Supplementary Material 1

# Animal feeding and diabetic model

All animal protocols conformed to the Public Health Service Guide for Care and Use of Laboratory Animals, which were approved by New York Institute of Technology College of Osteopathic Medicine (NYITCOM, Approval No. 2016-QL-01). FVB/N mice were initially purchased from the Jackson Laboratory and a breeding colony was maintained in a fully controlled animal facility at NYITCOM. Four mice were housed together in one cage at constant room temperature (20–22 °C) with free access to bottled tap water and food under a 12:12 h light:dark cycle. The type 2 diabetes was induced as follows: both male and female 2-month-old FVB/N mice were randomly divided into control and high-fat diet/streptozotocin (HFD-STZ)-induced diabetic groups. The control group was given a regular lab chow (5001 Rodent Diet, PMI Nutrition International, LLC, Brentwood, MO), while the HFD-STZ group was fed a high fat diet (HFD, D12492, 60% of calories derived from fat, 5.24 kcal/gm, Research Diets, New Brunswick, NJ) for 1 month, and then intraperitoneally injected with streptozotocin (STZ, Sigma, 30 mg/kg body weight, dissolved in 10 mM sodium citrate buffer, pH = 4.5) for 3 consecutive days. The mice were maintained on HFD for another 3 months. Blood glucose levels were determined using a TRUEtrack glucometer (NIPRO DIAGNOSTICS, Fort Lauderdale, FL), and a fasting blood glucose level of 250 mg/dL or greater was considered diabetic. Five control (all female) and five HFD-STZ (4 female and 1 male) mice were anesthetized with 2% isoflurane and the blood was taken from the right ventricle into 3.5 mL Vacutainer Plus Plastic Serum Tubes (BD-367983-1, MedexSupply, Passaic, NJ 07055) for serum separation, and the separated serum samples were immediately stored in −80 °C. The animal was perfused initially with cold KCl solution (25 mM in phosphate-buffered saline, PBS) through a syringe inserted into the left ventricle to arrest the heart at diastole and then with PBS to wash out KCl and residual blood from the organs. Tissue samples were collected into 2 mL cryovials, including liver, brain, ventricle, atrium, renal medulla, renal cortex, and spleen, and immediately snap-frozen in liquid nitrogen and stored in −80 °C until analysis.

# Echocardiography and hemodynamic measurement

A GE VIVID 7 echocardiographic suit and an in vivo hemodynamic monitoring system with pressure-volume catheter (Scisense Inc., Ontario, Canada) were used to examine cardiac geometry and function in mice. Two-dimensional images of the cardiac chamber were obtained from short-axis views of the left ventricle (LV) at the papillary muscle level. Fractional shortening (FS) and ejection fraction (EF) were calculated from left ventricular dimensions at the end of systole and diastole. Hemodynamic measurements in mice were performed through intraventricular catheterization. The maximal LV systolic and end-diastolic pressures (LVSP and LVEDP), maximal slope of systolic pressure increment (dP/dt-max), and diastolic pressure decrement (dP/dt-min) were recorded or calculated.

# HPLC conditions

An Atlantic T3 C18 column (2.1 × 150 mm, 3 µm, Waters, Milford, MA) was used for chromatographic separation. The column oven temperature was held at 40 °C, and the flow rate was kept at 200 μL/min, and the injection volume was set at 10 uL. The mobile phases consisted of (A) water with 5 mM ammonium acetate, (B) isopropanol, and (C) methanol.

The gradient elution program for ESI-positive mode was as below: the initial 1 min, 20% A, 10% B, 70% C; 1–11 min, 5% A, 65% B, 30% C; 11–20 min, 0% A, 75% B, 25% C; this ratio was maintained to 28 min; 28–28.5 min returned to initial gradient and kept to 30 min for re-equilibration. While the gradient elution program ESI-negative mode was as follows: the initial, 25% A, 40% B, 30% C; 0–1 min, 5% A, 60% B, 35% C, and keeping this ratio to 15 min; 15–27 min, 0% A, 65% B, 35% C; 27–28 min, returned to initial gradient within 1 min and kept to 30 min.

# Mass spectrometry parameters

The MS capillary voltage was set at 3.0 kV, the capillary temperature was kept at 330 °C, the sheath gas (nitrogen) flow was set to 50 psi, and the auxiliary gas (nitrogen) was set to 5 psi. The high-resolution MS data was obtained in Fourier Transform mode with resolving power of 60,000, and the scan ranges were set at *m/z* 150–1100 and *m/z* 220–1650 for ESI-positive and ESI-negative modes, respectively. The MS/MS data by collision-induced dissociation (CID) was acquired in data-dependent mode, with the normalized collision energy set at 35.0, activation Q value set at 0.25, and activation time set at 30 ms.

**Table S1.1** Echocardiographic and parameters in control and HFD-STZ diabetic mice

|  |  |  |
| --- | --- | --- |
|  | **Control**  | **HFD-STZ** |
| **Echocardiography** |  |  |
| N (animals) | 19 | 22 |
| Glucose (mg/dL) | 107 ± 29 | 427 ± 88 \* |
| LVESD (mm) | 1.93 ± 0.27 | 2.36 ± 0.28 \* |
| LVEDD (mm) | 3.54 ± 0.32 | 3.64 ± 0.37 |
| %EF | 82.4 ± 5.4 | 70.9 ± 5.0 \* |
| %FS | 45.6 ± 5.5 | 34.9 ± 4.0 \* |
| **Gravimetry** |  |  |
| n(animals) | 8 | 15 |
| BW (g) | 26.2 ± 3.5 | 26.1 ± 3.3 |
| HW (mg) | 140.8 ± 17.8 | 132.9 ± 15.8 |
| HW/BW | 5.4 ± 0.59 | 5.1 ± 0.53 |
| **Hemodynamics** |  |  |
| n(animals) | 8 | 15 |
| HR(bpm) | 443 ± 225 | 387 ± 204 |
| dP/dt max(mmHg/s) | 7502 ± 3857 | 5967 ± 3172 \* |
| dP/dt min(mmHg/s) | 6098 ± 3163 | 5013 ± 2733 \* |
| LVSP (mmHg) | 102.9 ± 52.3 | 91.5 ± 47.6 \* |
| LVEDP (mmHg) | 1.54 ± 1.25 | 3.48 ± 2.67 |

Results were expressed as mean ± SD and analyzed by two-tailed *t*-test. \* *P* < 0.05 vs control.

BW, body weight; %EF, % ejection fraction; %FS, % fractional shortening; HR, heart rate; HW/BW, heart weight/body weight; LVEDD, left ventricle end diastolic diameter; LVESD, left ventricle end systolic diameter; LVEDP, LV end diastolic pressure; LVSP, LV systolic pressure.

**Table S1.2** LC/MS data of the identified intact lipid species

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Lipid species | Formula | Diagnostic ion | RT | Calc. m/z | Exp. m/z | Δppm | Fragment | Fatty acyl(s) |
| TG42:0 | C45H86O6 | [M + NH4]+ | 13.37 | 740.6763 | 740.6764 | 0.14 | N/D | N/D |
| TG44:0 | C47H90O6 | [M + NH4]+ | 13.79 | 768.7076 | 768.7074 | −0.26 | N/D | N/D |
| TG46:0 | C49H94O6 | [M + NH4]+ | 14.18 | 796.7389 | 796.7383 | −0.75 | N/D | N/D |
| TG46:1 | C49H92O6 | [M + NH4]+ | 13.84 | 794.7232 | 794.7230 | −0.25 | N/D | N/D |
| TG46:2 | C49H90O6 | [M + NH4]+ | 13.52 | 792.7076 | 792.7075 | −0.13 | N/D | N/D |
| TG46:3 | C49H88O6 | [M + NH4]+ | 13.19 | 790.6919 | 790.6914 | −0.63 | N/D | N/D |
| TG48:0 | C51H98O6 | [M + NH4]+ | 14.54 | 824.7702 | 824.7701 | −0.12 | N/D | N/D |
| TG48:1 | C51H96O6 | [M + NH4]+ | 14.24 | 822.7545 | 822.7546 | 0.12 | 549,551523,549,577 | 16:0/16:1/16:014:0/18:1/16:0 |
| TG48:2 | C51H94O6 | [M + NH4]+ | 13.93 | 820.7389 | 820.7385 | −0.49 | 547,549521,549,575 | 16:0/16:1/16:114:0/18:1/16:1 |
| TG48:3 | C51H92O6 | [M + NH4]+ | 13.61 | 818.7232 | 818.7226 | −0.73 | 547521,547,573 | 16:1/16:1/16:114:0/18:2/16:1 |
| TG48:4 | C51H90O6 | [M + NH4]+ | 13.30 | 816.7076 | 816.7070 | −0.73 | 519,545,573 | 14:0/18:2/16:2 |
| TG50:0 | C53H102O6 | [M + NH4]+ | 14.91 | 852.8015 | 852.8015 | 0.00 | N/D | N/D |
| TG50:1 | C53H100O6 | [M + NH4]+ | 14.57 | 850.7858 | 850.7852 | −0.71 | 551,577 | 16:0/18:1/16:0 |
| TG50:2 | C53H98O6 | [M + NH4]+ | 14.29 | 848.7702 | 848.7700 | −0.24 | 549,575,577549,603 | 16:0/18:1/16:114:0/18:1/18:1 |
| TG50:3 | C53H96O6 | [M + NH4]+ | 14.00 | 846.7545 | 846.7540 | −0.59 | 547,575547,549,601 | 16:1/18:1/16:114:0/18:2/18:1 |
| TG50:4 | C53H94O6 | [M + NH4]+ | 13.72 | 844.7389 | 844.7385 | −0.47 | 547,573 | 16:1/18:2/16:1 |
| TG50:5 | C53H92O6 | [M + NH4]+ | 13.45 | 842.7232 | 842.7229 | −0.36 | 545,571,573 | 16:1/18:2/16:1 |
| TG50:6 | C53H90O6 | [M + NH4]+ | 13.19 | 840.7076 | 840.7071 | −0.59 | N/D | N/D |
| TG52:0 | C55H106O6 | [M + NH4]+ | 15.37 | 880.8328 | 880.8320 | −0.91 | 579,607 | 16:0/18:0/18:0 |
| TG52:1 | C55H104O6 | [M + NH4]+ | 14.96 | 878.8171 | 878.8166 | −0.57 | 577,579,605 | 16:0/18:1/18:0 |
| TG52:2 | C55H102O6 | [M + NH4]+ | 14.62 | 876.8015 | 876.8001 | −1.60 | 577,603 | 16:0/18:1/18:1 |
| TG52:3 | C55H100O6 | [M + NH4]+ | 14.38 | 874.7858 | 874.7842 | −1.83 | 575,603575,577,601 | 16:1/18:1/18:116:0/18:2/18:1 |
| TG52:4 | C55H98O6 | [M + NH4]+ | 14.09 | 872.7702 | 872.7692 | −1.15 | 573,575,601 | 16:1/18:2/18:1 |
| TG52:5 | C55H96O6 | [M + NH4]+ | 13.82 | 870.7545 | 870.7544 | −0.11 | 573,599 | 16:1/18:2/18:2 |
| TG52:6 | C55H94O6 | [M + NH4]+ | 13.54 | 868.7389 | 868.7389 | 0.00 | N/D | N/D |
| TG52:7 | C55H92O6 | [M + NH4]+ | 13.37 | 866.7232 | 866.7232 | 0.00 | N/D | N/D |
| TG54:0 | C57H110O6 | [M + NH4]+ | 15.83 | 908.8641 | 908.8630 | −1.21 | 607579,607,635 | 18:0/18:0/18:016:0/20:0/18:0 |
| TG54:1 | C57H108O6 | [M + NH4]+ | 15.43 | 906.8484 | 906.8471 | −1.43 | 605,607 | 18:0/18:1/18:0 |
| TG54:2 | C57H106O6 | [M + NH4]+ | 15.03 | 904.8328 | 904.8310 | −1.99 | 605,603 | 18:0/18:1/18:1 |
| TG54:3 | C57H104O6 | [M + NH4]+ | 14.78 | 902.8171 | 902.8151 | −2.22 | 603 | 18:1/18:1/18:1 |
| TG54:4 | C57H102O6 | [M + NH4]+ | 14.48 | 900.8015 | 900.7991 | −2.66 | 601,603 | 18:1/18:2/18:1 |
| TG54:5 | C57H100O6 | [M + NH4]+ | 14.18 | 898.7858 | 898.7847 | −1.22 | 599,601 | 18:1/18:2/18:2 |
| TG54:6 | C57H98O6 | [M + NH4]+ | 13.90 | 896.7702 | 896.7688 | −1.56 | 597,599,601 | 18:1/18:3/18:2 |
| TG54:7 | C57H96O6 | [M + NH4]+ | 13.65 | 894.7545 | 894.7540 | −0.56 | 597,599 | 18:2/18:3/18:2 |
| TG54:8 | C57H94O6 | [M + NH4]+ | 13.39 | 892.7389 | 892.7382 | −0.78 | N/D | N/D |
| TG54:9 | C57H92O6 | [M + NH4]+ | 13.28 | 890.7232 | 890.7227 | −0.56 | N/D | N/D |
| TG54:10 | C57H90O6 | [M + NH4]+ | 13.02 | 888.7076 | 888.7067 | −1.01 | N/D | N/D |
| TG56:4 | C59H106O6 | [M + NH4]+ | 14.86 | 928.8328 | 928.8299 | −3.12 | 631,601,629 | 18:1/20:1/18:2 |
| TG56:5 | C59H104O6 | [M + NH4]+ | 14.57 | 926.8171 | 926.8140 | −3.34 | N/D | N/D |
| TG56:6 | C59H102O6 | [M + NH4]+ | 14.45 | 924.8015 | 924.7977 | −4.11 | N/D | N/D |
| TG56:7 | C59H100O6 | [M + NH4]+ | 14.24 | 922.7858 | 922.7838 | −2.17 | N/D | N/D |
| TG56:8 | C59H98O6 | [M + NH4]+ | 13.97 | 920.7702 | 920.7682 | −2.17 | N/D | N/D |
| TG56:9 | C59H96O6 | [M + NH4]+ | 13.59 | 918.7545 | 918.7540 | −0.54 | N/D | N/D |
| TG56:10 | C59H94O6 | [M + NH4]+ | 13.34 | 916.7389 | 916.7383 | −0.65 | N/D | N/D |
| TG56:11 | C59H92O6 | [M + NH4]+ | 13.06 | 914.7232 | 914.7227 | −0.55 | N/D | N/D |
| TG58:6 | C61H106O6 | [M + NH4]+ | 14.84 | 952.8328 | 952.8301 | −2.83 | N/D | N/D |
| TG58:7 | C61H104O6 | [M + NH4]+ | 14.52 | 950.8171 | 950.8142 | −3.05 | N/D | N/D |
| TG58:8 | C61H102O6 | [M + NH4]+ | 14.27 | 948.8015 | 948.7989 | −2.74 | N/D | N/D |
| TG58:9 | C61H100O6 | [M + NH4]+ | 14.02 | 946.7858 | 946.7838 | −2.11 | N/D | N/D |
| TG58:10 | C61H98O6 | [M + NH4]+ | 13.75 | 944.7702 | 944.7688 | −1.48 | N/D | N/D |
| TG58:11 | C61H96O6 | [M + NH4]+ | 13.50 | 942.7545 | 942.7536 | −0.95 | N/D | N/D |
| TG58:12 | C61H94O6 | [M + NH4]+ | 13.25 | 940.7389 | 940.7379 | −1.06 | N/D | N/D |
| TG60:10 | C63H102O6 | [M + NH4]+ | 14.24 | 972.8015 | 972.7993 | −2.26 | N/D | N/D |
| TG60:11 | C63H100O6 | [M + NH4]+ | 13.97 | 970.7858 | 970.7838 | −2.06 | N/D | N/D |
| TG60:12 | C63H98O6 | [M + NH4]+ | 13.68 | 968.7702 | 968.7689 | −1.34 | N/D | N/D |
| TG60:13 | C63H96O6 | [M + NH4]+ | 13.43 | 966.7545 | 966.7534 | −1.14 | N/D | N/D |
| TG62:12 | C65H102O6 | [M + NH4]+ | 13.99 | 996.8015 | 996.8003 | −1.20 | N/D | N/D |
| TG62:13 | C65H100O6 | [M + NH4]+ | 13.86 | 994.7858 | 994.7841 | −1.71 | N/D | N/D |
| TG62:14 | C65H98O6 | [M + NH4]+ | 13.59 | 992.7702 | 992.7689 | −1.31 | N/D | N/D |
| TG62:15 | C65H96O6 | [M + NH4]+ | 13.36 | 990.7545 | 990.7533 | −1.21 | N/D | N/D |
| FFA16:0 | C16H32O2 | [M − H]− | 11.53 | 255.2330 | 255.2331 | 0.39 | N/A | 16:0 |
| FFA18:0 | C18H36O2 | [M − H]− | 13.34 | 283.2643 | 283.2640 | −1.06 | N/A | 18:0 |
| FFA18:1 | C18H34O2 | [M − H]− | 12.07 | 281.2486 | 281.2488 | 0.71 | N/A | 18:1 |
| FFA18:2 | C18H32O2 | [M − H]− | 10.78 | 279.2330 | 279.2332 | 0.72 | N/A | 18:2 |
| FFA18:3 | C18H30O2 | [M − H]− | 9.49 | 277.2173 | 277.2177 | 1.44 | N/A | 18:3 |
| FFA20:4 | C20H32O2 | [M − H]− | 10.76 | 303.2330 | 303.2328 | −0.66 | N/A | 20:4 |
| FFA20:5 | C20H30O2 | [M − H]− | 9.45 | 301.2173 | 301.2172 | −0.33 | N/A | 20:5 |
| FFA22:6 | C22H32O2 | [M − H]− | 10.36 | 327.2330 | 327.2334 | 1.22 | N/A | 22:6 |
| PC32:0 | C40H80O8NP | [M + H]+ | 9.52 | 734.5694 | 734.5699 | 0.68 | 478 | 16:0/16:0 |
| PC32:1 | C40H78O8NP | [M + H]+ | 8.69 | 732.5538 | 732.5537 | −0.14 | N/D | N/D |
| PC32:2 | C40H76O8NP | [M + H]+ | 8.43 | 730.5381 | 730.5378 | −0.41 | N/D | N/D |
| PC34:0 | C42H84O8NP | [M + H]+ | 10.95 | 762.6007 | 762.6010 | 0.39 | 478,506 | 16:0/18:0 |
| PC34:1 | C42H82O8NP | [M + H]+ | 9.58 | 760.5851 | 760.5841 | −1.31 | 478,504 | 16:0/18:1 |
| PC34:2 | C42H80O8NP | [M + H]+ | 9.13 | 758.5694 | 758.5697 | 0.40 | 478,502 | 16:0/18:2 |
| PC34:3 | C42H78O8NP | [M + H]+ | 8.57 | 756.5538 | 756.5536 | −0.26 | N/D | N/D |
| PC34:4 | C42H76O8NP | [M + H]+ | 8.33 | 754.5381 | 754.5386 | 0.66 | N/D | N/D |
| PC36:1 | C44H86O8NP | [M + H]+ | 11.82 | 788.6164 | 788.6144 | −2.54 | 504,506 | 18:0/18:1 |
| PC36:2 | C44H84O8NP | [M + H]+ | 9.98 | 786.6007 | 786.5997 | −1.27 | 502,506504 | 18:0/18:218:1/18:1 |
| PC36:3 | C44H82O8NP | [M + H]+ | 9.14 | 784.5851 | 784.5834 | −2.17 | 502,504 | 18:1/18:2 |
| PC36:4 | C44H80O8NP | [M + H]+ | 8.75 | 782.5694 | 782.5697 | 0.38 | 478,526 | 16:0/20:4 |
| PC36:5 | C44H78O8NP | [M + H]+ | 8.43 | 780.5538 | 780.5534 | −0.51 | 476,526 | 16:1/20:4 |
| PC36:6 | C44H76O8NP | [M + H]+ | 8.25 | 778.5381 | 778.5386 | 0.64 | N/D | N/D |
| PC38:4 | C46H84O8NP | [M + H]+ | 9.67 | 810.6007 | 810.5996 | −1.36 | 506,526 | 18:0/20:4 |
| PC38:5 | C46H82O8NP | [M + H]+ | 9.13 | 808.5851 | 808.5831 | −2.47 | 504,526 | 18:1/20:4 |
| PC38:6 | C46H80O8NP | [M + H]+ | 8.69 | 806.5694 | 806.5682 | −1.49 | 478,550 | 16:0/22:6 |
| PC38:7 | C46H78O8NP | [M + H]+ | 8.40 | 804.5538 | 804.5531 | −0.87 | 476,550 | 16:1/22:6 |
| PC40:6 | C48H84O8NP | [M + H]+ | 9.60 | 834.6007 | 834.5993 | −1.68 | 506,550 | 18:0/22:6 |
| PC40:7 | C48H82O8NP | [M + H]+ | 9.13 | 832.5851 | 832.5842 | −1.08 | 504,550 | 18:1/22:6 |
| PC40:8 | C48H80O8NP | [M + H]+ | 8.47 | 830.5694 | 830.5684 | −1.20 | 502,550 | 18:2/22:6 |
| PC42:10 | C50H80O8NP | [M + H]+ | 8.40 | 854.5694 | 854.5684 | −1.17 | N/D | N/D |
| PE34:0 | C39H78O8NP | [M − H]− | 17.10 | 718.5392 | 718.5408 | 2.23 | 255,480 | 16:0/18:0 |
| PE34:1 | C39H76O8NP | [M − H]− | 16.57 | 716.5236 | 716.5247 | 1.54 | N/D | N/D |
| PE36:0 | C41H82O8NP | [M − H]− | 17.92 | 746.5705 | 746.5718 | 1.74 | N/D | N/D |
| PE36:1 | C41H80O8NP | [M − H]− | 17.28 | 744.5549 | 744.5557 | 1.07 | 281,283,480 | 18:0/18:1 |
| PE36:2 | C41H78O8NP | [M − H]− | 16.69 | 742.5392 | 742.5399 | 0.94 | 279,283,480 | 18:0/18:2 |
| PE36:3 | C41H76O8NP | [M − H]− | 16.35 | 740.5236 | 740.5251 | 2.03 | 279,281,478 | 18:1/18:2 |
| PE38:4 | C43H78O8NP | [M − H]− | 16.75 | 766.5392 | 766.5413 | 2.74 | 283,303,480 | 18:0/20:4 |
| PE38:5 | C43H76O8NP | [M − H]− | 16.38 | 764.5236 | 764.5250 | 1.83 | 281,303,478 | 18:1/20:4 |
| PE38:6 | C43H74O8NP | [M − H]− | 16.06 | 762.5079 | 762.5064 | −1.97 | 279,303,476 | 18:2/20:4 |
| PE40:6 | C45H78O8NP | [M − H]− | 16.68 | 790.5392 | 790.5425 | 4.17 | 283,327,480 | 18:0/22:6 |
| PE40:7 | C45H76O8NP | [M − H]− | 16.26 | 788.5236 | 788.5242 | 0.76 | 281,327,478 | 18:1/22:6 |
| PI32:0 | C41H79O13P | [M − H]− | 14.50 | 809.5186 | 809.5179 | −0.86 | N/D | N/D |
| PI32:1 | C41H77O13P | [M − H]− | 13.98 | 807.5029 | 807.5021 | −0.99 | N/D | N/D |
| PI34:0 | C43H83O13P | [M − H]− | 15.20 | 837.5499 | 837.5497 | −0.24 | N/D | N/D |
| PI34:1 | C43H81O13P | [M − H]− | 14.67 | 835.5342 | 835.5341 | −0.12 | N/D | N/D |
| PI34:2 | C43H79O13P | [M − H]− | 14.25 | 833.5186 | 833.5171 | −1.80 | 255,279,391,553 | 16:0/18:2 |
| PI34:3 | C43H77O13P | [M − H]− | 13.77 | 831.5029 | 831.5021 | −0.96 | N/D | N/D |
| PI36:0 | C45H87O13P | [M − H]− | 15.86 | 865.5812 | 865.5806 | −0.69 | 283,419,581 | 18:0/18:0 |
| PI36:1 | C45H85O13P | [M − H]− | 15.41 | 863.5655 | 863.5655 | 0.00 | 281,283,419,581 | 18:0/18:1 |
| PI36:2 | C45H83O13P | [M − H]− | 14.95 | 861.5499 | 861.5498 | −0.12 | 281,417,579 | 18:0/18:2 |
| PI36:3 | C45H81O13P | [M − H]− | 14.43 | 859.5342 | 859.5343 | 0.12 | N/D | N/D |
| PI36:4 | C45H79O13P | [M − H]− | 14.30 | 857.5186 | 857.5181 | −0.58 | 255,303,391,553 | 16:0/20:4 |
| PI36:5 | C45H77O13P | [M − H]− | 13.87 | 855.5029 | 855.5026 | −0.35 | N/D | N/D |
| PI38:4 | C47H83O13P | [M − H]− | 15.02 | 885.5499 | 885.5490 | −1.02 | 283,303,419,581 | 18:0/20:4 |
| PI38:5 | C47H81O13P | [M − H]− | 14.50 | 883.5342 | 883.5330 | −1.36 | 281,303,417,579 | 18:1/20:4 |
| PI38:6 | C47H79O13P | [M − H]− | 14.29 | 881.5186 | 881.5168 | −2.04 | N/D | N/D |
| PI40:6 | C49H83O13P | [M − H]− | 14.93 | 909.5499 | 909.5464 | −3.85 | N/D | N/D |
| PI 40:7 | C49H81O13P | [M − H]− | 14.45 | 907.5342 | 907.5319 | −2.53 | N/D | N/D |
| PI 42:10 | C51H79O13P | [M − H]− | 13.32 | 929.5186 | 929.5179 | −0.75 | N/D | N/D |
| LPC16:0 | C24H50O7NP | [M + H]+ | 3.39 | 496.3398 | 496.3395 | −0.60 | N/A | 16:0 |
| LPC18:0 | C26H54O7NP | [M + H]+ | 4.48 | 524.3711 | 524.3701 | −1.91 | N/A | 18:0 |
| LPC18:1 | C26H52O7NP | [M + H]+ | 3.48 | 522.3554 | 522.3539 | −2.87 | N/A | 18:1 |
| LPC18:2 | C26H50O7NP | [M + H]+ | 2.88 | 520.3398 | 520.3398 | 0.00 | N/A | 18:2 |
| LPC18:3 | C26H48O7NP | [M + H]+ | 2.68 | 518.3241 | 518.3238 | −0.58 | N/A | 18:3 |
| LPC20:4 | C28H50O7NP | [M + H]+ | 3.31 | 544.3398 | 544.3392 | −1.10 | N/A | 20:4 |
| LPC20:5 | C28H48O7NP | [M + H]+ | 3.00 | 542.3241 | 542.3214 | −4.98 | N/A | 20:5 |
| LPC22:6 | C30H50O7NP | [M + H]+ | 2.72 | 568.3398 | 568.3392 | −1.06 | N/A | 22:6 |
| LPE16:0 | C21H44O7NP | [M − H]− | 9.91 | 452.2783 | 452.2785 | 0.44 | N/A | 16:0 |
| LPE18:0 | C23H48O7NP | [M − H]− | 11.67 | 480.3096 | 480.3096 | 0.00 | N/A | 18:0 |
| LPE18:1 | C23H46O7NP | [M − H]− | 10.41 | 478.2939 | 478.2942 | 0.63 | N/A | 18:1 |
| LPE18:2 | C23H44O7NP | [M − H]− | 9.27 | 476.2783 | 476.2797 | 2.94 | N/A | 18:2 |
| LPE18:3 | C23H42O7NP | [M − H]− | 8.19 | 474.2626 | 474.2624 | −0.42 | N/A | 18:3 |
| LPE20:4 | C25H44O7NP | [M − H]− | 9.34 | 500.2783 | 500.2787 | 0.80 | N/A | 20:4 |
| LPE20:5 | C25H42O7NP | [M − H]− | 8.29 | 498.2626 | 498.2620 | −1.20 | N/A | 20:5 |
| LPE22:6 | C27H44O7NP | [M − H]− | 9.34 | 524.2783 | 524.2790 | 1.34 | N/A | 22:6 |
| LPI16:0 | C25H49O12P | [M − H]− | 7.41 | 571.2889 | 571.2880 | −1.58 | N/A | 16:0 |
| LPI18:0 | C27H53O12P | [M − H]− | 9.25 | 599.3202 | 599.3202 | 0.00 | N/A | 18:0 |
| LPI18:1 | C27H51O12P | [M − H]− | 7.95 | 597.3045 | 597.3037 | −1.34 | N/A | 18:1 |
| LPI18:2 | C27H49O12P | [M − H]− | 6.64 | 595.2889 | 595.2887 | −0.34 | N/A | 18:2 |
| LPI20:4 | C29H49O12P | [M − H]− | 6.72 | 619.2889 | 619.2878 | −1.78 | N/A | 20:4 |
| CL68:2 | C77H146O17P2 | [M − H]− | 18.92 | 1403.9962 | 1403.9930 | −2.28 | N/D | N/D |
| CL68:3 | C77H144O17P2 | [M − H]− | 18.30 | 1401.9806 | 1401.9783 | −1.64 | N/D | N/D |
| CL68:4 | C77H142O17P2 | [M − H]− | 17.76 | 1399.9649 | 1399.9629 | −1.43 | N/D | N/D |
| CL68:5 | C77H140O17P2 | [M − H]− | 17.44 | 1397.9493 | 1397.9483 | −0.72 | N/D | N/D |
| CL68:6 | C77H138O17P2 | [M − H]− | 17.25 | 1395.9336 | 1395.9313 | −1.65 | N/D | N/D |
| CL70:3 | C79H148O17P2 | [M − H]− | 18.91 | 1430.0119 | 1430.0074 | −3.15 | N/D | N/D |
| CL70:4 | C79H146O17P2 | [M − H]− | 18.62 | 1427.9962 | 1427.9935 | −1.89 | N/D | N/D |
| CL70:5 | C79H144O17P2 | [M − H]− | 18.05 | 1425.9806 | 1425.9785 | −1.47 | N/D | N/D |
| CL70:6 | C79H142O17P2 | [M − H]− | 17.60 | 1423.9649 | 1423.9624 | −1.76 | N/D | N/D |
| CL70:7 | C79H140O17P2 | [M − H]− | 17.31 | 1421.9493 | 1421.9457 | −2.53 | N/D | N/D |
| CL72:4 | C81H150O17P2 | [M − H]− | 19.05 | 1456.0275 | 1456.0233 | −2.88 | 281,699 | (18:1)4 |
| CL72:5 | C81H148O17P2 | [M − H]− | 18.68 | 1454.0119 | 1454.0071 | −3.30 | 279,281,697,699 | (18:1)3(18:2)1 |
| CL72:6 | C81H146O17P2 | [M − H]− | 18.27 | 1451.9962 | 1451.9928 | −2.34 | 279,281,697 | (18:1)2(18:2)2 |
| CL72:7 | C81H144O17P2 | [M − H]− | 17.71 | 1449.9806 | 1449.9772 | −2.34 | 279,281,695,697 | (18:1)1(18:2)3 |
| CL72:8 | C81H142O17P2 | [M − H]− | 17.48 | 1447.9649 | 1447.9609 | −2.76 | 279,695 | (18:2)4 |
| CL72:9 | C81H140O17P2 | [M − H]− | 17.26 | 1445.9493 | 1445.9460 | −2.28 | N/D | N/D |
| CL74:5 | C83H152O17P2 | [M − H]− | 19.44 | 1482.0432 | 1482.0393 | −2.63 | N/D | N/D |
| CL74:6 | C83H150O17P2 | [M − H]− | 18.91 | 1480.0275 | 1480.0231 | −2.97 | N/D | N/D |
| CL74:7 | C83H148O17P2 | [M − H]− | 18.62 | 1478.0119 | 1478.0079 | −2.71 | N/D | N/D |
| CL74:8 | C83H146O17P2 | [M − H]− | 17.98 | 1475.9962 | 1475.9918 | −2.98 | N/D | N/D |
| CL74:9 | C83H144O17P2 | [M − H]− | 17.62 | 1473.9806 | 1473.9758 | −3.26 | 279,305,695,721 | (18:1)2(18:2)1(20:5)1(18:0)1(18:2)2(20:5)1 |
| CL74:10 | C83H142O17P2 | [M − H]− | 17.51 | 1471.9649 | 1471.9600 | −3.33 | N/D | N/D |
| CL74:11 | C83H140O17P2 | [M − H]− | 17.30 | 1469.9493 | 1469.9460 | −2.24 | N/D | N/D |
| CL76:7 | C85H152O17P2 | [M − H]− | 19.15 | 1506.0432 | 1506.0388 | −2.92 | N/D | N/D |
| CL76:8 | C85H150O17P2 | [M − H]− | 18.68 | 1504.0275 | 1504.0223 | −3.46 | N/D | N/D |
| CL76:9 | C85H148O17P2 | [M − H]− | 18.27 | 1502.0119 | 1502.0074 | −3.00 | N/D | N/D |
| CL76:10 | C85H146O17P2 | [M − H]− | 17.92 | 1499.9962 | 1499.9916 | −3.07 | N/D | N/D |
| CL76:11 | C85H144O17P2 | [M − H]− | 17.71 | 1497.9806 | 1497.9755 | −3.40 | 279,281,303,697,743 | (18:1)1(18:2)1(20:4)2 |
| CL76:12 | C85H142O17P2 | [M − H]− | 17.48 | 1495.9649 | 1495.9602 | −3.14 | N/D | N/D |
| CL78:10 | C87H150O17P2 | [M − H]− | 18.88 | 1528.0275 | 1528.0280 | 0.33 | N/D | N/D |
| CL78:11 | C87H148O17P2 | [M − H]− | 18.28 | 1526.0119 | 1526.0085 | −2.23 | N/D | N/D |
| CL78:12 | C87H146O17P2 | [M − H]− | 17.98 | 1523.9962 | 1523.9901 | −4.00 | N/D | N/D |
| CL78:13 | C87H144O17P2 | [M − H]− | 17.62 | 1521.9806 | 1521.9758 | −3.15 | N/D | N/D |

N/A: Not available (the lipid species contained only one fatty acyl, thus identical).

N/D: Not identified (we could not get the MS/MS data due to the low intensity).