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*Supplementary Materials*

# Stable isotope-labeled lipidomics to unravel the heterogeneous development lipotoxicity

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## Supplementary Materials

## Supplementary Tables

**Table S1.** Significant changes in metabolites produced by palmitic acid-treated (FA 16:0) HepG2 cells (in ESI-positive mode)

| ID | m/z | CON_4HR | CON_8HR | CON_16HR | CON_24HR | FA16:0_4HR | FA16:0_8HR | FA16:0_16HR | FA16:0_24HR | VIP 16:0 (16HR) | S-Plot 16:0 (16HR) | FA 16:0 P-value (16HR) |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| PC(32:0) | 734.5834 | 24691.7±1153.3 | 27339.0±1408.9 | 28110.2±2361.7 | 22855.4±694.3 | 364963.0±56529.1 | 781911.3±90400.4 | 935030.0±132598.1 | 686010.6±50028.2 | 16.81 | -0.99 | 3.31E-08 |
| DG(32:0) | 591.5063 | 3.5±10.6 | 0.0±0.0 | 13.2±30.5 | 0.0±0.0 | 12607.8±1720.6 | 38102.9±5615.1 | 66384.8±12540.1 | 50815.8±6556.5 | 4.52 | -0.98 | 2.48E-07 |
| PC(36:2) | 786.6069 | 69746.6±4876.9 | 73574.0±3341.9 | 75936.7±4271.8 | 75220.0±4247.1 | 50343.8±3712.0 | 39227.5±3117.0 | 18670.2±3815.4 | 8804.8±1134.6 | 4.25 | 0.98 | 1.72E-15 |
| PC(32:1) | 732.5675 | 79483.9±3415.6 | 89803.3±3453.2 | 104516.1±8222.2 | 110212.9±7997.9 | 91532.7±7892.1 | 134392.3±8126.8 | 169217.6±33023.7 | 172518.1±14801.4 | 4.10 | -0.82 | 0.0003 |
| PC(34:3) | 756.5590 | 0.0±0.0 | 0.0±0.0 | 10.2±30.6 | 5.3±16.0 | 12197.3±3268.7 | 41992.1±7255.3 | 52537.9±11588.1 | 30804.8±2764.3 | 4.00 | -0.97 | 8.22E-07 |
| TG(48:1) | 822.7662 | 9264.1±835.0 | 9650.5±1758.9 | 10796.9±1862.2 | 10367.5±1652.7 | 27619.3±4552.5 | 40287.3±9300.8 | 58718.1±16568.7 | 78618.0±38348.0 | 3.72 | -0.91 | 2.17E-05 |
| TG(50:1) | 850.8030 | 29585.0±11971.7 | 32632.6±4718.9 | 25574.7±14775.2 | 27504.9±12631.2 | 70014.0±18945.2 | 88392.5±24498.8 | 68192.0±22530.2 | 62405.4±49855.4 | 3.22 | -0.77 | 0.0002 |
| DG(32:0)Fragment | 313.2760 | 12.9±10.9 | 15.5±12.6 | 28.5±21.6 | 19.6±21.2 | 4199.4±552.4 | 12523.2±1045.2 | 23270.9±5806.1 | 16238.7±1885.6 | 2.65 | -0.96 | 2.13E-06 |
| PC(34:2) | 758.5779 | 20933.8±3166.1 | 21873.1±1557.1 | 27586.5±1728.5 | 36324.9±5152.7 | 12828.2±2012.8 | 10753.8±920.6 | 5770.5±2836.6 | 5519.1±1104.5 | 2.61 | 0.97 | 1.21E-12 |
| Unknown | 551.5065 | 343.1±68.1 | 365.4±67.3 | 321.5±43.7 | 292.3±83.8 | 3779.6±471.5 | 11177.4±1655.4 | 18243.2±4160.7 | 13581.7±1472.7 | 2.33 | -0.97 | 1.22E-06 |
| TG(50:2) | 848.7869 | 19857.6±713.4 | 21855.0±4038.1 | 28224.3±3044.5 | 27046.5±3991.7 | 32164.7±2887.3 | 36541.8±3099.0 | 41103.1±7239.7 | 56213.3±9468.4 | 1.78 | -0.76 | 0.0005 |
| SM | 703.5786 | 14187.6±958.3 | 15595.0±1686.5 | 16674.7±1212.0 | 13995.0±5313.1 | 12807.0±1785.2 | 11664.8±834.7 | 7707.7±1476.2 | 6741.6±624.6 | 1.66 | 0.95 | 1.96E-10 |
| TG(50:4) | 827.7192 | 0.0±0.0 | 39.3±87.5 | 94.5±172.8 | 51.7±102.7 | 2955.2±1095.4 | 5128.3±891.0 | 7248.5±1758.0 | 8709.6±4435.5 | 1.47 | -0.96 | 1.66E-06 |
| PC(36:1) | 788.6203 | 5272.3±1095.3 | 7404.4±1194.3 | 8882.5±1569.5 | 5315.5±983.2 | 3283.7±1059.4 | 4987.3±1226.0 | 2930.5±1128.1 | 1241.0±458.6 | 1.32 | 0.91 | 8.18E-08 |
| PC(36:4) | 782.5732 | 2538.4±1431.4 | 1950.8±537.5 | 1152.1±665.5 | 636.0±212.9 | 5986.0±1800.2 | 9207.8±942.1 | 7186.9±2216.7 | 4821.2±596.4 | 1.31 | -0.90 | 2.02E-05 |
| PC(34:0) | 762.6043 | 23.5±46.9 | 57.6±62.1 | 32.2±66.9 | 0.0±0.0 | 365.5±218.2 | 3972.2±1138.3 | 4964.1±2259.5 | 1398.9±815.7 | 1.16 | -0.88 | 0.0002 |
| Unknown | 607.4617 | 36.2±46.4 | 69.4±78.7 | 36.3±59.5 | 89.6±82.2 | 1560.9±326.1 | 2622.1±287.0 | 3670.1±516.8 | 3266.9±618.2 | 1.06 | -0.99 | 2.02E-08 |

Samples were analyzed using LC–TOFMS in the ESI-positive mode and demonstrated by peak area. Metabolites were selected when VIP values were >1.0, p value was <0.001, and S-plot [p(corr)] value was >0.75 and <–0.75, based on the results of control cells versus 16-hr FA (16:0)-treated cells.

**Table S2.** Significant changes in metabolites produced by palmitic acid-treated (FA16:0) HepG2 cells (in ESI-negative mode)

| ID | m/z | Con_4HR | Con_8HR | Con_16HR | Con_24HR | FA16:0_4HR | FA16:0_8HR | FA16:0_16HR | FA16:0_24HR | VIP 16:0 (16Hr) | S-Plot 16:0 (16Hr) | FA 16:0 P-value (16Hr) |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| PC(32:0) | 778.5676 | 817.2±212.4 | 771.0±328.1 | 950.3±274.4 | 781.8±300.5 | 28964.7±5837.3 | 64428.0±9529.7 | 69997.9±9882.7 | 50269.1±3140.9 | 12.84 | -0.99 | 2.77E-08 |
| PC(36:2) | 830.5960 | 4743.9±739.0 | 5883.5±773.4 | 6184.3±1208.3 | 5792.8±364.6 | 3150.5±769.2 | 2187.9±597.1 | 413.5±248.3 | 48.1±42.5 | 3.67 | 0.97 | 2.92E-07 |
| PC(32:1) | 776.5490 | 5200.8±1431.9 | 6672.3±690.6 | 8367.7±1513.5 | 8655.0±973.2 | 7484.5±1866.1 | 12066.8±2163.5 | 14002.7±3149.8 | 13805.8±1215.1 | 3.25 | -0.75 | 0.0002 |
| PE(36:2) | 742.5421 | 1128.1±370.8 | 1814.6±524.2 | 2401.3±427.8 | 1874.4±550.5 | 1018.8±444.4 | 716.5±381.1 | 37.0±32.6 | 44.4±50.0 | 2.36 | 0.98 | 1.60E-07 |
| Cer(d18:1/16:0) | 582.5118 | 0.0±0.0 | 0.0±0.0 | 3.7±11.0 | 0.0±0.0 | 75.9±78.1 | 816.8±244.7 | 1952.1±547.9 | 1586.6±574.4 | 2.11 | -0.95 | 5.20E-06 |
| PE(38:4) | 766.5427 | 3028.4±975.6 | 3396.6±601.9 | 3211.0±918.7 | 2070.2±507.3 | 2211.6±644.1 | 2937.6±809.2 | 1266.0±698.9 | 617.6±292.2 | 1.93 | 0.80 | 0.0001 |
| PE(38:5) | 764.5281 | 989.3±410.9 | 1323.0±289.3 | 1349.5±394.0 | 785.8±265.6 | 747.2±211.2 | 915.8±484.4 | 229.9±238.6 | 42.0±61.9 | 1.55 | 0.87 | 1.80E-06 |
| PC(34:2) | 802.5648 | 566.9±255.8 | 619.6±370.3 | 1072.6±404.4 | 1618.0±431.1 | 332.0±329.1 | 135.4±154.4 | 34.6±53.8 | 15.9±32.0 | 1.50 | 0.89 | 5.06E-05 |
| Cer(d18:1/24:1) | 692.6219 | 99.2±99.6 | 81.2±77.5 | 157.2±99.1 | 170.8±142.1 | 63.5±91.0 | 340.3±200.1 | 893.5±452.8 | 666.8±277.1 | 1.17 | -0.79 | 0.0009 |
| SM(d18:1/16:0) | 747.5687 | 632.2±178.5 | 805.5±255.3 | 713.3±244.3 | 762.9±370.5 | 599.1±252.4 | 625.7±241.8 | 106.4±80.0 | 125.9±142.2 | 1.13 | 0.88 | 3.95E-05 |
| PI(38:4) | 885.5551 | 812.0±257.1 | 865.3±305.3 | 644.1±239.6 | 321.6±310.0 | 667.7±278.7 | 653.8±276.0 | 55.3±92.1 | 186.4±143.7 | 1.11 | 0.88 | 3.68E-05 |

Samples were analyzed using LC–TOFMS in the ESI-negative mode and demonstrated by peak area. Metabolites were selected when VIP values were >1.0, p value was <0.001, and S-plot [p(corr)] value was >0.75) and <−0.75, based on the results of control cells versus 16-hr FA (16:0)-treated cells.

**Table S3.** Significant changes in metabolites produced by palmitoleic acid-treated (FA 16:1) HepG2 cells (in ESI-positive mode)

| ID | m/z | CON_4HR | CON_8HR | CON_16HR | CON_24HR | FA16:1_4HR | FA16:1_8HR | FA16:1_16HR | FA16:1_24HR | VIP 16:1 (16HR) | S-Plot 16:1 (16HR) | FA 16:1 P-value (16HR) |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| TG(48:3) | 818.7439 | 0.0±0.0 | 0.0±0.0 | 78.7±236.0 | 11.8±35.5 | 367162.6±46153.9 | 716009.0±199528.9 | 1077280.1±114992.2 | 1232628.4±138803.0 | 10.97 | -0.99 | 2.78E-09 |
| PC(32:2) | 730.5557 | 9.3±27.9 | 28.9±43.5 | 187.8±111.6 | 843.7±405.9 | 263883.5±16622.2 | 484101.9±24051.0 | 786079.0±80829.7 | 830999.9±65305.6 | 9.38 | -0.99 | 2.07E-09 |
| TG(50:3) | 846.7766 | 0.0±0.0 | 13.7±41.1 | 5205.8±10646.1 | 2728.3±7955.0 | 181411.1±16649.5 | 375873.9±106497.2 | 621077.2±83427.3 | 760821.2±50163.5 | 8.27 | -0.99 | 1.28E-08 |
| PC(34:1) | 760.6002 | 278665.7±14007.0 | 312040.0±18403.3 | 331564.7±26612.7 | 291665.3±20267.4 | 189759.5±16927.4 | 116532.5±9527.5 | 65276.4±8468.4 | 52262.8±5325.4 | 5.46 | 0.99 | 1.28E-10 |
| TG(48:2) | 820.7564 | 64.0±115.4 | 202.5±322.3 | 2601.4±3917.8 | 1503.3±3025.3 | 86035.1±12676.5 | 164619.8±58477.5 | 251458.2±31969.7 | 291774.9±24156.2 | 5.26 | -0.99 | 8.54E-09 |
| PC(32:1) | 732.5675 | 79483.9±3415.6 | 89803.3±3453.2 | 104516.1±8222.2 | 110212.9±7997.9 | 181771.7±16502.1 | 211236.7±15886.5 | 279813.5±37710.0 | 307584.7±32882.5 | 4.36 | -0.97 | 3.39E-07 |

| | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| PC(34:2) | 758.5779 | 20933.8±3166.1 | 21873.1±1557.1 | 27586.5±1728.5 | 36324.9±5152.7 | 70211.0±5318.3 | 89081.6±6660.8 | 141285.8±26257.3 | 169560.6±15879.7 | 3.50 | -0.97 | 1.10E-06 |
| TG(50:2) | 848.7869 | 19857.6±713.4 | 21855.0±4038.1 | 28224.3±3044.5 | 27046.5±3991.7 | 65965.7±8821.1 | 105294.7±32443.4 | 129290.1±23259.7 | 152140.5±9983.8 | 3.30 | -0.96 | 8.96E-07 |
| Unknown | 663.4700 | 799568.6±50590.3 | 748757.8±41446.1 | 712553.4±12742.9 | 724388.5±39594.9 | 781494.9±17919.9 | 787933.0±25870.7 | 806877.0±27431.1 | 776469.6±45240.7 | 3.13 | -0.92 | 1.17E-06 |
| TG(50:6) | 823.7055 | 0.0±0.0 | 0.0±0.0 | 0.0±0.0 | 0.0±0.0 | 44266.2±1848.7 | 54724.4±19343.8 | 86378.1±18990.2 | 106811.0±14235.9 | 3.06 | -0.96 | 8.01E-07 |
| PC(36:2) | 786.6069 | 69746.6±4876.9 | 73574.0±3341.9 | 75936.7±4271.8 | 75220.0±4247.1 | 48508.2±3437.8 | 25630.9±2778.6 | 6687.1±3483.4 | 5350.5±1447.1 | 2.79 | 0.99 | 4.67E-17 |
| PC(34:5) | 752.5308 | 0.0±0.0 | 0.0±0.0 | 0.0±0.0 | 0.0±0.0 | 10487.6±1185.4 | 25048.7±1745.3 | 51101.6±7717.4 | 60074.8±6155.3 | 2.38 | -0.98 | 4.30E-08 |
| TG(52:6) | 851.7229 | 0.0±0.0 | 0.0±0.0 | 0.0±0.0 | 0.0±0.0 | 21177.6±1480.6 | 25055.5±9595.1 | 33283.6±2549.0 | 31723.8±3582.4 | 1.93 | -0.99 | 1.98E-10 |
| PC(32:0) | 734.5834 | 24691.7±1153.3 | 27339.0±1408.9 | 28110.2±2361.7 | 22855.4±694.3 | 6387.0±864.7 | 4392.1±1050.3 | 2345.0±996.9 | 2713.5±789.3 | 1.70 | 0.99 | 9.59E-12 |
| Unknown | 547.4798 | 3.6±10.7 | 0.1±0.3 | 3.1±9.4 | 0.0±0.1 | 4917.3±855.8 | 11952.8±4200.1 | 19665.0±2820.3 | 24361.5±4434.6 | 1.48 | -0.99 | 2.87E-08 |
| TG(46:2) | 792.7162 | 0.0±0.0 | 0.0±0.0 | 0.0±0.0 | 6.9±20.7 | 3707.0±710.7 | 9357.8±3724.4 | 18936.4±3447.0 | 24989.2±3494.9 | 1.44 | -0.98 | 1.85E-07 |
| TG(54:3) | 902.8331 | 25915.6±9851.4 | 30433.3±5880.7 | 37430.3±12674.6 | 39931.7±11616.3 | 28905.3±2619.0 | 23884.9±4941.7 | 14630.0±1127.9 | 12311.5±1107.7 | 1.44 | 0.77 | 0.0006 |
| Unknown | 550.6327 | 125116.8±9407.2 | 118161.6±8962.9 | 110114.6±5635.4 | 116011.9±5920.7 | 124734.0±4189.7 | 125828.7±6165.7 | 130605.2±6787.1 | 122276.3±7393.7 | 1.42 | -0.87 | 3.17E-06 |
| PC(30:0) | 706.5420 | 8858.9±487.9 | 12793.9±694.9 | 17418.2±1328.8 | 14600.5±4574.1 | 1049.5±463.8 | 107.1±98.2 | 29.1±58.3 | 0.0±0.0 | 1.40 | 0.99 | 1.84E-10 |
| Unknown | 845.7478 | 0.0±0.0 | 0.0±0.0 | 0.0±0.0 | 0.0±0.0 | 5857.5±698.9 | 9020.4±3490.4 | 12943.5±1123.5 | 13517.7±779.9 | 1.21 | -1.00 | 5.37E-10 |
| Unknown | 839.6623 | 0.0±0.0 | 0.0±0.0 | 0.0±0.0 | 0.0±0.0 | 8614.8±651.1 | 9876.5±3743.9 | 12443.1±790.1 | 11916.2±648.6 | 1.18 | -0.99 | 4.45E-11 |
| Unknown | 685.4397 | 115411.3±8263.3 | 107016.9±6173.2 | 102738.3±3241.3 | 105055.5±7083.1 | 113082.3±2514.1 | 112498.1±4602.1 | 116834.0±5707.9 | 112247.4±7656.1 | 1.16 | -0.85 | 8.14E-06 |
| TG(52:5) | 853.7338 | 682.4±656.1 | 1270.9±608.0 | 1988.6±1359.4 | 2680.7±1121.6 | 8963.2±1606.1 | 10749.3±3693.3 | 12987.6±989.1 | 13420.5±1567.9 | 1.10 | -0.99 | 1.28E-12 |
| TG(50:5) | 825.7069 | 0.0±0.0 | 0.0±0.0 | 17.3±51.9 | 0.0±0.0 | 9068.2±1002.6 | 10869.0±4265.5 | 11548.7±4572.5 | 12542.3±1593.2 | 1.07 | -0.90 | 6.50E-05 |
| Unknown | 707.4953 | 112909.2±7529.7 | 105143.7±5190.7 | 100492.3±3647.6 | 102071.8±5580.9 | 109586.4±3986.4 | 112255.4±4089.8 | 112835.0±5315.6 | 108636.8±7810.9 | 1.07 | -0.83 | 3.02E-05 |
| Unknown | 522.6005 | 88313.0±5014.0 | 82282.2±5019.8 | 78640.1±1698.9 | 80146.2±5061.0 | 86482.6±2150.7 | 87747.9±3126.4 | 89225.3±3325.2 | 85906.9±6027.6 | 1.04 | -0.90 | 2.49E-07 |

Samples were analyzed by LC–TOFMS in the ESI-positive mode and demonstrated by peak area. Metabolites were selected when the VIP values were >1.0), p value was <0.001, and S-plot [p(corr)] was >0.75 and <−0.75, based on the results of control cells versus 16-hr FA (16:1)-treated cells.

**Table S4.** Significant changes in metabolites produced by palmitoleic acid-treated (FA 16:1) HepG2 cells (in ESI-negative mode)

| ID | | Con_4HR | Con_8HR | Con_16HR | Con_24HR | FA16:1_4HR | FA16:1_8HR | FA16:1_16HR | FA16:1_24HR | VIP 16:1 (16Hr) | S-Plot 16:1 (16Hr) | FA 16:1 P-value (16Hr) |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| PC(32:2) | 774.5402 | 0.0±0.0 | 0.0±0.0 | 0.0±0.0 | 0.0±0.0 | 16945.1±1691.8 | 30765.9±5410.2 | 51421.7±10287.2 | 55065.7±3237.7 | 9.92 | -0.97 | 3.86E-07 |
| PC(34:1) | 804.5809 | 24676.9±2774.5 | 26436.3±1595.5 | 27414.5±3075.6 | 25221.5±1956.2 | 15470.6±1286.9 | 9371.6±1673.5 | 3400.0±1386.7 | 1901.8±261.1 | 6.84 | 0.99 | 2.22E-10 |
| PC(34:2) | 802.5648 | 566.9±255.8 | 619.6±370.3 | 1072.6±404.4 | 1618.0±431.1 | 5155.7±594.0 | 7654.5±1840.2 | 12206.9±2930.7 | 13908.3±938.4 | 4.56 | -0.95 | 2.52E-06 |
| PC(32:1) | 776.5490 | 5200.8±1431.9 | 6672.3±690.6 | 8367.7±1513.5 | 8655.0±973.2 | 12440.2±1252.7 | 14161.2±2511.2 | 17272.9±3876.7 | 18536.5±1323.5 | 3.87 | -0.85 | 6.44E-05 |
| PC(36:2) | 830.5960 | 4743.9±739.0 | 5883.5±773.4 | 6184.3±1208.3 | 5792.8±364.6 | 2061.2±374.7 | 656.6±312.3 | 22.3±26.9 | 14.2±21.4 | 3.44 | 0.98 | 3.28E-07 |
| PE(34:2) | 714.5107 | 5.8±17.4 | 0.0±0.0 | 102.4±101.2 | 42.0±55.0 | 428.0±318.5 | 1652.7±779.0 | 5882.2±1943.2 | 7378.6±613.7 | 3.23 | -0.92 | 1.93E-05 |
| PE(32:2) | 686.4791 | 0.0±0.0 | 0.0±0.0 | 0.0±0.0 | 0.0±0.0 | 122.4±79.4 | 969.3±277.6 | 3006.4±977.6 | 3405.1±333.4 | 2.34 | -0.93 | 1.54E-05 |
| PE(36:2) | 742.5421 | 1128.1±370.8 | 1814.6±524.2 | 2401.3±427.8 | 1874.4±550.5 | 748.2±139.0 | 301.5±148.5 | 149.4±168.3 | 56.0±53.6 | 2.07 | 0.98 | 2.67E-08 |
| PE(38:5) | 764.5281 | 989.3±410.9 | 1323.0±289.3 | 1349.5±394.0 | 785.8±265.6 | 1135.3±321.4 | 558.9±198.5 | 271.4±219.0 | 280.2±132.6 | 1.37 | 0.87 | 2.21E-06 |
| PC(32:0) | 778.5676 | 817.2±212.4 | 771.0±328.1 | 950.3±274.4 | 781.8±300.5 | 36.8±51.9 | 3.2±9.6 | 12.2±24.2 | 9.4±18.6 | 1.32 | 0.93 | 6.45E-06 |

Samples were analyzed by LC–TOFMS in the ESI-negative mode and demonstrated by peak area. Metabolites were selected when the VIP values were >1.0, p value was <0.001, and S-plot [p(corr)] was >0.75 and <−0.75, based on the results of control cells versus 16-hr FA (16:1)-treated cells.

**Table S5.** Stable isotope-labeled metabolites in 13C16-palmitic acid (isoFA 16:0)- and 13C16-palmitoleic acid (isoFA 16:1)-treated HepG2 cells

| ID | Adduct | m/z | Con_4hr | IsoFA_4hr | Con_8hr | IsoFA_8hr | Con_16hr | IsoFA_16hr | Source_Mode |
|---|---|---|---|---|---|---|---|---|---|
| Cer(d18:0/16:0) | M+H | 540.5368 | 10.0±0.0 | 10.0±0.0 | 10.0±0.0 | 10.0±0.0 | 10.0±0.0 | 12.0±6.1 | C16:0_POS |
| Cer(d18:0/16:0)+16 | | 556.5900 | 10.0±0.0 | 10.0±0.0 | 10.0±0.0 | 67.2±41.5 | 10.0±0.0 | 570.5±201.4 | C16:0_POS |
| Cer(d18:0/16:0)+32 | | 572.6449 | 10.0±0.0 | 10.0±0.0 | 10.0±0.0 | 2602.0±388.1 | 10.0±0.0 | 5665.3±562.5 | C16:0_POS |
| Cer(d18:1/16:0) | M+Na | 560.5035 | 13.8±11.4 | 10.0±0.0 | 22.6±25.2 | 22.4±28.5 | 14.2±12.5 | 148.2±188.1 | C16:0_POS |
| Cer(d18:1/16:0)+16 | | 576.5558 | 10.0±0.0 | 983.7±176.1 | 10.0±0.0 | 2206.3±400.4 | 10.0±0.0 | 3119.0±513.7 | C16:0_POS |
| Cer(d18:1/16:0)+32 | | 592.6093 | 10.0±0.0 | 10.0±0.0 | 10.0±0.0 | 719.0±432.8 | 10.0±0.0 | 2595.1±678.2 | C16:0_POS |
| DG(32:0) | M+Na | 591.5009 | 32.8±37.2 | 22.7±19.5 | 40.7±47.2 | 50.0±48.4 | 22.5±20.9 | 23.3±39.9 | C16:0_POS |

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|---|---|---|---|---|---|---|---|---|---|
| DG(32:0)+16 | | 607.5494 | 10.0±0.0 | 3066.0±946.7 | 10.0±0.0 | 10250.4±561.1 | 34.4±40.0 | 10520.0±1232.1 | C16:0_POS |
| DG(32:0)+32 | | 623.6092 | 22.0±36.1 | 34571.9±2646.5 | 10.0±0.0 | 78315.2±4868.8 | 75.9±152.7 | 72488.9±9143.8 | C16:0_POS |
| Palmitoylcarnitine | M+H | 400.3426 | 21.4±12.8 | 10.7±2.0 | 138.2±82.0 | 24.5±17.9 | 21.9±20.0 | 16.8±20.5 | C16:0_POS |
| Palmitoylcarnitine+16 | | 416.3970 | 10.0±0.0 | 1983.7±654.2 | 10.0±0.0 | 3636.0±274.7 | 10.0±0.0 | 3161.3±412.6 | C16:0_POS |
| LysoPC(16:0) | M+H | 496.3425 | 559.9±163.1 | 2425.1±218.6 | 938.5±108.6 | 3169.1±297.4 | 1041.6±220.7 | 2824.5±333.6 | C16:0_POS |
| LysoPC(16:0)+16 | | 512.3983 | 12.6±7.9 | 3807.3±231.4 | 10.0±0.0 | 11477.0±645.4 | 10.0±0.0 | 14848.5±1430.2 | C16:0_POS |
| PC(30:0) | M+H | 706.5519 | 74787.4±13074.2 | 35500.5±2830.7 | 97698.6±11396.6 | 31924.2±1317.9 | 117557.3±11476.7 | 25488.0±2423.8 | C16:0_POS |
| PC(30:0)+16 | | 722.6000 | 10.0±0.0 | 16888.1±921.9 | 10.0±0.0 | 47835.3±2075.4 | 10.0±0.0 | 76511.2±2610.0 | C16:0_POS |
| PC(32:0) | M+H | 734.5852 | 163331.5±27744.0 | 70026.1±5853.4 | 180209.6±24506.5 | 64799.9±3500.6 | 184835.0±22658.4 | 60313.7±8229.6 | C16:0_POS |
| PC(32:0)+16 | | 750.6413 | 4410.9±6627.2 | 275207.3±26907.2 | 10.0±0.0 | 555069.0±25538.4 | 150.7±266.3 | 628466.7±63314.6 | C16:0_POS |
| PC(32:0)+32 | | 766.6970 | 16367.0±24575.1 | 797537.6±58026.6 | 381.8±511.5 | 1782316.9±88497.7 | 2009.1±2955.7 | 1990163.6±190498.4 | C16:0_POS |
| PC(34:0) | M+H | 762.6056 | 15951.0±3124.8 | 10256.9±1257.0 | 19516.1±2782.9 | 13648.0±1010.7 | 18213.6±2748.4 | 9914.3±1091.7 | C16:0_POS |
| PC(34:0)+16 | | 778.6593 | 10.0±0.0 | 8224.1±731.9 | 10.0±0.0 | 29634.3±1646.4 | 10.0±0.0 | 36073.8±4215.6 | C16:0_POS |
| PC(34:1) | M+H | 760.6054 | 1169330.2±75071.1 | 866152.1±61126.8 | 1149825.8±99006.5 | 667168.0±31426.0 | 1289932.6±71374.6 | 523559.5±22612.3 | C16:0_POS |
| PC(34:1)+16 | | 776.6590 | 10.0±0.0 | 293350.6±22659.4 | 10.0±0.0 | 768481.8±24480.9 | 10.0±0.0 | 1153439.7±40080.8 | C16:0_POS |
| PC(34:2) | M+H | 758.5771 | 67936.8±6033.5 | 45225.4±2348.7 | 68093.3±9479.2 | 30949.7±1760.3 | 74997.2±5847.6 | 26406.4±1723.0 | C16:0_POS |
| PC(34:2)+16 | | 774.6299 | 10.0±0.0 | 19950.3±1317.2 | 10.0±0.0 | 39363.5±1277.7 | 10.0±0.0 | 57265.7±3493.8 | C16:0_POS |
| PC(34:3) | M+H | 756.5633 | 17986.3±3761.8 | 312.8±318.6 | 19999.6±2288.4 | 80.6±85.8 | 20271.6±1899.6 | 77.5±50.5 | C16:0_POS |
| PC(34:3)+16 | | 772.6163 | 119.4±203.6 | 8803.2±1510.8 | 14.8±14.4 | 9399.8±1687.7 | 41.0±53.3 | 8543.1±1751.8 | C16:0_POS |
| PC(34:3)+32 | | 788.6731 | 2137.9±3222.4 | 71088.4±4899.4 | 10.0±0.0 | 110785.7±8034.0 | 10.0±0.0 | 100343.4±7429.9 | C16:0_POS |
| PC(34:4) | M+H | 754.5436 | 50325.9±3864.7 | 27032.3±1281.1 | 53672.6±4669.6 | 12915.7±1380.0 | 65063.3±2984.2 | 6213.3±515.8 | C16:0_POS |
| PC(34:4)+16 | | 770.5928 | 172.5±204.5 | 14256.7±1144.6 | 323.9±280.7 | 25803.6±1550.8 | 292.8±150.5 | 31748.3±915.0 | C16:0_POS |
| PC(34:4)+32 | | 786.6461 | 10.0±0.0 | 10548.5±1171.7 | 10.0±0.0 | 18196.3±713.2 | 10.0±0.0 | 26526.2±2064.5 | C16:0_POS |
| PC(36:3) | M+H | 784.5896 | 20258.5±1438.3 | 14502.6±1180.3 | 18012.7±2570.3 | 9609.4±1123.2 | 18360.1±1485.5 | 8709.4±342.2 | C16:0_POS |
| PC(36:3)+16 | | 800.6433 | 10.0±0.0 | 5455.6±486.8 | 10.0±0.0 | 11864.4±518.8 | 10.0±0.0 | 17214.3±692.9 | C16:0_POS |
| PC(36:4) | M+H | 782.5753 | 17575.3±959.3 | 3876.4±501.9 | 19827.5±2454.3 | 2066.9±805.2 | 18058.6±1159.8 | 2014.1±740.5 | C16:0_POS |

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|---|---|---|---|---|---|---|---|---|---|
| PC(36:4)+16 | | 798.6296 | 10.0±0.0 | 13627.1±1192.9 | 10.0±0.0 | 21727.7±1263.0 | 10.0±0.0 | 29142.2±1455.9 | C16:0_POS |
| PC(38:6) | M+H | 806.5744 | 6066.5±871.1 | 516.7±421.1 | 6678.8±1504.5 | 114.9±133.7 | 5895.7±660.0 | 96.8±133.8 | C16:0_POS |
| PC(38:6)+16 | | 822.6280 | 10.0±0.0 | 3651.1±629.7 | 10.0±0.0 | 7049.6±358.6 | 10.0±0.0 | 9114.9±490.4 | C16:0_POS |
| SM(d18:1/16:0) | M+H | 703.5923 | 220582.8±30495.9 | 195576.0±12880.1 | 253114.8±28417.6 | 201590.3±16795.6 | 279210.8±23394.4 | 165626.8±14622.4 | C16:0_POS |
| SM(d18:1/16:0)+32 | | 735.6562 | 10.0±0.0 | 303.2±140.2 | 10.0±0.0 | 5508.7±1052.9 | 10.0±0.0 | 9578.7±1503.3 | C16:0_POS |
| TG(50:1) | M+NH4 | 850.7936 | 15662.6±1121.2 | 11080.9±853.2 | 17412.0±2467.0 | 9635.8±665.7 | 15498.8±1175.0 | 4401.1±1060.6 | C16:0_POS |
| TG(50:1)+16 | | 866.8460 | 10.0±0.0 | 169.8±264.7 | 10.0±0.0 | 1247.0±615.7 | 10.0±0.0 | 667.5±552.9 | C16:0_POS |
| TG(50:2) | M+NH4 | 848.7792 | 22422.6±1363.4 | 22496.7±1459.3 | 25650.7±2251.4 | 19675.8±733.5 | 22872.7±3050.0 | 12900.9±755.6 | C16:0_POS |
| TG(50:2)+16 | | 864.8303 | 10.0±0.0 | 754.0±381.1 | 10.0±0.0 | 1890.5±608.0 | 10.0±0.0 | 2410.6±738.8 | C16:0_POS |
| TG(52:2) | M+NH4 | 876.8211 | 87856.8±8686.5 | 72794.5±4502.0 | 93177.2±9616.4 | 63522.7±4714.9 | 80807.6±13766.4 | 36621.1±2541.0 | C16:0_POS |
| TG(52:2)+16 | | 892.8635 | 10.0±0.0 | 2362.3±575.3 | 10.0±0.0 | 5949.8±912.7 | 10.0±0.0 | 6619.9±1093.2 | C16:0_POS |
| LysoPE(16:0) | M-H | 452.2783 | 10.0±0.0 | 108.5±102.2 | 15.0±15.1 | 269.9±99.3 | 10.0±0.0 | 318.8±170.1 | C16:0_NEG |
| LysoPE(16:0)+16 | | 468.3328 | 10.0±0.0 | 172.0±85.7 | 10.0±0.0 | 1202.8±452.5 | 10.0±0.0 | 1777.1±202.0 | C16:0_NEG |
| LysoPA(16:0) | M-H | 409.2330 | 10.0±0.0 | 22.46±2.22 | 10.0±0.0 | 29.58±2.45 | 10.0±0.0 | 31.17±9.65 | C16:0_NEG |
| LysoPA(16:0)+16 | | 425.2876 | 10.0±0.0 | 262.95±18.59 | 10.0±0.0 | 342.94±32.70 | 10.0±0.0 | 378.62±131.12 | C16:0_NEG |
| PC(32:1) | M+FA-H | 776.5524 | 56275.0±5746.6 | 41267.2±3979.5 | 61714.9±3496.1 | 33376.0±3080.2 | 71078.6±6763.5 | 25298.8±1916.9 | C16:0_NEG |
| PC(32:1)+16 | | 792.6031 | 10.0±0.0 | 17486.2±1417.8 | 10.0±0.0 | 37603.0±3518.0 | 10.0±0.0 | 55051.3±4080.7 | C16:0_NEG |
| PC(32:1)+32 | | 808.6571 | 10.0±0.0 | 12313.9±1440.0 | 10.0±0.0 | 23141.6±2632.1 | 10.0±0.0 | 40263.6±4825.4 | C16:0_NEG |
| PC(36:3) | M+FA-H | 828.5793 | 2851.1±330.2 | 1363.5±370.9 | 2376.7±635.4 | 483.9±202.1 | 2285.7±424.2 | 342.6±137.9 | C16:0_NEG |
| PC(36:3)+16 | | 844.6332 | 10.0±0.0 | 384.2±204.7 | 10.0±0.0 | 1844.4±435.0 | 10.0±0.0 | 3534.1±629.7 | C16:0_NEG |
| PE(32:0) | M-H | 690.5093 | 10.0±0.0 | 10.0±0.0 | 10.0±0.0 | 10.0±0.0 | 10.0±0.0 | 10.0±0.0 | C16:0_NEG |
| PE(32:0)+32 | | 722.6169 | 10.0±0.0 | 731.0±360.0 | 10.0±0.0 | 3338.6±454.9 | 10.0±0.0 | 3059.1±1421.0 | C16:0_NEG |
| PE(34:0) | M-H | 718.5415 | 80.3±73.2 | 10.0±0.0 | 55.1±30.7 | 10.0±0.0 | 130.7±77.0 | 10.0±0.0 | C16:0_NEG |
| PE(34:0)+32 | | 750.6495 | 10.0±0.0 | 1505.3±302.7 | 10.0±0.0 | 5733.5±730.4 | 10.0±0.0 | 6936.0±837.5 | C16:0_NEG |
| PE(34:1) | M-H | 716.5256 | 15749.6±1264.2 | 12387.9±1008.8 | 18937.8±1223.1 | 14811.6±1441.1 | 19612.8±1185.9 | 11543.3±409.7 | C16:0_NEG |
| PE(34:1)+16 | | 732.5796 | 10.0±0.0 | 4036.9±525.4 | 10.0±0.0 | 11859.4±1006.6 | 10.0±0.0 | 17463.5±1101.1 | C16:0_NEG |

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|---|---|---|---|---|---|---|---|---|---|
| PE(36:4) | M-H | 738.5101 | 6663.0±690.5 | 6419.1±798.5 | 7138.2±570.9 | 6288.8±707.4 | 7466.5±820.6 | 4552.2±467.6 | C16:0_NEG |
| PE(36:4)+16 | | 754.5640 | 10.0±0.0 | 2624.2±482.1 | 10.0±0.0 | 6504.8±1072.1 | 10.0±0.0 | 9003.6±559.6 | C16:0_NEG |
| PI(32:0) | M-H | 809.5215 | 10.0±0.0 | 10.0±0.0 | 10.0±0.0 | 10.0±0.0 | 10.0±0.0 | 10.0±0.0 | C16:0_NEG |
| PI(32:0)+32 | | 841.6296 | 10.0±0.0 | 75.6±92.4 | 10.0±0.0 | 2182.8±335.9 | 10.0±0.0 | 1535.0±588.7 | C16:0_NEG |
| PI(34:1) | M-H | 835.5378 | 646.7±380.7 | 212.9±111.1 | 1695.0±372.9 | 974.2±371.8 | 2726.9±454.5 | 823.1±706.0 | C16:0_NEG |
| PI(34:1)+16 | | 851.5912 | 10.0±0.0 | 1762.1±471.2 | 10.0±0.0 | 7823.9±1283.2 | 10.0±0.0 | 7861.0±3280.9 | C16:0_NEG |
| PI(36:4) | M-H | 857.5224 | 336.6±169.6 | 190.4±89.0 | 647.0±225.5 | 77.7±81.0 | 702.2±221.4 | 58.9±81.0 | C16:0_NEG |
| PI(36:4)+16 | | 873.5765 | 10.0±0.0 | 397.9±209.1 | 10.0±0.0 | 2687.9±634.4 | 10.0±0.0 | 2054.2±1123.0 | C16:0_NEG |
| DG(32:2) | M+Na | 587.4669 | 10.0±0.0 | 10.0±0.0 | 10.0±0.0 | 10.0±0.0 | 10.0±0.0 | 10.0±0.0 | C16:1_POS |
| DG(32:2)+16 | | 603.4402 | 10.0±0.0 | 10.0±0.0 | 10.0±0.0 | 10.0±0.0 | 10.0±0.0 | 10.0±0.0 | C16:1_POS |
| DG(32:2)+32 | | 619.5742 | 10.0±0.0 | 10.0±0.0 | 10.0±0.0 | 1914.7±671.2 | 10.0±0.0 | 4762.6±1163.7 | C16:1_POS |
| PC(32:1) | M+H | 732.5704 | 261362.6±20069.0 | 137800.2±20248.3 | 267691.0±6580.3 | 63903.1±12781.2 | 399882.2±19686.4 | 49645.2±5791.7 | C16:1_POS |
| PC(32:1)+16 | | 748.6245 | 10.0±0.0 | 198972.1±21074.0 | 10.0±0.0 | 250079.6±42882.3 | 10.0±0.0 | 706240.8±93155.4 | C16:1_POS |
| PC(32:2) | M+H | 730.5546 | 4132.9±955.2 | 348.0±150.3 | 4238.2±23.6 | 10.0±0.0 | 10564.1±655.2 | 10.0±0.0 | C16:1_POS |
| PC(32:2)+16 | | 746.5989 | 10.0±0.0 | 22240.5±3012.6 | 10.0±0.0 | 29161.0±5412.1 | 10.0±0.0 | 69359.9±8237.4 | C16:1_POS |
| PC(32:2)+32 | | 762.6665 | 10.0±0.0 | 307009.6±24299.2 | 10.0±0.0 | 470442.1±78570.2 | 10.0±0.0 | 1357526.2±160707.8 | C16:1_POS |
| PC(34:1) | M+H | 760.6043 | 694019.7±36635.0 | 457586.7±53195.6 | 712287.9±8487.7 | 230274.5±52238.0 | 954359.2±74985.4 | 169310.5±22954.7 | C16:1_POS |
| PC(34:1)+16 | | 776.6444 | 10.0±0.0 | 3624.4±1169.6 | 10.0±0.0 | 6377.5±1933.0 | 10.0±0.0 | 26144.6±3498.1 | C16:1_POS |
| PC(34:4) | M+H | 754.5421 | 6072.8±1163.6 | 941.4±866.0 | 6567.6±230.9 | 90.2±113.5 | 13498.4±1828.6 | 546.2±204.4 | C16:1_POS |
| PC(34:4)+16 | | 770.5947 | 10.0±0.0 | 5557.7±1793.0 | 10.0±0.0 | 8151.4±2175.4 | 10.0±0.0 | 31120.9±4601.3 | C16:1_POS |
| PC(34:5) | M+H | 752.5324 | 10.0±0.0 | 10.0±0.0 | 10.0±0.0 | 10.0±0.0 | 16.5±9.2 | 10.0±0.0 | C16:1_POS |
| PC(34:5)+32 | | 784.6444 | 10.0±0.0 | 13616.9±3265.2 | 10.0±0.0 | 27261.1±6651.6 | 10.0±0.0 | 97049.1±13202.9 | C16:1_POS |
| TG(48:3) | M+NH4 | 818.7466 | 10.0±0.0 | 10.0±0.0 | 10.0±0.0 | 10.0±0.0 | 10.0±0.0 | 10.0±0.0 | C16:1_POS |
| TG(48:3)+32 | | 850.8450 | 10.0±0.0 | 8247.6±245.2 | 10.0±0.0 | 13449.3±1296.0 | 10.0±0.0 | 44074.3±11518.0 | C16:1_POS |
| TG(48:3)+48 | | 866.9099 | 10.0±0.0 | 209471.5±2955.9 | 10.0±0.0 | 302325.2±24208.9 | 10.0±0.0 | 642343.0±153250.4 | C16:1_POS |
| TG(48:2) | M+NH4 | 820.7564 | 6304.0±442.6 | 5628.8±977.9 | 6966.2±264.7 | 2714.7±213.5 | 8008.6±1445.2 | 2603.6±1280.4 | C16:1_POS |

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| TG(48:2)+32 | | 852.8639 | 10.0±0.0 | 40790.6±1755.3 | 10.0±0.0 | 62950.3±3779.4 | 10.0±0.0 | 147369.7±36567.1 | C16:1_POS |
| TG(50:2) | M+NH4 | 848.7876 | 34175.6±3890.3 | 24212.4±2662.3 | 37990.5±892.4 | 14237.3±1022.2 | 54913.4±7560.3 | 16490.6±4412.7 | C16:1_POS |
| TG(50:2)+32 | | 880.8791 | 146.7±122.5 | 4775.6±473.9 | 151.2±47.9 | 5135.8±804.8 | 327.2±354.6 | 13901.9±4095.9 | C16:1_POS |
| TG(52:3) | M+NH4 | 874.7981 | 18727.3±2060.6 | 10092.5±751.2 | 20131.3±334.8 | 3458.6±742.9 | 27896.2±4341.3 | 2223.5±1316.0 | C16:1_POS |
| TG(52:3)+16 | | 890.8469 | 10.0±0.0 | 2325.9±257.3 | 10.0±0.0 | 2764.2±544.4 | 10.0±0.0 | 7901.2±3237.8 | C16:1_POS |
| PC(34:2) | M+FA-H | 802.5661 | 12485.7±2060.9 | 3848.3±649.8 | 11458.3±1150.9 | 861.1±341.5 | 17435.3±2776.4 | 138.0±61.3 | C16:1_NEG |
| PC(34:2)+16 | | 818.6198 | 10.0±0.0 | 7413.4±1276.2 | 10.0±0.0 | 10463.1±565.9 | 10.0±0.0 | 13776.8±1018.3 | C16:1_NEG |
| PC(34:2)+32 | | 834.6735 | 10.0±0.0 | 1821.7±309.0 | 10.0±0.0 | 4812.2±392.0 | 10.0±0.0 | 12632.8±1285.1 | C16:1_NEG |
| PE(34:1) | M-H | 716.5273 | 4345.6±791.8 | 2208.6±918.2 | 4181.5±834.7 | 2256.3±605.3 | 7225.9±1459.7 | 2181.5±501.6 | C16:1_NEG |
| PE(34:1)+16 | | 732.5809 | 10.0±0.0 | 130.5±44.5 | 10.0±0.0 | 513.9±329.5 | 10.0±0.0 | 3232.9±431.3 | C16:1_NEG |
| PE(34:2) | M-H | 714.5121 | 2494.0±566.3 | 892.6±122.4 | 2679.9±264.7 | 163.1±166.0 | 4400.5±1177.0 | 173.4±74.2 | C16:1_NEG |
| PE(34:2)+16 | | 730.5658 | 10.0±0.0 | 1529.3±632.8 | 10.0±0.0 | 2998.6±855.1 | 10.0±0.0 | 6384.1±169.7 | C16:1_NEG |
| PE(34:2)+32 | | 746.6192 | 10.0±0.0 | 188.9±88.8 | 10.0±0.0 | 792.1±368.3 | 10.0±0.0 | 3581.4±217.9 | C16:1_NEG |
| PI(34:1) | M-H | 835.5392 | 10.0±0.0 | 10.0±0.0 | 10.0±0.0 | 10.0±0.0 | 37.3±47.3 | 10.0±0.0 | C16:1_NEG |
| PI(34:1)+16 | M-H | 851.5922 | 10.0±0.0 | 10.0±0.0 | 10.0±0.0 | 232.3±196.1 | 10.0±0.0 | 1351.0±53.3 | C16:1_NEG |

Samples were analyzed by LC–TOFMS in the ESI-positive or negative mode and demonstrated by peak area.

**Table S6.** In-house database.

| Neutral mass | Compound Id | Description | Formula |
|---|---|---|---|
| 268.2402 | Fatty acid | 10E-heptadecenoic acid | C17H32O2 |
| 254.2246 | Fatty acid | 9Z-hexadecenoic acid | C16H30O2 |
| 282.2559 | Fatty acid | 9Z-octadecenoic acid | C18H34O2 |
| 282.2559 | Fatty acid | 9E-octadecenoic acid | C18H34O2 |
| 310.2872 | Fatty acid | 11Z-eicosenoic acid | C20H38O2 |
| 338.3185 | Fatty acid | 13Z-docosenoic acid | C22H42O2 |
| 366.3498 | Fatty acid | 15Z-tetracosenoic acid | C24H46O2 |

| | | | |
|---|---|---|---|
| 256.2402 | Fatty acid | hexadecanoic acid | C16H32O2 |
| 270.2559 | Fatty acid | heptadecanoic acid | C17H34O2 |
| 284.2715 | Fatty acid | octadecanoic acid | C18H36O2 |
| 312.3028 | Fatty acid | Eicosanoic acid | C20H40O2 |
| 340.3341 | Fatty acid | docosanoic acid | C22H44O2 |
| 368.3654 | Fatty acid | tetracosanoic acid | C24H48O2 |
| 396.3967 | Fatty acid | hexacosanoic acid | C26H52O2 |
| 278.2246 | Fatty acid | 9Z,12Z,15Z-octadecatrienoic acid | C18H30O2 |
| 302.2246 | Fatty acid | 5Z,8Z,11Z,14Z,17Z-eicosapentaenoic acid | C20H30O2 |
| 280.2402 | Fatty acid | 9Z,12Z-octadecadienoic acid | C18H32O2 |
| 304.2402 | Fatty acid | 5Z,8Z,11Z,14Z-eicosatetraenoic acid | C20H32O2 |
| 312.2896 | Fatty acid | 5Z,8Z,11Z,14Z-eicosatetraenoic acid (5,6,8,9,11,12,14,15-d8) | C20H24D8O2 |
| 328.2402 | Fatty acid | 4Z,7Z,10Z,13Z,16Z,19Z-docosahexaenoic acid | C22H32O2 |
| 330.2559 | Fatty acid | 4,7,10,13,16-docosapentaenoic acid | C22H34O2 |
| 330.2559 | Fatty acid | 7,10,13,16,19-docosapentaenoic acid | C22H34O2 |
| 306.2559 | Fatty acid | 8Z,11Z,14Z-eicosatrienoic acid | C20H34O2 |
| 306.2559 | Fatty acid | 5Z,8Z,11Z-eicosatrienoic acid | C20H34O2 |
| 332.2715 | Fatty acid | 7Z,10Z,13Z,16Z-docosatetraenoic acid | C22H36O2 |
| 635.4526 | Phosphatidylethanolamine | PE 28:0 | $C_{33}H_{66}NO_8P$ |
| 663.4839 | Phosphatidylethanolamine | PE 30:0 | $C_{35}H_{70}N_1O_8P$ |
| 699.5203 | Phosphatidylethanolamine | PEp 34:2 | C39H74NO7P |
| 701.5359 | Phosphatidylethanolamine | PEp 34:1 | C39H76NO7P |
| 703.5516 | Phosphatidylethanolamine | PEp 34:0 | C39H78NO7P |
| 715.5152 | Phosphatidylethanolamine | PE 34:2 | C39H74NO8P |
| 717.5309 | Phosphatidylethanolamine | PE 34:1 | C39H76NO8P |
| 719.5465 | Phosphatidylethanolamine | PE 34:0 | C39H78NO8P |
| 721.5046 | Phosphatidylethanolamine | PEp 36:5 | C41H72NO7P |
| 723.5203 | Phosphatidylethanolamine | PEp 36:4 | C41H74NO7P |

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|---|---|---|---|
| 727.5516 | Phosphatidylethanolamine | PEp 36:2 | C41H78NO7P |
| 729.5672 | Phosphatidylethanolamine | PEp 36:1 | C41H80NO7P |
| 737.4996 | Phosphatidylethanolamine | PE 36:5 | C41H72NO8P |
| 737.4996 | Phosphatidylethanolamine | PE 36:5 | C41H72NO8P |
| 739.5152 | Phosphatidylethanolamine | PE 36:4 | C41H74NO8P |
| 741.5309 | Phosphatidylethanolamine | PE 36:3 | C41H76NO8P |
| 743.5465 | Phosphatidylethanolamine | PE 36:2 | C41H78NO8P |
| 745.5622 | Phosphatidylethanolamine | PE 36:1 | C41H80NO8P |
| 747.5203 | Phosphatidylethanolamine | PEp 38:6 | C43H74NO7P |
| 749.5359 | Phosphatidylethanolamine | PEp 38:5 | C43H76NO7P |
| 749.5359 | Phosphatidylethanolamine | PEp 38:5 | $C_{43}H_{76}NO_7P$ |
| 751.5516 | Phosphatidylethanolamine | PEp 38:4 | C43H78NO7P |
| 751.5516 | Phosphatidylethanolamine | PEp 38:4 | C43H78NO7P |
| 753.5672 | Phosphatidylethanolamine | PEp 38:3 | C43H80NO7P |
| 755.5829 | Phosphatidylethanolamine | PEp 38:2 | C43H82NO7P |
| 757.5985 | Phosphatidylethanolamine | PEp 38:1 | C43H84NO7P |
| 763.5152 | Phosphatidylethanolamine | PE 38:6 | C43H74NO8P |
| 763.5152 | Phosphatidylethanolamine | PE 38:6 | C43H74NO8P |
| 765.5309 | Phosphatidylethanolamine | PE 38:5 | $C_{45}H_{76}NO_8P$ |
| 765.5309 | Phosphatidylethanolamine | PE 38:5 | C43H76NO8P |
| 767.5465 | Phosphatidylethanolamine | PE 38:4 | C43H78NO8P |
| 773.5359 | Phosphatidylethanolamine | PEp 40:7 | C45H76NO7P |
| 775.5516 | Phosphatidylethanolamine | PEp 40:6 | C45H78NO7P |
| 777.5672 | Phosphatidylethanolamine | PEp 40:5 | $C_{45}H_{80}NO_7P$ |
| 779.5829 | Phosphatidylethanolamine | PEp 40:4 | C45H82NO7P |
| 781.5985 | Phosphatidylethanolamine | PEp 40:3 | $C_{45}H_{84}NO_7P$ |
| 783.6142 | Phosphatidylethanolamine | PEp 40:2 | $C_{45}H_{86}NO_7P$ |
| 785.6298 | Phosphatidylethanolamine | PEp 40:1 | C45H88NO7P |

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|---|---|---|---|
| 789.5309 | Phosphatidylethanolamine | PE 40:7 | C45H76NO8P |
| 791.5465 | Phosphatidylethanolamine | PE 40:6 | $C_{45}H_{78}NO_8P$ |
| 791.5465 | Phosphatidylethanolamine | PE 40:6 | C45H78NO8P |
| 793.5622 | Phosphatidylethanolamine | PE 40:5 | $C_{45}H_{80}NO_8P$ |
| 795.5778 | Phosphatidylethanolamine | PE 40:4 | $C_{45}H_{84}NO_8P$ |
| 797.5935 | Phosphatidylethanolamine | PE 40:3 | $C_{45}H_{84}NO_8P$ |
| 799.6091 | Phosphatidylethanolamine | PE 40:2 | $C_{45}H_{86}NO_8P$ |
| 465.2855 | Lysophosphatidylethanolamine | LPE 17:1 | C22H44NO7P |
| 425.2542 | Lysophosphatidylethanolamine | LPE 14:0 | C19H40NO7P |
| 451.2699 | Lysophosphatidylethanolamine | LPE 16:1 | C21H42NO7P |
| 453.2855 | Lysophosphatidylethanolamine | LPE 16:0 | C21H44NO7P |
| 479.3012 | Lysophosphatidylethanolamine | LPE 18:1 | C23H46NO7P |
| 481.3168 | Lysophosphatidylethanolamine | LPE 18:0 | C23H48NO7P |
| 501.2855 | Lysophosphatidylethanolamine | LPE 20:4 | C25H44NO7P |
| 503.3012 | Lysophosphatidylethanolamine | LPE 20:3 | C25H46NO7P |
| 505.3168 | Lysophosphatidylethanolamine | LPE 20:2 | C25H48NO7P |
| 507.3325 | Lysophosphatidylethanolamine | LPE 20:1 | C25H50NO7P |
| 509.3481 | Lysophosphatidylethanolamine | LPE 20:0 | C25H52NO7P |
| 499.2699 | Lysophosphatidylethanolamine | LPE 20:5 | C25H42NO7P |
| 525.2855 | Lysophosphatidylethanolamine | LPE 22:6 | C27H44NO7P |
| 527.3012 | Lysophosphatidylethanolamine | LPE 22:5 | $C_{27}H_{46}NO_7P$ |
| 529.3168 | Lysophosphatidylethanolamine | LPE 22:4 | C27H48NO7P |
| 666.4472 | Phosphatidylglycerol | PG 28:0 | C34H67O10P |
| 720.4941 | Phosphatidylglycerol | PG 32:1 | C38H73O10P |
| 722.5098 | Phosphatidylglycerol | PG 32:0 | C38H75O10P |
| 746.5098 | Phosphatidylglycerol | PG 34:2 | C40H75O10P |
| 748.5254 | Phosphatidylglycerol | PG 34:1 | C40H77O10P |
| 750.5411 | Phosphatidylglycerol | PG 34:0 | C40H79O10P |

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|---|---|---|---|
| 770.5098 | Phosphatidylglycerol | PG 36:4 | C42H75O10P |
| 772.5254 | Phosphatidylglycerol | PG 36:3 | C42H77O10P |
| 774.5411 | Phosphatidylglycerol | PG 36:2 | $C_{42}H_{79}O_{10}P$ |
| 776.5567 | Phosphatidylglycerol | PG 36:1 | C42H81O10P |
| 778.5724 | Phosphatidylglycerol | PG 36:0 | C42H83O10P |
| 794.5098 | Phosphatidylglycerol | PG 38:6 | C44H75O10P |
| 796.5254 | Phosphatidylglycerol | PG 38:5 | C44H77O10P |
| 798.5411 | Phosphatidylglycerol | PG 38:4 | C44H79O10P |
| 800.5567 | Phosphatidylglycerol | PG 38:3 | C44H81O10P |
| 820.5254 | Phosphatidylglycerol | PG 40:7 | C46H77O10P |
| 822.5411 | Phosphatidylglycerol | PG 40:6 | C46H79O10P |
| 824.5567 | Phosphatidylglycerol | PG 40:5 | $C_{46}H_{81}O_{10}P$ |
| 826.5724 | Phosphatidylglycerol | PG 40:4 | C46H83O10P |
| 810.5258 | Phosphatidylinositol | PI 32:0 | C41H79O13P |
| 808.5102 | Phosphatidylinositol | PI 32:1 | C41H77O13P |
| 806.4945 | Phosphatidylinositol | PI 32:2 | C41H75O13P |
| 838.5571 | Phosphatidylinositol | PI 34:0 | C43H83O13P |
| 836.5415 | Phosphatidylinositol | PI 34:1 | C43H81O13P |
| 834.5258 | Phosphatidylinositol | PI 34:2 | C43H79O13P |
| 866.5884 | Phosphatidylinositol | PI 36:0 | C45H87O13P |
| 864.5728 | Phosphatidylinositol | PI 36:1 | C45H85O13P |
| 862.5571 | Phosphatidylinositol | PI 36:2 | C45H83O13P |
| 860.5415 | Phosphatidylinositol | PI 36:3 | C45H81O13P |
| 858.5258 | Phosphatidylinositol | PI 36:4 | C45H79O13P |
| 856.5102 | Phosphatidylinositol | PI 36:5 | C45H77O13P |
| 890.5884 | Phosphatidylinositol | PI 38:2 | C47H87O13P |
| 888.5728 | Phosphatidylinositol | PI 38:3 | C47H85O13P |
| 886.5571 | Phosphatidylinositol | PI 38:4 | C47H83O13P |

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|---|---|---|---|
| 884.5415 | Phosphatidylinositol | PI 38:5 | C47H81O13P |
| 882.5258 | Phosphatidylinositol | PI 38:6 | C47H79O13P |
| 914.5884 | Phosphatidylinositol | PI 40:4 | C49H87O13P |
| 912.5728 | Phosphatidylinositol | PI 40:5 | $C_{49}H_{85}O_{13}P$ |
| 910.5571 | Phosphatidylinositol | PI 40:6 | C49H83O13P |
| 908.5415 | Phosphatidylinositol | PI 40:7 | C49H81O13P |
| 679.4424 | Phosphatidylserine | PS 28:0 | C34H66NO10P |
| 759.5050 | Phosphatidylserine | PS 34:2 | C40H74NO10P |
| 761.5207 | Phosphatidylserine | PS 34:1 | C40H76NO10P |
| 763.5363 | Phosphatidylserine | PS 34:0 | C40H78NO10P |
| 781.4894 | Phosphatidylserine | PS 36:5 | C42H72NO10P |
| 783.5050 | Phosphatidylserine | PS 36:4 | C42H74NO10P |
| 785.5207 | Phosphatidylserine | PS 36:3 | C42H76NO10P |
| 787.5363 | Phosphatidylserine | PS 36:2 | C42H78NO10P |
| 789.5520 | Phosphatidylserine | PS 36:1 | C42H80NO10P |
| 807.5050 | Phosphatidylserine | PS 38:6 | C44H74NO10P |
| 809.5207 | Phosphatidylserine | PS 38:5 | C44H76NO10P |
| 811.5363 | Phosphatidylserine | PS 38:4 | C44H78NO10P |
| 813.5520 | Phosphatidylserine | PS 38:3 | C44H80NO10P |
| 815.5676 | Phosphatidylserine | PS 38:2 | C44H82NO10P |
| 817.5833 | Phosphatidylserine | PS 38:1 | C44H84NO10P |
| 833.5207 | Phosphatidylserine | PS 40:7 | C46H76NO10P |
| 835.5363 | Phosphatidylserine | PS 40:6 | C46H78NO10P |
| 837.5520 | Phosphatidylserine | PS 40:5 | C46H80NO10P |
| 839.5676 | Phosphatidylserine | PS 40:4 | C46H82NO10P |
| 841.5833 | Phosphatidylserine | PS 40:3 | C46H84NO10P |
| 843.5989 | Phosphatidylserine | PS 40:2 | C46H86NO10P |
| 723.4591 | Sulfatide | C12 Sulfatide | $C_{36}H_{69}NO_{11}S$ |

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|---|---|---|---|
| 779.5217 | Sulfatide | C16 Sulfatide | C40H77NO11S |
| 795.5167 | Sulfatide | C16-OH Sulfatide | C40H77NO12S |
| 807.5530 | Sulfatide | C18 Sulfatide | C42H81NO11S |
| 823.5480 | Sulfatide | C18-OH Sulfatide | C42H81NO12S |
| 835.5843 | Sulfatide | C20 Sulfatide | C44H85NO11S |
| 851.5793 | Sulfatide | C20-OH Sulfatide | C44H85NO12S |
| 863.6156 | Sulfatide | C22 Sulfatide | C46H89NO11S |
| 879.6106 | Sulfatide | C22-OH Sulfatide | C46H89NO12S |
| 889.6313 | Sulfatide | C24:1 Sulfatide | C48H91NO11S |
| 905.6262 | Sulfatide | C24:1-OH Sulfatide | C48H91NO12S |
| 891.6469 | Sulfatide | C24 Sulfatide | C48H93NO11S |
| 907.6419 | Sulfatide | C24-OH Sulfatide | C48H93NO12S |
| 677.4996 | Phosphatidylcholine | PC 28:0 | C36H72NO8P |
| 731.5465 | Phosphatidylcholine | PC 32:1 | C40H78NO8P |
| 733.5622 | Phosphatidylcholine | PC 32:0 | C40H80NO8P |
| 755.5465 | Phosphatidylcholine | PC 34:3 | C42H78NO8P |
| 757.5622 | Phosphatidylcholine | PC 34:2 | C42H80NO8P |
| 759.5778 | Phosphatidylcholine | PC 34:1 | C42H82NO8P |
| 761.5935 | Phosphatidylcholine | PC 34:0 | C42H84NO8P |
| 779.5465 | Phosphatidylcholine | PC 36:5 | C44H78NO8P |
| 779.5465 | Phosphatidylcholine | PC 36:5 | C44H78NO8P |
| 781.5622 | Phosphatidylcholine | PC 36:4 | C44H80NO8P |
| 783.5778 | Phosphatidylcholine | PC 36:3 | C44H82NO8P |
| 785.5935 | Phosphatidylcholine | PC 36:2 | C44H84NO8P |
| 787.6091 | Phosphatidylcholine | PC 36:1 | C44H86NO8P |
| 789.6248 | Phosphatidylcholine | PC 36:0 | C44H88NO8P |
| 803.5465 | Phosphatidylcholine | PC 38:7 | C46H78NO8P |
| 805.5622 | Phosphatidylcholine | PC 38:6 | C46H80NO8P |

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|---|---|---|---|
| 807.5778 | Phosphatidylcholine | PC 38:5 | C46H82NO8P |
| 807.5778 | Phosphatidylcholine | PC 38:5 | C46H82NO8P |
| 807.5778 | Phosphatidylcholine | PC 38:5 | C46H82NO8P |
| 809.5935 | Phosphatidylcholine | PC 38:4 | C46H84NO8P |
| 829.5622 | Phosphatidylcholine | PC 40:8 | C48H80NO8P |
| 831.5778 | Phosphatidylcholine | PC 40:7 | C48H82NO8P |
| 833.5935 | Phosphatidylcholine | PC 40:6 | C48H84NO8P |
| 835.6091 | Phosphatidylcholine | PC 40:5 | C48H86NO8P |
| 837.6248 | Phosphatidylcholine | PC 40:4 | C48H88NO8P |
| 507.3325 | Lysophosphatidylcholine | LPC 17:1 | C25H50NO7P |
| 509.3481 | Lysophosphatidylcholine | LPC 17:0 | C25H52NO7P |
| 467.3012 | Lysophosphatidylcholine | LPC 14:0 | C22H46NO7P |
| 493.3168 | Lysophosphatidylcholine | LPC 16:1 | C24H48NO7P |
| 495.3325 | Lysophosphatidylcholine | LPC 16:0 | C24H50NO7P |
| 519.3325 | Lysophosphatidylcholine | LPC 18:2 | C26H50NO7P |
| 521.3481 | Lysophosphatidylcholine | LPC 18:1 | C26H52NO7P |
| 523.3638 | Lysophosphatidylcholine | LPC 18:0 | C26H54NO7P |
| 541.3168 | Lysophosphatidylcholine | LPC 20:5 | C28H48NO7P |
| 543.3325 | Lysophosphatidylcholine | LPC 20:4 | C28H50NO7P |
| 545.3481 | Lysophosphatidylcholine | LPC 20:3 | C28H52NO7P |
| 547.3638 | Lysophosphatidylcholine | LPC 20:2 | C28H54NO7P |
| 549.3794 | Lysophosphatidylcholine | LPC 20:1 | C28H56NO7P |
| 551.3951 | Lysophosphatidylcholine | LPC 20:0 | C28H58NO7P |
| 567.3325 | Lysophosphatidylcholine | LPC 22:6 | C30H50NO7P |
| 646.5050 | Sphingomyelin | C12 Sphingomyelin | C35H71N2O6P |
| 702.5676 | Sphingomyelin | C16 Sphingomyelin | C39H79N2O6P |
| 716.5832 | Sphingomyelin | C17 Sphingomyelin | C40H81N2O6P |
| 730.5989 | Sphingomyelin | C18 Sphingomyelin | C41H83N2O6P |

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|---|---|---|---|
| 758.6302 | Sphingomyelin | C20 Sphingomyelin | C43H87N2O6P |
| 784.6458 | Sphingomyelin | C22:1 Sphingomyelin | $C_{45}H_{89}N_2O_6P$ |
| 786.6615 | Sphingomyelin | C22 Sphingomyelin | C45H91N2O6P |
| 812.6771 | Sphingomyelin | C24:1 Sphingomyelin | C47H93N2O6P |
| 814.6928 | Sphingomyelin | C24 Sphingomyelin | C47H95N2O6P |
| 842.7241 | Sphingomyelin | C26 Sphingomyelin | C49H99N2O6P |
| 840.7084 | Sphingomyelin | C26:1 Sphingomyelin | C49H97N2O6P |
| 704.5832 | Sphingomyelin | C16DH Sphingomyelin | C39H81N2O6P |
| 732.6145 | Sphingomyelin | C18DH Sphingomyelin | C41H85N2O6P |
| 760.6458 | Sphingomyelin | C20DH Sphingomyelin | C43H89N2O6P |
| 800.6407 | Sphingomyelin | C22:1DH Sphingomyelin | $C_{45}H_{89}N_2O_7P$ |
| 788.6771 | Sphingomyelin | C22DH Sphingomyelin | C45H93N2O6P |
| 814.6928 | Sphingomyelin | C24:1DH Sphingomyelin | C47H95N2O6P |
| 816.7084 | Sphingomyelin | C24DH Sphingomyelin | C47H97N2O6P |
| 842.7241 | Sphingomyelin | C26:1DH Sphingomyelin | C49H99N2O6P |
| 844.7397 | Sphingomyelin | C26DH Sphingomyelin | C49H101N2O6P |
| 481.4495 | Ceramide | C12 Cer; N-(dodecanoyl)-ceramide; N-(dodecanoyl)-ceramide | C30H59NO3 |
| 509.4808 | Ceramide | C14 Cer; N-(tetradecanoyl)-ceramide; N-(myristoyl)-ceramide | C32H63NO3 |
| 537.5121 | Ceramide | C16 Cer; N-(hexadecanoyl)-ceramide; N-(palmitoyl)-ceramide; N-palmitoyl-sphingosine | C34H67NO3 |
| 549.5121 | Ceramide | C17 Cer; N-(heptadecanoyl)-ceramide | C35H67NO3 |
| 565.5434 | Ceramide | C18 Cer; N-(octadecanoyl)-ceramide; N-(stearoyl)-ceramide | C36H71NO3 |
| 593.5747 | Ceramide | C20 Cer; N-(eicosanoyl)-ceramide; N-(eicosanoyl)-ceramide | C38H75NO3 |
| 621.6060 | Ceramide | C22 Cer; N-(docosanoyl)-ceramide; N-(docosanoyl)-ceramide; N-behenoyl-sphingosine | C40H79NO3 |
| 647.6216 | Ceramide | C24:1 Cer; N-(15Z-tetracosenoyl)-ceramide; N-(15Z-tetracosenoyl)-ceramide; N-nervonyl-sphingosine | C42H81NO3 |
| 649.6373 | Ceramide | C24 Cer; N-(tetracosanoyl)-ceramide; N-(tetracosanoyl)-ceramide; N-lignoceroyl-sphingosine | C42H83NO3 |
| 675.6529 | Ceramide | C26:1 Cer; N-(17Z-hexacosenoyl)-ceramide; N-(17Z-hexacosenoyl)-ceramide | C44H85NO3 |
| 677.6686 | Ceramide | C26 Cer; N-(hexacosanoyl)-ceramide; N-(hexacosanoyl)-ceramide | C44H87NO3 |

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|---|---|---|---|
| 539.5277 | Ceramide | C16DH Cer; N-(hexadecanoyl)-dihydroceramide; N-(palmitoyl)-dihydroceramide | C34H69NO3 |
| 567.5590 | Ceramide | C18DH Cer; N-(octadecanoyl)-dihydroceramide; N-(stearoyl)-dihydroceramide | C36H73NO3 |
| 595.5903 | Ceramide | C20DH Cer; N-(eicosanoyl)-dihydroceramide; N-(eicosanoyl)-dihydroceramide | C38H77NO3 |
| 623.6216 | Ceramide | C22DH Cer; N-(docosanoyl)-dihydroceramide; N-(docosanoyl)-dihydroceramide | C40H81NO3 |
| 651.6529 | Ceramide | C24DH Cer; N-(tetracosanoyl)-dihydroceramide; N-(tetracosanoyl)-dihydroceramide | C42H85NO3 |
| 649.6373 | Ceramide | C24:1DH Cer; N-(15Z-tetracosenoyl)-dihydroceramide; N-(15Z-tetracosenoyl)-dihydroceramide; N-nervonyl-sphinganine | C42H83NO3 |
| 679.6842 | Ceramide | C26DH Cer; N-(hexacosanoyl)-dihydroceramide; N-(hexacosanoyl)-dihydroceramide | C44H89NO3 |
| 677.6686 | Ceramide | C26:1DH Cer; N-(17Z-hexacosenoyl)-dihydroceramide; N-(17Z-hexacosenoyl)-dihydroceramide | C44H87NO3 |
| 638.6001 | Cholesteryl Ester | 17:0 Cholesteryl ester | $C_{44}H_{78}O_2$ |
| 666.6315 | Cholesteryl Ester | 19:0 Cholesteryl ester | C46H82O2 |
| 624.5845 | Cholesteryl Ester | 16:0 Cholesteryl ester | C43H76O2 |
| 652.6158 | Cholesteryl Ester | 18:0 Cholesteryl ester | C45H80O2 |
| 650.6002 | Cholesteryl Ester | 18:1 Cholesteryl ester | C45H78O2 |
| 648.5845 | Cholesteryl Ester | 18:2 Cholesteryl ester | C45H76O2 |
| 646.5689 | Cholesteryl Ester | 18:3 Cholesteryl ester | C45H74O2 |
| 674.6002 | Cholesteryl Ester | 20:3 Cholesteryl ester | C47H78O2 |
| 672.5845 | Cholesteryl Ester | 20:4 Cholesteryl ester | C47H76O2 |
| 670.5689 | Cholesteryl Ester | 20:5 Cholesteryl ester | C47H74O2 |
| 700.6158 | Cholesteryl Ester | 22:4 Cholesteryl ester | C49H80O2 |
| 698.6002 | Cholesteryl Ester | 22:5 Cholesteryl ester | C49H78O2 |
| 698.6002 | Cholesteryl Ester | 22:5 Cholesteryl ester | $C_{49}H_{78}O_2$ |
| 696.5845 | Cholesteryl Ester | 22:6 Cholesteryl ester | C49H76O2 |
| 386.3549 | Cholesterol | Cholesterol | C27H46O |
| 806.7363 | Triacylglycerol | TG 48:0 | C51H98O6 |
| 802.7050 | Triacylglycerol | TG (48:2) | C51H94O6 |
| 804.7207 | Triacylglycerol | TG (48:1) | C51H96O6 |

| | | | |
|---|---|---|---|
| 834.7676 | Triacylglycerol | TG (50:0) | C53H102O6 |
| 832.7520 | Triacylglycerol | TG (50:1) | C53H100O6 |
| 830.7363 | Triacylglycerol | TG (50:2) | C53H98O6 |
| 828.7207 | Triacylglycerol | TG (50:3) | C53H96O6 |
| 826.7050 | Triacylglycerol | TG (50:4) | C53H94O6 |
| 860.7832 | Triacylglycerol | TG (52:1) | C55H104O6 |
| 858.7676 | Triacylglycerol | TG (52:2) | C55H102O6 |
| 856.7520 | Triacylglycerol | TG (52:3) | C55H100O6 |
| 854.7363 | Triacylglycerol | TG (52:4) | C55H98O6 |
| 852.7207 | Triacylglycerol | TG (52:5) | C55H96O6 |
| 886.7989 | Triacylglycerol | TG (54:2) | C57H106O6 |
| 884.7832 | Triacylglycerol | TG 54:3) | C57H104O6 |
| 882.7676 | Triacylglycerol | TG (54:4) | C57H102O6 |
| 880.7520 | Triacylglycerol | TG (54:5) | C57H100O6 |
| 878.7363 | Triacylglycerol | TG 54:6 ) | C57H98O6 |
| 906.7676 | Triacylglycerol | TG (56:6) | C59H102O6 |
| 908.7832 | Triacylglycerol | TG (56:5) | C59H104O6 |
| 910.7989 | Triacylglycerol | TG (56:4) | C59H106O6 |
| 912.8145 | Triacylglycerol | TG (56:3) | C59H108O6 |

**Supplementary Figure**

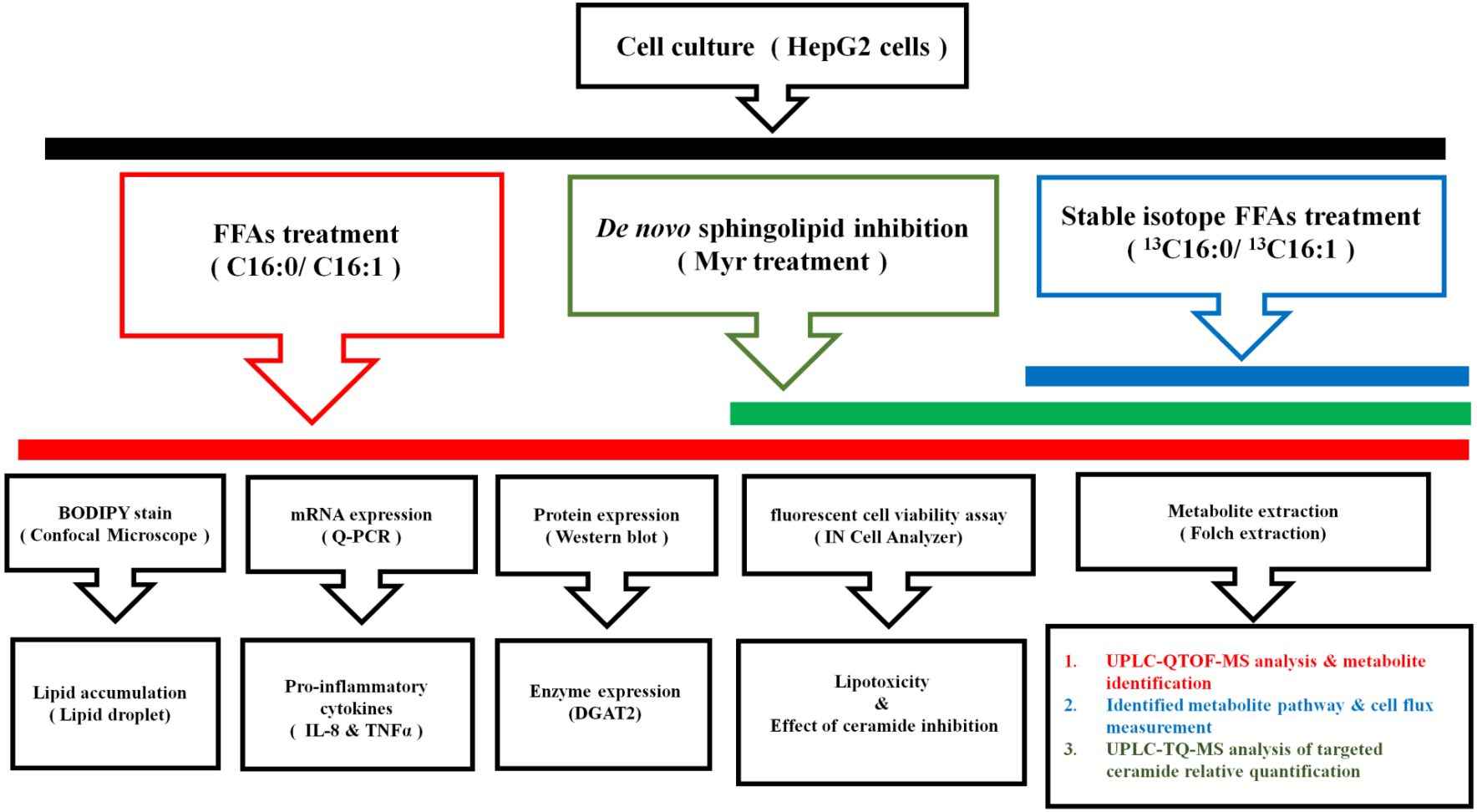


**Figure S1.** The workflow of FFAs treated HepG2 cell experiments

## Supplementary materials and methods

*Sample preparation for aqueous phase*

In brief, aqueous phase was extracted from FFAs treated $10^6$ HepG2 cells using the modified Folch method. The aqueous phase extract (upper layer) was dissolved in isopropanol/acetonitrile/water (2:1:1, V/V/V) mixture. After vortexing (30 sec, 4 times) and centrifuging (12,000 rpm, for 20 min at 4°C) the mixture, the supernatant was transferred into a vial for LC–MS analysis. [Samples per group were biological triplicates (n= total number of biological replicates) and each of biological triplicates was detected three times for technical triplicates (triplicates).]

*Aqueous phase analyzed by LC-MS*

Mass spectrometry analysis was performed using the ultra-performance liquid chromatography (UPLC) system coupled with time-of-flight mass spectrometry (TOF-MS; Waters, USA). Chromatographic separation was performed on an ACQUITY UPLC BEH Amide column (2.1 mm × 150 mm × 1.7 μm). Column temperature was maintained at 45°C. For metabolite profiling, the mobile phase A was water with 0.1% formic acid and the mobile phase B was acetonitrile with 0.1% formic acid. The flow rate was 0.4 mL/min, and the solvent gradient was as follows: 0–0.1 min, 99% solvent B; 0.1–7 min, 99%–30% solvent B; 7–7.2 min, 30%–99% solvent B; 7.2–10 min.

Mass spectrometric analysis was performed using the Waters Synapt HDMS system operating in positive- and negative-ion ESI mode. The capillary voltage was set at 2,700 V in ESI-positive mode and 2,000 V in ESI-negative mode and cone voltage was set at 35 V, respectively. Desolvation gas flow rate was set at 700 L/hr, and cone gas flow was maintained at 25 L/hr. The desolvation and source temperatures were set at 80°C. MS data were collected in centroid mode over a range of 20–990 m/z at a rate of 0.1 scan/sec. Leucine-enkephalin was used as the reference compound. LockSpray frequency was set at 0.5 sec and was averaged over 10 scans for correction.

Data matrices were determined utilizing the Progenesis QI software (Waters) by the extracted m/z value, retention time (RT), and ion intensity. Metabolite identification was performed by searching the extracted data against the METLIN (http://metlin.scripps.edu/index.php), LIPID MAPS (http://www.lipidmaps.org/), Human Metabolome Database (HMDB) (http://www.hmdb.ca/), and in-house database (Table S6).