 |
| 754.5604 9 | PC O-35:4 | 25.16 | 16.03 | 56.24 | 67.84 | 79.04 | 117.35 | 22.48 | 9.51 |
| 752.5557 9 | PC O-35:5 | 161.57 | 190.33 | 52.06 | 35.46 | 177.66 | 182.17 | 37.33 | 9.74 |
| 750.5628 1 | PC O-35:6 | 29.19 | 19.10 | 51.54 | 49.14 | 32.69 | 20.39 | 32.44 | 12.16 |
| 748.5390 6 | PC O-35:7 | 44.86 | 33.72 | 23.27 | 13.70 | 480.86 | 1306.16 | 50.71 | 22.20 |
| 766.5722 7 | PC O-36:5 | 295.53 | 251.66 | 153.61 | 83.77 | 627.41 | 530.12 | 160.62 | 79.54 |
| 764.5623 2 | PC O-36:6 | 752.47 | 904.73 | 279.21 | 175.81 | 1765.27 | 1844.28 | 361.11 | 218.09 |
| 760.5327 8 | PC O-36:8 | 521.97 | 921.53 | 48.96 | 25.11 | 149.71 | 127.32 | 51.84 | 27.82 |
| 758.5013 4 | PC O-36:9 | 67.10 | 98.05 | 8.59 | 3.83 | 17.62 | 14.05 | 13.46 | 2.36 |
| 788.6534 4 | PC O-37:1 | 3476.58 | 913.67 | 1070.49 | 622.37 | 10870.2 8 | 15171.2 9 | 1041.16 | 292.17 |
| 776.5792 2 | PC O-37:7 | 69.55 | 53.83 | 44.17 | 55.48 | 80.15 | 56.87 | 40.47 | 24.91 |
| 774.5658 | PC O-37:8 | 193.44 | 130.88 | 125.26 | 95.13 | 1887.08 | 5214.15 | 207.87 | 98.45 |
| 772.5537 1 | PC O-37:9 | 177.63 | 168.65 | 26.11 | 17.18 | 95.70 | 75.51 | 111.37 | 187.16 |
| 792.5913 7 | PC O-38:6 | 324.29 | 296.90 | 177.56 | 111.12 | 651.84 | 549.49 | 142.89 | 32.64 |
| 790.5744 | PC O-38:7 | 138.01 | 175.60 | 54.13 | 26.12 | 124.48 | 60.79 | 44.38 | 13.55 |
| 788.5567 | PC O-38:8 | 251.34 | 275.43 | 74.60 | 45.65 | 192.41 | 149.18 | 57.66 | 17.38 |
| 798.5613 4 | PC O-39:10 | 101.17 | 62.64 | 57.93 | 42.19 | 165.65 | 109.53 | 129.53 | 69.24 |
| 804.5929 6 | PC O-39:7 | 55.58 | 39.30 | 28.28 | 17.60 | 170.23 | 195.87 | 43.55 | 21.76 |
| 800.573 | PC O-39:9 | 48.95 | 29.86 | 34.19 | 21.70 | 100.43 | 104.72 | 58.03 | 8.94 |
| 826.6740 1 | PC O-40:3 | 79.16 | 45.18 | 86.27 | 48.80 | 234.49 | 210.70 | 67.06 | 2.57 |

| Mass <i>m/z</i> | Metabolite name | CTR | | SCH | | NF | | PNF | |
|--------------------|----------------------|-------------|------------|-------------|------------|--------------|--------------|-------------|------------|
| | | <i>mean</i> | <i>dev</i> | <i>mean</i> | <i>dev</i> | <i>mean</i> | <i>dev</i> | <i>mean</i> | <i>dev</i> |
| 818.6030 9 | PC O-40:7 | 126.73 | 125.73 | 18.49 | 22.19 | 74.12 | 86.96 | 56.44 | 93.12 |
| 816.5921 | PC O-40:8 | 90.32 | 95.69 | 60.68 | 59.33 | 155.51 | 120.01 | 36.08 | 7.78 |
| 814.6005 2 | PC O-40:9 | 89.29 | 65.61 | 38.80 | 58.28 | 58.56 | 56.72 | 45.50 | 41.41 |
| 826.5802 | PC O-41:10 | 172.87 | 176.24 | 48.90 | 52.76 | 116.04 | 79.88 | 41.14 | 18.68 |
| 834.6409 3 | PC O-41:6 | 837.23 | 526.26 | 172.99 | 113.78 | 1085.43 | 1198.09 | 208.50 | 119.79 |
| 858.7319 3 | PC O-42:1 | 29.38 | 12.65 | 13.50 | 7.58 | 34.84 | 24.97 | 43.03 | 53.13 |
| 840.5955 8 | PC O-42:10 | 137.11 | 193.29 | 33.75 | 20.02 | 93.78 | 78.05 | 25.90 | 7.05 |
| 838.5736 1 | PC O-42:11 | 66.43 | 84.06 | 13.80 | 6.80 | 35.98 | 23.99 | 14.13 | 3.95 |
| 846.6355 | PC O-42:7 | 11.91 | 3.61 | 16.96 | 10.81 | 68.76 | 58.97 | 22.97 | 6.31 |
| 844.6132 8 | PC O-42:8 | 377.19 | 467.94 | 110.05 | 88.72 | 276.96 | 176.91 | 58.58 | 25.60 |
| 842.5967 4 | PC O-42:9 | 81.62 | 105.08 | 17.06 | 6.85 | 42.33 | 23.47 | 25.71 | 9.76 |
| 874.6699 2 | PC O-44:7 | 23.64 | 11.51 | 40.93 | 35.76 | 108.09 | 94.25 | 41.58 | 14.74 |
| 538.3507 7 | PE 21:0 | 120.89 | 204.44 | 9.31 | 12.76 | 17.30 | 10.09 | 40.51 | 40.80 |
| 536.3351 4 | PE 21:1 | 2578.37 | 4820.83 | 41.44 | 22.36 | 162.29 | 147.00 | 721.59 | 803.21 |
| 530.2850 3 | PE 21:4 | 590.72 | 883.85 | 51.79 | 59.23 | 131.65 | 111.68 | 248.79 | 236.62 |
| 558.3178 7 | PE 23:4 PE 7:0_16:4 | 4139.06 | 4393.48 | 324.16 | 291.14 | 762.80 | 1010.80 | 458.59 | 264.74 |
| 592.4101 6 | PE 25:1 | 63.90 | 97.73 | 5.76 | 5.09 | 19.20 | 34.97 | 11.78 | 9.22 |
| 586.3488 2 | PE 25:4 | 204.00 | 331.36 | 15.18 | 12.28 | 31.44 | 25.92 | 31.54 | 26.30 |
| 664.4861 5 | PE 30:0 | 18.08 | 11.89 | 15.78 | 12.16 | 40.21 | 24.13 | 21.91 | 11.93 |
| 662.4729 6 | PE 30:1 PE 14:0_16:1 | 44.93 | 42.13 | 28.45 | 16.90 | 144.94 | 236.69 | 44.66 | 25.25 |
| 688.4972 5 | PE 32:2 | 73.60 | 71.94 | 72.82 | 98.72 | 167.17 | 294.01 | 68.70 | 34.85 |
| 688.4944 5 | PE 32:2 PE 16:1_16:1 | 126.61 | 154.99 | 160.62 | 283.78 | 138.72 | 82.56 | 449.01 | 680.87 |
| 686.4758 9 | PE 32:3 | 20.82 | 12.01 | 20.21 | 13.99 | 32.72 | 20.50 | 12.55 | 7.18 |
| 714.5139 8 | PE 34:3 PE 16:1_18:2 | 66.91 | 51.41 | 60.92 | 32.46 | 212.71 | 167.83 | 116.55 | 80.09 |
| 712.4906 6 | PE 34:4 | 195.38 | 177.08 | 92.45 | 74.65 | 230.75 | 118.27 | 155.67 | 114.89 |
| 742.5544 4 | PE 36:3 PE 18:1_18:2 | 4700.25 | 4301.88 | 2473.54 | 1757.92 | 16993.0 2 | 15859.2 7 | 4274.01 | 3134.80 |
| 740.5274 | PE 36:4 | 121.56 | 117.75 | 88.58 | 60.29 | 327.64 | 424.61 | 150.20 | 76.34 |

| Mass m/z | Metabolite name | CTR | | SCH | | NF | | PNF | |
|---------------|--------------------------|---------|---------|--------|--------|---------|---------|--------|---------|
| | | mean | dev | mean | dev | mean | dev | mean | dev |
| 738.5100 1 | PE 36:5 PE 16:1_20:4 | 190.50 | 153.53 | 126.21 | 90.66 | 283.71 | 159.09 | 242.37 | 199.43 |
| 736.5190 4 | PE 36:6 | 57.61 | 39.05 | 226.50 | 361.88 | 69.56 | 38.19 | 28.46 | 13.85 |
| 760.5824 | PE 37:1 | 296.12 | 189.38 | 75.12 | 86.66 | 127.44 | 84.56 | 49.04 | 21.54 |
| 756.5400 4 | PE 37:3 | 161.60 | 38.30 | 35.27 | 36.98 | 350.84 | 440.21 | 54.17 | 57.22 |
| 766.5376 | PE 38:5 | 154.46 | 105.20 | 48.57 | 34.54 | 149.97 | 42.40 | 51.04 | 25.38 |
| 764.5330 2 | PE 38:6 PE 18:2_20:4 | 479.83 | 252.88 | 304.61 | 211.84 | 804.81 | 427.61 | 240.84 | 111.97 |
| 762.5076 9 | PE 38:7 PE 16:1_22:6 | 244.43 | 116.39 | 303.25 | 228.30 | 622.42 | 497.92 | 236.98 | 186.34 |
| 778.5482 2 | PE 39:6 | 68.07 | 32.55 | 29.27 | 15.76 | 185.84 | 214.74 | 27.22 | 10.42 |
| 796.5859 4 | PE 40:4 PE 18:0_22:4 | 2056.45 | 1254.16 | 749.14 | 553.88 | 5298.69 | 7429.46 | 733.50 | 440.75 |
| 788.5179 4 | PE 40:8 PE 18:2_22:6 | 225.43 | 129.93 | 158.47 | 131.90 | 385.12 | 266.80 | 114.55 | 52.81 |
| 812.5294 8 | PE 42:10 PE 20:4_22:6 | 250.89 | 159.44 | 64.93 | 38.75 | 201.56 | 121.22 | 78.34 | 61.32 |
| 852.5485 8 | PE 45:11 | 128.29 | 84.54 | 119.92 | 91.47 | 270.89 | 181.32 | 92.53 | 61.73 |
| 572.3681 | PE O-25:4 | 298.16 | 306.77 | 61.47 | 42.48 | 86.02 | 55.77 | 64.17 | 49.77 |
| 668.4688 7 | PE O-32:5 | 13.61 | 10.88 | 11.03 | 9.10 | 131.02 | 371.17 | 7.87 | 3.04 |
| 724.5223 4 | PE O-36:5 | 48.66 | 18.58 | 41.97 | 28.19 | 436.79 | 534.77 | 71.08 | 34.54 |
| 746.5178 2 | PE O-38:8 | 38.16 | 25.91 | 280.61 | 683.08 | 37.13 | 28.40 | 16.08 | 7.86 |
| 772.5300 9 | PE O-40:9 | 347.28 | 254.85 | 132.66 | 201.43 | 281.60 | 228.85 | 148.75 | 111.15 |
| 782.5004 3 | PE O-41:11 | 100.91 | 78.03 | 52.77 | 26.71 | 108.77 | 62.76 | 52.68 | 29.78 |
| 620.4619 8 | PE P-28:0 PE P-16:0_12:0 | 36.12 | 48.21 | 10.90 | 5.59 | 61.39 | 84.42 | 43.26 | 52.02 |
| 674.5112 3 | PE P-32:1 PE P-16:0_16:1 | 447.05 | 716.36 | 95.31 | 113.66 | 912.16 | 877.92 | 964.73 | 1262.15 |
| 682.4885 9 | PE P-33:4 PE P-13:0_20:4 | 56.66 | 43.07 | 46.04 | 25.18 | 156.04 | 195.23 | 46.95 | 22.02 |
| 696.5006 7 | PE P-34:4 PE P-14:0_20:4 | 76.69 | 48.24 | 31.84 | 20.75 | 125.51 | 116.08 | 30.73 | 12.97 |
| 730.5676 3 | PE P-36:1 PE P-18:0_18:1 | 18.62 | 32.70 | 1.03 | 0.59 | 2.94 | 4.03 | 15.21 | 25.99 |
| 722.5211 2 | PE P-36:5 PE P-16:0_20:5 | 50.35 | 49.88 | 62.81 | 139.68 | 63.36 | 121.46 | 19.65 | 5.67 |
| 722.5087 9 | PE P-36:5 PE P-16:1_20:4 | 81.93 | 75.17 | 65.74 | 47.54 | 215.17 | 178.31 | 70.30 | 40.88 |
| 748.5320 4 | PE P-38:6 PE P-18:2_20:4 | 276.33 | 244.56 | 211.55 | 110.01 | 454.36 | 247.39 | 196.63 | 81.87 |
| 742.4926 1 | PE P-38:9 PE P-16:3_22:6 | 46.12 | 26.60 | 41.62 | 36.20 | 208.38 | 311.45 | 22.38 | 9.77 |

| Mass m/z | Metabolite name | CTR | | SCH | | NF | | PNF | |
|---------------|----------------------------|---------------|---------------|--------------|--------------|---------------|--------------|--------------|--------------|
| | | mean | dev | mean | dev | mean | dev | mean | dev |
| 766.5742 8 | PE P-39:4 PE P-17:0_22:4 | 195.74 | 137.34 | 163.88 | 126.19 | 771.30 | 922.16 | 115.70 | 77.26 |
| 776.5568 2 | PE P-40:6 PE P-18:0_22:6 | 80.51 | 59.61 | 39.85 | 33.41 | 79.63 | 57.63 | 25.41 | 4.56 |
| 830.6158 4 | PE P-44:7 PE P-22:1_22:6 | 14.05 | 3.56 | 29.73 | 22.89 | 102.63 | 100.17 | 23.69 | 11.40 |
| 788.5416 3 | PG 36:4 PG 18:2_18:2 | 45.77 | 44.68 | 28.66 | 25.07 | 53.61 | 42.94 | 19.60 | 6.71 |
| 814.5617 7 | PG 38:5 PG 18:1_20:4 | 171.12 | 204.04 | 42.99 | 21.07 | 87.66 | 41.46 | 38.49 | 15.26 |
| 595.3843 4 | SM 27:6;2O | 186.06 | 219.99 | 31.29 | 26.95 | 64.98 | 45.65 | 43.02 | 27.06 |
| 619.4830 3 | SM 28:1;2O | 47.91 | 44.62 | 52.16 | 54.72 | 47.88 | 24.50 | 40.34 | 21.46 |
| 647.4846 8 | SM 29:2;3O | 146.26 | 106.03 | 186.62 | 297.38 | 154.82 | 97.90 | 81.18 | 36.05 |
| 649.5268 6 | SM 30:0;2O | 37.30 | 34.50 | 31.38 | 39.56 | 59.76 | 44.51 | 90.54 | 92.31 |
| 647.5131 8 | SM 30:1;2O SM 16:1;2O/14:0 | 6964.25 | 6554.18 | 10847.1 0 | 26420.0 1 | 3808.68 | 2281.18 | 4384.14 | 3810.27 |
| 645.5009 8 | SM 30:2;2O SM 15:0;2O/15:2 | 40.17 | 37.04 | 27.79 | 14.54 | 51.05 | 21.42 | 48.31 | 33.28 |
| 661.4922 5 | SM 30:2;3O | 103.63 | 112.87 | 15.89 | 9.61 | 42.87 | 31.84 | 31.69 | 9.47 |
| 661.5284 4 | SM 31:1;2O SM 18:1;2O/13:0 | 1429.87 | 1454.26 | 1059.25 | 1223.02 | 1732.22 | 1830.24 | 1322.05 | 1098.09 |
| 677.5213 6 | SM 31:1;3O | 10.01 | 8.56 | 6.36 | 6.06 | 149.16 | 423.38 | 8.53 | 3.38 |
| 677.5632 9 | SM 32:0;2O | 3638.40 | 3063.05 | 3746.37 | 4671.72 | 5524.75 | 4253.32 | 8770.90 | 9300.49 |
| 675.5463 9 | SM 32:1;2O | 130.72 | 119.93 | 107.82 | 132.13 | 185.66 | 121.20 | 106.59 | 52.56 |
| 675.5441 9 | SM 32:1;2O SM 16:1;2O/16:0 | 160449. 52 | 168108. 32 | 87707.8 1 | 88752.8 2 | 143301. 42 | 88339.9 3 | 84722.9 2 | 55135.0 7 |
| 691.5391 2 | SM 32:1;3O | 195.26 | 252.03 | 75.20 | 97.72 | 1377.95 | 3254.85 | 119.58 | 77.08 |
| 673.5301 5 | SM 32:2;2O SM 18:2;2O/14:0 | 5309.25 | 5093.67 | 3080.83 | 2781.59 | 3517.74 | 1707.73 | 4583.73 | 3672.42 |
| 689.5279 5 | SM 32:2;3O | 55.48 | 44.72 | 48.98 | 90.36 | 28.00 | 16.21 | 19.92 | 9.54 |
| 667.4750 4 | SM 32:5;2O | 103.41 | 62.53 | 49.29 | 69.34 | 85.54 | 55.56 | 34.22 | 31.69 |
| 679.4479 4 | SM 32:7;3O | 59.47 | 47.69 | 160.10 | 383.72 | 34.38 | 21.26 | 24.05 | 2.72 |
| 691.5780 6 | SM 33:0;2O | 2049.32 | 2010.19 | 2221.98 | 3330.46 | 2239.55 | 1568.06 | 965.98 | 581.91 |
| 707.5729 4 | SM 33:0;3O | 6076.15 | 3130.14 | 2245.87 | 1296.99 | 6745.20 | 5402.77 | 3183.85 | 1590.45 |
| 689.5603 | SM 33:1;2O SM 17:1;2O/16:0 | 42664.1 7 | 41073.7 1 | 52119.6 5 | 71675.7 6 | 52115.0 2 | 39073.3 0 | 24603.6 7 | 15404.4 8 |

| Mass <i>m/z</i> | Metabolite name | CTR | | SCH | | NF | | PNF | |
|--------------------|----------------------------|---------------|---------------|--------------|---------------|---------------|---------------|--------------|--------------|
| | | <i>mean</i> | <i>dev</i> | <i>mean</i> | <i>dev</i> | <i>mean</i> | <i>dev</i> | <i>mean</i> | <i>dev</i> |
| 689.5649 4 | SM 33:1;2O SM 18:1;2O/15:0 | 444.84 | 593.69 | 198.08 | 216.94 | 385.37 | 279.83 | 135.93 | 47.73 |
| 689.5597 5 | SM 33:1;2O SM 21:1;2O/12:0 | 402.84 | 529.74 | 204.57 | 227.79 | 337.10 | 207.32 | 129.67 | 48.28 |
| 705.5553 | SM 33:1;3O | 20.09 | 17.99 | 13.78 | 14.41 | 194.05 | 520.53 | 27.15 | 20.69 |
| 687.5441 9 | SM 33:2;2O SM 17:2;2O/16:0 | 368.79 | 356.35 | 298.47 | 371.01 | 318.10 | 178.85 | 187.02 | 139.62 |
| 703.5365 6 | SM 33:2;3O | 757.33 | 676.61 | 276.79 | 491.70 | 191.13 | 174.18 | 254.42 | 220.93 |
| 721.5852 1 | SM 34:0;3O | 40.49 | 40.20 | 28.32 | 36.99 | 195.97 | 347.67 | 189.23 | 228.99 |
| 703.5761 1 | SM 34:1;2O | 10815.1 9 | 13553.1 5 | 4663.83 | 5472.89 | 5899.19 | 2871.25 | 3320.63 | 1853.57 |
| 703.5733 6 | SM 34:1;2O SM 18:1;2O/16:0 | 1496.98 | 981.94 | 2378.29 | 3545.14 | 2483.01 | 1692.63 | 2079.86 | 1854.83 |
| 719.5721 4 | SM 34:1;3O | 53472.1 6 | 68091.3 0 | 13584.4 7 | 13718.2 1 | 87717.6 6 | 90745.6 6 | 25615.8 7 | 9404.19 |
| 701.5598 1 | SM 34:2;2O SM 18:1;2O/16:1 | 746.10 | 665.22 | 1139.36 | 2063.05 | 1233.79 | 1142.76 | 289.22 | 96.22 |
| 701.5601 2 | SM 34:2;2O SM 18:2;2O/16:0 | 188625. 85 | 234383. 05 | 94385.0 3 | 103433. 49 | 173115. 56 | 142220. 35 | 69231.6 0 | 41424.7 9 |
| 717.5568 2 | SM 34:2;3O | 365.53 | 517.87 | 125.39 | 122.10 | 472.33 | 625.18 | 314.53 | 257.65 |
| 719.6052 2 | SM 35:0;2O | 1085.72 | 651.56 | 1131.73 | 1916.05 | 5092.51 | 7617.22 | 981.40 | 827.94 |
| 733.5839 8 | SM 35:1;3O | 24.90 | 30.70 | 18.14 | 30.22 | 449.70 | 1341.40 | 14.26 | 7.21 |
| 715.5795 9 | SM 35:2;2O SM 17:1;2O/18:1 | 11562.5 2 | 11838.6 0 | 9639.60 | 15372.4 0 | 6799.29 | 4025.35 | 4070.05 | 2577.84 |
| 731.5670 2 | SM 35:2;3O | 1803.85 | 1317.38 | 1436.38 | 1222.53 | 3436.94 | 1699.81 | 1757.97 | 763.06 |
| 711.5413 8 | SM 35:4;2O | 572.40 | 491.08 | 1696.71 | 2396.94 | 1790.77 | 2148.90 | 448.48 | 340.04 |
| 723.5056 2 | SM 35:6;3O | 56.09 | 46.54 | 57.29 | 52.64 | 55.48 | 39.94 | 31.84 | 16.94 |
| 747.6046 1 | SM 36:1;3O | 1131.20 | 1274.47 | 849.86 | 1422.01 | 5363.04 | 8886.49 | 744.80 | 401.37 |
| 745.5866 7 | SM 36:2;3O | 343.35 | 210.81 | 243.63 | 161.94 | 1610.51 | 1706.17 | 544.49 | 544.60 |
| 727.5777 | SM 36:3;2O | 98.79 | 62.74 | 313.70 | 528.34 | 130.31 | 78.81 | 92.82 | 45.28 |
| 727.5752 | SM 36:3;2O SM 18:2;2O/18:1 | 493.66 | 273.99 | 1723.95 | 2835.62 | 698.65 | 419.41 | 280.54 | 125.20 |
| 743.5672 | SM 36:3;3O | 94.57 | 97.69 | 70.31 | 92.55 | 147.03 | 146.14 | 45.01 | 13.10 |
| 737.5145 3 | SM 36:6;3O | 15.70 | 8.17 | 20.21 | 10.31 | 48.00 | 29.01 | 19.66 | 6.81 |
| 719.5365 | SM 36:7;2O | 201.58 | 197.07 | 437.24 | 1175.98 | 57.60 | 50.33 | 60.92 | 34.49 |
| 755.6051 6 | SM 38:3;2O SM 18:2;2O/20:1 | 100.29 | 50.53 | 118.17 | 108.58 | 383.83 | 321.92 | 115.08 | 60.72 |
| 751.5592 | SM 38:5;2O | 253.45 | 332.68 | 67.10 | 115.88 | 30.58 | 66.93 | 151.75 | 192.93 |
| 749.5592 | SM 38:6;2O | 55.50 | 38.01 | 91.46 | 135.10 | 96.34 | 96.84 | 38.49 | 12.52 |

| Mass m/z | Metabolite name | CTR | | SCH | | NF | | PNF | |
|---------------|--------------------------------|---------------|---------------|--------------|---------------|---------------|---------------|--------------|--------------|
| | | mean | dev | mean | dev | mean | dev | mean | dev |
| 765.5490 1 | SM 38:6;3O | 239.83 | 213.09 | 116.04 | 69.58 | 465.50 | 373.09 | 109.90 | 54.89 |
| 789.6451 4 | SM 39:1;3O | 16.54 | 7.10 | 8.53 | 3.30 | 27.36 | 15.39 | 12.76 | 3.29 |
| 757.5452 9 | SM 39:9;2O | 64.47 | 60.64 | 41.11 | 27.94 | 65.54 | 38.74 | 34.66 | 15.86 |
| 801.6528 9 | SM 40:2;3O | 34.78 | 48.70 | 11.15 | 13.02 | 15.55 | 8.57 | 14.55 | 10.52 |
| 777.5725 1 | SM 40:6;2O SM 18:2;2O/22:4 | 125.29 | 84.43 | 145.88 | 203.62 | 67.08 | 60.24 | 74.94 | 31.21 |
| 793.5969 8 | SM 40:6;3O | 140.82 | 108.86 | 86.27 | 53.04 | 342.32 | 285.22 | 76.72 | 20.54 |
| 791.5846 6 | SM 40:7;3O | 328.53 | 492.07 | 92.44 | 53.73 | 365.50 | 348.80 | 88.33 | 27.23 |
| 813.6869 5 | SM 42:2;2O | 73.21 | 49.99 | 82.11 | 125.88 | 43.52 | 16.44 | 55.12 | 57.50 |
| 813.6796 9 | SM 42:2;2O SM 18:1;2O/24:1 | 423251. 77 | 143565. 90 | 97005.2 9 | 101907. 71 | 275881. 67 | 327906. 39 | 69820.4 1 | 34874.1 7 |
| 829.6794 4 | SM 42:2;3O | 104.82 | 74.35 | 50.45 | 60.68 | 91.76 | 49.17 | 60.93 | 20.11 |
| 827.6651 6 | SM 42:3;3O | 52.12 | 39.45 | 25.50 | 38.96 | 28.72 | 12.36 | 24.50 | 13.49 |
| 799.5741 | SM 42:9;2O | 73.64 | 62.11 | 31.10 | 30.29 | 57.98 | 34.19 | 54.21 | 50.78 |
| 827.6002 8 | SM 44:9;2O | 86.13 | 67.96 | 25.90 | 29.93 | 61.53 | 26.24 | 42.81 | 28.59 |
| 859.6474 | SM 45:8;3O | 21.72 | 23.14 | 13.97 | 12.49 | 18.47 | 13.18 | 18.12 | 5.22 |
| 859.6383 7 | SM 45:8;3O SM 31:6;2O(FA 14:1) | 52.34 | 32.46 | 24.69 | 13.72 | 73.09 | 59.53 | 22.20 | 9.89 |
| 861.6718 8 | SM 46:6;2O SM 18:1;2O/28:5 | 149.14 | 92.11 | 88.69 | 95.63 | 107.11 | 112.26 | 135.08 | 45.91 |
| 385.3472 | ST 27:2;O | 4467.27 | 6642.39 | 1666.91 | 2478.60 | 2941.50 | 3868.77 | 1940.33 | 2511.61 |
| 423.3475 6 | ST 28:1;O | 1303.54 | 1804.06 | 67.66 | 62.89 | 1987.63 | 5516.27 | 1052.49 | 2077.93 |
| 421.3508 9 | ST 28:2;O | 36.52 | 24.00 | 38.41 | 44.09 | 240.64 | 220.40 | 23.40 | 8.65 |
| 419.3172 6 | ST 28:3;O | 1484.73 | 1498.73 | 1486.62 | 2944.32 | 2140.10 | 2006.81 | 523.52 | 91.94 |
| 377.3269 7 | ST 28:4;O | 76.44 | 45.51 | 108.12 | 154.12 | 803.96 | 792.94 | 57.10 | 25.17 |
| 437.3805 5 | ST 29:1;O | 28.36 | 21.11 | 27.73 | 37.95 | 99.26 | 111.41 | 14.01 | 4.27 |
| 435.3472 9 | ST 29:2;O | 3481.98 | 2537.06 | 141.28 | 134.31 | 3752.13 | 10401.5 2 | 1296.57 | 2529.56 |
| 488.3967 | TG 24:0 TG 8:0_8:0_8:0 | 11795.9 3 | 10102.6 9 | 668.33 | 983.73 | 4527.50 | 6043.32 | 1271.40 | 2241.32 |
| 516.4274 3 | TG 26:0 TG 8:0_8:0_10:0 | 20062.7 9 | 14467.9 9 | 1631.29 | 2100.05 | 8873.93 | 9128.93 | 2250.81 | 3732.90 |
| 535.3982 5 | TG 27:0 TG 9:0_9:0_9:0 | 40.21 | 48.08 | 48.35 | 85.14 | 32.78 | 25.54 | 136.65 | 159.70 |
| 626.5360 7 | TG 34:1 TG 8:0_8:0_18:1 | 195.06 | 186.15 | 25.82 | 11.89 | 280.69 | 470.38 | 8332.98 | 16629.3 2 |

| Mass <i>m/z</i> | Metabolite name | CTR | | SCH | | NF | | PNF | |
|--------------------|---------------------------------|--------------|--------------|-------------|------------|--------------|--------------|--------------|--------------|
| | | <i>mean</i> | <i>dev</i> | <i>mean</i> | <i>dev</i> | <i>mean</i> | <i>dev</i> | <i>mean</i> | <i>dev</i> |
| 661.5330 8 | TG 36:0 TG 12:0_12:0_12:0 | 169.89 | 189.94 | 73.16 | 66.22 | 213.70 | 145.51 | 62.65 | 10.62 |
| 652.5514 5 | TG 36:2 TG 8:0_10:0_18:2 | 54.08 | 40.38 | 8.58 | 3.73 | 77.97 | 118.44 | 4392.42 | 8775.57 |
| 726.5763 5 | TG 39:2;2O TG 8:0_16:1_15:1;2O | 8.73 | 4.56 | 3.98 | 4.59 | 7.38 | 6.54 | 60.40 | 116.63 |
| 740.6713 3 | TG 42:0 TG 12:0_14:0_16:0 | 1592.11 | 1553.59 | 108.48 | 79.04 | 3816.13 | 8555.81 | 3088.92 | 6083.90 |
| 752.6370 8 | TG 42:2;1O TG 16:1_18:1_8:0;1O | 39.38 | 32.09 | 3.80 | 2.36 | 17.10 | 20.01 | 279.62 | 549.91 |
| 750.6251 2 | TG 42:3;1O TG 9:0_16:0_17:3;1O | 88.46 | 37.87 | 50.51 | 37.12 | 150.93 | 135.14 | 148.55 | 200.46 |
| 755.6223 1 | TG 43:2 TG 11:0_16:1_16:1 | 23.85 | 16.35 | 177.09 | 409.51 | 24.56 | 48.97 | 11.16 | 8.13 |
| 750.6565 6 | TG 43:2 TG 14:0_14:1_15:1 | 462.90 | 471.25 | 7.07 | 3.16 | 510.74 | 965.32 | 1833.37 | 3657.65 |
| 760.6485 6 | TG 44:4 TG 8:0_16:0_20:4 | 196.56 | 188.29 | 6.74 | 3.85 | 84.75 | 134.04 | 1304.88 | 2602.11 |
| 760.6433 7 | TG 44:4 TG 8:0_18:2_18:2 | 808.36 | 760.36 | 10.19 | 8.78 | 151.12 | 283.50 | 2983.52 | 5954.91 |
| 778.6886 | TG 45:2 TG 16:0_13:1_16:1 | 837.63 | 776.48 | 19.85 | 8.07 | 1038.06 | 2201.44 | 3220.81 | 6414.83 |
| 776.6675 4 | TG 45:3 TG 11:0_16:1_18:2 | 139.67 | 123.56 | 2.71 | 2.05 | 90.98 | 144.42 | 818.45 | 1633.68 |
| 813.6808 5 | TG 47:1 TG 13:0_15:0_19:1 | 98.97 | 99.80 | 17.79 | 18.41 | 42.88 | 103.03 | 100.15 | 186.75 |
| 806.7239 4 | TG 47:2 TG 15:0_14:1_18:1 | 2097.70 | 2259.58 | 107.50 | 46.60 | 3294.58 | 5757.33 | 7932.22 | 15743.4 7 |
| 804.7028 8 | TG 47:3 TG 14:1_16:1_17:1 | 603.86 | 515.00 | 7.45 | 3.09 | 397.23 | 722.77 | 2979.38 | 5949.77 |
| 838.7394 4 | TG 48:1;1O TG 16:0_16:1_16:0;1O | 68.82 | 77.20 | 1.60 | 1.62 | 47.80 | 97.01 | 1296.79 | 2592.16 |
| 822.7587 9 | TG 48:1 TG 14:0_16:0_18:1 | 25123.9 9 | 15737.3 6 | 5440.23 | 4821.43 | 32380.3 5 | 58433.5 1 | 18047.2 4 | 32992.0 2 |
| 816.7170 4 | TG 48:4 TG 14:1_16:1_18:2 | 1956.12 | 1512.03 | 20.57 | 25.44 | 480.60 | 922.90 | 3049.34 | 6086.18 |
| 814.6844 5 | TG 48:5 TG 12:0_18:2_18:3 | 483.34 | 542.59 | 9.34 | 6.50 | 515.87 | 1283.73 | 2183.68 | 4355.85 |
| 812.6884 2 | TG 48:6 TG 14:1_14:1_20:4 | 129.48 | 106.84 | 6.26 | 8.67 | 39.69 | 81.34 | 398.28 | 792.64 |
| 834.7418 8 | TG 49:2 TG 14:0_16:1_19:1 | 157.36 | 153.11 | 3.98 | 5.56 | 34.23 | 62.20 | 270.48 | 528.81 |
| 832.7357 8 | TG 49:3 TG 15:0_16:1_18:2 | 2001.33 | 1512.39 | 32.20 | 17.45 | 2290.71 | 4877.64 | 6963.03 | 13895.9 9 |
| 830.7157 6 | TG 49:4 TG 14:1_17:1_18:2 | 228.88 | 195.81 | 5.16 | 4.97 | 146.55 | 344.62 | 958.59 | 1912.06 |
| 857.7504 3 | TG 50:0 TG 16:0_16:0_18:0 | 458.65 | 398.74 | 2.60 | 2.86 | 135.79 | 275.31 | 4301.13 | 8596.07 |
| 866.7794 2 | TG 50:1;1O TG 16:0_16:1_18:0;1O | 412.50 | 505.13 | 1.81 | 1.97 | 130.50 | 267.08 | 4484.67 | 8966.60 |
| 864.7634 9 | TG 50:2;1O TG 16:0_16:1_18:1;1O | 576.65 | 696.12 | 2.09 | 1.41 | 244.66 | 511.83 | 9623.51 | 19244.5 4 |

| Mass m/z | Metabolite name | CTR | | SCH | | NF | | PNF | |
|---------------|---|--------------|--------------|---------|---------|--------------|--------------|--------------|--------------|
| | | mean | dev | mean | dev | mean | dev | mean | dev |
| 862.7507 3 | TG 50:3;1O TG 16:1_18:1_16:1;1O | 267.58 | 253.63 | 3.31 | 3.49 | 143.76 | 294.54 | 4574.51 | 9144.01 |
| 844.7439 6 | TG 50:4 TG 16:1_16:1_18:2 | 5024.62 | 3905.01 | 131.56 | 191.26 | 2413.01 | 4848.23 | 7732.11 | 15441.0 6 |
| 842.7189 3 | TG 50:5 TG 14:1_18:2_18:2 | 3249.95 | 2623.52 | 22.59 | 20.53 | 1391.03 | 2908.61 | 9126.67 | 18241.9 7 |
| 869.7431 | TG 51:1 TG 16:0_16:0_19:1 | 65.79 | 52.13 | 1.91 | 1.51 | 39.75 | 72.39 | 231.53 | 460.82 |
| 864.7940 7 | TG 51:1 TG 16:0_17:0_18:1 | 6048.39 | 4630.96 | 239.87 | 262.86 | 13591.0 5 | 39210.8 1 | 8189.90 | 16265.7 8 |
| 862.7800 3 | TG 51:2 TG 16:0_17:1_18:1 | 15118.4 1 | 11702.6 8 | 707.79 | 635.95 | 22494.0 0 | 60003.2 8 | 13168.0 5 | 26067.1 4 |
| 858.7528 1 | TG 51:4 TG 16:1_17:1_18:2 | 1286.18 | 1214.15 | 21.60 | 15.80 | 1326.03 | 3387.62 | 2622.30 | 5229.88 |
| 894.8255 | TG 52:1;1O TG 16:0_18:1_18:0;1O | 346.35 | 334.33 | 1.27 | 1.05 | 72.13 | 151.96 | 1750.82 | 3499.81 |
| 883.7764 3 | TG 52:1 TG 16:0_18:0_18:1 | 815.85 | 858.91 | 3.81 | 2.96 | 58.80 | 108.15 | 924.05 | 1842.88 |
| 892.7854 | TG 52:2;1O TG 16:0_18:1_18:1;1O | 600.78 | 678.36 | 3.40 | 2.66 | 220.65 | 510.20 | 10539.2 0 | 21076.3 8 |
| 888.7572 | TG 52:4;1O TG 16:0_18:2_18:2;1O | 273.92 | 243.32 | 2.55 | 2.00 | 205.73 | 547.75 | 3260.78 | 6518.85 |
| 870.7542 1 | TG 52:5 TG 16:1_18:2_18:2 | 18550.2 2 | 13528.5 9 | 543.43 | 481.45 | 15871.2 2 | 40081.5 6 | 25399.2 8 | 50588.1 3 |
| 868.7343 8 | TG 52:6 TG 16:1_16:1_20:4 | 2414.39 | 1873.26 | 38.34 | 33.83 | 1328.60 | 2982.11 | 5746.82 | 11478.0 7 |
| 873.6986 7 | TG 52:6 TG 18:0_16:1_18:5 | 70.75 | 46.19 | 3.60 | 2.63 | 50.43 | 105.79 | 26.23 | 50.75 |
| 866.7236 3 | TG 52:7 TG 16:0_14:1_22:6 | 1187.75 | 864.79 | 8.62 | 8.56 | 216.34 | 524.08 | 2245.55 | 4487.22 |
| 890.8096 3 | TG 53:2 TG 16:0_18:1_19:1 | 16104.3 5 | 16190.0 9 | 238.03 | 243.17 | 27068.3 4 | 80235.0 9 | 13816.1 0 | 27537.1 2 |
| 890.8297 1 | TG 53:2 TG 17:0_18:1_18:1 | 19345.7 7 | 17364.5 4 | 305.56 | 349.33 | 18715.0 2 | 53983.0 8 | 6235.82 | 12367.8 6 |
| 888.7948 | TG 53:3 TG 17:1_18:1_18:1 | 11301.7 7 | 10841.3 1 | 258.69 | 263.65 | 14427.7 9 | 40568.9 7 | 8976.74 | 17853.9 7 |
| 918.7718 5 | TG 53:4;2O TG 18:1_18:1_17:2;2O | 5219.50 | 7319.07 | 16.97 | 21.67 | 147.43 | 367.07 | 712.12 | 1418.47 |
| 882.7577 5 | TG 53:6 TG 15:0_18:2_20:4 | 122.29 | 85.02 | 6.81 | 6.89 | 57.81 | 134.81 | 375.47 | 748.34 |
| 906.8416 7 | TG 54:1 TG 16:0_20:0_18:1 | 3343.51 | 3175.34 | 236.30 | 225.41 | 16641.2 5 | 51204.4 1 | 25702.8 2 | 51283.7 5 |
| 920.8300 8 | TG 54:2;1O TG 16:0_18:1_20:1;1O | 95.17 | 97.80 | 0.95 | 1.03 | 33.28 | 79.78 | 612.80 | 1224.11 |
| 918.8234 3 | TG 54:3;1O TG 18:1_18:1_18:1;1O | 79.17 | 66.95 | 1.64 | 1.14 | 53.58 | 135.47 | 640.94 | 1279.80 |
| 898.7857 7 | TG 54:5 TG 18:1_18:2_18:2 | 15972.4 3 | 10422.9 5 | 3974.27 | 7690.30 | 8475.04 | 18187.1 2 | 8406.02 | 16557.8 5 |
| 896.7722 8 | TG 54:6 TG 18:2_18:2_18:2 | 10441.1 2 | 7074.91 | 779.94 | 724.81 | 12291.0 2 | 32820.4 0 | 17165.4 9 | 34161.4 0 |
| 894.7523 8 | TG 54:7 TG 18:2_18:2_18:3 | 6629.82 | 4487.28 | 122.61 | 145.74 | 1799.88 | 4200.89 | 9767.05 | 19507.3 6 |
| 948.8181 8 | TG 55:3;O2 TG 14:1_14:1_15:0;O(FA 12:0) | 59.40 | 66.46 | 4.10 | 4.27 | 8.76 | 17.18 | 10.43 | 18.12 |

| Mass <i>m/z</i> | Metabolite name | CTR | | SCH | | NF | | PNF | |
|--------------------|--|--------------|--------------|-------------|------------|--------------|--------------|--------------|--------------|
| | | <i>mean</i> | <i>dev</i> | <i>mean</i> | <i>dev</i> | <i>mean</i> | <i>dev</i> | <i>mean</i> | <i>dev</i> |
| 916.8241 | TG 55:3 TG 18:1_18:1_19:1 | 3791.06 | 3395.53 | 34.82 | 45.06 | 4663.23 | 13601.1 1 | 4361.98 | 8708.49 |
| 914.8129 3 | TG 55:4 TG 18:1_19:1_18:2 | 1069.57 | 1038.52 | 34.58 | 60.19 | 1079.94 | 3149.45 | 801.02 | 1594.62 |
| 912.8018 2 | TG 55:5 TG 18:1_18:2_19:2 | 126.37 | 127.70 | 16.28 | 25.31 | 84.15 | 208.45 | 86.79 | 167.88 |
| 932.8555 9 | TG 56:2 TG 20:0_18:1_18:1 | 2147.73 | 2081.32 | 180.76 | 236.20 | 12140.1 3 | 37529.4 0 | 22418.6 8 | 44771.4 8 |
| 928.8342 9 | TG 56:4 TG 18:1_18:1_20:2 | 8215.41 | 8537.96 | 1252.08 | 2380.58 | 3659.86 | 10137.9 1 | 685.88 | 1231.03 |
| 926.8135 4 | TG 56:5 TG 16:0_18:1_22:4 | 19633.0 6 | 13855.8 0 | 2225.34 | 4557.87 | 10657.4 3 | 27845.6 7 | 12760.4 9 | 25426.3 0 |
| 926.8221 4 | TG 56:5 TG 18:1_18:1_20:3 | 13844.0 6 | 9918.14 | 1513.94 | 3115.38 | 9965.45 | 26538.2 9 | 9261.72 | 18427.2 4 |
| 924.8044 4 | TG 56:6 TG 18:1_18:1_20:4 | 16301.7 5 | 12615.7 2 | 2688.56 | 5334.67 | 9497.76 | 23451.0 9 | 8564.79 | 16937.8 5 |
| 920.7686 8 | TG 56:8 TG 16:0_18:2_22:6 | 8836.12 | 8065.60 | 338.35 | 618.58 | 3349.70 | 9298.93 | 5879.47 | 11719.3 8 |
| 942.8374 6 | TG 57:4 TG 18:1_19:1_20:2 | 63.29 | 43.84 | 8.05 | 15.18 | 53.64 | 152.57 | 102.43 | 202.89 |
| 944.7741 7 | TG 58:10 TG 18:2_18:2_22:6 | 243.66 | 252.63 | 24.59 | 36.56 | 75.52 | 197.11 | 41.00 | 72.98 |
| 942.7661 7 | TG 58:11 TG 18:2_18:3_22:6 | 36.62 | 29.50 | 4.35 | 3.71 | 6.45 | 11.07 | 40.83 | 77.07 |
| 958.8725 | TG 58:3 TG 22:0_18:1_18:2 | 456.25 | 385.83 | 77.64 | 134.70 | 1510.21 | 4597.48 | 5142.97 | 10267.3 9 |
| 954.8493 | TG 58:5 TG 18:1_18:1_22:3 | 1747.55 | 1233.50 | 382.62 | 783.04 | 1136.75 | 3177.95 | 1336.81 | 2650.11 |
| 952.8277 | TG 58:6 TG 18:1_18:1_22:4 | 4228.60 | 3222.95 | 605.49 | 1309.57 | 2541.58 | 7126.49 | 2381.66 | 4737.29 |
| 946.7902 8 | TG 58:9 TG 18:1_18:2_22:6 | 2154.53 | 2315.95 | 184.92 | 378.40 | 1133.02 | 3250.58 | 1159.81 | 2301.59 |
| 951.7508 5 | TG 58:9 TG 18:1_20:4_20:4 | 59.89 | 55.66 | 5.46 | 9.59 | 23.67 | 59.63 | 9.51 | 17.98 |
| 970.8789 7 | TG 59:4 TG 18:1_23:1_18:2 | 2.71 | 1.69 | 2.32 | 3.01 | 8.27 | 24.24 | 40.00 | 78.91 |
| 972.8034 7 | TG 60:10 TG 18:1_20:3_22:6 | 97.09 | 75.88 | 47.01 | 109.04 | 23.94 | 47.50 | 19.87 | 33.35 |
| 972.8065 2 | TG 60:10 TG 18:1_20:4_22:5 | 75.60 | 68.11 | 23.78 | 52.07 | 26.55 | 59.69 | 46.78 | 89.46 |
| 982.8746 3 | TG 60:5 TG 18:1_18:2_24:2 | 26.03 | 19.45 | 43.05 | 83.13 | 38.31 | 71.65 | 164.37 | 324.00 |
| 980.8649 9 | TG 60:6 TG 18:1_20:1_22:4 | 158.28 | 106.34 | 84.74 | 173.15 | 105.27 | 230.44 | 164.61 | 319.43 |
| 976.8314 2 | TG 60:8 TG 18:1_20:3_22:4 | 30.17 | 20.97 | 73.57 | 171.10 | 13.23 | 20.76 | 4.97 | 3.30 |
| 1000.836 06 | TG 62:10 TG 18:0_22:4_22:6 | 26.82 | 8.10 | 42.13 | 99.98 | 7.28 | 9.34 | 5.99 | 8.10 |
| 1126.994 02 | TG 68:5;O2 TG 16:1_18:1_18:2;O(FA 16:0) | 0.41 | 0.22 | 0.06 | 0.05 | 1.13 | 3.41 | 37.27 | 74.54 |
| 479.3726 2 | TG O-24:0 TG O-8:0_8:0_8:0 | 837.49 | 649.16 | 120.43 | 239.81 | 492.68 | 904.26 | 150.63 | 261.33 |

| Mass m/z | Metabolite name | CTR | | SCH | | NF | | PNF | |
|---------------|--------------------------------|---------|---------|--------|--------|---------|---------|---------|--------------|
| | | mean | dev | mean | dev | mean | dev | mean | dev |
| 488.4208 4 | TG O-25:0 TG O-9:0_8:0_8:0 | 742.99 | 374.85 | 67.65 | 69.27 | 388.25 | 235.46 | 98.73 | 141.21 |
| 521.4187 6 | TG O-27:0 TG O-10:0_8:0_9:0 | 32.03 | 10.37 | 33.39 | 28.04 | 185.88 | 151.35 | 109.54 | 98.45 |
| 521.4201 7 | TG O-27:0 TG O-9:0_9:0_9:0 | 32.15 | 14.82 | 39.97 | 35.57 | 194.80 | 158.07 | 150.78 | 145.57 |
| 577.4810 2 | TG O-31:0 TG O-9:0_11:0_11:0 | 17.10 | 8.45 | 21.39 | 18.36 | 104.75 | 88.13 | 49.14 | 16.51 |
| 619.5257 6 | TG O-34:0 TG O-16:0_9:0_9:0 | 234.72 | 191.38 | 108.28 | 99.80 | 378.39 | 467.20 | 171.06 | 151.39 |
| 709.5866 7 | TG O-41:4 TG O-19:4_11:0_11:0 | 45.76 | 62.09 | 101.94 | 187.84 | 47.66 | 41.47 | 28.02 | 19.35 |
| 724.6695 6 | TG O-42:1 TG O-16:1_12:0_14:0 | 527.76 | 510.65 | 31.06 | 76.71 | 185.17 | 336.82 | 349.19 | 685.49 |
| 723.6138 3 | TG O-42:4 TG O-20:4_11:0_11:0 | 149.83 | 297.98 | 90.86 | 215.49 | 1.69 | 4.79 | 0.67 | 0.78 |
| 736.6669 3 | TG O-43:2 TG O-17:1_8:0_18:1 | 4249.58 | 3745.41 | 22.39 | 18.27 | 1504.51 | 3342.91 | 5278.41 | 10540.3 9 |
| 794.7550 7 | TG O-47:1 TG O-15:0_16:0_16:1 | 116.12 | 85.86 | 6.58 | 5.00 | 117.29 | 237.52 | 92.60 | 179.59 |
| 829.7456 1 | TG O-49:0 TG O-17:0_16:0_16:0 | 517.66 | 680.64 | 2.13 | 2.29 | 37.23 | 69.62 | 598.29 | 1190.90 |
| 816.7463 4 | TG O-49:4 TG O-15:1_16:1_18:2 | 373.05 | 278.90 | 8.95 | 7.12 | 169.53 | 369.51 | 212.71 | 416.91 |
| 839.7476 8 | TG O-50:2 TG O-20:2_15:0_15:0 | 44.37 | 47.35 | 1.05 | 1.30 | 31.63 | 60.92 | 769.02 | 1537.29 |
| 858.7910 2 | TG O-52:4 TG O-16:0_16:0_20:4 | 93.67 | 76.08 | 30.74 | 58.54 | 169.41 | 488.78 | 38.40 | 71.06 |
| 884.8108 5 | TG O-54:5 TG O-16:0_18:1_20:4 | 57.42 | 39.01 | 68.54 | 146.37 | 85.19 | 232.13 | 17.55 | 29.06 |
| 889.7728 9 | TG O-54:5 TG O-16:0_19:0_19:5 | 172.89 | 148.16 | 1.88 | 1.95 | 133.16 | 359.43 | 1447.64 | 2893.06 |
| 922.8206 2 | TG O-57:7 TG O-21:5_18:1_18:1 | 928.17 | 553.06 | 134.22 | 206.47 | 600.79 | 1373.08 | 290.40 | 540.22 |
| 970.8014 5 | TG O-61:11 TG O-19:1_20:4_22:6 | 292.62 | 231.20 | 79.79 | 193.12 | 31.12 | 60.02 | 75.77 | 144.44 |
| 469.3893 4 | VAE 12:0 | 59.11 | 33.62 | 66.91 | 69.66 | 356.75 | 325.74 | 233.78 | 236.01 |
| 599.5039 7 | VAE 22:5 | 53.79 | 25.75 | 73.04 | 87.01 | 209.01 | 234.66 | 62.54 | 41.01 |
| 357.2801 5 | VAE 4:0 | 24.15 | 28.20 | 80.13 | 161.32 | 32.25 | 38.69 | 3.69 | 0.74 |

Table S2. List of all the single lipid species identified using an untargeted lipidomics approach across each histotype. Each lipid was identified with monoisotopic molecular adducts in negative electrospray ionization (m/z), name, and mass intensities scaled for protein content in each group.

| Average m/z | Metabolite name | CTR | | SCH | | NF | | PNF | |
|------------------|-----------------------------------|--------------|----------|---------|----------|---------|-------------|---------|---------|
| | | mean | dev | mean | dev | mean | dev | mean | dev |
| 482.2933 | BA 24:1;O2;T | 148.85 | 233.85 | 58.14 | 110.68 | 41.56 | 60.79 | 42.84 | 14.24 |
| 498.2871 7 | BA 24:1;O3;T | 21.60 | 12.87 | 38.01 | 39.21 | 84.19 | 83.46 | 99.75 | 55.31 |
| 528.2729 5 | BA 24:1;O4;G;S | 24539.5 8 | 28569.99 | 2961.82 | 2850.82 | 4303.17 | 5486.0 4 | 3927.19 | 1999.87 |
| 514.2904 1 | BA 24:1;O4;T | 3.76 | 3.73 | 281.49 | 887.06 | 3.13 | 4.72 | 1.22 | 0.64 |
| 619.4231 6 | CL 56:0 CL 14:0_14:0_14:0_14:0 | 130.41 | 208.72 | 61.18 | 111.06 | 28.88 | 23.74 | 28.70 | 19.48 |
| 618.4151 6 | CL 56:1 CL 12:0_12:0_16:0_16:1 | 18.46 | 34.24 | 2.91 | 4.40 | 1.85 | 2.27 | 2.56 | 2.12 |
| 623.4049 7 | CL 57:3 CL 12:0_15:1_15:1_15:1 | 250.13 | 255.88 | 3960.81 | 11053.51 | 112.53 | 184.29 | 108.91 | 54.90 |
| 628.3909 3 | CL 58:5 CL 14:1_14:1_14:1_16:2 | 206.57 | 171.99 | 113.85 | 89.71 | 111.44 | 124.89 | 85.60 | 26.18 |
| 647.4606 3 | CL 60:0 CL 12:0_16:0_16:0_16:0 | 384.94 | 302.75 | 286.31 | 283.15 | 191.11 | 156.86 | 107.85 | 45.57 |
| 644.4240 7 | CL 60:3 CL 12:0_12:0_18:1_18:2 | 19.09 | 26.96 | 11.08 | 19.28 | 5.51 | 5.67 | 4.23 | 1.78 |
| 643.4246 2 | CL 60:4 CL 14:1_14:1_14:1_18:1 | 97.83 | 77.67 | 64.53 | 48.59 | 66.61 | 88.33 | 29.02 | 16.88 |
| 657.4195 6 | CL 62:4 CL 14:1_16:1_16:1_16:1 | 165.90 | 156.21 | 56.27 | 40.82 | 61.52 | 112.12 | 84.10 | 32.59 |
| 667.4549 6 | CL 63:1 CL 16:0_16:0_16:0_15:1 | 479.23 | 508.97 | 361.18 | 404.10 | 273.48 | 275.38 | 217.51 | 68.92 |
| 675.4863 9 | CL 64:0 CL 16:0_16:0_16:0_16:0 | 163.57 | 253.23 | 70.70 | 92.34 | 104.98 | 217.17 | 49.72 | 44.81 |
| 673.4705 8 | CL 64:2 CL 12:0_16:0_18:1_18:1 | 46.17 | 52.24 | 15.44 | 23.19 | 55.99 | 135.33 | 8.25 | 6.48 |
| 673.4722 9 | CL 64:2 CL 16:0_16:0_16:0_16:2 | 83.55 | 101.08 | 16.87 | 24.27 | 88.57 | 221.39 | 13.56 | 10.78 |
| 669.4238 9 | CL 64:6 CL 16:0_14:1_14:1_20:4 | 323.26 | 197.62 | 157.85 | 101.11 | 245.79 | 130.27 | 160.73 | 48.07 |
| 680.4822 4 | CL 65:2 CL 16:0_16:0_16:0_17:2 | 85.88 | 106.00 | 37.56 | 24.17 | 91.82 | 196.71 | 41.05 | 27.55 |
| 677.4482 4 | CL 65:5 CL 16:1_16:1_16:1_17:2 | 439.97 | 728.89 | 1416.49 | 3319.23 | 30.34 | 35.47 | 30.71 | 43.40 |
| 689.5026 9 | CL 66:0 CL 16:0_16:0_17:0_17:0 | 184.08 | 322.46 | 46.76 | 24.93 | 60.25 | 75.12 | 45.01 | 15.68 |
| 695.4991 5 | CL 67:1 CL 16:0_16:0_17:0_18:1 | 16.37 | 8.79 | 60.04 | 100.78 | 43.47 | 99.92 | 13.94 | 9.34 |
| 700.4890 7 | CL 68:3 CL 14:0_16:1_18:1_20:1 | 36.63 | 34.59 | 88.93 | 184.19 | 123.66 | 131.17 | 110.91 | 108.70 |
| 699.4624 6 | CL 68:4 CL 14:1_18:1_18:1_18:1 | 170.98 | 142.98 | 136.57 | 179.83 | 66.31 | 44.03 | 35.86 | 14.66 |
| 694.4304 2 | CL 68:9 CL 16:1_16:2_16:2_20:4 | 492.44 | 497.34 | 133.93 | 75.35 | 145.97 | 188.45 | 229.25 | 73.84 |

| Average <i>m/z</i> | Metabolite name | CTR | | SCH | | NF | | PNF | |
|-----------------------|------------------------------------|-------------|------------|-------------|------------|-------------|-------------|-------------|------------|
| | | <i>mean</i> | <i>dev</i> | <i>mean</i> | <i>dev</i> | <i>mean</i> | <i>dev</i> | <i>mean</i> | <i>dev</i> |
| 707.5009 8 | CL 69:3 CL 24:0_15:1_15:1_15:1 | 283.00 | 252.56 | 828.97 | 1496.21 | 160.22 | 403.78 | 323.41 | 284.94 |
| 705.4832 8 | CL 69:5 CL 15:0_16:0_16:0_22:5 | 9.58 | 7.58 | 32.47 | 68.37 | 5.21 | 11.21 | 6.70 | 2.89 |
| 1434.037 35 | CL 70:1 CL 37:0_33:1 | 64.48 | 37.59 | 59.15 | 60.10 | 64.53 | 37.82 | 74.81 | 49.62 |
| 714.4977 4 | CL 70:3 CL 16:0_16:0_16:0_22:3 | 46.07 | 30.33 | 114.43 | 204.39 | 50.23 | 85.91 | 34.45 | 22.41 |
| 714.4933 5 | CL 70:3 CL 16:0_18:1_18:1_18:1 | 7.16 | 5.52 | 17.00 | 19.63 | 9.03 | 15.79 | 3.75 | 1.16 |
| 713.4887 1 | CL 70:4 CL 16:1_18:1_18:1_18:1 | 6.71 | 3.91 | 54.23 | 61.68 | 13.16 | 17.14 | 13.90 | 6.66 |
| 712.4798 6 | CL 70:5 CL 16:1_18:1_18:1_18:2 | 13.20 | 9.90 | 102.20 | 143.13 | 26.86 | 32.19 | 22.15 | 8.30 |
| 711.4651 5 | CL 70:6 CL 16:0_16:0_16:0_22:6 | 66.90 | 40.15 | 511.41 | 1300.54 | 104.03 | 247.38 | 31.76 | 12.63 |
| 711.4721 1 | CL 70:6 CL 16:1_18:1_18:2_18:2 | 29.05 | 32.42 | 80.93 | 86.98 | 40.83 | 35.15 | 37.57 | 7.51 |
| 1423.955 32 | CL 70:6 CL 34:3_36:3 | 55.62 | 52.85 | 122.82 | 154.58 | 100.11 | 147.54 | 45.15 | 25.56 |
| 721.5143 4 | CL 71:3 CL 17:0_18:1_18:1_18:1 | 33.88 | 26.43 | 102.30 | 223.00 | 22.10 | 23.67 | 28.26 | 22.52 |
| 721.5063 5 | CL 71:3 CL 26:0_15:1_15:1_15:1 | 13.92 | 13.12 | 35.85 | 59.36 | 9.08 | 12.65 | 13.94 | 5.25 |
| 719.4981 1 | CL 71:5 CL 16:0_17:0_18:1_20:4 | 47.92 | 33.61 | 197.12 | 394.46 | 17.79 | 20.10 | 44.81 | 30.15 |
| 717.4694 8 | CL 71:7 CL 15:0_18:0_16:1_22:6 | 22.20 | 32.76 | 22.18 | 41.54 | 3.55 | 4.11 | 4.82 | 2.99 |
| 717.4940 8 | CL 71:7 CL 18:1_17:2_18:2_18:2 | 56.47 | 65.44 | 49.58 | 68.96 | 32.76 | 32.83 | 52.57 | 25.07 |
| 730.5269 2 | CL 72:1 CL 16:0_16:0_20:0_20:1 | 716.14 | 435.88 | 662.86 | 592.71 | 2839.97 | 3488.8 5 | 537.10 | 321.34 |
| 730.5380 9 | CL 72:1 CL 18:0_18:0_18:0_18:1 | 168.16 | 139.55 | 102.08 | 43.30 | 246.85 | 200.05 | 179.51 | 172.65 |
| 1462.061 04 | CL 72:1 CL 33:0_39:1 | 65.23 | 48.36 | 53.16 | 40.96 | 58.52 | 64.77 | 55.23 | 51.15 |
| 721.4584 4 | CL 72:10 CL 14:1_18:1_20:4_20:4 | 286.00 | 216.22 | 170.31 | 165.86 | 138.10 | 102.38 | 83.07 | 33.77 |
| 728.5180 7 | CL 72:3 CL 18:0_18:1_18:1_18:1 | 2373.35 | 2280.30 | 1494.22 | 2021.19 | 4740.27 | 6999.7 6 | 2690.49 | 4052.51 |
| 726.5057 4 | CL 72:5 CL 18:1_18:1_18:1_18:2 | 191.70 | 127.67 | 1652.61 | 2956.08 | 639.93 | 1829.1 0 | 462.53 | 523.00 |
| 725.4893 2 | CL 72:6 CL 18:0_18:2_18:2_18:2 | 334.01 | 259.68 | 179.22 | 178.20 | 199.86 | 123.98 | 134.63 | 41.85 |
| 725.4881 6 | CL 72:6 CL 18:1_18:1_18:2_18:2 | 152.35 | 148.20 | 488.11 | 500.42 | 179.71 | 173.87 | 117.80 | 81.91 |
| 724.4856 6 | CL 72:7 CL 18:1_18:2_18:2_18:2 | 177.55 | 199.11 | 348.34 | 324.55 | 183.98 | 166.57 | 189.53 | 86.25 |
| 723.4753 4 | CL 72:8 CL 18:2_18:2_18:2_18:2 | 303.15 | 457.13 | 180.87 | 146.12 | 176.98 | 111.66 | 110.55 | 26.91 |

| Average <i>m/z</i> | Metabolite name | CTR | | SCH | | NF | | PNF | |
|-----------------------|------------------------------------|-------------|------------|-------------|------------|-------------|-------------|-------------|------------|
| | | <i>mean</i> | <i>dev</i> | <i>mean</i> | <i>dev</i> | <i>mean</i> | <i>dev</i> | <i>mean</i> | <i>dev</i> |
| 722.4592 9 | CL 72:9 CL 18:0_14:1_20:4_20:4 | 112.75 | 109.88 | 40.27 | 33.45 | 63.51 | 91.08 | 47.59 | 18.28 |
| 735.5212 4 | CL 73:3 CL 28:0_15:1_15:1_15:1 | 87.77 | 94.68 | 242.59 | 405.91 | 67.09 | 170.96 | 115.23 | 77.01 |
| 1470.024 9 | CL 73:4 CL 35:1_38:3 | 74.07 | 93.06 | 23.14 | 16.81 | 43.24 | 25.96 | 26.98 | 24.87 |
| 733.5175 2 | CL 73:5 CL 16:0_18:0_18:0_21:5 | 611.24 | 697.90 | 1239.53 | 2037.62 | 270.32 | 596.69 | 745.21 | 659.84 |
| 732.5181 9 | CL 73:6 CL 16:0_18:1_18:1_21:4 | 104.64 | 154.17 | 99.68 | 98.63 | 58.31 | 62.15 | 61.94 | 55.93 |
| 731.4914 6 | CL 73:7 CL 16:0_18:0_17:1_22:6 | 34.04 | 29.15 | 163.00 | 309.11 | 18.81 | 32.97 | 51.26 | 39.55 |
| 731.5006 1 | CL 73:7 CL 17:1_18:1_18:1_20:4 | 171.57 | 256.97 | 101.50 | 118.16 | 32.08 | 46.06 | 92.62 | 68.79 |
| 730.5020 1 | CL 73:8 CL 16:1_18:1_18:1_21:5 | 374.49 | 660.36 | 101.93 | 134.11 | 57.27 | 76.26 | 210.58 | 181.62 |
| 745.5525 5 | CL 74:0 CL 16:0_16:0_16:0_26:0 | 1842.14 | 1091.13 | 729.28 | 384.70 | 1626.95 | 561.65 | 1016.27 | 425.61 |
| 733.4512 9 | CL 74:12 CL 14:0_20:4_20:4_20:4 | 52.98 | 34.33 | 273.26 | 594.23 | 35.81 | 47.53 | 53.28 | 38.53 |
| 1488.100 95 | CL 74:2 CL 35:1_39:1 | 239.69 | 124.23 | 154.85 | 125.92 | 181.17 | 186.45 | 156.92 | 138.44 |
| 1486.077 51 | CL 74:3 CL 33:0_41:3 | 500.16 | 349.74 | 291.10 | 223.86 | 383.43 | 477.60 | 368.90 | 405.05 |
| 739.5090 9 | CL 74:6 CL 16:0_20:0_18:2_20:4 | 420.62 | 254.42 | 340.35 | 331.06 | 782.99 | 1636.4 8 | 411.23 | 412.79 |
| 1480.030 27 | CL 74:6 CL 38:1_36:5 | 117.76 | 90.83 | 45.21 | 35.79 | 60.94 | 87.28 | 49.02 | 43.69 |
| 738.4977 4 | CL 74:7 CL 18:1_18:1_18:2_20:3 | 46.47 | 45.68 | 118.29 | 112.41 | 52.11 | 52.00 | 34.65 | 20.20 |
| 1478.016 36 | CL 74:7 CL 34:3_40:4 | 174.68 | 209.10 | 27.06 | 24.09 | 22.96 | 12.80 | 29.73 | 23.34 |
| 1477.999 39 | CL 74:7 CL 38:2_36:5 | 44.21 | 42.49 | 97.62 | 158.98 | 61.66 | 66.69 | 22.70 | 17.11 |
| 737.4905 4 | CL 74:8 CL 16:0_16:0_22:3_20:5 | 251.08 | 224.89 | 69.10 | 49.39 | 142.94 | 152.91 | 90.30 | 41.20 |
| 737.4864 5 | CL 74:8 CL 18:1_18:2_18:2_20:3 | 82.79 | 103.71 | 123.71 | 132.99 | 92.24 | 145.61 | 53.21 | 22.82 |
| 736.4815 7 | CL 74:9 CL 18:2_18:2_18:2_20:3 | 268.73 | 408.18 | 128.88 | 125.42 | 112.05 | 116.28 | 51.42 | 16.84 |
| 739.4505 | CL 75:13 CL 15:1_20:4_20:4_20:4 | 132.94 | 203.89 | 92.41 | 112.27 | 15.80 | 18.06 | 29.41 | 35.03 |
| 1498.054 93 | CL 75:4 CL 41:0_34:4 | 1555.10 | 2099.49 | 482.26 | 390.76 | 401.61 | 270.41 | 503.55 | 477.37 |
| 1490.041 75 | CL 75:8 CL 38:1_37:7 | 53.96 | 34.04 | 22.55 | 15.92 | 52.51 | 62.73 | 31.47 | 23.36 |
| 759.5670 2 | CL 76:0 CL 16:0_16:0_16:0_28:0 | 133.83 | 213.07 | 726.83 | 2008.32 | 131.09 | 98.68 | 136.53 | 106.54 |
| 749.4873 | CL 76:10 CL 18:2_18:2_20:3_20:3 | 62.07 | 94.31 | 22.87 | 21.55 | 38.30 | 82.94 | 11.00 | 0.57 |

| Average <i>m/z</i> | Metabolite name | CTR | | SCH | | NF | | PNF | |
|-----------------------|------------------------------------|-------------|------------|-------------|------------|-------------|-------------|-------------|------------|
| | | <i>mean</i> | <i>dev</i> | <i>mean</i> | <i>dev</i> | <i>mean</i> | <i>dev</i> | <i>mean</i> | <i>dev</i> |
| 756.5598 8 | CL 76:3 CL 18:0_18:0_18:0_22:3 | 1040.24 | 1753.45 | 272.36 | 178.59 | 1134.90 | 1383.4 6 | 1614.27 | 2344.36 |
| 756.5624 4 | CL 76:3 CL 28:0_16:1_16:1_16:1 | 820.02 | 922.62 | 847.94 | 1339.50 | 194.09 | 237.34 | 237.42 | 171.25 |
| 754.5349 7 | CL 76:5 CL 18:0_18:0_18:1_22:4 | 706.51 | 624.34 | 1559.71 | 3146.92 | 2225.02 | 2999.4 7 | 1381.73 | 2056.49 |
| 752.5211 2 | CL 76:7 CL 18:1_18:1_18:2_22:3 | 264.15 | 329.46 | 187.25 | 160.72 | 265.14 | 397.51 | 152.34 | 130.07 |
| 751.5057 4 | CL 76:8 CL 18:0_18:2_20:2_20:4 | 9.95 | 6.95 | 18.66 | 18.64 | 9.49 | 9.19 | 7.29 | 1.98 |
| 765.5722 7 | CL 77:1 CL 16:0_16:0_27:0_18:1 | 3161.55 | 2480.66 | 2249.42 | 1294.29 | 2997.04 | 1564.6 6 | 2092.47 | 1752.31 |
| 763.5514 5 | CL 77:3 CL 28:0_16:1_16:1_17:1 | 2677.90 | 3632.24 | 3880.16 | 9083.29 | 4155.97 | 8974.3 1 | 3115.55 | 3149.43 |
| 759.5372 3 | CL 77:7 CL 16:0_24:0_18:1_19:6 | 323.96 | 499.44 | 82.15 | 56.65 | 122.35 | 135.41 | 112.69 | 106.56 |
| 773.5851 4 | CL 78:0 CL 18:0_18:0_18:0_24:0 | 535.39 | 376.59 | 275.49 | 131.50 | 561.51 | 219.47 | 327.40 | 139.23 |
| 770.5742 8 | CL 78:3 CL 24:0_18:1_18:1_18:1 | 2011.67 | 2844.58 | 14155.44 | 30819.09 | 1245.18 | 1235.7 4 | 3439.89 | 4751.81 |
| 769.5467 5 | CL 78:4 CL 16:0_16:0_26:0_20:4 | 34.08 | 22.24 | 53.60 | 98.32 | 55.17 | 123.14 | 14.63 | 4.95 |
| 769.5551 8 | CL 78:4 CL 24:0_18:1_18:1_18:2 | 4497.48 | 5689.31 | 1086.73 | 664.58 | 2134.09 | 1711.5 4 | 1730.60 | 1143.13 |
| 768.5415 | CL 78:5 CL 24:0_18:1_18:2_18:2 | 1066.12 | 976.93 | 514.40 | 328.09 | 814.37 | 774.06 | 468.18 | 293.35 |
| 766.5309 4 | CL 78:7 CL 24:0_16:1_18:2_20:4 | 696.46 | 827.35 | 196.66 | 164.63 | 1655.14 | 4866.8 6 | 129.13 | 86.98 |
| 765.5382 1 | CL 78:8 CL 14:0_24:0_20:4_20:4 | 388.79 | 339.26 | 252.68 | 127.46 | 334.06 | 203.82 | 256.12 | 45.93 |
| 765.5255 1 | CL 78:8 CL 18:0_18:1_21:3_21:4 | 245.43 | 235.33 | 111.27 | 78.12 | 139.66 | 272.67 | 74.81 | 46.56 |
| 764.5210 6 | CL 78:9 CL 18:0_16:1_21:4_23:4 | 481.85 | 413.64 | 238.13 | 161.78 | 282.85 | 529.74 | 146.21 | 83.11 |
| 772.5393 7 | CL 79:8 CL 17:0_18:0_22:4_22:4 | 418.04 | 220.37 | 244.86 | 242.84 | 602.00 | 1210.5 8 | 102.92 | 46.63 |
| 777.5383 3 | CL 80:10 CL 16:0_24:0_20:5_20:5 | 67.21 | 61.86 | 73.23 | 60.63 | 42.95 | 53.86 | 52.65 | 38.15 |
| 784.5892 9 | CL 80:3 CL 26:0_18:1_18:1_18:1 | 40.31 | 51.63 | 291.60 | 642.00 | 29.60 | 25.59 | 57.06 | 74.05 |
| 782.5540 8 | CL 80:5 CL 26:0_18:1_18:2_18:2 | 66.49 | 60.59 | 141.43 | 242.65 | 58.69 | 56.44 | 59.61 | 53.75 |
| 781.5513 3 | CL 80:6 CL 26:0_18:2_18:2_18:2 | 105.03 | 107.41 | 416.93 | 783.32 | 160.40 | 181.44 | 206.01 | 213.66 |
| 779.5524 3 | CL 80:8 CL 18:0_18:0_22:4_22:4 | 399.53 | 338.71 | 378.39 | 480.79 | 241.69 | 205.76 | 166.94 | 53.18 |
| 782.5246 6 | CL 81:12 CL 15:1_22:3_22:4_22:4 | 147.16 | 126.10 | 65.32 | 47.47 | 304.72 | 270.45 | 104.22 | 31.89 |
| 801.6024 2 | CL 82:0 CL 18:0_18:0_18:0_28:0 | 3185.17 | 2100.43 | 7103.00 | 15978.67 | 2643.63 | 956.88 | 1889.58 | 749.60 |

| Average <i>m/z</i> | Metabolite name | CTR | | SCH | | NF | | PNF | |
|-----------------------|------------------------------------|-------------|------------|-------------|------------|-------------|-------------|-------------|------------|
| | | <i>mean</i> | <i>dev</i> | <i>mean</i> | <i>dev</i> | <i>mean</i> | <i>dev</i> | <i>mean</i> | <i>dev</i> |
| 784.4952 4 | CL 82:17 CL 16:2_22:5_22:5_22:5 | 149.60 | 72.77 | 85.93 | 68.57 | 278.42 | 222.95 | 136.74 | 113.53 |
| 799.6072 4 | CL 82:2 CL 18:0_18:0_28:0_18:2 | 174.32 | 225.52 | 2172.29 | 5092.30 | 163.83 | 152.29 | 296.27 | 381.69 |
| 797.5917 4 | CL 82:4 CL 18:0_18:0_26:0_20:4 | 4208.61 | 3706.03 | 2671.22 | 4946.50 | 4461.15 | 4000.7 3 | 1295.43 | 509.06 |
| 793.5440 1 | CL 82:8 CL 16:0_26:0_20:4_20:4 | 6982.97 | 7573.31 | 1771.64 | 1187.82 | 2138.78 | 2104.8 9 | 1413.27 | 538.18 |
| 793.5551 8 | CL 82:8 CL 18:0_24:0_20:4_20:4 | 4246.16 | 5850.74 | 2001.17 | 1275.63 | 2757.35 | 2104.4 7 | 1581.98 | 319.99 |
| 792.5505 4 | CL 82:9 CL 24:0_18:2_18:2_22:5 | 661.69 | 492.89 | 326.04 | 170.83 | 423.23 | 190.12 | 280.56 | 124.19 |
| 795.5360 7 | CL 83:13 CL 17:1_22:4_22:4_22:4 | 426.61 | 281.55 | 206.67 | 120.34 | 306.52 | 144.61 | 136.78 | 24.47 |
| 791.4849 2 | CL 83:17 CL 17:2_22:5_22:5_22:5 | 116.74 | 55.76 | 94.45 | 80.02 | 244.01 | 140.89 | 74.17 | 38.67 |
| 803.5386 4 | CL 84:12 CL 24:0_20:4_20:4_20:4 | 112.79 | 131.56 | 43.94 | 25.47 | 62.84 | 50.88 | 44.74 | 39.17 |
| 802.5477 9 | CL 84:13 CL 18:1_22:4_22:4_22:4 | 532.77 | 262.50 | 791.86 | 1540.71 | 738.58 | 989.82 | 387.92 | 274.08 |
| 800.5235 | CL 84:15 CL 18:0_22:3_22:6_22:6 | 3124.17 | 5367.33 | 428.38 | 215.76 | 977.33 | 923.14 | 464.39 | 271.05 |
| 807.5477 9 | CL 84:8 CL 28:0_18:2_18:2_20:4 | 662.43 | 867.91 | 1044.78 | 1997.37 | 925.08 | 1497.9 4 | 858.30 | 882.89 |
| 817.5641 5 | CL 86:12 CL 26:0_20:4_20:4_20:4 | 789.66 | 548.62 | 971.16 | 1006.26 | 1134.27 | 936.17 | 727.79 | 524.55 |
| 814.5487 1 | CL 86:15 CL 24:0_18:3_22:6_22:6 | 393.76 | 389.54 | 393.69 | 418.33 | 745.14 | 1541.4 6 | 247.89 | 94.33 |
| 814.5469 4 | CL 86:15 CL 26:0_20:5_20:5_20:5 | 122.28 | 67.65 | 1155.01 | 2533.66 | 247.93 | 294.25 | 92.18 | 42.11 |
| 821.6057 7 | CL 86:8 CL 18:0_24:0_22:4_22:4 | 222.26 | 148.93 | 159.20 | 98.52 | 330.97 | 264.42 | 171.88 | 59.69 |
| 820.5612 8 | CL 86:9 CL 28:0_18:1_20:4_20:4 | 521.50 | 366.95 | 283.01 | 174.53 | 3474.69 | 9050.4 2 | 634.60 | 411.26 |
| 822.5179 4 | CL 88:21 CL 22:5_22:5_22:5_22:6 | 252.88 | 197.30 | 93.76 | 155.18 | 64.82 | 48.27 | 71.26 | 69.65 |
| 821.4917 | CL 88:22 CL 22:5_22:5_22:6_22:6 | 1189.18 | 2290.07 | 28.09 | 21.29 | 22.37 | 17.04 | 10.40 | 4.07 |
| 835.5969 2 | CL 88:8 CL 18:0_26:0_20:4_24:4 | 114.56 | 135.36 | 89.11 | 106.60 | 235.98 | 145.36 | 175.98 | 75.01 |
| 846.5828 9 | CL 90:11 CL 18:0_28:0_22:5_22:6 | 172.17 | 158.76 | 330.59 | 698.33 | 91.51 | 94.95 | 62.69 | 25.56 |
| 850.6194 5 | CL 90:7 CL 24:0_24:0_22:3_20:4 | 196.06 | 271.39 | 85.78 | 88.75 | 203.80 | 520.84 | 62.42 | 62.40 |
| 884.7133 8 | CL 94:1 CL 26:0_26:0_26:0_16:1 | 1845.27 | 2427.93 | 1266.91 | 1522.26 | 2247.22 | 2976.1 9 | 3511.62 | 4192.30 |
| 227.2038 3 | FA 14:0 | 1449.82 | 986.82 | 1397.34 | 1762.56 | 1119.17 | 1753.4 0 | 562.09 | 123.08 |
| 243.1993 9 | FA 14:0;(2OH) | 23.72 | 20.36 | 114.19 | 256.39 | 29.22 | 31.21 | 12.43 | 4.78 |

| Average <i>m/z</i> | Metabolite name | CTR | | SCH | | NF | | PNF | |
|-----------------------|-----------------|---------------|---------------|---------------|---------------|--------------|--------------|--------------|--------------|
| | | <i>mean</i> | <i>dev</i> | <i>mean</i> | <i>dev</i> | <i>mean</i> | <i>dev</i> | <i>mean</i> | <i>dev</i> |
| 243.1971 7 | FA 14:0;O | 23.64 | 20.44 | 110.21 | 242.50 | 29.30 | 31.27 | 12.36 | 4.79 |
| 225.1859 1 | FA 14:1 | 148.31 | 206.70 | 76.13 | 168.39 | 63.44 | 124.94 | 38.06 | 60.32 |
| 257.1751 1 | FA 14:1;2O | 44.71 | 29.89 | 97.67 | 218.10 | 45.63 | 22.22 | 44.06 | 36.74 |
| 241.2168 4 | FA 15:0 | 274.09 | 217.99 | 191.89 | 165.27 | 797.32 | 2150.8 6 | 103.79 | 18.71 |
| 257.2130 7 | FA 15:0;(2OH) | 9.76 | 5.19 | 442.86 | 1307.84 | 5.23 | 4.39 | 3.90 | 1.97 |
| 239.2014 6 | FA 15:1 | 59.10 | 54.14 | 39.56 | 46.53 | 148.91 | 424.18 | 18.81 | 3.09 |
| 255.2336 6 | FA 16:0 | 98809.3 3 | 81237.26 | 87439.34 | 121522.8 1 | 66548.5 3 | 54669. 24 | 46934.5 6 | 15033.0 6 |
| 271.2244 6 | FA 16:0;(2OH) | 169.27 | 164.41 | 132.94 | 127.30 | 151.11 | 136.08 | 92.64 | 25.97 |
| 287.2248 5 | FA 16:0;2O | 49.40 | 50.20 | 159.70 | 332.87 | 30.02 | 23.95 | 32.88 | 25.40 |
| 271.2263 8 | FA 16:0;O | 346.06 | 274.95 | 1110.78 | 2013.24 | 2160.70 | 5593.5 9 | 472.82 | 181.71 |
| 253.2169 3 | FA 16:1 | 7993.12 | 9277.98 | 9133.61 | 14912.25 | 1840.57 | 1704.6 5 | 2017.82 | 2459.26 |
| 285.2076 7 | FA 16:1;2O | 779.31 | 806.96 | 205.83 | 92.76 | 233.58 | 348.50 | 282.86 | 84.99 |
| 269.2134 7 | FA 16:1;O | 381.50 | 342.14 | 451.44 | 996.24 | 189.64 | 159.89 | 154.16 | 58.25 |
| 251.2008 8 | FA 16:2 | 64.39 | 46.12 | 1571.58 | 4414.84 | 33.98 | 16.45 | 16.07 | 6.02 |
| 263.1678 8 | FA 16:4;(2OH) | 42.69 | 37.00 | 98.75 | 243.29 | 17.73 | 17.42 | 15.36 | 4.99 |
| 269.2488 7 | FA 17:0 | 398.86 | 448.88 | 504.19 | 754.53 | 617.84 | 1406.5 0 | 150.09 | 33.50 |
| 285.2430 1 | FA 17:0;(2OH) | 30.88 | 39.06 | 98.48 | 244.12 | 496.64 | 1520.1 2 | 20.37 | 6.29 |
| 267.2325 1 | FA 17:1 | 374.50 | 297.96 | 943.02 | 1775.63 | 378.05 | 848.67 | 102.57 | 26.72 |
| 265.2140 8 | FA 17:2 | 9.61 | 7.59 | 17.96 | 22.68 | 37.46 | 107.82 | 2.74 | 0.95 |
| 281.2113 | FA 17:2;O | 91.62 | 129.67 | 204.25 | 388.53 | 59.48 | 79.15 | 8.42 | 10.44 |
| 279.1951 9 | FA 17:3;O | 404.77 | 487.82 | 1039.52 | 2024.60 | 245.10 | 318.07 | 15.64 | 11.38 |
| 261.1872 3 | FA 17:4 | 6.03 | 6.70 | 22.24 | 65.04 | 2.34 | 2.66 | 1.97 | 1.05 |
| 277.1806 9 | FA 17:4;O | 20.61 | 24.26 | 8451.61 | 25034.18 | 9.79 | 15.25 | 14.89 | 7.08 |
| 283.2627 | FA 18:0 | 119945. 46 | 124985.5 0 | 100917.7 0 | 126684.5 9 | 74685.4 4 | 65882. 59 | 56912.3 0 | 18138.2 5 |
| 299.2571 1 | FA 18:0;(2OH) | 223.89 | 227.20 | 689.95 | 1599.18 | 1051.98 | 2838.8 9 | 182.77 | 33.82 |
| 315.2539 7 | FA 18:0;2O | 478.98 | 511.28 | 683.77 | 1180.53 | 285.28 | 334.69 | 286.55 | 219.35 |

| Average <i>m/z</i> | Metabolite name | CTR | | SCH | | NF | | PNF | |
|-----------------------|-----------------|---------------|---------------|---------------|---------------|--------------|--------------|--------------|--------------|
| | | <i>mean</i> | <i>dev</i> | <i>mean</i> | <i>dev</i> | <i>mean</i> | <i>dev</i> | <i>mean</i> | <i>dev</i> |
| 299.2577 5 | FA 18:0;O | 1090.26 | 1052.62 | 1490.79 | 3481.27 | 406.01 | 422.41 | 416.70 | 173.26 |
| 281.2484 1 | FA 18:1 | 220841. 33 | 198187.8 7 | 382603.0 0 | 730466.0 7 | 81322.7 9 | 61281. 78 | 44347.9 7 | 18758.2 8 |
| 297.2433 8 | FA 18:1;(2OH) | 212.68 | 180.29 | 317.53 | 674.62 | 156.82 | 195.10 | 101.23 | 20.16 |
| 313.2386 8 | FA 18:1;2O | 131.52 | 113.88 | 148.11 | 238.71 | 83.57 | 77.39 | 75.39 | 69.23 |
| 297.2434 7 | FA 18:1;O | 449.33 | 237.11 | 450.00 | 387.97 | 347.50 | 486.60 | 511.64 | 636.76 |
| 279.2324 2 | FA 18:2 | 59145.5 0 | 64852.65 | 59589.15 | 87988.06 | 29706.3 0 | 38608. 37 | 12651.0 3 | 7070.09 |
| 295.2294 | FA 18:2;(2OH) | 178.03 | 212.56 | 38.26 | 43.92 | 44.79 | 51.10 | 24.34 | 32.15 |
| 311.2250 1 | FA 18:2;2O | 120.71 | 70.67 | 91.26 | 81.12 | 156.63 | 90.86 | 228.72 | 208.24 |
| 295.2261 | FA 18:2;O | 562.06 | 593.59 | 627.99 | 967.46 | 3558.68 | 10707. 00 | 115.79 | 158.82 |
| 277.2174 4 | FA 18:3 | 943.29 | 868.57 | 1383.10 | 1939.17 | 506.20 | 333.56 | 202.53 | 160.95 |
| 341.1874 4 | FA 18:3;4O | 44.79 | 41.17 | 3820.71 | 11538.11 | 25.69 | 27.52 | 28.24 | 8.25 |
| 293.2103 6 | FA 18:3;O | 27.44 | 23.18 | 30.00 | 57.83 | 61.13 | 148.11 | 9.58 | 8.65 |
| 275.2112 4 | FA 18:4 | 42.03 | 63.07 | 242.84 | 696.87 | 6.24 | 10.90 | 5.53 | 2.22 |
| 273.1888 1 | FA 18:5 | 375.48 | 362.16 | 122.90 | 111.77 | 87.89 | 133.85 | 121.41 | 29.60 |
| 297.2804 9 | FA 19:0 | 88.78 | 102.86 | 84.97 | 109.55 | 161.91 | 325.52 | 42.74 | 13.67 |
| 295.2634 6 | FA 19:1 | 197.47 | 185.77 | 703.85 | 1562.80 | 169.89 | 325.27 | 57.10 | 28.99 |
| 293.2483 8 | FA 19:2 | 38.81 | 41.37 | 146.24 | 271.98 | 38.71 | 87.08 | 8.93 | 3.49 |
| 325.2359 | FA 19:2;2O | 318.88 | 335.42 | 352.94 | 571.50 | 159.86 | 193.78 | 71.24 | 37.50 |
| 291.2297 4 | FA 19:3 | 26.77 | 26.88 | 425.01 | 1226.92 | 57.44 | 148.47 | 7.64 | 5.31 |
| 307.2251 | FA 19:3;O | 41.54 | 49.10 | 88.43 | 160.97 | 28.09 | 42.15 | 2.14 | 1.65 |
| 289.2136 8 | FA 19:4 | 8.81 | 6.53 | 46.14 | 88.25 | 7.31 | 12.02 | 3.37 | 1.19 |
| 305.2097 2 | FA 19:4;O | 3.43 | 4.05 | 59.46 | 189.40 | 0.91 | 0.71 | 0.74 | 0.17 |
| 311.2942 8 | FA 20:0 | 1246.41 | 1265.21 | 1003.50 | 1218.97 | 1016.59 | 1682.3 9 | 637.17 | 180.92 |
| 309.2802 1 | FA 20:1 | 3608.07 | 3442.20 | 24654.13 | 56483.32 | 1237.12 | 1025.0 4 | 950.75 | 677.16 |
| 307.2626 | FA 20:2 | 3686.77 | 4475.36 | 15029.19 | 33901.86 | 1216.08 | 1065.5 0 | 1211.42 | 966.60 |
| 355.2455 4 | FA 20:2;3O | 46.26 | 66.20 | 43.21 | 78.87 | 67.20 | 184.28 | 4.53 | 2.23 |
| 323.2576 6 | FA 20:2;O | 30.79 | 30.52 | 60.19 | 83.52 | 98.39 | 244.06 | 4.50 | 3.62 |

| Average <i>m/z</i> | Metabolite name | CTR | | SCH | | NF | | PNF | |
|-----------------------|-----------------|---------------|----------------|----------------|----------------|---------------|--------------|--------------|--------------|
| | | <i>mean</i> | <i>dev</i> | <i>mean</i> | <i>dev</i> | <i>mean</i> | <i>dev</i> | <i>mean</i> | <i>dev</i> |
| 305.2494 8 | FA 20:3 | 37313.1 5 | 59042.91 | 55503.46 | 115255.9 1 | 5909.01 | 5412.0 0 | 3719.14 | 3199.90 |
| 337.2373 7 | FA 20:3;2O | 162.52 | 124.76 | 91.55 | 83.94 | 109.84 | 77.04 | 77.26 | 22.61 |
| 353.2227 8 | FA 20:3;3O | 209.94 | 289.06 | 1784.55 | 5753.67 | 64.72 | 118.27 | 64.76 | 46.83 |
| 369.2263 8 | FA 20:3;4O | 1555.47 | 2390.90 | 1034.72 | 1290.32 | 482.06 | 599.36 | 61.87 | 26.25 |
| 321.2406 9 | FA 20:3;O | 202.66 | 323.90 | 115.88 | 201.33 | 506.59 | 1408.6 2 | 7.13 | 6.82 |
| 303.2316 9 | FA 20:4 | 791140. 07 | 1180482. 19 | 1010215. 82 | 1980468. 52 | 132260. 21 | 96783. 12 | 84969.7 8 | 52870.3 8 |
| 319.2259 5 | FA 20:4;(2OH) | 38.03 | 60.56 | 57.78 | 96.61 | 27.20 | 66.37 | 3.57 | 0.42 |
| 335.2220 2 | FA 20:4;2O | 234.85 | 349.79 | 113.73 | 242.67 | 104.64 | 225.35 | 11.06 | 5.41 |
| 351.215 | FA 20:4;3O | 408.39 | 469.30 | 401.06 | 423.22 | 926.72 | 2527.3 9 | 26.82 | 19.41 |
| 319.2270 5 | FA 20:4;O | 3898.16 | 6068.66 | 958.81 | 1666.45 | 4749.45 | 10336. 35 | 95.91 | 128.30 |
| 301.2168 | FA 20:5 | 4306.48 | 5795.44 | 8428.03 | 13726.01 | 2111.90 | 3653.7 3 | 1003.78 | 1135.89 |
| 317.2097 2 | FA 20:5;(2OH) | 63.82 | 95.40 | 40.98 | 81.94 | 99.98 | 174.09 | 3.76 | 3.60 |
| 333.2038 | FA 20:5;2O | 115.42 | 99.11 | 132.99 | 136.36 | 318.35 | 734.57 | 14.50 | 8.51 |
| 349.2015 1 | FA 20:5;3O | 110.62 | 169.01 | 105.19 | 267.26 | 38.07 | 62.91 | 9.31 | 5.22 |
| 317.2117 3 | FA 20:5;O | 79.93 | 100.01 | 114.46 | 153.16 | 28.08 | 31.25 | 4.65 | 4.55 |
| 325.3082 6 | FA 21:0 | 191.54 | 212.70 | 363.21 | 762.34 | 340.05 | 766.09 | 124.40 | 124.71 |
| 341.3017 9 | FA 21:0;(2OH) | 1.23 | 1.29 | 2.16 | 4.89 | 39.31 | 119.56 | 0.75 | 0.26 |
| 341.3036 5 | FA 21:0;O | 166.52 | 126.45 | 168.77 | 466.71 | 82.18 | 191.32 | 67.59 | 117.13 |
| 323.2914 7 | FA 21:1 | 10.09 | 8.14 | 67.66 | 146.68 | 13.94 | 32.40 | 4.62 | 2.74 |
| 321.2774 | FA 21:2 | 4.94 | 4.65 | 41.56 | 91.18 | 8.26 | 20.32 | 1.57 | 0.85 |
| 319.2618 1 | FA 21:3 | 26.57 | 24.16 | 457.30 | 1283.26 | 18.07 | 37.65 | 5.34 | 2.39 |
| 317.2467 | FA 21:4 | 9.40 | 8.82 | 378.22 | 887.34 | 3.56 | 5.00 | 2.46 | 1.35 |
| 315.2451 5 | FA 21:5 | 49.59 | 69.45 | 318.16 | 921.81 | 10.64 | 15.67 | 9.47 | 2.65 |
| 339.3228 8 | FA 22:0 | 2775.33 | 2502.18 | 1571.29 | 2022.92 | 4555.66 | 11719. 99 | 1076.55 | 304.61 |
| 403.3054 8 | FA 22:0;4O | 165.81 | 196.84 | 686.82 | 1509.73 | 120.89 | 89.40 | 43.19 | 5.13 |
| 337.3085 3 | FA 22:1 | 415.12 | 463.00 | 1639.20 | 3590.98 | 251.44 | 318.69 | 145.85 | 113.84 |
| 335.2931 8 | FA 22:2 | 231.48 | 201.31 | 1261.64 | 2588.94 | 110.27 | 129.38 | 86.49 | 56.13 |

| Average <i>m/z</i> | Metabolite name | CTR | | SCH | | NF | | PNF | |
|-----------------------|-----------------|---------------|---------------|---------------|---------------|--------------|--------------|--------------|--------------|
| | | <i>mean</i> | <i>dev</i> | <i>mean</i> | <i>dev</i> | <i>mean</i> | <i>dev</i> | <i>mean</i> | <i>dev</i> |
| 333.2770 1 | FA 22:3 | 586.48 | 551.54 | 5100.40 | 13317.30 | 163.08 | 204.08 | 75.75 | 32.16 |
| 365.2690 4 | FA 22:3;2O | 24.48 | 7.36 | 20.62 | 25.28 | 63.06 | 39.37 | 77.59 | 73.66 |
| 381.2610 5 | FA 22:3;3O | 14.92 | 12.65 | 58.62 | 89.94 | 26.57 | 57.21 | 2.54 | 1.75 |
| 349.2714 2 | FA 22:3;O | 21.19 | 23.00 | 87.32 | 223.60 | 8.78 | 13.51 | 7.53 | 2.13 |
| 331.2637 3 | FA 22:4 | 46646.2 5 | 63984.10 | 114747.3 0 | 250912.2 3 | 6303.99 | 5703.7 2 | 3782.98 | 2338.08 |
| 347.2572 3 | FA 22:4;O | 67.14 | 90.10 | 45.48 | 58.33 | 70.72 | 104.81 | 4.83 | 6.39 |
| 329.2481 7 | FA 22:5 | 26227.5 9 | 37314.44 | 63357.40 | 130178.5 9 | 2464.54 | 2308.9 1 | 1778.83 | 881.98 |
| 409.2249 5 | FA 22:5;4O | 685.98 | 1093.20 | 240.37 | 287.78 | 258.71 | 386.82 | 137.29 | 70.63 |
| 345.2405 4 | FA 22:5;O | 110.03 | 160.00 | 63.82 | 103.80 | 97.20 | 210.38 | 5.44 | 5.80 |
| 327.2315 7 | FA 22:6 | 161453. 26 | 240087.6 9 | 366129.5 4 | 929409.6 0 | 19579.0 6 | 12346. 85 | 15860.5 8 | 13711.8 1 |
| 343.2248 5 | FA 22:6;(2OH) | 344.21 | 526.06 | 141.39 | 275.99 | 390.05 | 853.75 | 13.27 | 10.74 |
| 391.2046 8 | FA 22:6;4O | 1752.18 | 1012.02 | 849.84 | 545.72 | 1444.55 | 754.16 | 861.08 | 266.20 |
| 353.3383 8 | FA 23:0 | 155.85 | 113.18 | 109.96 | 140.13 | 1176.14 | 3160.6 4 | 92.76 | 35.43 |
| 369.3329 5 | FA 23:0;(2OH) | 6.66 | 6.72 | 23.78 | 36.14 | 338.17 | 1048.5 4 | 6.68 | 4.00 |
| 351.3248 9 | FA 23:1 | 48.17 | 42.30 | 1137.70 | 2798.75 | 52.14 | 96.76 | 45.73 | 52.81 |
| 367.3534 5 | FA 24:0 | 876.23 | 582.76 | 696.76 | 749.17 | 9695.80 | 28626. 30 | 556.01 | 186.06 |
| 383.3482 1 | FA 24:0;(2OH) | 156.55 | 158.93 | 301.13 | 356.24 | 15470.3 9 | 48350. 88 | 156.45 | 84.14 |
| 365.3392 3 | FA 24:1 | 1718.19 | 1674.13 | 4483.43 | 8215.95 | 1359.44 | 1889.0 2 | 639.80 | 353.02 |
| 381.3348 7 | FA 24:1;O | 3.88 | 2.91 | 36.47 | 88.27 | 3.29 | 1.55 | 1.91 | 0.50 |
| 363.3251 3 | FA 24:2 | 71.58 | 88.92 | 312.03 | 563.73 | 52.44 | 62.32 | 32.93 | 23.33 |
| 361.3109 7 | FA 24:3 | 90.53 | 112.13 | 737.59 | 1814.85 | 16.42 | 17.09 | 8.96 | 5.45 |
| 359.293 | FA 24:4 | 1131.41 | 1168.17 | 4340.11 | 10212.57 | 621.95 | 594.37 | 391.07 | 293.76 |
| 357.2774 | FA 24:5 | 575.74 | 621.71 | 2608.48 | 5282.93 | 153.62 | 123.75 | 126.13 | 96.33 |
| 355.2615 7 | FA 24:6 | 485.04 | 630.60 | 1746.68 | 4443.59 | 128.31 | 87.09 | 143.09 | 159.03 |
| 381.3687 7 | FA 25:0 | 97.30 | 62.21 | 56.39 | 37.19 | 2755.69 | 8371.7 0 | 97.93 | 92.23 |
| 397.3654 2 | FA 25:0;O | 28.06 | 21.97 | 32.03 | 36.02 | 2820.47 | 8809.0 0 | 22.97 | 3.98 |

| Average <i>m/z</i> | Metabolite name | CTR | | SCH | | NF | | PNF | |
|-----------------------|-----------------|--------------|---------------|---------------|---------------|--------------|--------------|--------------|------------|
| | | <i>mean</i> | <i>dev</i> | <i>mean</i> | <i>dev</i> | <i>mean</i> | <i>dev</i> | <i>mean</i> | <i>dev</i> |
| 379.3537 9 | FA 25:1 | 14.96 | 10.41 | 53.46 | 89.66 | 33.65 | 79.08 | 11.16 | 3.34 |
| 395.3859 9 | FA 26:0 | 1088.20 | 810.22 | 690.38 | 387.88 | 11860.4 8 | 35718. 63 | 637.05 | 168.70 |
| 411.3793 3 | FA 26:0;(2OH) | 10.06 | 4.18 | 16.03 | 21.61 | 3653.02 | 11447. 86 | 14.47 | 10.03 |
| 411.3821 1 | FA 26:0;O | 32.29 | 24.22 | 62.30 | 49.48 | 74.99 | 40.02 | 92.32 | 50.70 |
| 393.3693 8 | FA 26:1 | 109.68 | 77.29 | 404.01 | 641.69 | 165.02 | 316.63 | 65.52 | 53.79 |
| 409.3620 3 | FA 26:1;(2OH) | 7.54 | 6.12 | 18.00 | 22.07 | 399.66 | 1247.3 9 | 5.54 | 2.60 |
| 391.3516 5 | FA 26:2 | 39.45 | 35.47 | 188.23 | 274.97 | 31.82 | 36.77 | 24.17 | 22.26 |
| 389.3391 7 | FA 26:3 | 87.10 | 102.09 | 662.99 | 1311.55 | 32.49 | 38.89 | 21.05 | 11.74 |
| 387.3237 9 | FA 26:4 | 113.76 | 127.70 | 415.20 | 808.71 | 73.88 | 73.97 | 45.30 | 33.05 |
| 385.3092 3 | FA 26:5 | 210.05 | 197.56 | 521.16 | 712.40 | 69.88 | 59.36 | 56.78 | 45.33 |
| 383.2916 | FA 26:6 | 63.62 | 82.25 | 163.24 | 304.90 | 25.73 | 21.59 | 28.75 | 31.53 |
| 381.2788 7 | FA 26:7 | 7698.02 | 6501.54 | 317.70 | 326.03 | 817.06 | 1006.0 7 | 838.85 | 1270.11 |
| 397.2716 7 | FA 26:7;O | 287.41 | 201.04 | 27.52 | 42.30 | 41.71 | 57.14 | 147.39 | 292.01 |
| 409.3973 7 | FA 27:0 | 174.18 | 200.46 | 50.85 | 21.52 | 2688.23 | 8272.0 0 | 63.64 | 59.54 |
| 425.3919 1 | FA 27:0;(2OH) | 1.33 | 1.18 | 2.20 | 2.97 | 358.11 | 1117.7 3 | 2.11 | 1.93 |
| 423.4160 2 | FA 28:0 | 63.87 | 35.47 | 110.42 | 277.29 | 148.14 | 168.02 | 44.90 | 37.14 |
| 439.4103 7 | FA 28:0;O | 18.49 | 20.59 | 44.13 | 108.19 | 310.26 | 951.36 | 17.41 | 4.98 |
| 421.3991 7 | FA 28:1 | 16.65 | 10.49 | 49.74 | 53.80 | 137.78 | 404.87 | 9.96 | 3.93 |
| 415.3564 1 | FA 28:4 | 10.44 | 10.24 | 59.52 | 84.62 | 11.00 | 14.31 | 7.24 | 4.54 |
| 413.3402 1 | FA 28:5 | 27.79 | 27.29 | 65.95 | 70.68 | 14.78 | 21.79 | 12.72 | 10.34 |
| 427.3177 8 | FA 28:6;O | 15.15 | 15.12 | 45.46 | 99.94 | 33.34 | 64.62 | 6.97 | 3.11 |
| 409.3081 4 | FA 28:7 | 87280.6 8 | 120224.0 8 | 201512.7 8 | 543645.5 2 | 22270.4 6 | 37453. 15 | 12810.2 7 | 3694.72 |
| 425.3012 4 | FA 28:7;O | 373.30 | 331.48 | 5271.66 | 15346.77 | 143.68 | 221.11 | 176.14 | 83.61 |
| 437.4299 | FA 29:0 | 24.61 | 18.99 | 11.72 | 6.73 | 532.04 | 1606.2 2 | 15.09 | 6.78 |
| 435.4127 2 | FA 29:1 | 10.68 | 12.92 | 7.15 | 8.45 | 43.03 | 126.03 | 5.02 | 4.45 |
| 451.4442 7 | FA 30:0 | 836.80 | 704.81 | 488.58 | 305.70 | 1590.80 | 3646.9 3 | 550.42 | 284.88 |

| Average <i>m/z</i> | Metabolite name | CTR | | SCH | | NF | | PNF | |
|-----------------------|-----------------|-------------|------------|-------------|------------|-------------|------------|-------------|------------|
| | | <i>mean</i> | <i>dev</i> | <i>mean</i> | <i>dev</i> | <i>mean</i> | <i>dev</i> | <i>mean</i> | <i>dev</i> |
| 435.3182 7 | FA 30:8 | 116.23 | 178.11 | 503.26 | 1446.51 | 12.26 | 18.29 | 16.13 | 10.77 |
| 465.4607 8 | FA 31:0 | 157.55 | 137.19 | 103.38 | 176.00 | 192.60 | 159.15 | 81.02 | 47.66 |
| 463.4485 8 | FA 31:1 | 21.70 | 32.26 | 23.62 | 60.47 | 4.10 | 4.61 | 5.87 | 3.27 |
| 479.4810 8 | FA 32:0 | 709.70 | 672.95 | 525.93 | 419.69 | 536.58 | 541.06 | 485.57 | 238.02 |
| 471.4288 6 | FA 32:4 | 2.30 | 1.66 | 14.56 | 40.00 | 1.24 | 1.62 | 2.08 | 0.80 |
| 469.4108 6 | FA 32:5 | 6.45 | 5.41 | 29.35 | 82.59 | 2.10 | 3.42 | 2.36 | 0.53 |
| 463.3676 5 | FA 32:8 | 6.12 | 4.69 | 7.09 | 9.23 | 90.90 | 272.74 | 6.21 | 7.69 |
| 493.4906 6 | FA 33:0 | 148.33 | 119.95 | 93.77 | 157.09 | 138.65 | 105.31 | 65.41 | 26.32 |
| 507.5110 8 | FA 34:0 | 475.90 | 333.14 | 487.59 | 245.36 | 412.97 | 245.62 | 464.94 | 47.34 |
| 505.4894 1 | FA 34:1 | 14.25 | 10.10 | 25.07 | 39.16 | 285.62 | 850.29 | 12.95 | 4.27 |
| 521.5224 | FA 35:0 | 21.95 | 15.61 | 57.13 | 87.05 | 16.95 | 16.79 | 26.13 | 7.57 |
| 519.5102 5 | FA 35:1 | 4.35 | 4.63 | 24.79 | 59.52 | 18.42 | 49.62 | 3.65 | 1.26 |
| 535.5357 1 | FA 36:0 | 318.81 | 282.88 | 261.94 | 177.66 | 197.00 | 108.02 | 191.39 | 74.57 |
| 533.5233 8 | FA 36:1 | 10.05 | 6.51 | 27.09 | 41.69 | 198.50 | 592.85 | 13.39 | 4.43 |
| 531.5086 7 | FA 36:2 | 3.93 | 3.30 | 19.76 | 44.33 | 59.94 | 179.50 | 3.56 | 0.20 |
| 527.4878 5 | FA 36:4 | 8.81 | 7.94 | 42.06 | 109.82 | 7.63 | 11.29 | 9.25 | 1.45 |
| 525.4708 3 | FA 36:5 | 16.57 | 13.69 | 98.90 | 272.13 | 6.11 | 8.63 | 9.01 | 2.62 |
| 521.4283 4 | FA 36:7 | 31.34 | 49.75 | 46.77 | 120.67 | 4.82 | 5.11 | 3.55 | 2.52 |
| 519.4318 2 | FA 36:8 | 28.53 | 28.40 | 14.13 | 11.97 | 42.51 | 99.05 | 41.70 | 63.47 |
| 549.5519 4 | FA 37:0 | 145.45 | 143.88 | 117.91 | 227.44 | 197.43 | 175.34 | 79.56 | 43.65 |
| 563.5658 6 | FA 38:0 | 165.30 | 148.48 | 134.51 | 123.18 | 108.60 | 67.02 | 88.42 | 45.11 |
| 561.5535 9 | FA 38:1 | 7.92 | 5.09 | 22.65 | 41.69 | 68.54 | 200.61 | 6.18 | 3.43 |
| 543.4305 4 | FA 38:10 | 5.86 | 4.43 | 41.79 | 120.37 | 7.43 | 6.77 | 2.66 | 1.97 |
| 555.5173 3 | FA 38:4 | 2.86 | 2.30 | 23.66 | 63.46 | 1.34 | 1.70 | 2.34 | 1.54 |
| 553.4866 3 | FA 38:5 | 73.49 | 91.21 | 99.44 | 234.07 | 47.33 | 30.66 | 23.76 | 5.87 |
| 547.4613 | FA 38:8 | 33.19 | 36.78 | 17.79 | 20.57 | 23.64 | 29.69 | 38.26 | 55.21 |

| Average <i>m/z</i> | Metabolite name | CTR | | SCH | | NF | | PNF | |
|-----------------------|-----------------|-------------|------------|-------------|------------|-------------|-------------|-------------|------------|
| | | <i>mean</i> | <i>dev</i> | <i>mean</i> | <i>dev</i> | <i>mean</i> | <i>dev</i> | <i>mean</i> | <i>dev</i> |
| 577.5831 3 | FA 39:0 | 94.36 | 96.80 | 103.58 | 200.34 | 105.09 | 80.40 | 52.38 | 21.30 |
| 591.5986 9 | FA 40:0 | 104.69 | 103.84 | 131.88 | 272.24 | 137.67 | 115.31 | 62.33 | 32.57 |
| 589.5858 2 | FA 40:1 | 2.80 | 2.86 | 25.27 | 65.38 | 1.31 | 2.02 | 1.59 | 0.64 |
| 571.4664 3 | FA 40:10 | 241.22 | 175.62 | 238.10 | 322.90 | 391.93 | 262.02 | 112.27 | 42.34 |
| 569.4490 4 | FA 40:11 | 58.45 | 39.09 | 125.64 | 143.08 | 99.98 | 53.02 | 65.86 | 28.06 |
| 575.4923 7 | FA 40:8 | 29.31 | 30.10 | 9.72 | 14.75 | 20.29 | 36.24 | 17.55 | 25.52 |
| 619.6315 3 | FA 42:0 | 85.78 | 85.42 | 122.60 | 235.68 | 88.56 | 60.49 | 58.56 | 31.52 |
| 599.4935 9 | FA 42:10 | 849.86 | 431.68 | 2178.78 | 4096.90 | 1729.09 | 1287.5 6 | 632.76 | 220.25 |
| 597.4816 3 | FA 42:11 | 183.69 | 106.97 | 282.78 | 446.38 | 248.49 | 82.69 | 94.49 | 46.56 |
| 609.5626 2 | FA 42:5 | 8.22 | 7.93 | 47.42 | 132.16 | 3.80 | 2.80 | 3.40 | 1.15 |
| 601.5088 5 | FA 42:9 | 1112.44 | 694.56 | 2891.95 | 4877.67 | 4096.42 | 4787.1 1 | 3730.54 | 2149.35 |
| 633.6458 1 | FA 43:0 | 105.03 | 94.53 | 138.35 | 266.96 | 122.24 | 83.00 | 66.56 | 42.38 |
| 647.6630 9 | FA 44:0 | 21.47 | 13.80 | 22.85 | 18.85 | 22.29 | 18.08 | 15.03 | 3.00 |
| 627.5236 8 | FA 44:10 | 3246.79 | 1073.35 | 5174.13 | 5046.87 | 5158.56 | 2869.0 1 | 2004.12 | 1139.37 |
| 625.5127 | FA 44:11 | 1548.15 | 904.15 | 7643.16 | 14641.58 | 1620.28 | 1611.5 5 | 841.03 | 532.96 |
| 623.4813 2 | FA 44:12 | 46.97 | 50.25 | 37.74 | 36.46 | 18.86 | 14.76 | 9.07 | 3.82 |
| 631.5397 3 | FA 44:8 | 40.45 | 63.26 | 14.19 | 20.49 | 23.90 | 14.67 | 9.95 | 10.74 |
| 629.5421 1 | FA 44:9 | 65.75 | 50.59 | 258.24 | 355.75 | 518.64 | 597.70 | 96.76 | 58.73 |
| 1123.677 49 | GM3 32:1;2O | 37.28 | 50.53 | 13.67 | 10.52 | 18.97 | 10.76 | 14.77 | 5.31 |
| 1153.706 05 | GM3 34:0;2O | 47.22 | 52.14 | 22.15 | 23.38 | 16.85 | 12.26 | 19.40 | 13.77 |
| 1177.719 73 | GM3 36:2;2O | 22.37 | 25.98 | 24.43 | 29.14 | 11.37 | 9.18 | 5.99 | 1.09 |
| 1235.795 29 | GM3 40:1;2O | 200.06 | 187.50 | 114.20 | 72.88 | 398.12 | 618.61 | 246.05 | 337.98 |
| 1249.797 97 | GM3 41:1;2O | 33.08 | 18.99 | 67.00 | 61.92 | 67.29 | 83.55 | 31.45 | 21.93 |
| 1263.824 71 | GM3 42:1;2O | 534.96 | 554.19 | 238.93 | 135.65 | 411.95 | 362.57 | 297.99 | 359.16 |
| 381.1953 1 | LPA 14:0 | 145.30 | 235.04 | 39.94 | 43.98 | 40.73 | 56.44 | 22.19 | 10.91 |

| Average <i>m/z</i> | Metabolite name | CTR | | SCH | | NF | | PNF | |
|-----------------------|-----------------|-------------|------------|-------------|------------|-------------|-------------|-------------|------------|
| | | <i>mean</i> | <i>dev</i> | <i>mean</i> | <i>dev</i> | <i>mean</i> | <i>dev</i> | <i>mean</i> | <i>dev</i> |
| 395.2250 4 | LPA 15:0 | 121.57 | 86.58 | 100.84 | 127.70 | 64.09 | 38.97 | 37.08 | 13.33 |
| 423.2429 2 | LPA 17:0 | 56.99 | 89.62 | 12.86 | 8.32 | 24.27 | 36.91 | 12.23 | 4.73 |
| 435.2492 7 | LPA 18:1 | 14.68 | 13.88 | 67.46 | 108.71 | 8.36 | 17.67 | 3.76 | 1.48 |
| 451.2760 9 | LPA 19:0 | 1.80 | 1.01 | 336.65 | 803.65 | 1.39 | 1.20 | 0.98 | 0.55 |
| 485.2637 3 | LPA 22:4 | 298.15 | 214.51 | 312.63 | 567.81 | 177.09 | 79.21 | 132.18 | 82.02 |
| 543.3375 9 | LPA 26:3 | 3.81 | 2.76 | 43.14 | 108.83 | 4.72 | 3.53 | 2.33 | 0.87 |
| 537.2940 7 | LPA 26:6 | 38.22 | 49.67 | 72.02 | 149.83 | 8.94 | 8.92 | 12.56 | 17.02 |
| 483.2703 6 | LPG 16:0 | 934.87 | 1612.42 | 44.37 | 35.34 | 43.84 | 52.09 | 36.36 | 13.78 |
| 511.3039 9 | LPG 18:0 | 1345.40 | 2449.57 | 43.52 | 37.46 | 55.05 | 77.14 | 30.10 | 12.56 |
| 509.2860 7 | LPG 18:1 | 486.67 | 431.64 | 615.78 | 896.95 | 422.70 | 410.73 | 353.59 | 140.39 |
| 507.2702 3 | LPG 18:2 | 554.67 | 823.45 | 441.14 | 509.67 | 197.93 | 224.71 | 163.48 | 98.19 |
| 537.3161 6 | LPG 20:1 | 32.40 | 33.63 | 25.19 | 26.56 | 29.59 | 48.91 | 13.24 | 14.95 |
| 535.3147 6 | LPG 20:2 | 11.88 | 13.07 | 34.14 | 65.07 | 7.52 | 5.58 | 6.91 | 4.17 |
| 531.2697 1 | LPG 20:4 | 219.11 | 248.83 | 141.32 | 161.52 | 88.85 | 66.91 | 67.11 | 33.77 |
| 559.3002 3 | LPG 22:4 | 47.38 | 34.34 | 54.07 | 59.58 | 29.90 | 23.85 | 19.05 | 6.19 |
| 557.2875 4 | LPG 22:5 | 182.27 | 123.56 | 191.67 | 235.71 | 101.36 | 94.40 | 97.11 | 57.39 |
| 555.2671 5 | LPG 22:6 | 600.37 | 837.60 | 337.21 | 356.16 | 291.17 | 181.60 | 286.33 | 212.61 |
| 441.2496 3 | LPG O-14:0 | 159.36 | 105.46 | 95.88 | 86.74 | 121.25 | 61.80 | 82.57 | 39.47 |
| 479.2787 5 | LPG O-17:2 | 19.24 | 8.83 | 25.75 | 24.28 | 21.46 | 8.43 | 16.61 | 5.76 |
| 495.3090 5 | LPG O-18:1 | 31.04 | 40.64 | 1141.58 | 3150.58 | 9.56 | 12.03 | 6.05 | 2.99 |
| 521.3301 4 | LPG O-20:2 | 9.32 | 9.05 | 86.98 | 220.75 | 2.56 | 2.42 | 2.34 | 0.53 |
| 533.3328 2 | LPG O-21:3 | 12.15 | 10.94 | 117.18 | 303.43 | 4.23 | 3.29 | 4.59 | 2.78 |
| 595.3425 9 | LPG O-26:7 | 3.45 | 2.10 | 30.73 | 95.27 | 3.09 | 3.83 | 2.09 | 0.89 |
| 599.3147 6 | LPI 18:0 | 468.59 | 470.84 | 96.10 | 66.88 | 493.61 | 1202.3 6 | 55.38 | 29.61 |
| 597.3023 7 | LPI 18:1 | 144.83 | 197.00 | 28.66 | 28.92 | 60.88 | 104.87 | 13.53 | 8.46 |

| Average <i>m/z</i> | Metabolite name | CTR | | SCH | | NF | | PNF | |
|-----------------------|----------------------|--------------|------------|-------------|------------|--------------|--------------|--------------|--------------|
| | | <i>mean</i> | <i>dev</i> | <i>mean</i> | <i>dev</i> | <i>mean</i> | <i>dev</i> | <i>mean</i> | <i>dev</i> |
| 595.2825 3 | LPI 18:2 | 33.47 | 29.38 | 22.00 | 25.22 | 16.90 | 21.84 | 7.85 | 2.53 |
| 621.2991 3 | LPI 20:3 | 13.92 | 11.76 | 19.66 | 27.88 | 9.12 | 10.18 | 4.07 | 1.58 |
| 619.2838 1 | LPI 20:4 | 347.01 | 517.82 | 218.89 | 475.80 | 60.64 | 57.56 | 32.68 | 21.03 |
| 496.2645 9 | LPS 16:0 | 32.32 | 43.42 | 6.31 | 11.53 | 3.48 | 5.50 | 1.27 | 0.75 |
| 524.2981 | LPS 18:0 | 540.86 | 632.24 | 22.73 | 30.96 | 64.02 | 164.20 | 7.88 | 6.39 |
| 522.2840 6 | LPS 18:1 | 684.79 | 1178.06 | 178.87 | 319.70 | 97.76 | 257.71 | 11.00 | 9.56 |
| 520.2683 7 | LPS 18:2 | 21.08 | 24.00 | 16.08 | 23.31 | 7.56 | 11.74 | 2.23 | 1.82 |
| 536.3134 2 | LPS 19:1 | 13.05 | 17.65 | 153.16 | 463.64 | 4.86 | 3.87 | 12.06 | 12.01 |
| 546.2825 3 | LPS 20:3 | 32.27 | 37.43 | 59.06 | 102.53 | 5.30 | 5.80 | 2.08 | 1.15 |
| 544.2646 5 | LPS 20:4 | 69.52 | 95.52 | 26.08 | 33.54 | 11.60 | 21.43 | 2.69 | 1.35 |
| 572.2983 4 | LPS 22:4 | 43.94 | 66.87 | 33.51 | 58.04 | 4.37 | 3.51 | 2.43 | 0.99 |
| 570.2825 9 | LPS 22:5 | 73.35 | 110.67 | 21.89 | 17.55 | 11.62 | 10.11 | 9.42 | 7.48 |
| 568.2677 | LPS 22:6 | 91.50 | 144.10 | 41.73 | 58.52 | 12.88 | 19.33 | 2.98 | 1.14 |
| 721.5032 3 | PG 32:0 PG 16:0_16:0 | 4488.20 | 7892.24 | 508.94 | 352.46 | 869.74 | 1032.0 9 | 566.34 | 259.57 |
| 719.4782 7 | PG 32:1 PG 16:0_16:1 | 707.29 | 910.42 | 569.28 | 448.94 | 357.46 | 634.93 | 361.78 | 197.55 |
| 747.5087 9 | PG 34:1 PG 16:0_18:1 | 12117.3 7 | 14594.41 | 6984.09 | 5086.92 | 7053.54 | 6109.5 9 | 4571.80 | 2426.02 |
| 745.5026 9 | PG 34:2 PG 16:0_18:2 | 545.27 | 680.23 | 289.84 | 240.98 | 293.34 | 319.25 | 177.37 | 50.25 |
| 745.4940 8 | PG 34:2 PG 16:1_18:1 | 474.00 | 420.42 | 1176.92 | 1002.16 | 317.12 | 351.52 | 493.41 | 388.26 |
| 743.4826 | PG 34:3 PG 16:1_18:2 | 47.86 | 37.85 | 61.58 | 46.74 | 48.03 | 42.43 | 47.57 | 14.04 |
| 759.5277 7 | PG 35:2 PG 17:1_18:1 | 548.51 | 452.67 | 2558.64 | 3862.74 | 358.58 | 428.36 | 355.98 | 350.77 |
| 757.4912 1 | PG 35:3 PG 17:1_18:2 | 4.68 | 3.61 | 10.98 | 17.05 | 8.52 | 20.16 | 4.23 | 3.73 |
| 777.5551 1 | PG 36:0 PG 18:0_18:0 | 11574.5 3 | 11025.33 | 4089.04 | 2168.21 | 5100.82 | 2355.8 8 | 3285.47 | 1602.92 |
| 775.5470 6 | PG 36:1 PG 18:0_18:1 | 9452.38 | 11180.37 | 3075.03 | 1542.83 | 4293.68 | 3459.9 1 | 2508.44 | 735.89 |
| 773.5225 2 | PG 36:2 PG 18:1_18:1 | 18097.2 7 | 15599.71 | 23063.83 | 28370.36 | 15091.8 7 | 23392. 87 | 13261.0 1 | 12974.5 3 |
| 771.5197 1 | PG 36:3 PG 18:1_18:2 | 14531.0 5 | 12185.34 | 28285.94 | 33002.10 | 13515.1 1 | 14906. 75 | 13184.3 9 | 8724.19 |
| 769.4988 4 | PG 36:4 PG 16:0_20:4 | 868.45 | 1189.40 | 347.90 | 253.27 | 214.87 | 102.71 | 199.70 | 66.89 |
| 769.4988 4 | PG 36:4 PG 18:2_18:2 | 1079.34 | 1235.38 | 831.28 | 927.84 | 735.29 | 1072.3 2 | 455.69 | 266.33 |

| Average <i>m/z</i> | Metabolite name | CTR | | SCH | | NF | | PNF | |
|-----------------------|----------------------------|-------------|------------|-------------|------------|-------------|------------|-------------|------------|
| | | <i>mean</i> | <i>dev</i> | <i>mean</i> | <i>dev</i> | <i>mean</i> | <i>dev</i> | <i>mean</i> | <i>dev</i> |
| 815.4720 5 | PG 36:5;3O PG 18:3_18:2;3O | 32.78 | 57.53 | 29.39 | 64.70 | 12.44 | 17.74 | 7.28 | 4.19 |
| 767.4751 | PG 36:5 PG 16:1_20:4 | 8.92 | 6.36 | 15.51 | 13.29 | 6.39 | 4.61 | 8.23 | 2.26 |
| 767.4751 6 | PG 36:5 PG 18:2_18:3 | 7.97 | 8.54 | 17.94 | 35.76 | 8.10 | 14.56 | 3.93 | 2.77 |
| 785.5178 8 | PG 37:3 PG 19:1_18:2 | 449.85 | 794.47 | 102.42 | 87.29 | 105.78 | 117.55 | 53.11 | 20.16 |
| 803.5745 8 | PG 38:1 PG 18:0_20:1 | 602.53 | 447.13 | 339.24 | 240.59 | 614.53 | 677.21 | 316.59 | 132.72 |
| 801.5510 3 | PG 38:2 PG 18:1_20:1 | 1062.52 | 1471.09 | 743.36 | 895.51 | 649.77 | 818.46 | 362.85 | 286.72 |
| 799.5396 1 | PG 38:3 PG 18:0_20:3 | 321.97 | 392.17 | 75.70 | 41.27 | 142.82 | 86.93 | 64.83 | 10.12 |
| 799.5369 3 | PG 38:3 PG 18:1_20:2 | 701.15 | 393.61 | 1177.68 | 2219.05 | 526.76 | 659.87 | 411.23 | 232.91 |
| 797.5321 7 | PG 38:4 PG 18:0_20:4 | 741.68 | 481.16 | 1228.48 | 1740.81 | 727.54 | 728.63 | 554.89 | 82.34 |
| 797.5302 7 | PG 38:4 PG 18:1_20:3 | 771.83 | 497.81 | 1170.19 | 1521.96 | 681.35 | 588.83 | 501.36 | 79.49 |
| 797.5217 9 | PG 38:4 PG 18:2_20:2 | 2116.90 | 2203.58 | 6001.34 | 11543.07 | 2031.90 | 2238.14 | 2728.40 | 2724.05 |
| 795.5136 1 | PG 38:5 PG 18:1_20:4 | 4317.76 | 3352.31 | 6066.60 | 7322.11 | 2853.78 | 2998.68 | 2244.98 | 799.31 |
| 795.5063 5 | PG 38:5 PG 18:2_20:3 | 72.45 | 74.15 | 122.51 | 109.80 | 52.45 | 45.23 | 41.27 | 29.64 |
| 793.4921 9 | PG 38:6 PG 16:0_22:6 | 936.08 | 1557.19 | 250.98 | 191.14 | 141.50 | 148.15 | 121.04 | 67.64 |
| 793.4912 1 | PG 38:6 PG 18:2_20:4 | 280.07 | 344.61 | 284.25 | 354.37 | 120.30 | 162.81 | 108.73 | 126.64 |
| 791.4797 4 | PG 38:7 PG 16:1_22:6 | 14.40 | 14.85 | 25.17 | 41.63 | 11.46 | 10.41 | 13.67 | 11.94 |
| 791.4777 2 | PG 38:7 PG 18:2_20:5 | 11.75 | 14.64 | 15.96 | 27.44 | 6.94 | 9.62 | 3.94 | 3.34 |
| 809.5299 7 | PG 39:5 PG 18:1_21:4 | 117.37 | 101.03 | 128.70 | 103.14 | 59.13 | 72.94 | 60.33 | 51.18 |
| 829.6002 2 | PG 40:2 PG 20:1_20:1 | 90.23 | 52.16 | 114.57 | 118.76 | 154.38 | 76.35 | 130.38 | 62.69 |
| 825.5543 8 | PG 40:4 PG 18:1_22:3 | 1402.57 | 2459.11 | 278.09 | 278.73 | 293.55 | 181.53 | 195.13 | 137.11 |
| 823.5475 5 | PG 40:5 PG 18:1_22:4 | 3735.32 | 2936.07 | 4774.70 | 6373.23 | 2093.17 | 2897.04 | 1699.15 | 1671.94 |
| 823.5324 1 | PG 40:5 PG 20:2_20:3 | 279.18 | 242.83 | 468.08 | 396.02 | 181.68 | 184.85 | 168.81 | 104.45 |
| 821.5319 8 | PG 40:6 PG 18:1_22:5 | 1890.58 | 1933.27 | 2885.26 | 2899.96 | 1392.06 | 1661.37 | 925.62 | 475.69 |
| 821.5200 2 | PG 40:6 PG 18:2_22:4 | 92.30 | 89.56 | 218.46 | 344.15 | 67.11 | 61.91 | 56.45 | 44.35 |
| 819.5056 2 | PG 40:7 PG 18:1_22:6 | 1426.90 | 2094.21 | 1194.09 | 2017.30 | 558.12 | 653.37 | 468.58 | 495.01 |
| 819.5059 2 | PG 40:7 PG 18:2_22:5 | 198.77 | 187.19 | 255.19 | 252.99 | 159.04 | 102.39 | 147.20 | 67.27 |

| Average <i>m/z</i> | Metabolite name | CTR | | SCH | | NF | | PNF | |
|-----------------------|--------------------------|-------------|------------|-------------|------------|-------------|-------------|-------------|------------|
| | | <i>mean</i> | <i>dev</i> | <i>mean</i> | <i>dev</i> | <i>mean</i> | <i>dev</i> | <i>mean</i> | <i>dev</i> |
| 819.5153 8 | PG 40:7 PG 20:3_20:4 | 59.26 | 68.52 | 55.90 | 66.57 | 21.94 | 17.47 | 15.29 | 14.39 |
| 817.5021 4 | PG 40:8 PG 18:2_22:6 | 641.62 | 1032.77 | 543.12 | 1011.21 | 258.81 | 320.60 | 286.27 | 376.15 |
| 817.4910 3 | PG 40:8 PG 20:4_20:4 | 332.34 | 451.07 | 268.11 | 242.64 | 158.00 | 131.86 | 124.23 | 68.43 |
| 841.4901 1 | PG 42:10 PG 20:4_22:6 | 475.45 | 729.62 | 216.27 | 265.67 | 82.44 | 77.08 | 89.26 | 114.77 |
| 839.4719 2 | PG 42:11 PG 20:5_22:6 | 94.30 | 117.66 | 57.73 | 54.28 | 35.88 | 23.48 | 23.99 | 13.15 |
| 851.5803 2 | PG 42:5 PG 20:1_22:4 | 1113.29 | 1808.72 | 271.26 | 215.17 | 308.27 | 221.51 | 265.00 | 211.32 |
| 849.5507 2 | PG 42:6 PG 20:2_22:4 | 143.64 | 106.37 | 206.74 | 200.41 | 91.69 | 44.70 | 82.45 | 51.48 |
| 847.5336 3 | PG 42:7 PG 20:2_22:5 | 412.95 | 556.99 | 894.63 | 1357.33 | 182.60 | 162.23 | 244.56 | 216.51 |
| 845.5302 7 | PG 42:8 PG 20:3_22:5 | 531.54 | 518.44 | 1027.76 | 979.40 | 432.85 | 381.62 | 468.13 | 252.46 |
| 845.5196 5 | PG 42:8 PG 20:4_22:4 | 77.57 | 74.37 | 95.37 | 116.30 | 33.09 | 22.67 | 36.74 | 38.10 |
| 843.5040 3 | PG 42:9 PG 20:3_22:6 | 110.29 | 164.83 | 76.61 | 95.46 | 26.87 | 24.02 | 24.13 | 27.86 |
| 843.5133 7 | PG 42:9 PG 20:4_22:5 | 194.27 | 223.46 | 123.38 | 124.33 | 38.79 | 25.45 | 55.02 | 55.19 |
| 869.5308 2 | PG 44:10 PG 22:4_22:6 | 137.23 | 163.02 | 71.55 | 70.58 | 44.48 | 33.62 | 38.15 | 25.29 |
| 869.5329 | PG 44:10 PG 22:5_22:5 | 1056.05 | 1000.35 | 983.67 | 1497.96 | 446.79 | 641.42 | 620.30 | 502.33 |
| 867.5213 | PG 44:11 PG 22:5_22:6 | 602.63 | 934.78 | 179.37 | 200.64 | 67.07 | 69.60 | 120.83 | 173.79 |
| 865.4909 7 | PG 44:12 PG 22:6_22:6 | 906.52 | 1606.65 | 426.81 | 724.68 | 136.01 | 164.44 | 198.29 | 302.75 |
| 873.5592 7 | PG 44:8 PG 22:4_22:4 | 372.05 | 300.99 | 427.75 | 718.16 | 134.63 | 98.93 | 122.87 | 117.87 |
| 871.5437 6 | PG 44:9 PG 22:4_22:5 | 440.19 | 463.40 | 725.97 | 712.84 | 162.94 | 159.09 | 347.32 | 446.49 |
| 937.6557 | PG 48:4 PG 24:2_24:2 | 80.05 | 40.17 | 122.23 | 132.54 | 80.73 | 42.12 | 66.39 | 15.87 |
| 705.5089 7 | PG O-32:1 PG O-16:1_16:0 | 22.44 | 16.06 | 65.34 | 76.78 | 32.81 | 37.65 | 19.23 | 4.64 |
| 703.4860 2 | PG O-32:2 PG O-16:1_16:1 | 8.51 | 4.30 | 49.96 | 59.66 | 12.19 | 17.10 | 8.68 | 5.67 |
| 731.5230 7 | PG O-34:2 PG O-16:1_18:1 | 80.54 | 47.54 | 223.33 | 246.38 | 133.60 | 103.80 | 92.45 | 55.24 |
| 731.5379 6 | PG O-34:2 PG O-18:2_16:0 | 377.37 | 296.65 | 319.08 | 249.67 | 624.59 | 1104.1 9 | 220.18 | 60.10 |
| 729.5060 4 | PG O-34:3 PG O-16:2_18:1 | 21.53 | 12.63 | 86.35 | 104.57 | 34.12 | 39.64 | 22.90 | 13.47 |
| 729.5264 3 | PG O-34:3 PG O-17:2_17:1 | 152.29 | 71.66 | 390.64 | 575.95 | 460.93 | 1161.3 8 | 168.54 | 123.66 |
| 727.4841 9 | PG O-34:4 PG O-16:1_18:3 | 23.27 | 20.00 | 45.38 | 77.17 | 17.74 | 16.04 | 21.01 | 11.15 |
| 727.5015 3 | PG O-34:4 PG O-16:2_18:2 | 125.86 | 144.78 | 74.51 | 109.56 | 140.13 | 225.45 | 59.46 | 43.53 |

| Average <i>m/z</i> | Metabolite name | CTR | | SCH | | NF | | PNF | |
|-----------------------|--------------------------|--------------|------------|-------------|------------|--------------|--------------|--------------|------------|
| | | <i>mean</i> | <i>dev</i> | <i>mean</i> | <i>dev</i> | <i>mean</i> | <i>dev</i> | <i>mean</i> | <i>dev</i> |
| 761.5700 7 | PG O-36:1 PG O-18:1_18:0 | 1619.51 | 2674.40 | 414.59 | 537.01 | 837.46 | 865.07 | 1108.11 | 1349.40 |
| 759.5486 5 | PG O-36:2 PG O-18:1_18:1 | 101.44 | 53.04 | 204.67 | 147.19 | 96.95 | 58.89 | 132.08 | 76.76 |
| 757.5361 3 | PG O-36:3 PG O-18:1_18:2 | 56.61 | 32.13 | 146.11 | 96.54 | 129.05 | 80.15 | 92.17 | 82.54 |
| 755.5231 3 | PG O-36:4 PG O-18:2_18:2 | 37.85 | 33.62 | 78.35 | 64.55 | 36.04 | 33.26 | 36.33 | 32.58 |
| 753.5059 2 | PG O-36:5 PG O-18:3_18:2 | 85.87 | 75.11 | 98.42 | 117.66 | 60.08 | 102.93 | 38.05 | 12.49 |
| 753.5189 2 | PG O-36:5 PG O-20:4_16:1 | 154.79 | 166.42 | 147.47 | 253.81 | 142.46 | 243.13 | 105.06 | 74.83 |
| 789.6007 1 | PG O-38:1 PG O-20:1_18:0 | 296.71 | 249.16 | 64.41 | 53.73 | 145.15 | 147.68 | 212.64 | 194.19 |
| 781.5354 | PG O-38:5 PG O-18:1_20:4 | 260.71 | 308.12 | 227.58 | 219.46 | 145.50 | 121.23 | 97.55 | 51.66 |
| 817.6311 | PG O-40:1 PG O-20:1_20:0 | 62.16 | 90.01 | 9.90 | 9.04 | 42.91 | 45.33 | 61.18 | 61.98 |
| 805.5240 5 | PG O-40:7 PG O-18:1_22:6 | 208.16 | 175.27 | 102.02 | 89.38 | 110.76 | 77.43 | 64.03 | 48.05 |
| 807.4959 1 | PI 32:1 PI 16:0_16:1 | 125.72 | 202.84 | 28.88 | 41.95 | 25.28 | 28.35 | 31.46 | 30.71 |
| 835.5360 7 | PI 34:1 PI 16:0_18:1 | 7281.89 | 10845.24 | 1182.38 | 1758.87 | 1263.62 | 1116.2 1 | 1001.89 | 762.71 |
| 833.5144 | PI 34:2 PI 16:0_18:2 | 2646.64 | 3316.50 | 1533.74 | 2408.83 | 1173.23 | 1785.1 7 | 634.67 | 508.66 |
| 833.5021 4 | PI 34:2 PI 16:1_18:1 | 94.00 | 126.29 | 56.94 | 79.18 | 36.19 | 44.83 | 43.62 | 54.90 |
| 863.5604 2 | PI 36:1 PI 18:0_18:1 | 1197.84 | 1005.21 | 393.67 | 441.46 | 988.65 | 1208.3 7 | 339.27 | 161.17 |
| 861.5426 | PI 36:2 PI 18:1_18:1 | 6246.73 | 7392.34 | 1032.32 | 1048.63 | 2358.71 | 2449.6 4 | 1319.89 | 933.20 |
| 859.5310 7 | PI 36:3 PI 16:0_20:3 | 472.57 | 534.83 | 398.30 | 718.10 | 375.79 | 461.46 | 172.34 | 111.94 |
| 857.5045 2 | PI 36:4 | 1039.51 | 923.98 | 869.69 | 1091.13 | 734.67 | 1314.3 9 | 438.33 | 317.81 |
| 857.5183 1 | PI 36:4 PI 16:0_20:4 | 2263.88 | 2143.63 | 1457.76 | 1863.75 | 2494.80 | 4530.8 3 | 1216.64 | 1381.80 |
| 857.5153 8 | PI 36:4 PI 18:2_18:2 | 45.05 | 39.27 | 37.98 | 39.58 | 38.25 | 24.41 | 23.28 | 16.18 |
| 855.5092 8 | PI 36:5 PI 16:0_20:5 | 411.80 | 346.10 | 245.11 | 217.83 | 261.88 | 146.68 | 213.25 | 99.95 |
| 855.4901 1 | PI 36:5 PI 16:1_20:4 | 11.28 | 13.46 | 10.45 | 12.55 | 23.39 | 41.14 | 12.61 | 17.02 |
| 871.5313 7 | PI 37:4 PI 17:0_20:4 | 860.29 | 767.91 | 540.74 | 783.48 | 575.16 | 628.20 | 217.59 | 78.82 |
| 887.5640 9 | PI 38:3 PI 18:0_20:3 | 2681.81 | 1644.60 | 2040.29 | 2673.96 | 2473.13 | 3250.8 0 | 612.22 | 238.18 |
| 885.5377 2 | PI 38:4 PI 18:0_20:4 | 70145.8 3 | 65204.75 | 21227.63 | 19904.48 | 48717.2 2 | 60798. 04 | 14534.3 7 | 6530.27 |
| 883.5345 5 | PI 38:5 | 27.87 | 27.39 | 14.74 | 20.27 | 14.59 | 9.93 | 9.27 | 7.32 |

| Average <i>m/z</i> | Metabolite name | CTR | | SCH | | NF | | PNF | |
|-----------------------|----------------------------|--------------|---------------|-------------|------------|--------------|--------------|--------------|--------------|
| | | <i>mean</i> | <i>dev</i> | <i>mean</i> | <i>dev</i> | <i>mean</i> | <i>dev</i> | <i>mean</i> | <i>dev</i> |
| 883.5204 5 | PI 38:5 PI 18:1_20:4 | 86871.0 0 | 110337.7 0 | 63803.77 | 92371.97 | 41596.7 7 | 68430. 54 | 28321.7 4 | 31569.6 0 |
| 881.5156 2 | PI 38:6 PI 16:0_22:6 | 207.45 | 209.50 | 101.41 | 99.19 | 78.04 | 68.93 | 48.83 | 20.11 |
| 881.5189 2 | PI 38:6 PI 18:2_20:4 | 60.96 | 69.36 | 52.44 | 70.39 | 63.29 | 84.17 | 22.96 | 24.21 |
| 913.5674 4 | PI 40:4 PI 18:0_22:4 | 830.10 | 592.83 | 282.41 | 246.37 | 690.80 | 909.39 | 179.48 | 94.89 |
| 911.5670 2 | PI 40:5 | 209.53 | 139.09 | 177.81 | 279.24 | 75.17 | 45.17 | 45.07 | 13.28 |
| 909.5375 4 | PI 40:6 | 135.14 | 107.59 | 149.45 | 187.04 | 253.51 | 475.56 | 75.36 | 53.38 |
| 909.5393 7 | PI 40:6 PI 18:1_22:5 | 139.22 | 151.86 | 187.95 | 332.76 | 55.50 | 51.04 | 45.24 | 39.55 |
| 907.5332 | PI 40:7 | 88.07 | 85.95 | 44.69 | 45.31 | 52.92 | 65.05 | 18.25 | 12.39 |
| 905.5153 8 | PI 40:8 PI 20:4_20:4 | 75.94 | 67.58 | 47.53 | 57.09 | 51.28 | 37.24 | 23.80 | 21.25 |
| 933.5295 4 | PI 42:8 | 154.24 | 221.76 | 52.23 | 67.64 | 36.31 | 34.75 | 28.60 | 22.54 |
| 953.5275 3 | PI 44:12 | 195.88 | 85.53 | 46.35 | 45.82 | 268.04 | 286.23 | 43.35 | 43.59 |
| 679.3801 9 | PI O-24:2 | 407.31 | 289.88 | 206.92 | 133.61 | 316.58 | 216.81 | 207.45 | 61.20 |
| 678.3964 2 | PS 27:1;O PS 10:0_17:1;O | 101.92 | 158.58 | 9.48 | 6.94 | 21.35 | 48.45 | 5.52 | 3.82 |
| 734.4902 3 | PS 32:0 PS 16:0_16:0 | 121.42 | 95.69 | 31.28 | 23.65 | 57.40 | 105.53 | 19.37 | 7.75 |
| 732.4841 3 | PS 32:1 PS 16:0_16:1 | 48.23 | 90.23 | 3.65 | 5.13 | 5.53 | 8.82 | 28.99 | 54.37 |
| 760.5046 4 | PS 34:1 PS 16:0_18:1 | 4976.32 | 9066.96 | 344.95 | 525.76 | 883.93 | 2241.5 0 | 241.00 | 180.45 |
| 806.4879 8 | PS 34:2;3O PS 16:0_18:2;3O | 213.95 | 220.26 | 53.26 | 94.69 | 59.83 | 132.18 | 23.84 | 22.65 |
| 758.4932 3 | PS 34:2 PS 16:0_18:2 | 462.18 | 852.37 | 114.92 | 149.71 | 59.68 | 80.02 | 47.97 | 42.70 |
| 786.4984 7 | PS 35:3;O PS 18:1_17:2;O | 27.28 | 8.46 | 40.26 | 34.61 | 111.52 | 93.39 | 26.02 | 21.73 |
| 788.5425 4 | PS 36:1 | 65.48 | 42.82 | 32.98 | 24.16 | 58.51 | 73.98 | 28.78 | 27.57 |
| 788.5353 4 | PS 36:1 PS 18:0_18:1 | 33972.8 6 | 55831.91 | 4963.17 | 6613.48 | 26174.4 4 | 70236. 02 | 2747.31 | 2161.42 |
| 818.5265 5 | PS 36:2;2O PS 18:2_18:0;2O | 117.08 | 62.40 | 143.95 | 168.10 | 73.14 | 28.01 | 33.81 | 7.30 |
| 834.5156 2 | PS 36:2;3O PS 18:0_18:2;3O | 1811.59 | 1354.95 | 480.34 | 325.49 | 1015.59 | 539.58 | 537.28 | 373.21 |
| 786.5225 2 | PS 36:2 PS 18:1_18:1 | 23371.3 8 | 45932.58 | 1204.97 | 2360.90 | 4147.24 | 11286. 49 | 717.10 | 873.65 |
| 784.5007 9 | PS 36:3 PS 18:1_18:2 | 1345.90 | 2590.37 | 101.64 | 194.92 | 94.69 | 142.92 | 38.47 | 30.82 |
| 782.4887 1 | PS 36:4 | 128.64 | 54.64 | 66.51 | 37.64 | 231.15 | 179.64 | 124.70 | 53.27 |

| Average <i>m/z</i> | Metabolite name | CTR | | SCH | | NF | | PNF | |
|-----------------------|--------------------------|--------------|------------|-------------|------------|-------------|--------------|-------------|------------|
| | | <i>mean</i> | <i>dev</i> | <i>mean</i> | <i>dev</i> | <i>mean</i> | <i>dev</i> | <i>mean</i> | <i>dev</i> |
| 782.4974 4 | PS 36:4 PS 16:0_20:4 | 420.36 | 627.86 | 241.77 | 355.12 | 68.24 | 98.25 | 52.06 | 21.69 |
| 816.5651 9 | PS 38:1 PS 20:0_18:1 | 659.00 | 1005.02 | 113.54 | 94.59 | 1200.62 | 3336.4 0 | 114.27 | 71.66 |
| 814.5456 5 | PS 38:2 | 16.52 | 22.38 | 4.90 | 5.82 | 15.44 | 33.15 | 3.76 | 2.91 |
| 814.5468 8 | PS 38:2 PS 18:1_20:1 | 1680.92 | 1860.15 | 843.49 | 852.42 | 4955.31 | 13268. 04 | 521.98 | 388.05 |
| 812.5496 8 | PS 38:3 | 499.58 | 203.77 | 5432.82 | 11854.71 | 1087.30 | 805.38 | 734.33 | 507.18 |
| 812.5781 9 | PS 38:3 PS 18:0_20:3 | 12536.1 7 | 8551.81 | 4611.67 | 2759.36 | 7931.18 | 3914.1 6 | 5253.25 | 2069.28 |
| 810.5378 4 | PS 38:4 PS 16:0_22:4 | 460.53 | 616.19 | 348.95 | 561.11 | 111.78 | 64.34 | 104.35 | 44.61 |
| 810.5217 3 | PS 38:4 PS 18:0_20:4 | 6941.32 | 9056.02 | 1633.20 | 3476.27 | 4341.59 | 11057. 19 | 459.89 | 458.86 |
| 810.5259 4 | PS 38:4 PS 18:1_20:3 | 987.30 | 1445.87 | 129.95 | 147.63 | 207.94 | 271.19 | 97.85 | 56.26 |
| 808.5056 8 | PS 38:5 PS 18:0_20:5 | 344.89 | 335.88 | 153.07 | 155.42 | 118.01 | 91.15 | 58.39 | 35.75 |
| 808.5087 9 | PS 38:5 PS 18:1_20:4 | 876.72 | 1475.55 | 102.33 | 146.04 | 207.95 | 433.44 | 55.74 | 37.86 |
| 840.5360 1 | PS 39:4;O PS 22:3_17:1;O | 118.95 | 108.45 | 80.04 | 53.34 | 218.54 | 149.14 | 107.51 | 79.17 |
| 842.5796 5 | PS 40:2 PS 18:1_22:1 | 627.94 | 981.53 | 223.91 | 373.62 | 3433.59 | 10394. 35 | 74.06 | 40.87 |
| 836.5412 | PS 40:5 PS 18:0_22:5 | 1876.55 | 1819.39 | 729.21 | 1464.13 | 640.17 | 1269.8 8 | 112.00 | 54.64 |
| 834.5257 6 | PS 40:6 | 177.39 | 179.76 | 61.01 | 64.86 | 78.64 | 65.29 | 35.41 | 19.33 |
| 834.5227 7 | PS 40:6 PS 18:0_22:6 | 4053.30 | 4077.80 | 1317.43 | 2447.46 | 1794.97 | 4266.4 9 | 176.44 | 100.27 |
| 832.5036 6 | PS 40:7 PS 18:1_22:6 | 597.53 | 983.66 | 379.86 | 690.80 | 114.44 | 205.47 | 61.34 | 60.07 |
| 870.6065 7 | PS 42:2 | 24.82 | 43.03 | 3.92 | 4.88 | 10.15 | 23.88 | 1.93 | 1.72 |
| 870.6077 9 | PS 42:2 PS 18:1_24:1 | 106.29 | 133.55 | 32.32 | 29.69 | 318.79 | 920.44 | 14.81 | 8.37 |
| 868.6016 2 | PS 42:3 | 1114.61 | 848.10 | 1395.30 | 2564.96 | 2624.96 | 3543.7 3 | 804.27 | 597.84 |
| 860.5307 | PS 42:7 PS 20:1_22:6 | 110.29 | 115.68 | 59.94 | 95.44 | 50.47 | 98.95 | 9.68 | 4.10 |
| 938.5905 2 | PS 48:10 | 39.35 | 59.91 | 5.82 | 6.39 | 6.91 | 6.45 | 2.26 | 0.82 |
| 744.508 | PS O-34:2 PS O-16:1_18:1 | 2551.37 | 4769.94 | 261.13 | 331.26 | 1118.61 | 3163.1 6 | 125.38 | 140.57 |
| 770.5244 8 | PS O-36:3 PS O-18:2_18:1 | 1079.71 | 1676.89 | 230.64 | 175.57 | 627.87 | 1287.9 1 | 268.96 | 248.90 |
| 786.5605 5 | PS O-37:2 PS O-19:1_18:1 | 3607.67 | 2744.38 | 1741.56 | 1463.91 | 6034.21 | 9952.5 6 | 2478.63 | 934.59 |
| 750.4824 2 | SHexCer 32:1;2O | 114.10 | 188.60 | 329.83 | 553.96 | 49.89 | 32.41 | 77.26 | 51.10 |

| Average <i>m/z</i> | Metabolite name | CTR | | SCH | | NF | | PNF | |
|-----------------------|-----------------|--------------|------------|-------------|------------|--------------|--------------|--------------|--------------|
| | | <i>mean</i> | <i>dev</i> | <i>mean</i> | <i>dev</i> | <i>mean</i> | <i>dev</i> | <i>mean</i> | <i>dev</i> |
| 778.5141 6 | SHexCer 34:1;2O | 2049.45 | 2688.75 | 11702.14 | 19146.34 | 1343.05 | 1053.6 9 | 1811.46 | 1176.11 |
| 794.5082 4 | SHexCer 34:1;3O | 459.26 | 504.94 | 555.94 | 634.44 | 369.52 | 185.79 | 295.07 | 158.14 |
| 776.4978 | SHexCer 34:2;2O | 379.32 | 575.60 | 1897.40 | 3485.05 | 284.65 | 282.85 | 262.66 | 175.68 |
| 810.5481 6 | SHexCer 35:0;3O | 218.73 | 192.25 | 1220.42 | 2191.04 | 233.57 | 303.02 | 186.11 | 186.92 |
| 792.5234 4 | SHexCer 35:1;2O | 1140.30 | 2104.18 | 5609.23 | 13765.46 | 271.06 | 327.38 | 891.70 | 796.82 |
| 824.5329 6 | SHexCer 36:0;3O | 4780.16 | 4397.58 | 3844.65 | 3106.04 | 2288.29 | 1664.2 8 | 3431.01 | 3166.92 |
| 806.5524 3 | SHexCer 36:1;2O | 361.44 | 561.47 | 202.19 | 326.11 | 311.41 | 796.07 | 166.54 | 218.46 |
| 804.5318 | SHexCer 36:2;2O | 3387.18 | 6017.68 | 11000.93 | 18160.44 | 1270.54 | 1083.0 1 | 2777.11 | 2253.87 |
| 838.5942 4 | SHexCer 37:0;3O | 13351.6 9 | 14059.79 | 3834.74 | 2642.62 | 7250.58 | 4561.0 3 | 4641.13 | 1944.46 |
| 820.5583 5 | SHexCer 37:1;2O | 18.26 | 9.77 | 27.67 | 29.29 | 21.09 | 16.76 | 35.76 | 37.21 |
| 834.5448 | SHexCer 37:2;3O | 1263.61 | 1237.41 | 620.81 | 974.28 | 300.49 | 265.59 | 150.28 | 31.61 |
| 814.5073 2 | SHexCer 37:4;2O | 143.12 | 89.84 | 118.38 | 65.93 | 406.03 | 1058.5 3 | 86.47 | 41.47 |
| 830.5312 5 | SHexCer 37:4;3O | 1716.70 | 3331.97 | 103.80 | 95.24 | 336.58 | 491.47 | 225.19 | 379.58 |
| 836.5886 8 | SHexCer 38:0;2O | 238.22 | 245.66 | 127.42 | 129.78 | 255.72 | 255.96 | 181.61 | 105.84 |
| 846.5402 8 | SHexCer 38:3;3O | 1479.23 | 893.69 | 731.75 | 488.90 | 1754.23 | 812.88 | 822.97 | 209.79 |
| 828.5440 7 | SHexCer 38:4;2O | 645.18 | 509.85 | 659.61 | 735.53 | 1083.75 | 2287.0 2 | 397.13 | 193.12 |
| 842.5246 | SHexCer 38:5;3O | 589.73 | 654.90 | 125.29 | 75.37 | 404.16 | 283.82 | 117.00 | 40.31 |
| 866.5941 8 | SHexCer 39:0;3O | 380.37 | 326.47 | 1109.22 | 2237.19 | 488.09 | 478.96 | 704.24 | 890.78 |
| 858.5353 4 | SHexCer 39:4;3O | 126.56 | 53.54 | 94.14 | 65.33 | 204.78 | 159.51 | 103.08 | 27.81 |
| 840.5262 5 | SHexCer 39:5;2O | 37.63 | 26.79 | 27.03 | 40.22 | 39.02 | 29.16 | 22.83 | 9.71 |
| 864.6144 4 | SHexCer 40:0;2O | 667.04 | 683.23 | 314.42 | 359.77 | 1491.23 | 2196.8 7 | 1597.29 | 1770.34 |
| 880.6032 7 | SHexCer 40:0;3O | 6337.04 | 5143.10 | 2501.68 | 1804.47 | 3837.49 | 1274.5 6 | 2367.01 | 1197.12 |
| 878.5898 4 | SHexCer 40:1;3O | 46397.4 9 | 50619.21 | 36701.73 | 75500.97 | 10175.3 5 | 18553. 51 | 15770.9 3 | 12272.3 8 |
| 874.5636 6 | SHexCer 40:3;3O | 184.49 | 182.02 | 131.70 | 76.37 | 224.05 | 106.83 | 88.67 | 54.35 |
| 852.5532 2 | SHexCer 40:6;2O | 241.78 | 254.97 | 110.98 | 90.21 | 59.12 | 64.02 | 107.70 | 85.52 |
| 850.5231 9 | SHexCer 40:7;2O | 49.11 | 54.64 | 19.85 | 12.87 | 39.06 | 34.17 | 24.74 | 7.68 |
| 894.6229 2 | SHexCer 41:0;3O | 1467.17 | 1175.42 | 1455.18 | 2071.23 | 1727.05 | 1908.9 3 | 1037.43 | 1034.02 |

| Average m/z | Metabolite name | CTR | | SCH | | NF | | PNF | |
|----------------|--------------------------------|--------------|---------------|---------------|---------------|--------------|--------------|---------------|---------------|
| | | mean | dev | mean | dev | mean | dev | mean | dev |
| 886.5814 8 | SHexCer 41:4;3O | 77.05 | 42.29 | 133.60 | 234.22 | 91.67 | 56.29 | 49.84 | 8.06 |
| 862.5089 1 | SHexCer 41:8;2O | 219.86 | 147.71 | 87.03 | 65.01 | 166.95 | 95.46 | 99.57 | 26.69 |
| 878.5072 6 | SHexCer 41:8;3O | 36.99 | 23.54 | 22.61 | 31.38 | 65.39 | 70.87 | 34.94 | 53.31 |
| 908.6323 9 | SHexCer 42:0;3O | 169.87 | 59.04 | 164.98 | 89.79 | 292.75 | 199.94 | 214.17 | 154.38 |
| 888.6233 5 | SHexCer 42:2;2O | 79020.2 0 | 124460.8 9 | 100670.5 0 | 170923.4 6 | 52057.5 3 | 49039. 94 | 137522. 10 | 125543. 53 |
| 886.6066 9 | SHexCer 42:3;2O | 11121.6 8 | 20452.75 | 23081.49 | 52548.51 | 4418.17 | 3476.0 5 | 5533.79 | 5133.23 |
| 884.5991 8 | SHexCer 42:4;2O | 898.00 | 1050.46 | 437.61 | 685.05 | 1355.73 | 1953.4 5 | 416.26 | 366.99 |
| 878.5309 4 | SHexCer 42:7;2O | 226.92 | 248.65 | 104.82 | 93.98 | 213.52 | 139.94 | 102.47 | 52.93 |
| 892.5161 7 | SHexCer 42:8;3O | 268.03 | 170.64 | 87.26 | 55.04 | 115.05 | 44.90 | 97.82 | 78.04 |
| 874.5312 5 | SHexCer 42:9;2O | 145.34 | 73.43 | 180.61 | 227.17 | 134.67 | 149.65 | 47.47 | 5.85 |
| 922.6536 9 | SHexCer 43:0;3O | 26215.8 4 | 20214.71 | 21809.23 | 23342.58 | 22691.0 7 | 19741. 28 | 18177.8 7 | 16608.6 2 |
| 920.6414 2 | SHexCer 43:1;3O | 4483.24 | 2354.07 | 5644.46 | 8460.65 | 3850.50 | 4006.9 8 | 2764.47 | 2539.31 |
| 900.6184 7 | SHexCer 43:3;2O | 1792.89 | 3164.77 | 1820.95 | 3756.83 | 280.97 | 366.59 | 556.89 | 349.40 |
| 912.6343 4 | SHexCer 44:4;2O | 10558.3 2 | 12017.76 | 3257.78 | 3182.03 | 14711.2 3 | 21022. 63 | 6387.96 | 6206.13 |
| 936.6049 8 | SHexCer 45:7;3O | 48.26 | 58.36 | 76.44 | 163.54 | 10.95 | 6.93 | 74.54 | 64.54 |
| 934.5958 9 | SHexCer 46:7;2O | 46.16 | 74.20 | 73.35 | 160.69 | 16.37 | 14.23 | 89.14 | 89.77 |
| 972.7300 4 | SHexCer 48:2;2O | 590.55 | 645.47 | 371.49 | 293.97 | 278.83 | 362.55 | 118.65 | 96.92 |
| 966.6886 | SHexCer 48:5;2O | 440.26 | 631.56 | 250.59 | 328.92 | 195.23 | 239.32 | 255.36 | 247.28 |
| 526.3222 | SL 28:4;2O | 30.06 | 13.77 | 336.61 | 952.05 | 12.13 | 19.32 | 18.69 | 13.87 |
| 784.6622 9 | SL 46:1;2O SL 16:0;O/30:1;O | 33.96 | 28.21 | 47.62 | 78.68 | 236.33 | 277.60 | 174.51 | 208.79 |
| 856.6832 3 | SL 53:6;O | 2051.06 | 2928.43 | 3221.13 | 5665.91 | 6810.80 | 8558.2 6 | 11451.9 2 | 16626.8 5 |
| 391.2813 1 | ST 24:1;O4 | 29.54 | 22.69 | 71.44 | 124.54 | 74.66 | 51.81 | 64.15 | 40.60 |
| 389.2732 2 | ST 24:2;O4 | 160.98 | 210.80 | 137.14 | 159.54 | 234.30 | 158.36 | 136.51 | 123.61 |
| 467.3268 1 | ST 27:0;O;S | 65.63 | 72.53 | 487.37 | 1413.66 | 139.60 | 404.00 | 17.63 | 4.88 |
| 465.2997 4 | ST 27:1;O;S | 2842.35 | 3329.33 | 2670.15 | 4385.75 | 31376.8 9 | 94321. 26 | 448.61 | 219.91 |
| 479.3160 1 | ST 28:1;O;S | 1396.57 | 2105.77 | 2710.79 | 5006.62 | 360.36 | 320.33 | 135.89 | 68.72 |

| Average <i>m/z</i> | Metabolite name | CTR | | SCH | | NF | | PNF | |
|-----------------------|-----------------|-------------|------------|-------------|------------|-------------|------------|-------------|------------|
| | | <i>mean</i> | <i>dev</i> | <i>mean</i> | <i>dev</i> | <i>mean</i> | <i>dev</i> | <i>mean</i> | <i>dev</i> |
| 493.3354 5 | ST 29:1;O;S | 1104.29 | 1533.48 | 1126.82 | 2036.93 | 419.52 | 208.73 | 199.98 | 91.28 |
| 491.3139 6 | ST 29:2;O;S | 144.40 | 207.72 | 180.70 | 303.87 | 50.21 | 37.33 | 24.32 | 10.87 |

Table S3. List of all the sphingolipids species identified using a targeted approach across each histotype. Each sphingolipid was identified with multiple reaction monitoring mass transition (MRM) in positive electrospray ionization, name, and concentration (pmol/mg protein) in each group. The MRM transition were recorded using an optimized declustering potential (DP) and collision energy (CE) for each sphingolipids subclasses: Cer (DP 40 eV, CE 30–40 eV); DHCer (DP 40 eV, CE 35–40 eV); SM (DP 60 eV, CE 40 eV); HexCer (DP 40 eV, CE 50 eV); LacCer (DP 60 eV, CE 60 eV) and GM3 (DP 70 eV, CE 60 eV).

| MRM <i>m/z</i> | Metabolite name | CTR | | SCH | | NF | | PNF | |
|-------------------|--------------------|--------------|--------------|-------------|-------------|--------------|--------------|--------------|--------------|
| | | <i>mean</i> | <i>dev</i> | <i>mean</i> | <i>dev</i> | <i>mean</i> | <i>dev</i> | <i>mean</i> | <i>dev</i> |
| 510.7 > 264.4 | Cer 14 | 14.85 | 28.51 | 12.99 | 10.30 | 68.59 | 85.90 | 23.69 | 14.65 |
| 538.8 > 264.4 | Cer 16 | 1159.30 | 1356.06 | 821.18 | 525.67 | 3335.88 | 3089.40 | 1110.10 | 627.66 |
| 564.8 > 264.4 | Cer 18 | 0.78 | 1.46 | 2.73 | 5.01 | 3.00 | 3.67 | 1.93 | 2.35 |
| 566.8 > 264.4 | Cer 18:1 | 424.69 | 507.21 | 472.74 | 364.87 | 702.88 | 611.04 | 348.80 | 245.85 |
| 594.8 > 264.4 | Cer 20 | 84.68 | 106.06 | 73.75 | 64.13 | 170.82 | 187.02 | 77.70 | 51.78 |
| 622.9 > 264.4 | Cer 22 | 127.15 | 174.37 | 108.02 | 89.72 | 330.01 | 337.85 | 137.03 | 80.31 |
| 648.9 > 264.4 | Cer 24 | 738.81 | 871.42 | 527.62 | 399.37 | 1548.31 | 1350.01 | 609.17 | 378.02 |
| 650.9 > 264.4 | Cer 24:1 | 790.48 | 906.77 | 606.92 | 505.58 | 1548.24 | 2010.38 | 576.26 | 287.85 |
| 540.4 > 266.4 | DHCer 16 | 45.31 | 68.24 | 16.42 | 22.31 | 221.63 | 246.67 | 83.73 | 87.06 |
| 566.5 > 266.4 | DHCer 18 | 21.51 | 23.51 | 7.63 | 7.24 | 24.07 | 25.63 | 8.93 | 12.75 |
| 568.5 > 266.4 | DHCer 18:1 | 11.56 | 25.49 | 6.49 | 13.35 | 35.80 | 61.60 | 9.33 | 7.58 |
| 650.5 > 266.4 | DHCer 24 | 41.41 | 70.51 | 31.03 | 34.51 | 112.46 | 127.36 | 37.69 | 31.07 |
| 652.5 > 266.4 | DHCer 24:1 | 73.00 | 187.49 | 12.23 | 25.91 | 28.87 | 43.25 | 12.50 | 11.66 |
| 703.5 > 184.1 | SM 16 | 26928.3 9 | 30334.7 8 | 9937.0 4 | 8115.3 0 | 39566.1 6 | 51380.6 3 | 11736.1 1 | 8280.05 |
| 731.6 > 184.1 | SM 18 | 16216.7 6 | 16587.7 4 | 7631.3 8 | 7561.2 3 | 16541.4 8 | 16789.1 0 | 7330.94 | 6442.53 |
| 729.6 > 184.1 | SM 18:1 | 2796.15 | 2762.65 | 2313.8 7 | 2237.9 7 | 3001.76 | 2303.99 | 1294.79 | 771.89 |
| 815.7 > 184.1 | SM 24 | 14091.3 6 | 14349.1 8 | 5901.9 7 | 7122.1 6 | 16578.4 1 | 22613.5 3 | 6037.50 | 5626.91 |
| 813.7 > 184.1 | SM 24:1 | 24283.3 4 | 27408.6 0 | 8311.8 9 | 8704.7 2 | 30529.5 0 | 39376.6 5 | 11044.2 1 | 11541.0 2 |
| 700.6 > 264.3 | HexCer 16 | 439.75 | 586.38 | 311.09 | 370.70 | 404.63 | 738.48 | 160.39 | 103.17 |
| 728.6 > 264.3 | HexCer 18 | 1533.50 | 1563.84 | 916.71 | 1301.5 5 | 493.68 | 513.05 | 1196.79 | 1443.86 |
| 726.6 > 264.3 | HexCer 18:1 | 8.40 | 12.72 | 12.43 | 16.34 | 0.02 | 0.06 | 21.21 | 17.57 |

| MRM <i>m/z</i> | Metabolite name | CTR | | SCH | | NF | | PNF | |
|-------------------|--------------------|-------------|--------------|-------------|-------------|-------------|------------|-------------|------------|
| | | <i>mean</i> | <i>dev</i> | <i>mean</i> | <i>dev</i> | <i>mean</i> | <i>dev</i> | <i>mean</i> | <i>dev</i> |
| 756.6 > 264.3 | HexCer 20 | 411.65 | 399.88 | 229.61 | 508.61 | 323.18 | 465.55 | 323.39 | 398.67 |
| 784.7 > 264.3 | HexCer 22 | 2669.25 | 3032.77 | 1288.6 3 | 2899.3 1 | 1224.13 | 1277.87 | 1710.23 | 2360.91 |
| 812.7 > 264.3 | HexCer 24 | 9667.29 | 11957.6 1 | 4400.2 1 | 9674.1 5 | 3783.70 | 3704.41 | 5361.49 | 7051.04 |
| 810.7 > 264.3 | HexCer 24:1 | 8613.90 | 9619.57 | 4472.0 7 | 8901.4 6 | 4062.86 | 3453.80 | 5441.51 | 6429.39 |
| 862.6 > 264.3 | LacCer 16 | 772.25 | 1187.62 | 175.08 | 89.63 | 655.47 | 948.18 | 213.14 | 114.43 |
| 890.7 > 264.3 | LacCer 18 | 48.48 | 79.25 | 50.56 | 51.48 | 35.43 | 47.55 | 17.11 | 9.38 |
| 888.7 > 264.3 | LacCer 18:1 | 0.00 | 0.00 | 0.03 | 0.14 | 0.00 | 0.00 | 0.00 | 0.00 |
| 918.7 > 264.3 | LacCer 20 | 24.09 | 49.25 | 12.49 | 23.62 | 14.23 | 24.66 | 5.67 | 6.43 |
| 946.7 > 264.3 | LacCer 22 | 186.06 | 308.85 | 85.65 | 75.72 | 181.48 | 287.62 | 32.61 | 22.99 |
| 974.8 > 264.3 | LacCer 24 | 309.16 | 384.12 | 269.82 | 293.26 | 511.69 | 929.61 | 62.03 | 27.17 |
| 972.7 > 264.3 | LacCer 24:1 | 984.55 | 1309.74 | 395.95 | 245.79 | 1005.67 | 1565.99 | 203.74 | 93.50 |
| 1153.7> 264.3 | GM3 16 | 564.44 | 898.74 | 221.45 | 115.71 | 518.41 | 561.00 | 286.29 | 150.00 |
| 1181.7> 264.3 | GM3 18 | 177.70 | 370.99 | 93.41 | 66.06 | 132.62 | 145.67 | 70.93 | 54.89 |
| 1179.8> 264.3 | GM3 18:1 | 0.00 | 0.00 | 0.53 | 1.43 | 0.00 | 0.00 | 0.00 | 0.00 |
| 1209.8> 264.3 | GM3 20 | 80.19 | 175.44 | 30.43 | 27.98 | 55.43 | 66.78 | 34.49 | 29.45 |
| 1237.8> 264.3 | GM3 22 | 435.71 | 650.27 | 227.59 | 161.14 | 322.10 | 265.08 | 195.76 | 146.05 |
| 1265.8> 264.3 | GM3 24 | 786.41 | 1017.83 | 572.17 | 518.81 | 581.60 | 593.26 | 306.10 | 204.12 |
| 1263.8> 264.3 | GM 24:1 | 991.20 | 1402.63 | 608.68 | 371.69 | 982.32 | 763.39 | 562.40 | 380.55 |