

Effects of endurance exercise and vitamin D supplementation on insulin resistance and plasma lipidome in middle-aged adults with type 2 diabetes

Supplemental tables

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Table S1. The protocol of endurance exercise training

| Stage | HRmax (%) | RPE | Time |
|-----------|-----------|-------|---|
| Week 1 | 65-70% | 11-13 | 60 min (including 5 min warm up, and 5 min recovery exercise) |
| Week 2-4 | 70-75% | 11-13 | 60 min (including 5 min warm up, and 5 min recovery exercise) |
| Week 5-8 | 75-80% | 12-13 | 60 min (including 5 min warm up, and 5 min recovery exercise) |
| Week 9-12 | 80% | 13 | 60 min (including 5 min warm up, and 5 min recovery exercise) |

Note: HRmax, Maximum heart rate; RPE, Rating of perceived exertion.

Table S2. Procedures of lipidomic measurement

| |
|--|
| 1) Sample preparation |
| A total of 100 μ L plasma samples was properly mixed with 800 μ L cold methyl tert-butyl ether, followed by adding 240 μ L methanol. The mixture was vortexed for 30 seconds, sonicated at 4°C for 20 min and was centrifuged (14000 g for 15 minutes at 10 °C). The upper organic layer containing lipids was then dried in a vacuum centrifuge for instrumental analyses. |
| 2) Lipid extraction |
| The lipid extracts were resuspended in 200 μ L isopropanol acetonitrile 9:1 (v/v). Chromatographic separation of 1 μ L of the extracted lipids was performed on ultra-high-performance liquid chromatography system LC-30A (Nexera). Analyses were conducted by Shanghai Applied Protein Technology Co., Ltd. In brief, lipids were separated on a Waters ACQUITY PREMIER CSH C18 Column (1.7 μ m, 2.1*100 mm), under the following chromatographic conditions: mobile phase A (acetonitrile: water = 6:4, v/v) and mobile phase B (acetonitrile: isopropanol = 1:9, v/v) at a flow rate of 300 μ L/min; column oven temperature at 45°C; gradients started with 30% of B for 2 min, then increased to 100% of B over 23 min. The gradient was returned to 30% B over 1 min, and was finally equilibrated for 9 min. |
| 3) Mass detection |
| The mass detection was performed using a Thermo Scientific™ Q Exactive mass spectrometer mass spectrometer, equipped with a jet stream electrospray ionization. Data were acquired in both positive and negative ion modes, respectively. Data-dependent acquisition method was used for MS/MS analyses of lipidome. Specifically, 10 MS2 scans were collected after each MS1 full scan. The resolution of MS1 is 70000 at m/z 200. The resolution of MS2 is 17500 at m/z 200. The ESI conditions are: Heater Temp 300 °C, Sheath Gas Flow rate 45 arb, Aux Gas Flow Rate 15 arb, Sweep Gas Flow Rate 1arb, spray voltage 3.0KV, Capillary Temp 350 °C, S-Lens RF Level 50%, MS1 scan ranges: 200-1800. |
| 4) Quality control |
| The quality control was performed throughout the dataset by including blanks, pure standard samples, extracted standard samples, and pooled plasma samples from this study. Lipidsearch 4.0 software was used for peak detection and lipids annotation. Main parameters are as follows: precursor tolerance 5 ppm, product tolerance 5 ppm, product ion threshold 5%. For the lipid species, fatty acyl chains were abbreviated Cx:y, where x represents the number of carbon atoms and y the number of double bonds of the fatty acyl chain. |

Table S3. Mean differences (95% CI) of blood parameters from the pre (0-week) with each group using 2×2 factorial ANOVA

| Variables | EX + VD | VD | EX | Con | Vitamin D effect | | Exercise effect | | Interaction effect | |
|-------------------------------------|-------------------------|-------------------------|--------------------------|--------------------------|------------------|------------------|-----------------|------------------|--------------------|------------------|
| | N=15 | N=15 | N=14 | N=15 | P | Partial η^2 | P | Partial η^2 | P | Partial η^2 |
| Δ Total body fat (%) ^a | -1.0 (-2.1, 0.2) | 0.4 (-0.7, 1.6) | -1.1 (-2.0, -0.2) | -0.5 (-1.2, 0.2) | 0.262 | 0.024 | 0.032 | 0.084 | 0.428 | 0.012 |
| Δ Apolipoprotein A (g/L) | 0.02 (-0.10, 0.15) | 0.03 (-0.07, 0.12) | 0.01 (-0.06, 0.07) | 0.09 (-0.02, 0.21) | 0.582 | 0.004 | 0.349 | 0.009 | 0.400 | 0.010 |
| Δ Apolipoprotein B (g/L) | 0.02 (-0.07, 0.12) | -0.02 (-0.10, 0.06) | 0.03 (-0.06, 0.12) | 0.07 (-0.01, 0.14) | 0.232 | 0.020 | 0.986 | 0.000 | 0.327 | 0.013 |
| Δ Low density lipoprotein (mmol/L) | -0.09 (-0.43, 0.25) | -0.25 (-0.57, 0.06) | -0.26 (-0.54, 0.01) | -0.09 (-0.23, 0.05) | 0.969 | 0.000 | 0.977 | 0.000 | 0.203 | 0.026 |
| Δ High density lipoprotein (mmol/L) | 0.06 (-0.05, 0.17) | 0.00 (-0.12, 0.13) | 0.01 (-0.12, 0.15) | -0.01 (-0.12, 0.10) | 0.563 | 0.009 | 0.455 | 0.018 | 0.777 | 0.000 |
| Δ Cholesterol (mmol/L) | 0.06 (-0.39, 0.51) | -0.19 (-0.29, 0.29) | -0.19 (-0.50, 0.12) | -0.07 (-0.31, 0.16) | 0.699 | 0.005 | 0.691 | 0.004 | 0.281 | 0.015 |
| Δ Triglyceride (mmol/L) | -0.04 (-0.26, 0.18) | -0.00 (-0.34, 0.33) | -0.24 (-0.66, 0.18) | 0.32 (0.04, 0.59) | 0.698 | 0.015 | 0.050 | 0.048 | 0.085 | 0.089 |
| Δ HbA1c (%) | -0.8 (-1.6, 0.1) | -0.3 (-1.0, 0.3) | -0.2 (-0.5, 0.2) | -0.5 (-1.3, 0.3) | 0.506 | 0.023 | 0.820 | 0.002 | 0.229 | 0.014 |
| Δ Fasting blood glucose (mmol/L) | -0.9 (-1.6, -0.2) | -0.9 (-1.8, -0.1) | -0.6 (-1.3, 0.2) | 0.4 (-1.8, 1.1) | 0.337 | 0.086 | 0.884 | 0.010 | 0.798 | 0.033 |
| Δ Fasting insulin (μU/mL) | -1.8 (-6.1, 2.5) | 1.3 (-1.3, 4.0) | 0.5 (-3.8, 4.8) | 0.5 (-3.6, 4.5) | 0.806 | 0.004 | 0.342 | 0.023 | 0.594 | 0.012 |
| Δ HOMA-IR | -0.9 (-2.4, 0.5) | -0.2 (-1.1, 0.7) | -0.2 (-1.6, 1.3) | 0.2 (-1.8, 2.3) | 0.447 | 0.026 | 0.273 | 0.027 | 0.754 | 0.000 |
| Δ Glucose AUC ^b | -78.1 (-225.8, 69.6) | -140.1 (-307.2, 27.0) | -75.9 (-201.7, 49.9) | 36.1 (-112.0, 184.2) | 0.197 | 0.032 | 0.716 | 0.003 | 0.208 | 0.031 |
| Δ Insulin AUC ^b | 515.8 (-1106.7, 2138.2) | 1018.1 (-128.1, 2164.3) | 1205.9 (-161.9, 2249.9) | -149.1 (-1979.0, 1680.9) | 0.724 | 0.002 | 0.529 | 0.008 | 0.173 | 0.036 |

Δ, changes from the endpoint to the pre; EX+VD, vitamin D supplementation and exercise training; VD, vitamin D supplementation; EX, exercise training; Con, control group; HOMA-IR, homeostasis model assessment of insulin resistance; HbA1c, glycated hemoglobin; AUC, area under the curves during oral glucose tolerance test; CI, confidence interval. ^a, n=14 in VD and Con; ^b, n=13 in VD and Con were included.

Table S4. Mean differences of glycemic control indicators at three time point with each group

| Variable | HbA1c (%) | Fasting glucose (mmol/L) | Fasting insulin (μ U/mL) | HOMA-IR |
|--------------------|---------------|--------------------------|-------------------------------|---------------|
| EX+VD | | | | |
| t1 | 7.0 \pm 1.9 | 6.7 \pm 1.4 | 12.6 \pm 8.6 | 3.9 \pm 3.0 |
| t2 | 6.3 \pm 0.7 | 5.9 \pm 1.0 | 10.8 \pm 6.2 | 3.0 \pm 2.2 |
| t3 | 6.3 \pm 0.9 | 6.2 \pm 1.3 | 10.6 \pm 6.0 | 3.0 \pm 2.0 |
| P _{t1-t2} | 0.064 | 0.016 | 0.389 | 0.086 |
| P _{t2-t3} | 0.200 | 0.123 | 0.430 | 0.222 |
| P _{t1-t3} | 0.067 | 0.250 | 0.737 | 0.549 |
| EX | | | | |
| t1 | 6.7 \pm 1.2 | 7.8 \pm 2.1 | 11.7 \pm 6.1 | 3.9 \pm 2.3 |
| t2 | 6.5 \pm 1.1 | 7.2 \pm 2.1 | 12.1 \pm 8.3 | 3.8 \pm 2.3 |
| t3 | 6.6 \pm 1.1 | 7.6 \pm 2.9 | 10.4 \pm 5.3 | 3.4 \pm 1.8 |
| P _{t1-t2} | 0.316 | 0.114 | 0.809 | 0.823 |
| P _{t2-t3} | 0.083 | 0.365 | 0.483 | 0.288 |
| P _{t1-t3} | 0.457 | 0.722 | 0.391 | 0.511 |
| VD | | | | |
| t1 | 6.9 \pm 1.4 | 7.4 \pm 1.9 | 9.7 \pm 5.6 | 3.4 \pm 2.6 |
| t2 | 6.6 \pm 0.8 | 6.5 \pm 0.8 | 11.0 \pm 8.9 | 3.2 \pm 2.7 |
| t3 | 6.8 \pm 1.1 | 7.2 \pm 1.8 | 12.7 \pm 10.1 | 4.5 \pm 4.6 |
| P _{t1-t2} | 0.318 | 0.032 | 0.294 | 0.649 |
| P _{t2-t3} | 0.471 | 0.223 | 0.248 | 0.183 |
| P _{t1-t3} | 0.538 | 0.217 | 0.083 | 0.205 |
| Con | | | | |
| t1 | 7.2 \pm 1.6 | 7.5 \pm 2.6 | 14.7 \pm 7.6 | 4.9 \pm 2.6 |
| t2 | 6.7 \pm 0.8 | 7.1 \pm 1.3 | 15.1 \pm 11.0 | 5.1 \pm 4.9 |
| t3 | 6.7 \pm 0.6 | 7.1 \pm 1.1 | 15.8 \pm 7.7 | 5.1 \pm 2.9 |
| P _{t1-t2} | 0.186 | 0.588 | 0.813 | 0.814 |
| P _{t2-t3} | 0.968 | 0.649 | 0.993 | 0.759 |
| P _{t1-t3} | 0.354 | 0.966 | 0.276 | 0.432 |

Data are mean \pm standard deviation (SD). EX+VD, vitamin D supplementation and exercise training; VD, vitamin D supplementation; EX, exercise training; Con, control group; HbA1c, glycated hemoglobin; HOMA-IR, homeostasis model assessment of insulin resistance; P_{t1-t2}, comparisons between baseline and endpoint with each group were assessed using paired t-test; P_{t2-t3}, comparisons between endpoint and flow-up with each group were assessed using paired t-test; P_{t1-t3}, comparisons between baseline and flow-up with each group were assessed using paired t-test. t1 and t2: EX+VD, n=15; EX, n=14; VD, n=15; Con, n=15; t3: EX+VD, n=13; EX, n=12; VD, n=11; Con, n=12.

Table S5. The 105 lipids that had pronounced changes between t2 and t1 sampling in VD, EX, or EX+VD and their corresponding module colors of WGCNA

[illegible]

[illegible]

[illegible]

| | | | | | | | | | | | | | | | |
|--------------------|---------------|-----|------|--------|--------|-------|--------|--------|--------|--------|--------|--------|--------|--------|--------|
| LPE(18:1e)+Na | LPE(18:1e)+Na | LPE | blue | 1.3e+0 | 7.5e+0 | 1.2e+ | 1.2e+0 | 1.2e+0 | 1.2e+0 | 1.3e+0 | 1.1e+0 | 6.4e+0 | 6.3e+0 | 8.1e+0 | 1.6e+0 |
| | | | | 7 | 6 | 07 | 7 | 7 | 7 | 7 | 7 | 6 | 6 | 6 | 7 |
| | | | | 1.2e+0 | 8.7e+0 | 1.2e+ | 9.9e+0 | 1.2e+0 | 9.0e+0 | 1.2e+0 | 1.1e+0 | 9.4e+0 | 8.8e+0 | 1.0e+0 | 1.3e+0 |
| | | | | 6 ± | 5 ± | 06 ± | 5 ± | 6 ± | 5 ± | 6 ± | 6 ± | 5 ± | 5 ± | 6 ± | 6 ± |
| | | | | 6.8e+0 | 6.6e+0 | 6.1e+ | 6.0e+0 | 7.3e+0 | 4.5e+0 | 5.9e+0 | 7.3e+0 | 4.3e+0 | 5.4e+0 | 5.8e+0 | 9.3e+0 |
| | | | | 5 | 5 | 05 | 5 | 5 | 5 | 5 | 5 | 5 | 5 | 5 | 5 |
| PI(18:3_18:2)+Na | PI(36:5)+Na | PI | blue | 4.9e+0 | 4.4e+0 | 4.7e+ | 3.9e+0 | 4.8e+0 | 4.5e+0 | 4.3e+0 | 4.3e+0 | 4.7e+0 | 4.4e+0 | 4.8e+0 | 5.1e+0 |
| | | | | 6 ± | 6 ± | 06 ± | 6 ± | 6 ± | 6 ± | 6 ± | 6 ± | 6 ± | 6 ± | 6 ± | 6 ± |
| | | | | 1.4e+0 | 1.3e+0 | 1.7e+ | 1.6e+0 | 2.3e+0 | 1.4e+0 | 1.4e+0 | 1.3e+0 | 1.4e+0 | 1.3e+0 | 1.6e+0 | 1.8e+0 |
| | | | | 6 | 6 | 06 | 6 | 6 | 6 | 6 | 6 | 6 | 6 | 6 | 6 |
| | | | | 7.9e+0 | 4.1e+0 | 8.7e+ | 4.7e+0 | 7.3e+0 | 4.5e+0 | 8.6e+0 | 6.5e+0 | 4.6e+0 | 3.5e+0 | 5.6e+0 | 7.9e+0 |
| | | | | 5 ± | 5 ± | 05 ± | 5 ± | 5 ± | 5 ± | 5 ± | 5 ± | 5 ± | 5 ± | 5 ± | 5 ± |
| LPC(18:1e)+Na | LPC(18:1e)+Na | LPC | blue | 7.8e+0 | 3.2e+0 | 8.6e+ | 3.8e+0 | 7.6e+0 | 4.5e+0 | 9.5e+0 | 5.8e+0 | 3.0e+0 | 2.6e+0 | 5.3e+0 | 7.6e+0 |
| | | | | 5 | 5 | 05 | 5 | 5 | 5 | 5 | 5 | 5 | 5 | 5 | 5 |
| | | | | 3.0e+0 | 2.6e+0 | 3.7e+ | 3.2e+0 | 2.9e+0 | 3.4e+0 | 3.7e+0 | 3.4e+0 | 2.5e+0 | 2.5e+0 | 3.1e+0 | 3.8e+0 |
| | | | | 7 ± | 7 ± | 07 ± | 7 ± | 7 ± | 7 ± | 7 ± | 7 ± | 7 ± | 7 ± | 7 ± | 7 ± |
| | | | | 1.6e+0 | 1.1e+0 | 1.8e+ | 1.8e+0 | 1.2e+0 | 2.4e+0 | 1.8e+0 | 1.9e+0 | 1.6e+0 | 1.3e+0 | 1.2e+0 | 2.1e+0 |
| | | | | 7 | 7 | 07 | 7 | 7 | 7 | 7 | 7 | 7 | 7 | 7 | 7 |
| LPC(18:0)-CH3 | LPC(18:0)-CH3 | LPC | blue | 6.4e+0 | 5.1e+0 | 8.6e+ | 6.3e+0 | 6.0e+0 | 5.7e+0 | 8.9e+0 | 7.2e+0 | 4.6e+0 | 4.9e+0 | 6.7e+0 | 7.0e+0 |
| | | | | 5 ± | 5 ± | 05 ± | 5 ± | 5 ± | 5 ± | 5 ± | 5 ± | 5 ± | 5 ± | 5 ± | 5 ± |
| | | | | 3.8e+0 | 2.6e+0 | 4.6e+ | 3.2e+0 | 2.8e+0 | 3.7e+0 | 4.8e+0 | 4.0e+0 | 2.2e+0 | 2.6e+0 | 2.9e+0 | 3.7e+0 |
| | | | | 5 | 5 | 05 | 5 | 5 | 5 | 5 | 5 | 5 | 5 | 5 | 5 |
| | | | | 4.1e+0 | 3.6e+0 | 4.0e+ | 3.3e+0 | 4.0e+0 | 3.6e+0 | 3.7e+0 | 3.8e+0 | 3.9e+0 | 3.6e+0 | 4.3e+0 | 4.4e+0 |
| | | | | 6 ± | 6 ± | 06 ± | 6 ± | 6 ± | 6 ± | 6 ± | 6 ± | 6 ± | 6 ± | 6 ± | 6 ± |
| PIP(18:3e_22:6)-H | PIP(40:9e)-H | PIP | blue | 1.2e+0 | 1.1e+0 | 1.2e+ | 1.4e+0 | 1.7e+0 | 1.5e+0 | 1.2e+0 | 1.3e+0 | 1.5e+0 | 1.2e+0 | 1.5e+0 | 1.6e+0 |
| | | | | 6 | 6 | 06 | 6 | 6 | 6 | 6 | 6 | 6 | 6 | 6 | 6 |
| | | | | 3.8e+0 | 2.3e+0 | 3.1e+ | 2.9e+0 | 3.9e+0 | 2.6e+0 | 3.0e+0 | 3.0e+0 | 3.6e+0 | 1.6e+0 | 3.9e+0 | 3.4e+0 |
| | | | | 6 ± | 6 ± | 06 ± | 6 ± | 6 ± | 6 ± | 6 ± | 6 ± | 6 ± | 6 ± | 6 ± | 6 ± |
| | | | | 3.4e+0 | 1.2e+0 | 2.3e+ | 2.2e+0 | 3.1e+0 | 2.0e+0 | 2.4e+0 | 2.3e+0 | 2.6e+0 | 6.4e+0 | 2.3e+0 | 2.5e+0 |
| | | | | 6 | 6 | 06 | 6 | 6 | 6 | 6 | 6 | 6 | 5 | 6 | 6 |
| PC(14:0_22:6)+HCOO | PC(36:6)+HCOO | PC | blue | 7.0e+0 | 7.0e+0 | 6.6e+ | 5.9e+0 | 7.0e+0 | 5.9e+0 | 7.3e+0 | 5.3e+0 | 6.8e+0 | 5.5e+0 | 8.6e+0 | 8.1e+0 |
| | | | | 6 ± | 6 ± | 06 ± | 6 ± | 6 ± | 6 ± | 6 ± | 6 ± | 6 ± | 6 ± | 6 ± | 6 ± |

| | | | | | | | | | | | | | | | |
|----------------------|---------------|-------|------|--------|--------|-------|--------|--------|--------|--------|--------|--------|--------|--------|--------|
| PC(16:0_18:1)+HCOO | PC(34:1)+HCOO | PC | blue | 6.0e+0 | 6.4e+0 | 4.6e+ | 3.8e+0 | 4.3e+0 | 4.5e+0 | 5.7e+0 | 4.0e+0 | 5.2e+0 | 3.8e+0 | 8.2e+0 | 6.1e+0 |
| | | | | 6 | 6 | 06 | 6 | 6 | 6 | 6 | 6 | 6 | 6 | 6 | 6 |
| | | | | 2.3e+0 | 1.9e+0 | 2.0e+ | 2.1e+0 | 2.4e+0 | 1.8e+0 | 2.4e+0 | 1.8e+0 | 2.1e+0 | 1.9e+0 | 2.5e+0 | 2.5e+0 |
| | | | | 8 ± | 8 ± | 08 ± | 8 ± | 8 ± | 8 ± | 8 ± | 8 ± | 8 ± | 8 ± | 8 ± | 8 ± |
| | | | | 8.6e+0 | 8.3e+0 | 7.5e+ | 8.7e+0 | 8.5e+0 | 8.5e+0 | 1.2e+0 | 4.8e+0 | 7.5e+0 | 6.2e+0 | 9.8e+0 | 1.1e+0 |
| | | | | 7 | 7 | 07 | 7 | 7 | 7 | 8 | 7 | 7 | 7 | 7 | 7 |
| TG(18:0_18:2_20:5)+H | TG(56:7)+H | TG | grey | 1.6e+0 | 1.0e+0 | 1.3e+ | 1.1e+0 | 1.6e+0 | 1.9e+0 | 1.9e+0 | 2.2e+0 | 1.6e+0 | 1.0e+0 | 3.4e+0 | 1.6e+0 |
| | | | | 7 ± | 7 ± | 07 ± | 7 ± | 7 ± | 7 ± | 7 ± | 7 ± | 7 ± | 7 ± | 7 ± | 7 ± |
| | | | | 1.6e+0 | 8.1e+0 | 1.2e+ | 1.0e+0 | 1.4e+0 | 2.5e+0 | 2.9e+0 | 2.6e+0 | 1.6e+0 | 8.5e+0 | 4.5e+0 | 1.4e+0 |
| | | | | 7 | 6 | 07 | 7 | 7 | 7 | 7 | 7 | 7 | 6 | 7 | 7 |
| OAHFA(47:6)-H | OAHFA(47:6)-H | OAHFA | grey | 1.6e+0 | 1.7e+0 | 1.6e+ | 1.5e+0 | 1.6e+0 | 1.7e+0 | 1.7e+0 | 1.7e+0 | 1.5e+0 | 1.6e+0 | 1.5e+0 | 1.7e+0 |
| | | | | 6 ± | 6 ± | 06 ± | 6 ± | 6 ± | 6 ± | 6 ± | 6 ± | 6 ± | 6 ± | 6 ± | 6 ± |
| | | | | 4.9e+0 | 6.0e+0 | 6.3e+ | 4.2e+0 | 5.0e+0 | 8.2e+0 | 7.8e+0 | 6.6e+0 | 2.5e+0 | 6.7e+0 | 4.1e+0 | 7.0e+0 |
| | | | | 5 | 5 | 05 | 5 | 5 | 5 | 5 | 5 | 5 | 5 | 5 | 5 |
| PE(37:3e)+Na | PE(37:3e)+Na | PE | grey | 5.8e+0 | 1.8e+0 | 2.9e+ | 1.9e+0 | 3.7e+0 | 2.2e+0 | 3.4e+0 | 2.0e+0 | 3.2e+0 | 2.5e+0 | 3.1e+0 | 2.4e+0 |
| | | | | 7 ± | 7 ± | 07 ± | 7 ± | 7 ± | 7 ± | 7 ± | 7 ± | 7 ± | 7 ± | 7 ± | 7 ± |
| | | | | 1.2e+0 | 1.2e+0 | 2.7e+ | 1.3e+0 | 4.6e+0 | 3.8e+0 | 3.0e+0 | 1.4e+0 | 3.2e+0 | 2.3e+0 | 3.0e+0 | 1.7e+0 |
| | | | | 8 | 7 | 07 | 7 | 7 | 7 | 7 | 7 | 7 | 7 | 7 | 7 |
| DG(26:6e)+Na | DG(26:6e)+Na | DG | grey | 6.4e+0 | 6.2e+0 | 4.5e+ | 3.9e+0 | 5.1e+0 | 5.1e+0 | 3.6e+0 | 2.6e+0 | 4.5e+0 | 5.1e+0 | 6.2e+0 | 5.0e+0 |
| | | | | 5 ± | 5 ± | 05 ± | 5 ± | 5 ± | 5 ± | 5 ± | 5 ± | 5 ± | 5 ± | 5 ± | 5 ± |
| | | | | 6.1e+0 | 4.8e+0 | 3.8e+ | 3.3e+0 | 4.1e+0 | 4.0e+0 | 2.3e+0 | 1.6e+0 | 3.4e+0 | 3.3e+0 | 5.5e+0 | 3.8e+0 |
| | | | | 5 | 5 | 05 | 5 | 5 | 5 | 5 | 5 | 5 | 5 | 5 | 5 |
| PA(17:0_18:2)-H | PA(35:2)-H | PA | grey | 6.1e+0 | 2.8e+0 | 5.9e+ | 5.4e+0 | 6.1e+0 | 3.2e+0 | 4.3e+0 | 4.1e+0 | 5.0e+0 | 2.8e+0 | 5.1e+0 | 5.6e+0 |
| | | | | 6 ± | 6 ± | 06 ± | 6 ± | 6 ± | 6 ± | 6 ± | 6 ± | 6 ± | 6 ± | 6 ± | 6 ± |
| | | | | 3.7e+0 | 2.0e+0 | 3.4e+ | 3.8e+0 | 4.0e+0 | 3.5e+0 | 3.7e+0 | 4.5e+0 | 4.3e+0 | 1.9e+0 | 4.2e+0 | 6.0e+0 |
| | | | | 6 | 6 | 06 | 6 | 6 | 6 | 6 | 6 | 6 | 6 | 6 | 6 |
| PC(22:4_21:1)+HCOO | PC(43:5)+HCOO | PC | grey | 8.6e+0 | 7.9e+0 | 9.9e+ | 8.2e+0 | 8.1e+0 | 6.8e+0 | 9.0e+0 | 7.9e+0 | 7.1e+0 | 6.8e+0 | 8.5e+0 | 9.1e+0 |
| | | | | 6 ± | 6 ± | 06 ± | 6 ± | 6 ± | 6 ± | 6 ± | 6 ± | 6 ± | 6 ± | 6 ± | 6 ± |
| | | | | 2.6e+0 | 3.9e+0 | 4.4e+ | 3.1e+0 | 3.6e+0 | 2.5e+0 | 4.0e+0 | 2.3e+0 | 1.6e+0 | 2.9e+0 | 2.7e+0 | 3.6e+0 |
| | | | | 6 | 6 | 06 | 6 | 6 | 6 | 6 | 6 | 6 | 6 | 6 | 6 |
| SM(d18:2_16:1)+H | SM(d34:3)+H | SM | grey | 3.4e+0 | 2.6e+0 | 3.4e+ | 2.8e+0 | 3.4e+0 | 2.6e+0 | 2.9e+0 | 3.2e+0 | 3.2e+0 | 2.6e+0 | 3.2e+0 | 3.8e+0 |
| | | | | 6 ± | 6 ± | 06 ± | 6 ± | 6 ± | 6 ± | 6 ± | 6 ± | 6 ± | 6 ± | 6 ± | 6 ± |

| | | | | | | | | | | | | | | | |
|---------------------------|-------------------------|---------|------|--------|--------|-------|--------|--------|--------|--------|--------|--------|--------|--------|--------|
| PC(37:6)+H | PC(37:6)+H | PC | grey | 2.0e+0 | 1.2e+0 | 1.9e+ | 1.4e+0 | 1.9e+0 | 1.5e+0 | 1.5e+0 | 1.6e+0 | 2.0e+0 | 8.2e+0 | 1.2e+0 | 2.1e+0 |
| | | | | 6 | 6 | 06 | 6 | 6 | 6 | 6 | 6 | 5 | 6 | 6 | |
| | | | | 3.3e+0 | 2.3e+0 | 3.3e+ | 2.6e+0 | 3.3e+0 | 2.7e+0 | 3.1e+0 | 3.0e+0 | 3.0e+0 | 2.4e+0 | 3.7e+0 | 4.2e+0 |
| | | | | 7 ± | 7 ± | 07 ± | 7 ± | 7 ± | 7 ± | 7 ± | 7 ± | 7 ± | 7 ± | 7 ± | 7 ± |
| | | | | 3.0e+0 | 2.0e+0 | 2.9e+ | 2.0e+0 | 2.7e+0 | 3.6e+0 | 2.3e+0 | 2.4e+0 | 2.7e+0 | 1.8e+0 | 3.0e+0 | 3.9e+0 |
| | | | | 7 | 7 | 07 | 7 | 7 | 7 | 7 | 7 | 7 | 7 | 7 | 7 |
| LPC(15:0)+H | LPC(15:0)+H | LPC | grey | 2.0e+0 | 1.7e+0 | 2.5e+ | 1.8e+0 | 2.0e+0 | 2.3e+0 | 2.5e+0 | 2.0e+0 | 1.5e+0 | 1.6e+0 | 2.1e+0 | 2.1e+0 |
| | | | | 7 ± | 7 ± | 07 ± | 7 ± | 7 ± | 7 ± | 7 ± | 7 ± | 7 ± | 7 ± | 7 ± | 7 ± |
| | | | | 1.6e+0 | 9.3e+0 | 1.6e+ | 1.3e+0 | 1.4e+0 | 1.6e+0 | 1.7e+0 | 1.4e+0 | 1.2e+0 | 8.8e+0 | 1.3e+0 | 1.5e+0 |
| | | | | 7 | 6 | 07 | 7 | 7 | 7 | 7 | 7 | 7 | 6 | 7 | 7 |
| TG(15:0_18:1_18:3)+N a | TG(51:4)+Na | TG | grey | 6.2e+0 | 4.3e+0 | 5.1e+ | 5.7e+0 | 6.2e+0 | 5.5e+0 | 5.5e+0 | 6.4e+0 | 5.4e+0 | 4.5e+0 | 7.0e+0 | 7.7e+0 |
| | | | | 6 ± | 6 ± | 06 ± | 6 ± | 6 ± | 6 ± | 6 ± | 6 ± | 6 ± | 6 ± | 6 ± | 6 ± |
| | | | | 4.0e+0 | 3.2e+0 | 3.9e+ | 3.5e+0 | 4.4e+0 | 3.9e+0 | 4.1e+0 | 4.2e+0 | 4.0e+0 | 2.5e+0 | 4.5e+0 | 4.4e+0 |
| | | | | 6 | 6 | 06 | 6 | 6 | 6 | 6 | 6 | 6 | 6 | 6 | 6 |
| PC(18:3e_22:0)+HCO O | PC(40:3e)+HCOO | PC | grey | 1.7e+0 | 1.3e+0 | 1.4e+ | 1.4e+0 | 1.5e+0 | 1.2e+0 | 1.5e+0 | 1.3e+0 | 1.4e+0 | 1.0e+0 | 1.5e+0 | 1.5e+0 |
| | | | | 7 ± | 7 ± | 07 ± | 7 ± | 7 ± | 7 ± | 7 ± | 7 ± | 7 ± | 7 ± | 7 ± | 7 ± |
| | | | | 8.9e+0 | 6.3e+0 | 5.1e+ | 6.7e+0 | 7.4e+0 | 6.7e+0 | 1.0e+0 | 6.1e+0 | 6.3e+0 | 3.1e+0 | 8.3e+0 | 6.8e+0 |
| | | | | 6 | 6 | 06 | 6 | 6 | 6 | 7 | 6 | 6 | 6 | 6 | 6 |
| Hex2Cer(m42:7)+HCO O | Hex2Cer(m42:7)+HCO O | Hex2Cer | grey | 1.6e+0 | 1.4e+0 | 1.8e+ | 1.6e+0 | 1.5e+0 | 1.2e+0 | 1.7e+0 | 1.4e+0 | 1.2e+0 | 1.3e+0 | 1.4e+0 | 1.5e+0 |
| | | | | 6 ± | 6 ± | 06 ± | 6 ± | 6 ± | 6 ± | 6 ± | 6 ± | 6 ± | 6 ± | 6 ± | 6 ± |
| | | | | 5.9e+0 | 4.8e+0 | 9.8e+ | 5.0e+0 | 7.3e+0 | 4.2e+0 | 8.1e+0 | 4.9e+0 | 3.4e+0 | 4.5e+0 | 5.2e+0 | 5.1e+0 |
| | | | | 5 | 5 | 05 | 5 | 5 | 5 | 5 | 5 | 5 | 5 | 5 | 5 |
| DG(16:0_20:5)+H | DG(36:5)+H | DG | grey | 4.6e+0 | 5.7e+0 | 4.7e+ | 4.2e+0 | 5.4e+0 | 5.2e+0 | 4.7e+0 | 4.1e+0 | 2.8e+0 | 4.3e+0 | 5.4e+0 | 4.6e+0 |
| | | | | 6 ± | 6 ± | 06 ± | 6 ± | 6 ± | 6 ± | 6 ± | 6 ± | 6 ± | 6 ± | 6 ± | 6 ± |
| | | | | 2.4e+0 | 3.8e+0 | 3.8e+ | 3.1e+0 | 3.9e+0 | 3.0e+0 | 3.2e+0 | 2.8e+0 | 1.8e+0 | 3.2e+0 | 3.9e+0 | 5.7e+0 |
| | | | | 6 | 6 | 06 | 6 | 6 | 6 | 6 | 6 | 6 | 6 | 6 | 6 |
| Cer(d44:5)+H | Cer(d44:5)+H | Cer | grey | 8.1e+0 | 6.7e+0 | 9.0e+ | 6.5e+0 | 7.8e+0 | 6.4e+0 | 8.3e+0 | 6.3e+0 | 5.7e+0 | 6.3e+0 | 7.8e+0 | 6.9e+0 |
| | | | | 7 ± | 7 ± | 07 ± | 7 ± | 7 ± | 7 ± | 7 ± | 7 ± | 7 ± | 7 ± | 7 ± | 7 ± |
| | | | | 3.6e+0 | 2.4e+0 | 6.0e+ | 1.8e+0 | 3.3e+0 | 2.0e+0 | 3.5e+0 | 2.1e+0 | 1.9e+0 | 2.9e+0 | 2.7e+0 | 2.3e+0 |
| | | | | 7 | 7 | 07 | 7 | 7 | 7 | 7 | 7 | 7 | 7 | 7 | 7 |
| AcCa(10:3)+H | AcCa(10:3)+H | AcCa | grey | 3.8e+0 | 2.7e+0 | 3.9e+ | 3.3e+0 | 3.7e+0 | 2.2e+0 | 4.0e+0 | 2.9e+0 | 3.1e+0 | 2.4e+0 | 3.4e+0 | 3.2e+0 |
| | | | | 6 ± | 6 ± | 06 ± | 6 ± | 6 ± | 6 ± | 6 ± | 6 ± | 6 ± | 6 ± | 6 ± | 6 ± |

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| | | | | | | | | | | | | | | | |
|------------------------|------------------------|------------|-----------|--------|--------|-------|--------|--------|--------|--------|--------|--------|--------|--------|--------|
| CerG2GNAc1(d36:3)-H | CerG2GNAc1(d36:3)-H | CerG2GNAc1 | turquoise | 2.1e+0 | 1.4e+0 | 2.8e+ | 1.8e+0 | 2.0e+0 | 3.2e+0 | 2.9e+0 | 2.6e+0 | 1.9e+0 | 2.0e+0 | 1.7e+0 | 2.5e+0 |
| | | | | 7 | 7 | 07 | 7 | 7 | 7 | 7 | 7 | 7 | 7 | 7 | 7 |
| | | | | 2.0e+0 | 1.8e+0 | 3.4e+ | 1.7e+0 | 1.9e+0 | 3.2e+0 | 2.8e+0 | 2.0e+0 | 1.7e+0 | 1.8e+0 | 2.6e+0 | 2.3e+0 |
| | | | | 6 ± | 6 ± | 06 ± | 6 ± | 6 ± | 6 ± | 6 ± | 6 ± | 6 ± | 6 ± | 6 ± | 6 ± |
| | | | | 1.9e+0 | 2.9e+0 | 2.7e+ | 1.6e+0 | 1.3e+0 | 4.5e+0 | 1.7e+0 | 2.0e+0 | 2.1e+0 | 2.7e+0 | 2.6e+0 | 1.6e+0 |
| CerG2GNAc1(d36:1)-H | CerG2GNAc1(d36:1)-H | CerG2GNAc1 | turquoise | 6 | 6 | 06 | 6 | 6 | 6 | 6 | 6 | 6 | 6 | 6 | 6 |
| | | | | 8.7e+0 | 7.6e+0 | 1.3e+ | 9.2e+0 | 8.7e+0 | 1.5e+0 | 1.3e+0 | 1.2e+0 | 7.4e+0 | 7.7e+0 | 9.9e+0 | 1.4e+0 |
| | | | | 6 ± | 6 ± | 07 ± | 6 ± | 6 ± | 7 ± | 7 ± | 7 ± | 6 ± | 6 ± | 6 ± | 7 ± |
| | | | | 8.4e+0 | 6.0e+0 | 1.1e+ | 8.9e+0 | 5.6e+0 | 2.0e+0 | 9.6e+0 | 1.3e+0 | 9.9e+0 | 8.0e+0 | 6.6e+0 | 1.4e+0 |
| | | | | 6 | 6 | 07 | 6 | 6 | 7 | 6 | 7 | 6 | 6 | 6 | 7 |
| GM3(m36:5)-H | GM3(m36:5)-H | GM3 | turquoise | 8.9e+0 | 8.2e+0 | 1.5e+ | 8.0e+0 | 9.0e+0 | 1.3e+0 | 1.4e+0 | 9.2e+0 | 7.5e+0 | 8.7e+0 | 1.2e+0 | 1.0e+0 |
| | | | | 5 ± | 5 ± | 06 ± | 5 ± | 5 ± | 6 ± | 6 ± | 5 ± | 5 ± | 5 ± | 6 ± | 6 ± |
| | | | | 6.7e+0 | 1.1e+0 | 1.0e+ | 6.1e+0 | 5.8e+0 | 1.4e+0 | 7.4e+0 | 7.6e+0 | 7.4e+0 | 1.0e+0 | 1.0e+0 | 6.6e+0 |
| | | | | 5 | 6 | 06 | 5 | 5 | 6 | 5 | 5 | 5 | 6 | 6 | 5 |
| | | | | 5.7e+0 | 5.2e+0 | 8.4e+ | 5.3e+0 | 5.7e+0 | 8.1e+0 | 7.8e+0 | 7.1e+0 | 4.6e+0 | 5.0e+0 | 6.5e+0 | 8.6e+0 |
| CerG2GNAc1(d38:4)+HCOO | CerG2GNAc1(d38:4)+HCOO | CerG2GNAc1 | turquoise | 6 ± | 6 ± | 06 ± | 6 ± | 6 ± | 6 ± | 6 ± | 6 ± | 6 ± | 6 ± | 6 ± | 6 ± |
| | | | | 4.7e+0 | 3.5e+0 | 6.0e+ | 3.2e+0 | 3.4e+0 | 8.5e+0 | 4.6e+0 | 6.2e+0 | 4.9e+0 | 4.4e+0 | 3.5e+0 | 7.1e+0 |
| | | | | 6 | 6 | 06 | 6 | 6 | 6 | 6 | 6 | 6 | 6 | 6 | 6 |
| | | | | 3.9e+0 | 3.5e+0 | 5.2e+ | 3.6e+0 | 3.8e+0 | 5.0e+0 | 5.0e+0 | 4.5e+0 | 2.9e+0 | 3.6e+0 | 3.9e+0 | 5.2e+0 |
| | | | | 6 ± | 6 ± | 06 ± | 6 ± | 6 ± | 6 ± | 6 ± | 6 ± | 6 ± | 6 ± | 6 ± | 6 ± |
| GM3(m38:6)+HCOO | GM3(m38:6)+HCOO | GM3 | turquoise | 2.6e+0 | 1.7e+0 | 2.6e+ | 1.8e+0 | 2.1e+0 | 4.4e+0 | 2.3e+0 | 3.3e+0 | 1.7e+0 | 2.3e+0 | 1.1e+0 | 2.7e+0 |
| | | | | 6 | 6 | 06 | 6 | 6 | 6 | 6 | 6 | 6 | 6 | 6 | 6 |
| | | | | 5.6e+0 | 4.3e+0 | 7.3e+ | 5.0e+0 | 5.4e+0 | 4.6e+0 | 6.1e+0 | 5.4e+0 | 4.4e+0 | 4.5e+0 | 5.6e+0 | 5.9e+0 |
| | | | | 6 ± | 6 ± | 06 ± | 6 ± | 6 ± | 6 ± | 6 ± | 6 ± | 6 ± | 6 ± | 6 ± | 6 ± |
| | | | | 1.8e+0 | 2.4e+0 | 5.2e+ | 1.8e+0 | 2.7e+0 | 2.5e+0 | 3.2e+0 | 2.2e+0 | 2.4e+0 | 2.6e+0 | 1.9e+0 | 2.5e+0 |
| GM3(d42:2)-H | GM3(d42:2)-H | GM3 | turquoise | 6 | 6 | 06 | 6 | 6 | 6 | 6 | 6 | 6 | 6 | 6 | 6 |
| | | | | 3.0e+0 | 2.5e+0 | 3.0e+ | 2.6e+0 | 3.1e+0 | 2.7e+0 | 3.0e+0 | 2.9e+0 | 2.8e+0 | 2.5e+0 | 3.5e+0 | 3.1e+0 |
| | | | | 7 ± | 7 ± | 07 ± | 7 ± | 7 ± | 7 ± | 7 ± | 7 ± | 7 ± | 7 ± | 7 ± | 7 ± |
| | | | | 1.8e+0 | 1.4e+0 | 1.8e+ | 1.5e+0 | 1.5e+0 | 1.8e+0 | 1.9e+0 | 1.4e+0 | 1.7e+0 | 1.0e+0 | 1.1e+0 | 2.1e+0 |
| | | | | 7 | 7 | 07 | 7 | 7 | 7 | 7 | 7 | 7 | 7 | 7 | 7 |
| PC(31:0)+H | PC(31:0)+H | PC | turquoise | 9.7e+0 | 7.1e+0 | 1.1e+ | 8.4e+0 | 9.9e+0 | 8.0e+0 | 8.1e+0 | 1.0e+0 | 8.4e+0 | 7.4e+0 | 1.1e+0 | 1.0e+0 |
| | | | | 6 ± | 6 ± | 07 ± | 6 ± | 6 ± | 6 ± | 6 ± | 7 ± | 6 ± | 6 ± | 7 ± | 7 ± |

| | | | | | | | | | | | | | | | |
|-----------------|---------------|-----|-----------|---------------|---------------|---------------|---------------|---------------|---------------|---------------|---------------|---------------|---------------|---------------|---------------|
| LPE(18:2)+H | LPE(18:2)+H | LPE | turquoise | 6.1e+0 6 | 3.4e+0 6 | 8.5e+ 06 | 5.3e+0 6 | 6.0e+0 6 | 6.0e+0 6 | 3.3e+0 6 | 4.9e+0 6 | 4.9e+0 6 | 2.4e+0 6 | 4.9e+0 6 | 5.6e+0 6 |
| | | | | 4.5e+0 7 ± | 4.9e+0 7 ± | 5.6e+ 07 ± | 4.3e+0 7 ± | 4.1e+0 7 ± | 7.0e+0 7 ± | 5.1e+0 7 ± | 4.9e+0 7 ± | 4.0e+0 7 ± | 4.7e+0 7 ± | 6.4e+0 7 ± | 6.6e+0 7 ± |
| | | | | 2.9e+0 7 | 4.8e+0 7 | 2.6e+ 07 | 4.1e+0 7 | 1.5e+0 7 | 7.1e+0 7 | 2.2e+0 7 | 5.9e+0 7 | 2.2e+0 7 | 4.1e+0 7 | 3.6e+0 7 | 6.7e+0 7 |
| LPC(16:2e)+H | LPC(16:2e)+H | LPC | turquoise | 8.8e+0 6 ± | 7.9e+0 6 ± | 1.1e+ 07 ± | 8.5e+0 6 ± | 9.1e+0 6 ± | 1.1e+0 7 ± | 1.1e+0 7 ± | 9.5e+0 6 ± | 7.7e+0 6 ± | 8.2e+0 6 ± | 9.7e+0 6 ± | 1.0e+0 7 ± |
| | | | | 4.1e+0 6 | 4.1e+0 6 | 6.0e+ 06 | 5.8e+0 6 | 6.8e+0 6 | 8.9e+0 6 | 6.0e+0 6 | 4.6e+0 6 | 6.4e+0 6 | 4.3e+0 6 | 3.8e+0 6 | 7.0e+0 6 |
| LPC(16:0)+H | LPC(16:0)+H | LPC | turquoise | 5.0e+0 9 ± | 4.0e+0 9 ± | 5.7e+ 09 ± | 4.3e+0 9 ± | 4.9e+0 9 ± | 5.6e+0 9 ± | 6.2e+0 9 ± | 4.8e+0 9 ± | 3.9e+0 9 ± | 4.2e+0 9 ± | 5.3e+0 9 ± | 5.2e+0 9 ± |
| | | | | 2.8e+0 9 | 1.7e+0 9 | 3.2e+ 09 | 2.8e+0 9 | 2.5e+0 9 | 3.9e+0 9 | 4.4e+0 9 | 2.7e+0 9 | 2.6e+0 9 | 2.4e+0 9 | 2.6e+0 9 | 3.1e+0 9 |
| PC(8:0e_10:0)+H | PC(18:0e)+H | PC | turquoise | 1.5e+0 9 ± | 1.3e+0 9 ± | 1.8e+ 09 ± | 1.5e+0 9 ± | 1.6e+0 9 ± | 1.9e+0 9 ± | 1.9e+0 9 ± | 1.8e+0 9 ± | 1.3e+0 9 ± | 1.2e+0 9 ± | 1.6e+0 9 ± | 2.0e+0 9 ± |
| | | | | 1.0e+0 9 | 7.1e+0 8 | 1.0e+ 09 | 1.0e+0 9 | 8.6e+0 8 | 1.7e+0 9 | 1.1e+0 9 | 1.5e+0 9 | 9.7e+0 8 | 7.4e+0 8 | 8.5e+0 8 | 1.4e+0 9 |
| WE(16:0)-H | WE(16:0)-H | WE | turquoise | 4.1e+0 6 ± | 3.5e+0 6 ± | 4.8e+ 06 ± | 4.0e+0 6 ± | 4.0e+0 6 ± | 4.1e+0 6 ± | 5.0e+0 6 ± | 4.5e+0 6 ± | 3.6e+0 6 ± | 3.3e+0 6 ± | 3.6e+0 6 ± | 4.3e+0 6 ± |
| | | | | 1.6e+0 6 | 1.7e+0 6 | 2.2e+ 06 | 1.7e+0 6 | 1.6e+0 6 | 1.9e+0 6 | 2.2e+0 6 | 2.1e+0 6 | 1.0e+0 6 | 1.2e+0 6 | 1.5e+0 6 | 2.1e+0 6 |
| LPC(18:2)-CH3 | LPC(18:2)-CH3 | LPC | turquoise | 2.9e+0 7 ± | 2.7e+0 7 ± | 4.0e+ 07 ± | 2.6e+0 7 ± | 2.5e+0 7 ± | 3.3e+0 7 ± | 3.3e+0 7 ± | 3.0e+0 7 ± | 2.3e+0 7 ± | 2.5e+0 7 ± | 3.4e+0 7 ± | 3.4e+0 7 ± |
| | | | | 1.9e+0 7 | 2.2e+0 7 | 3.0e+ 07 | 2.1e+0 7 | 9.6e+0 6 | 2.5e+0 7 | 1.3e+0 7 | 2.8e+0 7 | 1.2e+0 7 | 1.9e+0 7 | 1.4e+0 7 | 2.7e+0 7 |
| LPC(18:0)-CH3 | LPC(18:0)-CH3 | LPC | turquoise | 2.0e+0 6 ± | 1.9e+0 6 ± | 2.6e+ 06 ± | 2.1e+0 6 ± | 2.1e+0 6 ± | 2.3e+0 6 ± | 2.8e+0 6 ± | 2.5e+0 6 ± | 1.7e+0 6 ± | 1.7e+0 6 ± | 2.2e+0 6 ± | 3.0e+0 6 ± |
| | | | | 7.8e+0 5 | 6.3e+0 5 | 1.1e+ 06 | 9.0e+0 5 | 9.0e+0 5 | 1.4e+0 6 | 1.2e+0 6 | 1.1e+0 6 | 7.6e+0 5 | 4.9e+0 5 | 7.3e+0 5 | 2.0e+0 6 |
| GM3(m38:2)-2H | GM3(m38:2)-2H | GM3 | turquoise | 4.5e+0 6 ± | 3.9e+0 6 ± | 7.0e+ 06 ± | 4.4e+0 6 ± | 4.3e+0 6 ± | 5.1e+0 6 ± | 5.9e+0 6 ± | 4.6e+0 6 ± | 3.6e+0 6 ± | 3.6e+0 6 ± | 4.6e+0 6 ± | 5.5e+0 6 ± |

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| | | | | | | | | | | | | | | | |
|--------------|--------------|-----|-----------|--------|--------|-------|--------|--------|--------|--------|--------|--------|--------|--------|--------|
| | | | | 5.5e+0 | 5.9e+0 | 8.3e+ | 5.8e+0 | 7.3e+0 | 9.3e+0 | 8.6e+0 | 7.6e+0 | 8.6e+0 | 4.7e+0 | 7.6e+0 | 8.6e+0 |
| | | | | 5 | 5 | 05 | 5 | 5 | 5 | 5 | 5 | 5 | 5 | 5 | 5 |
| | | | | 6.2e+0 | 5.7e+0 | 6.8e+ | 5.8e+0 | 6.1e+0 | 6.4e+0 | 6.2e+0 | 6.5e+0 | 5.1e+0 | 5.6e+0 | 6.5e+0 | 6.3e+0 |
| LPC(16:0)+Na | LPC(16:0)+Na | LPC | turquoise | 8 ± | 8 ± | 08 ± | 8 ± | 8 ± | 8 ± | 8 ± | 8 ± | 8 ± | 8 ± | 8 ± | 8 ± |
| | | | | 2.2e+0 | 1.6e+0 | 2.4e+ | 1.9e+0 | 1.8e+0 | 1.7e+0 | 1.8e+0 | 2.1e+0 | 1.5e+0 | 1.6e+0 | 1.9e+0 | 2.3e+0 |
| | | | | 8 | 8 | 08 | 8 | 8 | 8 | 8 | 8 | 8 | 8 | 8 | 8 |

Metabolites after log transformation are presented as mean ± SD. WGCNA, weighted gene correlation network analysis; EX+VD, vitamin D supplementation and exercise training; VD, vitamin D supplementation; EX, exercise training; Con, control group; t1, time 1 (0-week); t2, time 2(12-week); t3, time 3 (24-week); TG, triglycerols; PC, phosphatidylcholine; Cer, ceramide; SM, sphingomyelin; PE, phosphatidylethanolamine; LPC, lyso-phosphatidylcholine; DG, diacylglycerols; PS, phosphatidylserine; AcCa, acyl carnitine; HexCer/Hex2Cer, hexosyl ceramide; GM3, ganglioside, monosialo trihexosyl ceramide; PIP, phosphatidylinositol(4)phosphate; CerG3GNAc1, dihexosyl N-acetylhexosyl ceramide; WE, wax exters; PIP2, phosphatidylinositol(4,5)bisphosphate; DGDG, digalactosyl diglyceride.

Table S6. Different co-expression modules of lipids from WGCNA

| ID | Time | Group | MEturquoise | MEblue | MEgrey |
|-------|------|-------|-------------|----------|----------|
| NO.9 | t2 | Con | -0.14902 | -0.21164 | -0.10501 |
| NO.11 | t2 | Con | -0.12497 | -0.17163 | 0.044051 |
| NO.7 | t2 | Con | -0.08231 | -0.1705 | -0.07593 |
| NO.64 | t2 | Con | -0.14548 | -0.12775 | 0.120497 |
| NO.14 | t2 | Con | -0.07593 | -0.09396 | -0.05323 |
| NO.57 | t2 | Con | -0.03385 | -0.06944 | -0.05637 |
| NO.42 | t2 | Con | 0.01436 | -0.00806 | -0.00889 |
| NO.36 | t2 | Con | 0.001078 | 0.000352 | 0.220759 |
| NO.38 | t2 | Con | -0.00037 | 0.005865 | 0.102853 |
| NO.41 | t2 | Con | -0.00819 | 0.025145 | -0.15752 |
| NO.20 | t2 | Con | 0.055918 | 0.038414 | 0.051209 |
| NO.34 | t2 | Con | -0.08257 | 0.050942 | -0.02604 |
| NO.59 | t2 | Con | 0.039487 | 0.056244 | 0.115969 |
| NO.39 | t2 | Con | 0.078848 | 0.151449 | -0.08364 |
| NO.56 | t2 | Con | 0.058312 | 0.153096 | 0.071819 |
| NO.15 | t2 | EX | 0.214057 | -0.33127 | -0.22934 |
| NO.5 | t2 | EX | -0.12099 | -0.14307 | -0.20828 |
| NO.61 | t2 | EX | 0.624663 | -0.09745 | -0.05146 |
| NO.4 | t2 | EX | 0.002245 | -0.08219 | 0.030735 |
| NO.52 | t2 | EX | 0.01043 | -0.08124 | -0.01524 |
| NO.40 | t2 | EX | -0.02237 | -0.03985 | -0.0574 |
| NO.63 | t2 | EX | -0.08475 | -0.00143 | -0.26457 |
| NO.18 | t2 | EX | 0.052397 | 0.00438 | 0.021825 |
| NO.48 | t2 | EX | 0.050366 | 0.009003 | -0.02017 |
| NO.27 | t2 | EX | 0.029604 | 0.014806 | 0.053752 |
| NO.13 | t2 | EX | 0.04413 | 0.05796 | 0.144222 |
| NO.49 | t2 | EX | 0.02013 | 0.07619 | 0.01099 |
| NO.25 | t2 | EX | 0.167324 | 0.203141 | 0.270766 |
| NO.43 | t2 | EX | 0.27969 | 0.309746 | -0.06524 |
| NO.16 | t2 | VD | -0.25667 | -0.13338 | -0.2095 |
| NO.54 | t2 | VD | -0.29076 | 0.157854 | 0.049957 |
| NO.50 | t2 | VD | -0.05998 | -0.11207 | 0.129471 |
| NO.33 | t2 | VD | -0.12463 | -0.09882 | 0.122718 |
| NO.60 | t2 | VD | -0.05812 | -0.0665 | -0.04066 |
| NO.62 | t2 | VD | -0.14805 | -0.05179 | 0.365859 |
| NO.1 | t2 | VD | 0.01411 | 0.0027 | -0.11476 |
| NO.45 | t2 | VD | 0.031488 | 0.084735 | 0.013738 |
| NO.47 | t2 | VD | 0.029508 | 0.089646 | -0.11039 |
| NO.26 | t2 | VD | -0.01676 | 0.125403 | 0.225281 |
| NO.17 | t2 | VD | 0.045495 | 0.11715 | -0.14742 |
| NO.22 | t2 | VD | -0.03488 | 0.121818 | 0.126183 |
| NO.6 | t2 | VD | 0.103333 | 0.136579 | -0.01837 |
| NO.19 | t2 | VD | 0.093501 | 0.172567 | 0.01401 |
| NO.31 | t2 | VD | 0.146504 | 0.219633 | -0.36501 |
| NO.28 | t2 | EX+VD | -0.09457 | -0.10412 | -0.03346 |
| NO.29 | t2 | EX+VD | 0.018104 | 0.03054 | -0.05845 |
| NO.10 | t2 | EX+VD | -0.06507 | 0.028361 | 0.015147 |

| | | | | | |
|-------|----|-------|----------|----------|----------|
| NO.2 | t2 | EX+VD | -0.01957 | 0.005179 | -0.04044 |
| NO.58 | t2 | EX+VD | -0.01884 | 0.003571 | 0.208005 |
| NO.55 | t2 | EX+VD | 0.008954 | 0.000775 | -0.12782 |
| NO.21 | t2 | EX+VD | 0.001452 | 0.005407 | -0.0147 |
| NO.12 | t2 | EX+VD | 0.085247 | 0.132154 | 0.103314 |
| NO.51 | t2 | EX+VD | 0.011978 | 0.05062 | 0.095735 |
| NO.24 | t2 | EX+VD | 0.100242 | 0.064908 | 0.057968 |
| NO.65 | t2 | EX+VD | 0.204589 | 0.181325 | 0.0036 |
| NO.53 | t2 | EX+VD | 0.102646 | 0.187004 | -0.02311 |
| NO.23 | t2 | EX+VD | 0.04235 | 0.196406 | -0.11416 |
| NO.32 | t2 | EX+VD | 0.195223 | 0.2017 | 0.086285 |
| NO.44 | t2 | EX+VD | 0.124677 | 0.216248 | 0.019867 |

WGCNA, weighted gene correlation network analysis; EX+VD, vitamin D supplementation and exercise training; VD, vitamin D supplementation; EX, exercise training; Con, control group; t1, time 1 (0-week); t2, time 2 (12-week).