

Subject	0	1	Significance, p
Index			0.143
Mean ± Standard deviation	29.5 ± 16.1	37.1 ± 22.3	
Median and [25%; 75%]	29.5 [17.3; 42.8]	44.0 [12.8; 56.3]	
Group			<0.001
Control	2 (4.3%)	8 (50.0%)	
Main	44 (95.7%)	8 (50.0%)	
Sex			0.319
Female	10 (21.7%)	6 (37.5%)	
Male	36 (78.3%)	10 (62.5%)	
Age, years			0.001
Mean ± Standard deviation	66.1 ± 11.3	52.1 ± 14.4	
Median and [25%; 75%]	68.0 [63.0; 72.8]	49.5 [41.0; 64.5]	
Smoking			0.111
0	24 (52.2%)	12 (75.0%)	
1	22 (47.8%)	4 (25.0%)	
Diabetes melitus			0.026
0	34 (73.9%)	16 (100.0%)	
1	12 (26.1%)	0 (0.0%)	
Arterial Hypertension			<0.001
0	3 (6.5%)	8 (50.0%)	
1	43 (93.5%)	8 (50.0%)	
Coronary heart disease			0.355
0	31 (67.4%)	13 (81.3%)	
1	15 (32.6%)	3 (18.8%)	
Ischemic Stroke			0.200
0	32 (69.6%)	14 (87.5%)	
1	14 (30.4%)	2 (12.5%)	
Sinus rhythm			
1	46 (100.0%)	16 (100.0%)	
Heart failure			0.565
0	42 (91.3%)	16 (100.0%)	
1	4 (8.7%)	0 (0.0%)	
Chronic Kidney Disease			0.422
0	7 (15.2%)	3 (18.8%)	
1	2 (4.3%)	3 (18.8%)	

2	17 (37.0%)	5 (31.3%)	
3a	18 (39.1%)	5 (31.3%)	
3b	2 (4.3%)	0 (0.0%)	
Chronic Kidney Failure			
0	46 (100.0%)	16 (100.0%)	
Hemoglobine g/l			0.541
Mean ± Standard deviation	134.1 ± 14.0	137.2 ± 18.3	
Median and [25%; 75%]	135.0 [124.3; 143.8]	137.5 [130.0; 145.5]	
RBC 10*12/l			0.916
Mean ± Standard deviation	4.6 ± 0.4	4.6 ± 0.5	
Median and [25%; 75%]	4.6 [4.3; 5.0]	4.6 [4.3; 4.8]	
WBC 10*9/l			0.334
Mean ± Standard deviation	7.4 ± 3.0	6.8 ± 2.2	
Median and [25%; 75%]	7.0 [5.7; 8.1]	6.3 [5.1; 7.6]	
PLT 10*9/l			0.954
Mean ± Standard deviation	254.9 ± 56.1	254.0 ± 53.3	
Median and [25%; 75%]	246.0 [213.4; 292.0]	242.5 [211.8; 299.1]	
ESR mm/h			0.077
Mean ± Standard deviation	24.0 ± 17.7	18.9 ± 22.5	
Median and [25%; 75%]	19.0 [11.0; 30.0]	9.0 [6.0; 20.5]	
Specific gravity			0.839
Mean ± Standard deviation	998.0 ± 135.3	1,017.4 ± 5.1	
Median and [25%; 75%]	1,017.0 [1,015.0; 1,020.0]	1,016.5 [1,015.0; 1,020.3]	
Erythrocyturia per field			0.315
0	41 (89.1%)	16 (100.0%)	
1	5 (10.9%)	0 (0.0%)	
Leukocyturia fer field			0.743
0	36 (78.3%)	12 (75.0%)	
1	10 (21.7%)	4 (25.0%)	
Bacteriuria			0.725
0	37 (80.4%)	12 (75.0%)	
1	9 (19.6%)	4 (25.0%)	
Glucosuria			>0.999
0	43 (97.7%)	15 (100.0%)	
1	1 (2.3%)	0 (0.0%)	
Proteinuria			0.453

0	45 (97.8%)	15 (93.8%)	
1	1 (2.2%)	1 (6.3%)	
Salts in urine			0.315
0	41 (89.1%)	16 (100.0%)	
1	5 (10.9%)	0 (0.0%)	
Total protein g/l			0.924
Mean ± Standard deviation	72.0 ± 4.5	72.1 ± 5.4	
Median and [25%; 75%]	72.0 [69.2; 74.6]	70.5 [68.8; 74.2]	
Creatinine µmol/l			0.558
Mean ± Standard deviation	101.3 ± 21.1	97.4 ± 23.0	
Median and [25%; 75%]	101.5 [87.0; 111.0]	92.0 [79.8; 116.5]	
CKD MDRD ml/min/1.73m2			0.454
Mean ± Standard deviation	65.7 ± 15.6	71.2 ± 19.6	
Median and [25%; 75%]	63.8 [54.3; 74.2]	63.9 [57.9; 85.7]	
Urea µmol/l			0.215
Mean ± Standard deviation	7.0 ± 2.2	6.2 ± 1.4	
Median and [25%; 75%]	6.6 [5.5; 7.9]	5.7 [5.5; 6.9]	
Uric acid µmol/l			0.484
Mean ± Standard deviation	343.1 ± 105.9	309.7 ± 86.8	
Median and [25%; 75%]	335.9 [288.8; 389.5]	334.4 [208.8; 361.6]	
Mean ± Standard deviation			0.816
Mean ± Standard deviation	8.2 ± 15.4	6.2 ± 7.6	
Median and [25%; 75%]	2.9 [1.2; 6.4]	2.6 [0.8; 9.8]	
Glucose µmol/l			0.949
Mean ± Standard deviation	5.7 ± 2.0	5.3 ± 0.5	
Median and [25%; 75%]	5.3 [4.9; 5.8]	5.2 [5.0; 5.5]	
AST points/l			0.897
Mean ± Standard deviation	22.4 ± 6.4	23.4 ± 9.7	
Median and [25%; 75%]	21.5 [18.3; 26.8]	19.5 [16.0; 30.0]	
ALT points/l			0.484
Mean ± Standard deviation	21.3 ± 8.4	26.9 ± 15.6	
Median and [25%; 75%]	19.5 [15.3; 26.0]	21.0 [15.0; 41.3]	
Total bilirubine µmol/l			0.974
Mean ± Standard deviation	11.8 ± 4.2	11.9 ± 4.9	
Median and [25%; 75%]	10.9 [9.7; 12.4]	10.9 [9.3; 14.0]	
Iron µmol/l			0.250

Mean ± Standard deviation	14.7 ± 7.9	17.5 ± 8.0	
Median and [25%; 75%]	12.7 [8.1; 21.7]	15.7 [11.7; 24.1]	
Fibrinogen g/l			0.068
Mean ± Standard deviation	3.9 ± 1.1	3.4 ± 1.5	
Median and [25%; 75%]	3.7 [3.3; 4.3]	3.1 [2.5; 4.0]	
APTT			0.477
Mean ± Standard deviation	1.1 ± 0.2	1.1 ± 0.1	
Median and [25%; 75%]	1.0 [1.0; 1.1]	1.0 [1.0; 1.1]	
INR			0.100
Mean ± Standard deviation	1.1 ± 0.1	1.0 ± 0.0	
Median and [25%; 75%]	1.1 [1.0; 1.1]	1.0 [1.0; 1.0]	
Quick's value			0.325
Mean ± Standard deviation	94.0 ± 10.7	96.6 ± 8.1	
Median and [25%; 75%]	93.0 [87.0; 101.0]	94.0 [91.0; 99.5]	
Total cholesterol µmol/l			0.257
Mean ± Standard deviation	4.6 ± 1.2	5.0 ± 1.2	
Median and [25%; 75%]	4.4 [4.0; 5.5]	4.7 [4.3; 5.4]	
Triglycerides µmol/l			0.607
Mean ± Standard deviation	1.6 ± 0.8	1.7 ± 0.9	
Median and [25%; 75%]	1.3 [1.1; 1.9]	1.6 [1.1; 2.0]	
LDL µmol/l			0.365
Mean ± Standard deviation	2.8 ± 0.9	3.1 ± 1.0	
Median and [25%; 75%]	2.8 [2.2; 3.5]	3.0 [2.4; 3.6]	
VLDL µmol/l			0.904
Mean ± Standard deviation	0.8 ± 0.5	0.7 ± 0.3	
Median and [25%; 75%]	0.7 [0.5; 0.9]	0.7 [0.5; 0.8]	
HDL µmol/l			0.174
Mean ± Standard deviation	1.2 ± 0.4	1.2 ± 0.3	
Median and [25%; 75%]	1.1 [0.9; 1.3]	1.2 [1.1; 1.4]	
Atherogenic coefficient			0.726
Mean ± Standard deviation	3.2 ± 1.3	3.1 ± 1.2	
Median and [25%; 75%]	3.2 [2.4; 4.2]	3.0 [2.1; 3.7]	
TSH µIU/l			0.693
Mean ± Standard deviation	1.9 ± 1.4	1.9 ± 1.2	
Median and [25%; 75%]	1.4 [1.1; 2.0]	1.5 [1.2; 2.7]	
C12.0_1_per cmol			<0.001

Mean ± Standard deviation	0.0 ± 0.0	0.0 ± 0.0	
Median and [25%; 75%]	0.0 [0.0; 0.0]	0.0 [0.0; 0.0]	
C14.0_1_percmol			<0.001
Mean ± Standard deviation	0.0 ± 0.0	0.0 ± 0.0	
Median and [25%; 75%]	0.0 [0.0; 0.0]	0.0 [0.0; 0.0]	
C16.0_1_percmol			0.598
Mean ± Standard deviation	0.2 ± 0.0	0.3 ± 0.0	
Median and [25%; 75%]	0.3 [0.2; 0.3]	0.3 [0.2; 0.3]	
C18.0_1_percmol			0.200
Mean ± Standard deviation	0.1 ± 0.0	0.1 ± 0.0	
Median and [25%; 75%]	0.1 [0.1; 0.1]	0.1 [0.1; 0.1]	
C20.0_1_percmol			0.384
Mean ± Standard deviation	0.0 ± 0.0	0.0 ± 0.0	
Median and [25%; 75%]	0.0 [0.0; 0.0]	0.0 [0.0; 0.0]	
C22.0_1_percmol			0.654
Mean ± Standard deviation	0.0 ± 0.0	0.0 ± 0.0	
Median and [25%; 75%]	0.0 [0.0; 0.0]	0.0 [0.0; 0.0]	
C24.0_1_percmol			0.319
Mean ± Standard deviation	0.0 ± 0.0	0.0 ± 0.0	
Median and [25%; 75%]	0.0 [0.0; 0.0]	0.0 [0.0; 0.0]	
C16.1_cis_1_percmol			0.496
Mean ± Standard deviation	0.0 ± 0.0	0.0 ± 0.0	
Median and [25%; 75%]	0.0 [0.0; 0.0]	0.0 [0.0; 0.0]	
C18.1_cis_1_percmol			0.916
Mean ± Standard deviation	0.3 ± 0.0	0.3 ± 0.0	
Median and [25%; 75%]	0.3 [0.2; 0.3]	0.3 [0.2; 0.3]	
C20.1_cis_1_percmol			0.703
Mean ± Standard deviation	0.0 ± 0.0	0.0 ± 0.0	
Median and [25%; 75%]	0.0 [0.0; 0.0]	0.0 [0.0; 0.0]	
C24.1_cis_1_percmol			0.001
Mean ± Standard deviation	0.0 ± 0.0	0.0 ± 0.0	
Median and [25%; 75%]	0.0 [0.0; 0.0]	0.0 [0.0; 0.0]	
C16.1_trans_1_percmol			0.250
Mean ± Standard deviation	0.0 ± 0.0	0.0 ± 0.0	
Median and [25%; 75%]	0.0 [0.0; 0.0]	0.0 [0.0; 0.0]	
C18.1_trans_1_percmol			0.883

Mean ± Standard deviation	0.0 ± 0.0	0.0 ± 0.0	
Median and [25%; 75%]	0.0 [0.0; 0.0]	0.0 [0.0; 0.0]	
C18.2_trans_1_percmol			0.883
Mean ± Standard deviation	0.0 ± 0.0	0.0 ± 0.0	
Median and [25%; 75%]	0.0 [0.0; 0.0]	0.0 [0.0; 0.0]	
C18.2_n_6_1_percmol			0.672
Mean ± Standard deviation	0.2 ± 0.0	0.2 ± 0.0	
Median and [25%; 75%]	0.2 [0.2; 0.3]	0.2 [0.2; 0.3]	
C18.3_n_6_1_percmol			0.366
Mean ± Standard deviation	0.0 ± 0.0	0.0 ± 0.0	
Median and [25%; 75%]	0.0 [0.0; 0.0]	0.0 [0.0; 0.0]	
C20.2_n_6_1_percmol			0.148
Mean ± Standard deviation	0.0 ± 0.0	0.0 ± 0.0	
Median and [25%; 75%]	0.0 [0.0; 0.0]	0.0 [0.0; 0.0]	
C20.3_n_6_1_percmol			0.635
Mean ± Standard deviation	0.0 ± 0.0	0.0 ± 0.0	
Median and [25%; 75%]	0.0 [0.0; 0.0]	0.0 [0.0; 0.0]	
C20.4_n_6_1_percmol			0.084
Mean ± Standard deviation	0.1 ± 0.0	0.1 ± 0.0	
Median and [25%; 75%]	0.1 [0.1; 0.1]	0.1 [0.0; 0.1]	
C22.4_n_6_1_percmol			0.411
Mean ± Standard deviation	0.0 ± 0.0	0.0 ± 0.0	
Median and [25%; 75%]	0.0 [0.0; 0.0]	0.0 [0.0; 0.0]	
C22.5_n_6_1_percmol			0.564
Mean ± Standard deviation	0.0 ± 0.0	0.0 ± 0.0	
Median and [25%; 75%]	0.0 [0.0; 0.0]	0.0 [0.0; 0.0]	
EPA_C20.5_n_3_1_percmol			>0.999
Mean ± Standard deviation	0.0 ± 0.0	0.0 ± 0.0	
Median and [25%; 75%]	0.0 [0.0; 0.0]	0.0 [0.0; 0.0]	
DHA_C22.6n3_2_percmol			0.077
Mean ± Standard deviation	0.0 ± 0.0	0.0 ± 0.0	
Median and [25%; 75%]	0.0 [0.0; 0.0]	0.0 [0.0; 0.0]	
SFA_rel			0.060
Mean ± Standard deviation	0.3 ± 0.0	0.4 ± 0.0	
Median and [25%; 75%]	0.3 [0.3; 0.3]	0.4 [0.3; 0.4]	
UFA_rel			0.060

Mean ± Standard deviation	0.7 ± 0.0	0.6 ± 0.0	
Median and [25%; 75%]	0.7 [0.7; 0.7]	0.6 [0.6; 0.7]	
MUFA_rel			0.970
Mean ± Standard deviation	0.3 ± 0.0	0.3 ± 0.0	
Median and [25%; 75%]	0.3 [0.3; 0.3]	0.3 [0.3; 0.3]	
PUFA_rel			0.159
Mean ± Standard deviation	0.4 ± 0.0	0.3 ± 0.0	
Median and [25%; 75%]	0.4 [0.3; 0.4]	0.3 [0.3; 0.4]	
HUFA_rel			0.069
Mean ± Standard deviation	0.1 ± 0.0	0.1 ± 0.0	
Median and [25%; 75%]	0.1 [0.1; 0.1]	0.1 [0.1; 0.1]	
omega_6_rel			0.280
Mean ± Standard deviation	0.3 ± 0.0	0.3 ± 0.0	
Median and [25%; 75%]	0.3 [0.3; 0.4]	0.3 [0.3; 0.3]	
omega_3_index_rel			0.212
Mean ± Standard deviation	0.0 ± 0.0	0.0 ± 0.0	
Median and [25%; 75%]	0.0 [0.0; 0.0]	0.0 [0.0; 0.0]	
AAEPA_rel			0.163
Mean ± Standard deviation	18.6 ± 12.4	13.9 ± 7.0	
Median and [25%; 75%]	16.6 [12.3; 20.4]	13.9 [8.2; 17.9]	
Omega_63_rel			0.691
Mean ± Standard deviation	15.7 ± 4.8	17.6 ± 7.0	
Median and [25%; 75%]	15.4 [12.6; 18.1]	15.2 [12.4; 22.5]	
PUFASFA_rel			0.038
Mean ± Standard deviation	1.0 ± 0.1	1.0 ± 0.1	
Median and [25%; 75%]	1.0 [1.0; 1.1]	1.0 [0.9; 1.0]	
TFA_index_rel			0.862
Mean ± Standard deviation	0.0 ± 0.0	0.0 ± 0.0	
Median and [25%; 75%]	0.0 [0.0; 0.0]	0.0 [0.0; 0.0]	
C18.2n6C20.3n6_rel			0.955
Mean ± Standard deviation	21.8 ± 7.9	22.0 ± 9.1	
Median and [25%; 75%]	20.2 [15.7; 26.5]	20.5 [16.4; 24.0]	
AHexCer 54:10;O3 AHexCer (O-22:3)32:7;O3__[M+H]__1.99			0.057
Mean ± Standard deviation	35,740.4 ± 37,551.4	53,031.3 ± 54,722.7	
Median and [25%; 75%]	18,872.5 [10,014.0; 47,180.8]	35,939.5 [25,071.8; 52,698.0]	
CAR 18:2__[M+H]__1.8			0.029

Mean ± Standard deviation	115,374.3 ± 241,614.2	53,799.9 ± 104,175.0	
Median and [25%; 75%]	36,133.5 [15,615.0; 77,330.5]	10,286.4 [1,807.8; 71,960.6]	
CE 18:2 [M+NH4] 11.25			0.270
Mean ± Standard deviation	211,747,964.2 ± 47,670,589.2	195,870,839.4 ± 48,275,291.0	
Median and [25%; 75%]	212,342,912.0 [177,134,490.0; 254,574,	202,797,026.0 [177,257,634.0; 224,531,878.0]	
CE 18:3 [M+NH4] 10.64			0.260
Mean ± Standard deviation	10,053,828.8 ± 6,456,818.5	11,660,529.7 ± 7,266,980.1	
Median and [25%; 75%]	8,321,357.0 [5,472,546.8; 13,101,340.1]	10,651,840.1 [7,993,123.3; 14,368,370.5]	
CE 20:3 [M+NH4] 10.81			0.262
Mean ± Standard deviation	7,201,344.1 ± 1,990,876.0	6,303,276.4 ± 2,867,314.8	
Median and [25%; 75%]	7,125,559.5 [5,984,816.1; 8,145,912.0]	6,452,061.9 [4,302,428.0; 8,762,202.1]	
CE 20:4 [M+NH4] 10.67			0.406
Mean ± Standard deviation	126,010,282.9 ± 38,946,581.3	113,356,764.5 ± 54,774,278.0	
Median and [25%; 75%]	124,507,796.0 [102,728,046.1; 146,404,	104,113,796.0 [89,607,185.0; 161,601,324.0]	
CE 20:5 [M+NH4] 9.96			0.442
Mean ± Standard deviation	7,867,237.0 ± 17,939,909.8	2,873,869.9 ± 7,124,150.2	
Median and [25%; 75%]	13,666.5 [2,805.5; 10,237,981.5]	7,790.1 [3,277.6; 413,372.5]	
CE 22:6 [M+NH4] 10.2			0.374
Mean ± Standard deviation	9,903,455.6 ± 11,518,138.7	7,090,440.6 ± 10,121,820.6	
Median and [25%; 75%]	7,696,127.0 [368.5; 16,159,955.5]	847,224.8 [240.1; 13,359,005.6]	
CL 75:4 [M+NH4] 5.26			0.132
Mean ± Standard deviation	1,535,051.9 ± 2,073,911.7	2,513,270.7 ± 2,841,084.5	
Median and [25%; 75%]	723,740.0 [68,375.5; 2,324,810.0]	1,593,721.1 [512,267.8; 3,617,124.3]	
Mean ± Standard deviation			0.131
Mean ± Standard deviation	25,694.7 ± 60,664.0	50,599.1 ± 70,323.8	
Median and [25%; 75%]	4,155.5 [1,212.6; 22,351.8]	21,173.1 [3,753.5; 59,035.5]	
Cer 40:1;O2 Cer 18:1;O2/22:0 [M+H] 7.82			<0.001
Mean ± Standard deviation	106,332.3 ± 63,435.4	269,366.8 ± 232,670.7	
Median and [25%; 75%]	85,061.5 [58,334.9; 155,465.5]	190,534.5 [144,841.9; 356,025.1]	
Cer 40:1;O2 Cer 19:0;O2/21:1 [M+Na] 7.83			0.050
Mean ± Standard deviation	143,147.8 ± 87,628.4	225,600.1 ± 173,625.4	
Median and [25%; 75%]	118,914.5 [71,066.4; 184,488.8]	203,285.3 [119,546.3; 260,504.6]	
Cer 41:8;O2 Cer 17:2;O2/24:6 [M+H-H2O] 6.86			0.006
Mean ± Standard deviation	17,056.5 ± 23,208.8	53,009.3 ± 55,569.3	
Median and [25%; 75%]	5,131.0 [2,673.0; 19,319.6]	32,543.4 [11,226.6; 90,400.9]	
Cer 42:1;O2 Cer 18:1;O2/24:0 [M+H] 8.6			<0.001

Mean ± Standard deviation	2,645,086.3 ± 914,818.0	4,166,126.6 ± 1,841,379.7	
Median and [25%; 75%]	2,566,870.0 [2,134,683.0; 3,044,938.3]	3,337,161.3 [3,025,400.8; 5,654,769.6]	
Cer 42:2;O2 Cer 17:1;O2/25:1__[M+Na]__7.98			0.913
Mean ± Standard deviation	377,041.6 ± 176,640.4	409,108.3 ± 315,757.9	
Median and [25%; 75%]	358,802.0 [262,764.5; 471,262.3]	325,666.9 [242,897.6; 504,363.3]	
Cer 42:2;O2 Cer 18:2;O2/24:0__[M+H]__7.97			0.027
Mean ± Standard deviation	303,819.8 ± 160,852.7	450,526.1 ± 282,864.8	
Median and [25%; 75%]	280,075.5 [212,116.5; 363,184.3]	365,771.0 [279,698.6; 534,695.6]	
Cer 44:7;O2 Cer 18:1;O2/26:6__[M+Na]__8.6			0.166
Mean ± Standard deviation	64,399.3 ± 37,819.0	83,704.5 ± 52,038.1	
Median and [25%; 75%]	54,900.5 [37,445.9; 87,919.5]	72,898.6 [48,423.6; 100,994.4]	
DG 13:0__[M+Na]__2.95			0.014
Mean ± Standard deviation	110,621.7 ± 57,911.2	65,386.6 ± 79,050.5	
Median and [25%; 75%]	105,860.0 [77,794.0; 141,120.3]	26,372.9 [726.1; 123,262.5]	
DG 18:1__[M+Na]__2.88			0.402
Mean ± Standard deviation	15,073.5 ± 27,371.7	6,200.6 ± 7,009.0	
Median and [25%; 75%]	3,417.0 [778.0; 11,264.9]	3,698.5 [98.3; 10,507.1]	
DG 26:5__[M+Na]__1.99			0.037
Mean ± Standard deviation	7,052,242.9 ± 2,443,788.6	8,990,108.0 ± 3,243,499.5	
Median and [25%; 75%]	6,473,784.0 [5,235,220.5; 9,187,238.3]	8,602,367.0 [7,432,060.3; 9,523,287.8]	
DG 28:3 OA1__[M+Na]__0.96			0.034
Mean ± Standard deviation	2,824,465.6 ± 3,567,058.8	2,136,645.0 ± 3,991,369.1	
Median and [25%; 75%]	1,781,832.5 [477,325.0; 3,897,307.1]	45,426.0 [0.0; 2,920,730.9]	
DG 28:3 OA2__[M+Na]__0.88			0.068
Mean ± Standard deviation	2,596,615.2 ± 3,377,011.7	2,186,837.4 ± 3,835,260.7	
Median and [25%; 75%]	1,726,196.3 [478,541.8; 3,472,654.2]	22,766.8 [0.0; 2,639,798.2]	
DG 28:3__[M+Na]__2.18			0.016
Mean ± Standard deviation	176,759.3 ± 82,716.5	250,986.7 ± 101,967.1	
Median and [25%; 75%]	171,912.3 [119,302.5; 236,872.1]	265,569.8 [173,935.3; 309,193.0]	
DG 28:6__[M+Na]__2.21			0.004
Mean ± Standard deviation	1,673,235.3 ± 604,840.6	2,513,199.4 ± 1,316,265.3	
Median and [25%; 75%]	1,620,267.5 [1,159,868.3; 1,906,205.3]	2,291,168.4 [1,745,742.8; 2,668,588.9]	
DG 31:0__[M+Na]__6.8			<0.001
Mean ± Standard deviation	27,044.2 ± 41,399.1	82,057.4 ± 92,458.1	
Median and [25%; 75%]	12,357.0 [3,725.8; 27,993.0]	45,535.9 [28,187.9; 84,609.5]	
DG 31:1__[M+Na]__6.24			0.006

Mean ± Standard deviation	8,670.7 ± 13,989.6	22,189.9 ± 21,748.8	
Median and [25%; 75%]	2,759.0 [1,218.6; 8,339.8]	9,812.5 [2,673.4; 40,211.0]	
DG 32:0 [M+Na] 6.68			0.018
Mean ± Standard deviation	244,959.5 ± 361,121.6	422,058.8 ± 460,374.5	
Median and [25%; 75%]	67,842.5 [26,528.8; 310,141.0]	192,848.6 [108,328.9; 652,997.3]	
DG 32:0 DG 16:0 16:0 [M+NH4] 6.68			<0.001
Mean ± Standard deviation	353,388.7 ± 496,289.8	1,133,830.5 ± 1,089,925.9	
Median and [25%; 75%]	117,117.3 [46,036.4; 414,687.5]	700,426.3 [420,321.3; 1,670,262.5]	
DG 32:1 DG 16:0 16:1 [M+NH4] 6.16			<0.001
Mean ± Standard deviation	136,959.2 ± 264,058.3	992,368.3 ± 1,333,088.1	
Median and [25%; 75%]	24,200.0 [6,805.9; 97,887.3]	482,218.8 [130,373.9; 1,320,206.8]	
DG 33:0 [M+Na] 7.48			<0.001
Mean ± Standard deviation	1,623.3 ± 2,426.4	10,714.8 ± 14,233.4	
Median and [25%; 75%]	605.0 [400.5; 1,703.8]	5,255.3 [1,439.6; 13,293.5]	
DG 33:1 [M+Na] 4.98			0.001
Mean ± Standard deviation	4,914.2 ± 3,576.2	10,517.5 ± 7,455.7	
Median and [25%; 75%]	3,897.0 [2,150.6; 6,890.3]	8,811.5 [5,575.0; 13,068.8]	
DG 33:3 [M+Na] 5.88			0.577
Mean ± Standard deviation	5,994.7 ± 10,413.9	11,002.8 ± 26,388.9	
Median and [25%; 75%]	937.5 [131.0; 4,587.0]	844.0 [0.0; 3,934.5]	
DG 34:0 OA4 [M+Na] 6.36			0.005
Mean ± Standard deviation	32,935.9 ± 60,109.6	115,081.2 ± 223,044.8	
Median and [25%; 75%]	7,436.0 [3,550.6; 38,717.0]	29,805.0 [13,113.9; 84,162.3]	
DG 34:1 OA1 [M+Na] 6.77			0.066
Mean ± Standard deviation	2,521,376.3 ± 2,513,557.6	3,593,761.4 ± 2,430,643.2	
Median and [25%; 75%]	1,345,436.8 [756,344.8; 3,739,911.0]	2,575,630.1 [2,140,250.5; 5,897,521.7]	
DG 34:1 OA2 [M+Na] 6.79			0.066
Mean ± Standard deviation	2,529,169.9 ± 2,507,106.6	3,593,741.3 ± 2,430,653.0	
Median and [25%; 75%]	1,345,157.0 [757,880.3; 3,739,757.3]	2,575,469.0 [2,140,250.5; 5,897,521.7]	
DG 34:1 OA3 [M+Na] 5.89			0.926
Mean ± Standard deviation	498,199.3 ± 904,883.2	1,020,133.4 ± 2,886,737.5	
Median and [25%; 75%]	68,657.0 [9,579.9; 521,899.1]	59,253.3 [12,416.8; 210,558.6]	
DG 34:1 DG 16:0 18:1 [M+NH4] 6.79			<0.001
Mean ± Standard deviation	7,073,736.8 ± 7,921,623.1	16,954,286.8 ± 12,662,816.1	
Median and [25%; 75%]	3,914,849.0 [1,595,636.5; 8,513,462.5]	13,322,309.8 [7,560,773.4; 21,994,317.5]	
DG 34:2 [M+Na] 6.29			0.899

Mean ± Standard deviation	393,901.7 ± 677,997.9	232,469.1 ± 320,368.1	
Median and [25%; 75%]	51,027.5 [9,861.5; 493,231.4]	64,558.0 [15,749.0; 317,756.0]	
DG 34:2 DG 16:0_18:2__[M+NH4]__6.28			0.016
Mean ± Standard deviation	4,123,876.2 ± 5,904,829.0	9,052,018.4 ± 9,339,872.4	
Median and [25%; 75%]	1,835,372.8 [468,258.5; 5,553,046.3]	6,332,455.0 [2,132,011.1; 13,433,427.4]	
DG 36:1__[M+Na]__7.48			<0.001
Mean ± Standard deviation	265,741.0 ± 388,900.2	906,305.1 ± 1,012,889.8	
Median and [25%; 75%]	87,120.0 [30,124.0; 260,826.5]	552,595.3 [151,819.1; 1,219,500.4]	
DG 36:1 DG 18:0_18:1__[M+NH4]__7.49			<0.001
Mean ± Standard deviation	250,736.5 ± 376,602.5	1,447,462.5 ± 1,585,094.1	
Median and [25%; 75%]	80,538.0 [23,183.0; 288,125.1]	807,143.3 [185,732.5; 2,161,835.6]	
DG 36:2__[M+Na]__6.85			0.422
Mean ± Standard deviation	673,094.7 ± 765,264.4	706,976.8 ± 635,011.5	
Median and [25%; 75%]	319,495.5 [173,356.8; 930,806.4]	452,122.8 [256,676.6; 997,428.3]	
DG 36:2 DG 18:1_18:1__[M+NH4]__6.86			0.002
Mean ± Standard deviation	3,476,318.3 ± 4,139,442.9	8,968,041.0 ± 8,122,973.2	
Median and [25%; 75%]	1,779,800.5 [731,178.1; 4,456,517.6]	6,178,164.5 [3,051,019.6; 12,932,142.6]	
DG 36:3__[M+Na]__6.35			0.755
Mean ± Standard deviation	183,528.7 ± 295,827.2	113,213.8 ± 178,691.0	
Median and [25%; 75%]	29,548.0 [9,781.0; 271,676.3]	37,992.8 [19,493.5; 90,262.1]	
DG 36:3 DG 18:1_18:2__[M+NH4]__6.36			0.025
Mean ± Standard deviation	5,731,712.9 ± 6,861,969.0	12,685,855.5 ± 16,196,278.4	
Median and [25%; 75%]	3,333,777.8 [884,852.8; 7,209,351.6]	7,366,340.9 [3,355,724.4; 15,883,050.3]	
DG 36:4__[M+Na]__5.9			0.899
Mean ± Standard deviation	62,550.6 ± 137,789.3	81,586.8 ± 191,166.5	
Median and [25%; 75%]	8,659.0 [2,683.4; 29,935.6]	12,496.1 [1,800.6; 34,026.1]	
DG 38:3__[M+Na]__10.65			0.188
Mean ± Standard deviation	434,159.7 ± 487,007.8	264,970.8 ± 365,720.8	
Median and [25%; 75%]	162,814.8 [72,657.5; 783,701.3]	120,880.4 [54,412.8; 324,713.8]	
DG 38:5 DG 18:1_20:4__[M+NH4]__6.24			0.980
Mean ± Standard deviation	177,146.2 ± 290,708.4	123,916.6 ± 118,920.3	
Median and [25%; 75%]	57,070.0 [29,650.3; 146,117.3]	116,567.5 [24,071.9; 200,280.3]	
DG 38:7__[M+Na]__7.48			<0.001
Mean ± Standard deviation	8,231.8 ± 12,392.5	32,862.2 ± 40,558.5	
Median and [25%; 75%]	3,486.0 [1,513.8; 8,111.3]	15,450.3 [5,494.5; 45,600.0]	
DG 39:1__[M+Na]__11.4			0.100

Mean ± Standard deviation	12,197.9 ± 9,100.0	8,109.3 ± 5,053.6	
Median and [25%; 75%]	9,489.5 [6,381.9; 12,406.0]	7,062.3 [4,751.7; 10,155.3]	
DG 40:4 [M+Na] 10.6			0.232
Mean ± Standard deviation	2,787,231.7 ± 1,465,981.9	2,342,799.9 ± 1,155,358.7	
Median and [25%; 75%]	2,793,084.5 [1,700,269.1; 3,926,140.6]	2,227,951.8 [1,599,347.3; 3,248,011.6]	
DG 40:5 [M+Na] 10.02			0.172
Mean ± Standard deviation	1,395,407.4 ± 901,691.7	1,068,770.2 ± 950,176.6	
Median and [25%; 75%]	1,360,442.0 [723,265.5; 2,038,230.0]	927,060.1 [407,766.6; 1,486,648.1]	
DG 41:3 [M+Na] 10.88			0.072
Mean ± Standard deviation	30,329.2 ± 22,707.2	18,566.6 ± 9,551.9	
Median and [25%; 75%]	22,972.8 [16,302.6; 35,162.8]	18,444.0 [10,048.6; 25,450.6]	
DG 41:4 [M+Na] 10.14			0.011
Mean ± Standard deviation	145,841.1 ± 126,271.9	61,975.8 ± 39,213.6	
Median and [25%; 75%]	106,763.5 [59,832.0; 189,037.5]	70,964.0 [31,210.1; 82,623.4]	
DG 42:1 [M+Na] 5.17			0.212
Mean ± Standard deviation	825,923.6 ± 717,669.1	913,361.7 ± 493,939.5	
Median and [25%; 75%]	639,120.5 [324,983.0; 954,171.0]	829,124.0 [579,732.1; 1,161,146.3]	
DG 42:6 [M+Na] 10.19			<0.001
Mean ± Standard deviation	1,298,982.7 ± 742,919.7	625,960.0 ± 364,781.6	
Median and [25%; 75%]	1,131,653.8 [914,640.0; 1,734,584.9]	760,778.3 [283,892.3; 866,841.1]	
DG 43:0 [M+Na] 6.01			0.003
Mean ± Standard deviation	21,794.7 ± 16,815.4	36,503.2 ± 20,647.2	
Median and [25%; 75%]	15,146.0 [9,310.5; 25,676.5]	34,292.0 [19,282.4; 44,024.1]	
DG 43:5 [M+Na] 10.33			<0.001
Mean ± Standard deviation	141,612.4 ± 138,202.9	38,258.5 ± 46,710.7	
Median and [25%; 75%]	102,040.0 [43,896.1; 191,837.8]	18,880.3 [9,772.4; 45,008.7]	
DG 43:7 [M+Na] 5.63			0.156
Mean ± Standard deviation	333,556.0 ± 204,927.4	417,904.7 ± 219,138.0	
Median and [25%; 75%]	287,078.0 [197,059.9; 453,700.3]	369,999.0 [277,623.1; 572,429.5]	
DG 44:3 [M+Na] 5.39			<0.001
Mean ± Standard deviation	2,364,393.4 ± 945,650.3	1,446,474.8 ± 328,203.5	
Median and [25%; 75%]	2,120,271.5 [1,720,384.4; 2,819,778.3]	1,516,540.6 [1,175,015.6; 1,701,303.3]	
DG 44:7 [M+Na] 6.02			0.002
Mean ± Standard deviation	813,934.2 ± 771,353.5	1,842,150.5 ± 1,642,656.3	
Median and [25%; 75%]	600,289.0 [409,069.5; 993,768.1]	1,225,658.3 [779,720.4; 2,174,484.6]	
DG 44:8 [M+Na] 5.52			0.003

Mean ± Standard deviation	1,644,815.7 ± 966,471.7	3,855,216.2 ± 3,556,040.6	
Median and [25%; 75%]	1,452,661.3 [909,143.1; 2,054,272.6]	2,210,168.3 [1,684,908.9; 4,817,279.0]	
DG 45:8 [M+Na] 8.74			<0.001
Mean ± Standard deviation	4,929,913.7 ± 2,555,199.6	10,208,644.8 ± 5,131,488.5	
Median and [25%; 75%]	4,822,925.8 [3,040,540.1; 6,184,767.8]	8,928,062.5 [7,728,493.9; 12,352,298.4]	
DG 46:0 [M+Na] 6.96			0.001
Mean ± Standard deviation	7,610,408.0 ± 5,177,980.2	11,778,405.6 ± 6,417,000.1	
Median and [25%; 75%]	6,110,469.5 [4,711,094.3; 8,029,842.5]	9,900,176.0 [7,726,101.3; 14,979,912.5]	
DG 46:6 [M+Na] 5.93			<0.001
Mean ± Standard deviation	848,310.6 ± 415,710.1	1,743,878.0 ± 915,749.4	
Median and [25%; 75%]	866,409.0 [609,823.3; 1,064,354.0]	1,720,575.3 [1,027,166.0; 1,944,697.1]	
DG 46:9 [M+Na] 4.98			>0.999
Mean ± Standard deviation	495,920.4 ± 477,189.2	489,547.8 ± 399,005.2	
Median and [25%; 75%]	314,518.0 [170,947.8; 667,639.6]	308,974.8 [151,137.4; 791,343.2]	
DG 47:0 [M+Na] 7.34			<0.001
Mean ± Standard deviation	3,460,097.3 ± 2,220,854.3	5,729,745.7 ± 2,442,226.0	
Median and [25%; 75%]	2,982,871.0 [2,021,202.0; 3,917,939.5]	5,592,478.8 [3,778,164.3; 7,584,378.5]	
DG 48:0 [M+Na] 7.72			0.003
Mean ± Standard deviation	7,047,858.1 ± 4,110,090.2	10,234,474.1 ± 4,903,197.7	
Median and [25%; 75%]	5,891,367.5 [4,338,599.3; 8,997,501.5]	7,783,057.3 [7,270,983.5; 12,408,960.1]	
DG 48:1 OA1 [M+Na] 6.91			0.025
Mean ± Standard deviation	31,533,381.1 ± 24,130,330.4	36,883,692.1 ± 11,128,628.2	
Median and [25%; 75%]	23,925,985.0 [16,614,539.0; 38,009,578]	39,527,859.0 [30,983,378.8; 42,415,624.1]	
DG 48:1 [M+Na] 7.14			<0.001
Mean ± Standard deviation	8,035,157.7 ± 5,201,167.6	11,496,018.1 ± 4,162,723.1	
Median and [25%; 75%]	6,102,565.0 [4,850,730.3; 9,179,904.5]	11,721,004.3 [8,196,746.0; 14,133,895.1]	
DG 48:2 [M+Na] 6.38			0.560
Mean ± Standard deviation	18,065,266.2 ± 10,191,517.5	17,085,845.8 ± 4,679,960.7	
Median and [25%; 75%]	15,720,322.0 [11,645,270.0; 20,573,925]	16,661,072.3 [14,384,642.3; 21,041,896.4]	
DG 49:0 [M+Na] 11.52			<0.001
Mean ± Standard deviation	211,975.9 ± 95,699.1	116,189.9 ± 85,676.8	
Median and [25%; 75%]	210,394.0 [148,842.5; 277,949.8]	70,159.3 [63,459.8; 156,588.9]	
DG 49:12 [M+Na] 4.72			0.009
Mean ± Standard deviation	215,868.2 ± 296,795.4	419,384.6 ± 363,406.0	
Median and [25%; 75%]	143,460.8 [64,578.1; 229,412.8]	276,904.3 [121,220.5; 609,699.1]	
DG 49:7 [M+Na] 5.94			0.002

Mean ± Standard deviation	128,277.4 ± 104,187.5	200,073.1 ± 108,369.4	
Median and [25%; 75%]	103,276.5 [60,367.4; 142,621.3]	169,478.1 [115,938.1; 237,159.3]	
DG 49:8 [M+Na] 7.11			<0.001
Mean ± Standard deviation	400,058.9 ± 330,831.7	879,052.0 ± 385,035.0	
Median and [25%; 75%]	355,622.0 [94,917.5; 622,749.5]	822,216.3 [571,872.4; 1,080,307.6]	
DG 49:9 [M+Na] 5.37			0.886
Mean ± Standard deviation	160,885,241.0 ± 62,669,081.6	162,409,542.4 ± 78,219,876.6	
Median and [25%; 75%]	144,569,848.0 [109,364,624.0; 193,826,	147,250,146.0 [110,806,135.0; 239,152,374.0]	
DG 50:5 [M+Na] 6.36			0.020
Mean ± Standard deviation	88,267.1 ± 65,870.4	46,025.2 ± 22,585.2	
Median and [25%; 75%]	70,091.0 [39,466.5; 119,550.6]	42,944.3 [29,506.3; 67,828.7]	
DG 51:11 [M+Na] 5.93			0.128
Mean ± Standard deviation	50,247,106.1 ± 23,085,917.5	65,824,255.1 ± 33,404,415.7	
Median and [25%; 75%]	42,487,614.0 [30,879,719.5; 65,423,978	65,531,223.5 [50,294,632.0; 79,346,761.5]	
DG 51:3 [M+Na] 10.9			0.064
Mean ± Standard deviation	154,423.4 ± 140,251.7	212,515.5 ± 115,284.1	
Median and [25%; 75%]	152,810.8 [1,231.3; 230,732.5]	203,892.3 [155,623.3; 252,403.1]	
DG 51:5 [M+Na] 11.04			<0.001
Mean ± Standard deviation	1,125,643.4 ± 1,058,271.5	3,688,329.0 ± 1,886,192.6	
Median and [25%; 75%]	935,002.8 [344,373.5; 1,524,869.8]	3,791,007.3 [2,619,467.1; 5,123,521.1]	
DG 51:6 [M+Na] 10.4			<0.001
Mean ± Standard deviation	217,375.7 ± 254,762.6	798,338.1 ± 381,436.1	
Median and [25%; 75%]	170,667.0 [24,312.8; 316,196.5]	920,963.8 [479,615.1; 1,023,756.5]	
DG 52:10 [M+Na] 6.83			0.023
Mean ± Standard deviation	909,394.9 ± 368,375.3	1,232,470.2 ± 573,532.3	
Median and [25%; 75%]	870,474.5 [651,437.9; 1,124,261.5]	1,163,066.8 [928,572.9; 1,428,120.1]	
DG O-35:1 DG O-17:0_18:1 [M+NH4] 6.8			0.004
Mean ± Standard deviation	935,884.1 ± 1,426,717.4	1,869,885.8 ± 1,563,221.1	
Median and [25%; 75%]	304,029.0 [96,840.6; 1,376,435.8]	1,272,163.3 [614,561.4; 2,979,479.0]	
DG O-37:1 DG O-17:1_20:0 [M+NH4] 11.22			0.545
Mean ± Standard deviation	160,744.0 ± 318,643.4	74,829.6 ± 93,677.2	
Median and [25%; 75%]	31,438.5 [1,945.8; 138,914.4]	37,812.6 [25,555.4; 88,879.5]	
DG O-37:2 DG O-19:1_18:1 [M+NH4] 6.86			0.021
Mean ± Standard deviation	362,778.8 ± 613,909.3	757,403.7 ± 833,632.6	
Median and [25%; 75%]	116,628.8 [38,503.9; 377,315.5]	469,720.3 [182,605.1; 1,074,267.1]	
DG O-37:4 DG O-19:2_18:2 [M+NH4] 5.9			0.072

Mean ± Standard deviation	101,296.6 ± 252,494.9	1,191,665.7 ± 4,197,965.6	
Median and [25%; 75%]	16,242.5 [5,301.5; 84,013.5]	54,113.6 [14,125.3; 137,789.5]	
DG O-39:3 DG O-19:3_20:0__ [M+NH4]__ 10.63			0.642
Mean ± Standard deviation	5,378,371.3 ± 4,079,835.0	5,756,086.0 ± 4,938,571.0	
Median and [25%; 75%]	4,457,293.3 [2,098,031.5; 7,024,504.1]	5,318,557.5 [3,887,564.0; 6,687,507.1]	
DG O-41:3 DG O-21:3_20:0__ [M+NH4]__ 11.47			0.090
Mean ± Standard deviation	2,736,621.7 ± 1,654,604.5	1,918,699.5 ± 909,068.7	
Median and [25%; 75%]	2,538,805.0 [1,430,978.4; 3,298,605.8]	1,865,277.3 [1,380,691.3; 2,602,686.3]	
LPC 14:0/0:0__ [M+H]__ 1.46			<0.001
Mean ± Standard deviation	1,081,585.0 ± 612,692.6	2,062,493.8 ± 697,855.4	
Median and [25%; 75%]	875,362.5 [637,478.9; 1,386,582.5]	2,026,085.8 [1,644,410.0; 2,443,340.4]	
LPC 15:0/0:0__ [M+H]__ 1.7			0.010
Mean ± Standard deviation	755,192.2 ± 453,123.6	1,059,643.5 ± 407,312.0	
Median and [25%; 75%]	706,843.0 [397,644.8; 961,553.3]	1,082,213.8 [668,191.6; 1,422,922.8]	
LPC 16:0__ [M+H]__ 2.0			0.059
Mean ± Standard deviation	168,848,371.5 ± 48,364,196.2	193,579,205.0 ± 44,472,647.5	
Median and [25%; 75%]	170,663,232.0 [131,375,274.0; 197,243,	183,946,644.0 [174,631,612.0; 209,432,362.0]	
LPC 16:0__ [M+Na]__ 2.0			0.339
Mean ± Standard deviation	5,971,073.8 ± 1,145,347.2	6,240,247.0 ± 864,580.6	
Median and [25%; 75%]	5,880,358.5 [5,062,908.5; 6,781,772.6]	6,229,864.3 [5,849,048.1; 6,564,592.5]	
LPC 16:1/0:0__ [M+H]__ 1.61			0.078
Mean ± Standard deviation	4,049,385.7 ± 1,844,160.9	5,092,375.6 ± 2,662,068.2	
Median and [25%; 75%]	3,363,072.0 [2,570,778.1; 4,609,750.8]	4,348,778.6 [3,719,557.4; 5,897,038.6]	
LPC 17:0/0:0__ [M+H]__ 2.33			0.013
Mean ± Standard deviation	3,372,429.2 ± 1,321,377.5	4,332,653.4 ± 1,211,682.0	
Median and [25%; 75%]	3,152,134.3 [2,450,612.8; 4,282,060.8]	4,352,474.8 [3,340,465.5; 5,057,298.5]	
LPC 18:0__ [M+H]__ 2.56			0.001
Mean ± Standard deviation	69,949,503.6 ± 21,128,295.5	92,124,697.6 ± 25,059,138.6	
Median and [25%; 75%]	71,625,120.0 [54,377,323.0; 85,600,176	87,431,126.0 [74,775,834.0; 103,602,068.0]	
LPC 18:0__ [M+Na]__ 2.56			0.239
Mean ± Standard deviation	5,857,406.0 ± 1,715,465.7	5,481,742.8 ± 1,954,553.8	
Median and [25%; 75%]	5,243,924.0 [4,712,976.0; 7,049,481.5]	4,901,568.3 [4,000,660.0; 5,862,464.0]	
LPC 18:1/0:0__ [M+H]__ 2.18			0.298
Mean ± Standard deviation	36,858,028.7 ± 11,000,354.3	45,927,970.8 ± 24,321,809.8	
Median and [25%; 75%]	35,206,581.0 [29,730,256.5; 42,949,786	37,652,521.5 [31,148,625.0; 57,245,720.0]	
LPC 18:1__ [M+Na]__ 2.2			<0.001

Mean ± Standard deviation	2,922,737.1 ± 1,194,825.5	3,943,104.3 ± 691,881.1	
Median and [25%; 75%]	2,814,707.3 [2,329,174.3; 3,602,079.5]	3,800,937.8 [3,480,429.3; 4,379,731.8]	
LPC 18:2/0:0 [M+H] 1.78			0.010
Mean ± Standard deviation	53,626,938.0 ± 24,106,153.9	76,570,400.5 ± 38,678,207.2	
Median and [25%; 75%]	46,316,780.0 [38,645,070.5; 60,601,226]	69,354,863.0 [47,639,766.0; 93,556,380.0]	
LPC 18:2 [M+H] 1.77			0.009
Mean ± Standard deviation	52,428,626.2 ± 22,683,841.9	75,412,656.3 ± 36,526,018.4	
Median and [25%; 75%]	45,376,790.0 [37,273,648.5; 60,223,101]	69,603,866.0 [48,636,608.8; 92,721,132.0]	
LPC 18:2 [M+Na] 1.77			0.044
Mean ± Standard deviation	2,831,662.0 ± 781,422.4	3,529,625.6 ± 1,131,135.6	
Median and [25%; 75%]	2,696,551.5 [2,321,498.3; 3,169,268.8]	3,134,354.8 [2,485,974.8; 4,563,887.1]	
LPC 18:3/0:0 [M+H] 1.51			0.006
Mean ± Standard deviation	187,472.6 ± 161,800.8	384,616.8 ± 321,186.2	
Median and [25%; 75%]	137,079.0 [83,777.9; 265,167.5]	285,384.3 [155,297.9; 438,724.4]	
LPC 20:1/0:0 [M+H] 2.92			0.833
Mean ± Standard deviation	493,510.9 ± 292,635.6	508,176.4 ± 307,102.8	
Median and [25%; 75%]	367,350.5 [284,724.1; 646,309.3]	378,147.5 [293,379.4; 623,768.1]	
LPC 20:2/0:0 [M+H] 2.38			0.820
Mean ± Standard deviation	637,554.3 ± 432,146.0	606,989.1 ± 377,264.4	
Median and [25%; 75%]	513,620.8 [357,166.8; 714,558.1]	503,525.3 [369,757.3; 712,678.4]	
LPC 20:4/0:0 [M+H] 1.81			0.704
Mean ± Standard deviation	18,054,607.1 ± 13,046,819.4	14,177,439.8 ± 5,761,277.7	
Median and [25%; 75%]	14,156,673.3 [9,902,012.5; 19,889,408.5]	14,001,472.0 [11,603,009.6; 18,869,676.3]	
LPC 20:4 [M+H] 1.71			0.583
Mean ± Standard deviation	13,363,462.7 ± 10,844,261.4	10,867,054.3 ± 6,792,887.9	
Median and [25%; 75%]	10,641,900.0 [6,385,481.6; 15,708,569.9]	10,169,912.3 [4,919,587.0; 18,452,913.3]	
LPC 20:4 [M+Na] 1.71			0.132
Mean ± Standard deviation	488,575.6 ± 470,956.4	317,801.9 ± 271,619.7	
Median and [25%; 75%]	296,992.5 [212,524.6; 661,887.3]	178,516.0 [124,437.4; 543,179.3]	
LPC 20:5/0:0 [M+H] 1.51			0.282
Mean ± Standard deviation	1,130,746.6 ± 1,215,851.1	1,499,946.9 ± 1,670,674.9	
Median and [25%; 75%]	758,229.5 [365,899.8; 1,485,578.3]	798,745.3 [541,605.9; 1,791,969.4]	
LPC 20:5 [M+Na] 1.51			0.820
Mean ± Standard deviation	108,803.6 ± 141,885.5	128,204.3 ± 180,638.2	
Median and [25%; 75%]	53,191.5 [21,490.3; 131,766.5]	52,604.6 [28,165.5; 183,761.0]	
LPC 22:4 [M+H] 2.3			0.926

Mean ± Standard deviation	132,928.6 ± 138,537.2	119,161.4 ± 98,296.1	
Median and [25%; 75%]	89,718.3 [36,979.6; 193,881.4]	80,889.8 [51,390.9; 175,035.0]	
LPC 22:5 [M+H] 1.91			0.704
Mean ± Standard deviation	238,390.6 ± 284,655.2	137,050.6 ± 139,986.9	
Median and [25%; 75%]	86,366.5 [40,983.1; 364,568.0]	83,958.3 [43,468.9; 176,931.1]	
LPC 22:6/0:0 [M+H] 1.73			0.052
Mean ± Standard deviation	5,735,115.4 ± 3,595,643.1	3,774,726.4 ± 2,174,730.6	
Median and [25%; 75%]	5,027,549.0 [3,443,991.3; 7,235,275.8]	3,137,453.4 [2,194,979.1; 4,861,692.3]	
LPC 22:6 [M+H] 1.64			0.537
Mean ± Standard deviation	4,647,966.7 ± 3,346,630.9	3,728,110.9 ± 2,229,868.4	
Median and [25%; 75%]	3,894,482.5 [2,289,051.6; 6,325,546.3]	3,137,453.4 [2,192,514.8; 4,861,692.3]	
LPC 22:6 [M+Na] 1.64			0.183
Mean ± Standard deviation	285,784.3 ± 217,671.6	199,620.2 ± 148,476.9	
Median and [25%; 75%]	251,453.0 [132,164.5; 405,079.3]	146,177.8 [104,115.4; 270,793.3]	
LPC O-16:0 [M+H] 2.25			0.055
Mean ± Standard deviation	346,303.9 ± 305,459.6	460,868.8 ± 263,614.1	
Median and [25%; 75%]	221,140.3 [132,985.9; 478,040.8]	392,334.4 [284,035.5; 594,031.1]	
LPC O-16:1 [M+H] 2.25			0.055
Mean ± Standard deviation	523,674.8 ± 373,499.2	761,405.4 ± 472,623.5	
Median and [25%; 75%]	397,960.0 [241,989.3; 719,432.3]	666,989.4 [444,930.5; 975,327.1]	
LPC O-18:0 [M+H] 3.04			0.225
Mean ± Standard deviation	378,305.9 ± 214,655.4	458,253.0 ± 259,506.9	
Median and [25%; 75%]	306,244.0 [243,715.0; 460,272.3]	374,190.0 [261,604.8; 569,452.4]	
LPC O-18:1 [M+H] 2.44			0.183
Mean ± Standard deviation	1,088,139.1 ± 627,888.5	839,187.5 ± 460,287.5	
Median and [25%; 75%]	876,645.3 [610,897.0; 1,422,840.3]	682,022.1 [570,761.9; 902,325.3]	
LPC O-19:0 OA1 [M+H] 2.57			0.151
Mean ± Standard deviation	471,282.8 ± 295,997.1	504,156.4 ± 170,258.1	
Median and [25%; 75%]	403,629.0 [292,725.0; 556,219.3]	475,501.5 [358,432.8; 635,766.8]	
LPC O-19:0 [M+H] 2.73			0.006
Mean ± Standard deviation	3,777,720.2 ± 2,855,808.6	5,236,553.8 ± 2,336,542.9	
Median and [25%; 75%]	3,510,795.0 [2,043,724.9; 4,198,416.3]	4,313,642.3 [3,804,415.3; 6,847,295.5]	
LPC O-24:0 [M+H] 4.57			0.008
Mean ± Standard deviation	158,487.8 ± 101,393.2	265,555.6 ± 163,244.2	
Median and [25%; 75%]	149,942.3 [85,511.8; 208,859.3]	261,283.3 [166,453.4; 299,384.0]	
LPC O-24:1 [M+H] 4.13			0.033

Mean ± Standard deviation	190,117.6 ± 93,815.8	263,814.3 ± 151,074.4	
Median and [25%; 75%]	176,706.0 [105,141.1; 223,412.8]	248,411.0 [191,824.0; 276,433.6]	
LPE 22:6 __[M+H]__ 1.73			0.002
Mean ± Standard deviation	103,277.3 ± 118,735.7	39,495.3 ± 52,163.2	
Median and [25%; 75%]	66,172.0 [36,002.3; 120,297.9]	19,305.6 [12,114.9; 54,821.3]	
NAE 17:1 __[M+H]__ 3.86			0.031
Mean ± Standard deviation	35,559.5 ± 86,958.2	63,346.1 ± 93,307.0	
Median and [25%; 75%]	1,355.0 [235.3; 41,025.8]	21,828.5 [2,711.1; 96,023.9]	
NAE 19:3 __[M+H]__ 3.79			0.128
Mean ± Standard deviation	252,334.1 ± 379,018.2	262,424.6 ± 303,691.1	
Median and [25%; 75%]	47,024.3 [10,675.0; 356,418.0]	111,322.0 [55,343.0; 353,132.3]	
NAE 22:5 __[M+H]__ 3.37			0.306
Mean ± Standard deviation	3,426.7 ± 6,094.8	2,325.0 ± 4,162.5	
Median and [25%; 75%]	1,042.5 [324.8; 3,694.3]	904.5 [124.9; 1,672.6]	
NAE 22:6 __[M+H]__ 2.88			0.733
Mean ± Standard deviation	4,804.1 ± 11,659.6	6,830.4 ± 15,151.0	
Median and [25%; 75%]	906.5 [218.0; 2,437.5]	896.0 [64.6; 2,859.4]	
NAE 26:7 __[M+H]__ 2.19			0.132
Mean ± Standard deviation	26,772.2 ± 46,042.6	14,028.8 ± 21,274.0	
Median and [25%; 75%]	14,802.0 [3,737.0; 30,014.4]	5,228.1 [2,439.0; 15,338.9]	
PC 17:0 __[M+H]__ 2.73			<0.001
Mean ± Standard deviation	371,652.9 ± 264,478.7	658,187.1 ± 299,947.0	
Median and [25%; 75%]	293,373.8 [192,639.5; 488,026.3]	664,645.3 [408,823.0; 777,271.9]	
PC 30:0 __[M+H]__ 5.04			<0.001
Mean ± Standard deviation	558,157.8 ± 755,123.3	2,432,620.9 ± 2,014,875.0	
Median and [25%; 75%]	320,049.5 [161,462.8; 565,687.3]	2,001,865.4 [1,012,226.9; 3,379,397.3]	
PC 32:0 __[M+H]__ 5.16			<0.001
Mean ± Standard deviation	34,195,179.6 ± 8,493,272.5	49,696,164.6 ± 11,918,230.6	
Median and [25%; 75%]	34,343,193.0 [28,815,429.5; 37,890,781]	48,256,849.0 [41,317,769.5; 59,874,047.0]	
PC 32:0 PC 16:0 16:0 __[M+H]__ 5.55			<0.001
Mean ± Standard deviation	34,178,550.7 ± 8,488,830.6	49,672,054.1 ± 11,919,366.5	
Median and [25%; 75%]	34,319,069.5 [28,796,828.0; 37,869,343]	48,236,569.0 [41,275,820.0; 59,841,582.0]	
PC 32:1 PC 16:0 16:1 __[M+H]__ 5.16			<0.001
Mean ± Standard deviation	15,211,223.0 ± 9,716,172.5	37,766,491.6 ± 18,490,161.0	
Median and [25%; 75%]	13,219,797.0 [8,165,024.6; 21,321,431.5]	33,202,595.5 [25,834,819.5; 43,865,374.5]	
PC 32:2 __[M+Na]__ 4.78			<0.001

Mean ± Standard deviation	169,153.4 ± 128,905.9	383,472.7 ± 173,602.0	
Median and [25%; 75%]	161,707.5 [75,623.5; 209,175.0]	368,344.0 [286,882.3; 439,456.6]	
PC 32:2 PC 14:0_18:2__[M+H]__4.79			<0.001
Mean ± Standard deviation	5,683,578.3 ± 3,159,215.7	14,974,294.0 ± 6,577,842.0	
Median and [25%; 75%]	5,272,930.0 [3,551,878.5; 6,835,926.1]	13,248,996.0 [10,655,184.6; 17,776,517.9]	
PC 33:1__[M+H]__5.6			0.225
Mean ± Standard deviation	508,911.7 ± 925,261.6	699,709.1 ± 1,971,163.6	
Median and [25%; 75%]	79,682.5 [50,528.3; 509,742.4]	143,076.8 [88,317.8; 242,037.6]	
PC 33:1 PC 15:0_18:1__[M+H]__5.41			<0.001
Mean ± Standard deviation	1,786,386.1 ± 987,707.8	5,045,753.1 ± 2,664,961.6	
Median and [25%; 75%]	1,535,989.5 [1,079,248.0; 2,210,975.0]	4,775,592.8 [3,221,437.8; 7,222,608.5]	
PC 33:2 PC 15:0_18:2__[M+H]__5.01			<0.001
Mean ± Standard deviation	6,209,869.1 ± 2,704,023.0	12,935,364.7 ± 7,038,217.9	
Median and [25%; 75%]	5,975,477.8 [4,210,589.3; 8,002,101.4]	10,620,746.6 [9,081,011.9; 17,154,372.9]	
PC 34:0__[M+H]__6.13			<0.001
Mean ± Standard deviation	8,483,195.4 ± 2,189,600.3	14,128,123.5 ± 3,941,865.6	
Median and [25%; 75%]	8,305,602.5 [6,740,679.3; 9,808,272.5]	13,650,697.0 [11,121,136.4; 17,620,170.9]	
PC 34:1__[M+Na]__5.66			0.384
Mean ± Standard deviation	269,872,707.4 ± 75,250,404.5	294,201,949.7 ± 99,420,585.4	
Median and [25%; 75%]	269,464,720.0 [221,488,339.0; 313,099,	308,962,056.0 [261,397,502.0; 365,497,188.0]	
PC 34:2__[M+H]__5.0			<0.001
Mean ± Standard deviation	517,512,900.8 ± 97,358,400.0	634,440,293.0 ± 82,018,820.3	
Median and [25%; 75%]	525,300,352.0 [458,094,916.0; 581,062,	621,880,368.0 [579,644,080.0; 675,385,236.0]	
PC 34:3 PC 16:0_18:3__[M+H]__5.01			<0.001
Mean ± Standard deviation	21,598,254.9 ± 9,132,360.0	44,922,051.2 ± 18,939,176.4	
Median and [25%; 75%]	20,995,317.5 [14,798,722.0; 26,875,647	39,928,502.0 [31,501,261.3; 55,074,175.5]	
PC 34:3 PC 16:1_18:2__[M+H]__4.89			<0.001
Mean ± Standard deviation	21,627,933.7 ± 9,311,503.3	45,221,578.1 ± 18,492,463.9	
Median and [25%; 75%]	20,996,381.5 [14,698,513.0; 26,676,451	39,220,072.5 [33,113,318.0; 56,400,535.5]	
PC 35:1__[M+H]__5.5			<0.001
Mean ± Standard deviation	692,747.1 ± 292,661.8	1,431,158.5 ± 795,410.3	
Median and [25%; 75%]	662,616.3 [473,822.8; 864,146.5]	1,284,743.0 [849,881.8; 1,621,228.8]	
PC 35:2__[M+H]__6.17			<0.001
Mean ± Standard deviation	24,789,214.9 ± 7,786,732.1	50,127,096.8 ± 26,000,893.0	
Median and [25%; 75%]	25,849,869.0 [19,335,744.3; 29,944,355	44,458,775.0 [34,374,537.3; 52,769,036.0]	
PC 35:2 PC 17:0_18:2__[M+H]__5.5			<0.001

Mean ± Standard deviation	24,766,740.8 ± 7,784,987.0	50,094,617.3 ± 25,992,615.0	
Median and [25%; 75%]	25,832,555.0 [19,322,067.5; 29,927,018]	44,428,064.5 [34,349,228.0; 52,739,312.0]	
PC 35:4 PC 15:0_20:4__[M+H]__4.98			0.151
Mean ± Standard deviation	2,806,305.1 ± 1,827,791.5	3,854,279.9 ± 2,339,099.0	
Median and [25%; 75%]	2,219,336.5 [1,620,589.5; 3,603,753.5]	2,961,084.5 [1,851,013.4; 5,900,533.4]	
PC 36:0 PC 18:0_18:0__[M+H]__6.25			<0.001
Mean ± Standard deviation	7,016,832.3 ± 2,335,836.6	15,561,623.4 ± 13,390,225.0	
Median and [25%; 75%]	6,704,849.0 [5,402,026.6; 7,644,986.1]	12,807,140.5 [8,554,858.4; 16,902,791.6]	
PC 36:1 PC 18:0_18:1__[M+H]__6.26			<0.001
Mean ± Standard deviation	120,895,050.2 ± 31,268,724.0	215,674,189.3 ± 82,741,079.5	
Median and [25%; 75%]	115,622,696.0 [101,141,358.0; 137,452,]	193,221,812.0 [156,319,796.0; 256,544,189.0]	
PC 36:2 PC 18:0_18:2__[M+H]__5.81			<0.001
Mean ± Standard deviation	424,350,852.5 ± 87,574,813.4	575,198,097.0 ± 78,918,679.8	
Median and [25%; 75%]	434,057,040.0 [371,895,880.0; 478,787,]	559,648,792.0 [535,531,920.0; 591,070,156.0]	
PC 36:3__[M+Na]__5.41			0.001
Mean ± Standard deviation	237,617,486.5 ± 45,349,745.9	291,321,316.3 ± 51,630,047.0	
Median and [25%; 75%]	236,759,376.0 [206,543,828.0; 272,326,]	291,142,260.0 [259,006,722.0; 314,354,726.0]	
PC 36:4 PC 18:2_18:2__[M+H]__4.96			<0.001
Mean ± Standard deviation	52,259,697.6 ± 29,907,989.8	128,969,847.6 ± 70,127,415.2	
Median and [25%; 75%]	45,210,970.0 [37,062,379.0; 57,763,775]	111,288,417.0 [73,325,812.0; 151,172,444.0]	
PC 36:5__[M+Na]__4.87			0.504
Mean ± Standard deviation	846,660.6 ± 466,515.1	777,914.6 ± 514,146.7	
Median and [25%; 75%]	760,463.0 [505,338.8; 1,116,447.5]	648,870.0 [430,402.0; 903,967.1]	
PC 36:5 PC 16:0_20:5__[M+H]__4.88			0.002
Mean ± Standard deviation	54,066,524.2 ± 41,991,193.7	99,663,389.0 ± 59,785,346.9	
Median and [25%; 75%]	50,392,778.0 [26,626,548.5; 61,289,982]	81,099,052.0 [53,286,576.0; 138,388,511.0]	
PC 36:5 PC 18:2_18:3__[M+H]__4.64			0.003
Mean ± Standard deviation	54,377,750.7 ± 41,900,132.6	99,533,696.6 ± 59,712,132.0	
Median and [25%; 75%]	50,917,118.0 [26,762,684.0; 61,634,409]	80,980,660.0 [53,063,189.8; 138,132,066.0]	
PC 36:6__[M+H]__4.53			<0.001
Mean ± Standard deviation	725,867.5 ± 986,101.2	1,510,011.3 ± 1,278,714.9	
Median and [25%; 75%]	391,265.5 [132,453.3; 832,641.5]	1,018,092.0 [765,028.9; 1,753,603.9]	
PC 36:6 PC 14:0_22:6__[M+H]__4.62			<0.001
Mean ± Standard deviation	716,424.5 ± 954,245.4	1,502,583.5 ± 1,272,932.6	
Median and [25%; 75%]	390,729.5 [131,961.3; 828,429.9]	1,013,771.8 [762,254.8; 1,748,621.8]	
PC 37:1__[M+H]__6.56			<0.001

Mean ± Standard deviation	181,169.3 ± 80,486.6	538,643.2 ± 551,926.1	
Median and [25%; 75%]	181,561.5 [122,514.3; 226,411.5]	335,951.0 [293,598.7; 426,764.6]	
PC 37:3 __[M+H]__ 5.63			<0.001
Mean ± Standard deviation	472,297.4 ± 444,729.5	965,951.5 ± 509,338.9	
Median and [25%; 75%]	310,072.5 [191,673.3; 540,313.8]	972,506.8 [621,326.5; 1,163,659.9]	
PC 37:4 __[M+H]__ 6.15			0.080
Mean ± Standard deviation	12,690,430.6 ± 5,152,342.2	16,252,489.6 ± 7,180,875.3	
Median and [25%; 75%]	11,418,138.0 [9,329,314.5; 15,652,353.0]	16,404,445.3 [11,058,314.3; 23,575,285.1]	
PC 37:4 PC 17:0_20:4 __[M+H]__ 5.47			0.080
Mean ± Standard deviation	12,600,647.7 ± 5,160,793.7	16,179,202.6 ± 7,159,072.7	
Median and [25%; 75%]	11,359,828.0 [9,091,092.5; 15,601,030.3]	16,325,009.5 [11,006,787.4; 23,510,101.4]	
PC 37:5 __[M+H]__ 5.63			0.239
Mean ± Standard deviation	1,502,230.5 ± 1,201,209.3	1,706,022.2 ± 822,454.3	
Median and [25%; 75%]	1,246,261.0 [681,282.5; 1,938,897.3]	1,634,159.8 [1,292,233.3; 2,212,782.6]	
PC 37:6 __[M+H]__ 5.35			0.029
Mean ± Standard deviation	1,234,035.6 ± 667,014.4	1,740,067.0 ± 838,136.5	
Median and [25%; 75%]	1,185,923.0 [743,754.5; 1,514,269.4]	1,817,757.8 [1,156,416.0; 2,239,883.2]	
PC 37:6 PC 15:0_22:6 __[M+H]__ 4.82			0.027
Mean ± Standard deviation	1,226,081.7 ± 661,465.6	1,736,502.7 ± 837,119.0	
Median and [25%; 75%]	1,183,102.0 [741,944.3; 1,511,735.4]	1,813,868.5 [1,154,316.1; 2,235,182.0]	
PC 38:1 __[M+H]__ 6.84			0.003
Mean ± Standard deviation	570,389.2 ± 369,206.0	1,014,139.8 ± 700,518.4	
Median and [25%; 75%]	507,114.0 [386,641.6; 678,951.3]	733,859.8 [595,696.0; 1,102,016.6]	
PC 38:2 OA1 __[M+H]__ 5.96			0.003
Mean ± Standard deviation	9,414,164.6 ± 4,718,697.7	14,511,014.3 ± 6,135,101.3	
Median and [25%; 75%]	8,876,921.0 [5,646,281.4; 11,411,705.9]	12,762,794.8 [10,093,085.6; 17,331,065.9]	
PC 38:2 __[M+H]__ 6.31			0.001
Mean ± Standard deviation	9,344,557.0 ± 4,655,625.9	14,567,698.7 ± 6,023,157.7	
Median and [25%; 75%]	8,852,544.0 [5,657,980.6; 11,166,803.8]	13,036,900.8 [10,134,836.4; 17,391,062.0]	
PC 38:3 OA1 __[M+H]__ 5.62			<0.001
Mean ± Standard deviation	132,201,199.4 ± 52,650,699.2	204,825,541.8 ± 64,388,591.3	
Median and [25%; 75%]	126,086,756.0 [98,464,906.0; 163,302,700.0]	194,634,992.0 [151,178,912.0; 251,247,322.0]	
PC 38:3 __[M+H]__ 6.19			<0.001
Mean ± Standard deviation	128,777,964.8 ± 49,976,329.2	201,241,234.8 ± 61,922,461.5	
Median and [25%; 75%]	127,122,320.0 [96,399,764.0; 157,021,500.0]	190,388,928.0 [153,923,376.0; 245,154,828.0]	
PC 38:3 PC 18:0_20:3 __[M+H]__ 5.95			<0.001

Mean ± Standard deviation	130,950,660.9 ± 51,144,125.5	207,586,227.5 ± 62,969,237.5	
Median and [25%; 75%]	131,022,884.0 [99,298,354.0; 156,908,1	199,399,946.0 [159,425,494.0; 250,064,162.0]	
PC 38:4 [M+H] 5.36			<0.001
Mean ± Standard deviation	30,581,383.0 ± 12,741,215.7	46,760,957.3 ± 18,204,219.0	
Median and [25%; 75%]	27,526,055.0 [19,197,921.5; 36,160,920	41,395,396.0 [35,053,029.0; 55,340,356.0]	
PC 38:4 PC 16:0_22:4 [M+H] 5.52			<0.001
Mean ± Standard deviation	19,304,753.8 ± 15,774,180.2	39,451,377.2 ± 19,332,157.7	
Median and [25%; 75%]	17,974,938.5 [2,606,641.8; 30,673,889.0	33,768,166.8 [26,176,203.8; 50,478,402.0]	
PC 38:4 PC 18:0_20:4 [M+H] 5.76			0.248
Mean ± Standard deviation	288,475,405.3 ± 53,854,980.2	317,876,447.8 ± 93,042,940.9	
Median and [25%; 75%]	282,696,032.0 [255,534,958.0; 317,618,	302,463,560.0 [248,493,929.0; 405,414,364.0]	
PC 38:5 PC 16:0_22:5 [M+H] 5.17			0.002
Mean ± Standard deviation	33,476,840.1 ± 12,555,590.4	48,045,358.5 ± 17,229,897.7	
Median and [25%; 75%]	31,935,471.0 [23,824,551.0; 39,999,146	41,367,990.0 [37,819,119.5; 54,448,078.0]	
PC 38:5 PC 18:1_20:4 [M+H] 5.34			0.005
Mean ± Standard deviation	75,847,845.6 ± 40,892,025.7	103,424,486.6 ± 36,134,205.4	
Median and [25%; 75%]	66,045,189.0 [51,613,341.5; 91,826,014	112,120,632.0 [70,255,925.5; 131,996,413.0]	
PC 38:6 PC 18:2_20:4 [M+H] 4.93			0.014
Mean ± Standard deviation	258,851,366.5 ± 54,946,396.8	312,986,325.8 ± 73,234,603.6	
Median and [25%; 75%]	250,315,720.0 [230,825,804.0; 301,524,	301,147,042.0 [271,250,512.0; 358,289,532.0]	
PC 39:4 [M+H] 6.06			0.013
Mean ± Standard deviation	489,090.2 ± 235,805.6	697,267.3 ± 326,512.4	
Median and [25%; 75%]	450,536.0 [354,933.0; 604,554.9]	615,138.3 [511,901.3; 857,030.4]	
PC 39:6 [M+H] 5.31			0.267
Mean ± Standard deviation	377,186.5 ± 370,122.9	472,176.6 ± 383,734.3	
Median and [25%; 75%]	256,251.5 [133,600.3; 489,559.9]	366,450.5 [184,576.0; 744,123.7]	
PC 40:4 PC 18:0_22:4 [M+H] 6.13			0.002
Mean ± Standard deviation	8,419,047.2 ± 4,401,570.1	14,813,453.2 ± 8,107,489.1	
Median and [25%; 75%]	7,469,740.5 [4,943,366.6; 9,770,541.8]	13,926,809.5 [8,287,211.5; 19,919,196.3]	
PC 40:5 [M+H] 5.98			0.001
Mean ± Standard deviation	3,920,276.5 ± 3,053,772.9	8,717,713.4 ± 7,011,257.3	
Median and [25%; 75%]	3,449,844.0 [1,535,015.5; 4,931,707.5]	6,249,138.0 [4,335,132.0; 9,305,417.7]	
PC 40:5 PC 18:0_22:5 OA1 [M+H] 5.98			0.001
Mean ± Standard deviation	3,995,835.3 ± 3,038,577.2	8,768,001.3 ± 7,001,574.4	
Median and [25%; 75%]	3,449,844.0 [1,586,874.9; 5,157,097.0]	6,249,138.0 [4,335,132.0; 9,305,417.7]	
PC 40:5 PC 18:0_22:5 [M+H] 5.71			0.007

Mean ± Standard deviation	5,599,962.6 ± 2,644,547.8	8,132,631.2 ± 3,850,239.0	
Median and [25%; 75%]	5,202,176.5 [3,904,794.3; 6,475,210.6]	6,889,683.5 [5,955,693.9; 9,457,590.9]	
PC 40:6 [M+H] 5.35			0.016
Mean ± Standard deviation	120,026,639.9 ± 37,414,394.0	150,736,241.8 ± 45,815,772.2	
Median and [25%; 75%]	110,671,988.0 [90,134,746.0; 142,094,7	153,669,376.0 [137,594,307.0; 166,808,593.0]	
PC 40:7 PC 18:1_22:6 [M+H] 5.15			0.078
Mean ± Standard deviation	7,819,612.0 ± 3,366,645.0	10,308,011.6 ± 5,552,092.4	
Median and [25%; 75%]	7,142,071.5 [5,327,694.8; 9,822,894.4]	9,689,348.3 [7,317,289.6; 11,734,062.9]	
PC 40:8 [M+H] 4.81			0.001
Mean ± Standard deviation	1,327,850.9 ± 741,825.9	2,143,160.9 ± 990,322.4	
Median and [25%; 75%]	1,118,006.0 [893,739.5; 1,800,099.0]	1,838,797.3 [1,419,057.1; 2,677,445.4]	
PC 40:8 PC 20:4_20:4 [M+H] 4.86			<0.001
Mean ± Standard deviation	1,237,909.7 ± 572,084.5	2,168,218.6 ± 989,679.0	
Median and [25%; 75%]	1,154,851.5 [813,358.1; 1,531,277.0]	1,988,822.3 [1,400,874.8; 2,705,398.5]	
PC 43:5 [M+H] 7.51			0.146
Mean ± Standard deviation	621,337.9 ± 279,145.9	869,333.5 ± 517,286.9	
Median and [25%; 75%]	533,029.5 [428,442.5; 868,277.5]	726,996.9 [570,443.5; 973,861.5]	
PC O-31:0 [M+H] 5.08			0.009
Mean ± Standard deviation	678,572.3 ± 341,707.0	1,282,282.5 ± 829,640.6	
Median and [25%; 75%]	627,603.5 [431,584.5; 874,915.5]	1,209,394.8 [615,653.4; 1,601,182.4]	
PC O-32:0 PC O-16:0_16:0 [M+H] 5.93			0.037
Mean ± Standard deviation	3,460,020.3 ± 1,975,331.0	4,429,735.8 ± 1,817,941.9	
Median and [25%; 75%]	3,117,513.5 [2,193,301.4; 4,519,050.0]	4,137,403.8 [3,570,519.3; 5,561,001.8]	
PC O-32:1 [M+H] 5.89			0.011
Mean ± Standard deviation	2,313,975.2 ± 1,229,029.0	3,230,681.0 ± 1,234,978.2	
Median and [25%; 75%]	2,129,465.5 [1,410,576.3; 2,736,948.3]	2,920,611.1 [2,073,290.9; 4,157,257.4]	
PC O-32:1 PC O-16:1_16:0 [M+H] 5.91			0.011
Mean ± Standard deviation	2,302,325.0 ± 1,238,449.8	3,230,719.5 ± 1,234,974.7	
Median and [25%; 75%]	2,129,465.5 [1,362,591.8; 2,736,948.3]	2,920,919.1 [2,073,290.9; 4,157,257.4]	
PC O-33:1 [M+H] 5.61			0.161
Mean ± Standard deviation	5,917,070.3 ± 2,023,859.7	7,041,481.6 ± 2,563,852.8	
Median and [25%; 75%]	5,389,843.5 [4,403,451.0; 7,173,576.5]	6,617,247.0 [5,156,622.9; 9,152,650.8]	
PC O-33:2 [M+H] 4.79			<0.001
Mean ± Standard deviation	1,914,084.2 ± 1,993,333.0	4,908,627.7 ± 3,043,643.9	
Median and [25%; 75%]	1,232,601.3 [785,458.9; 1,896,157.3]	4,003,082.6 [2,991,094.2; 5,714,821.1]	
PC O-34:2 PC O-16:0_18:2 [M+H] 5.0			0.011

Mean ± Standard deviation	1,145,092.8 ± 678,361.1	1,921,058.1 ± 1,167,463.0	
Median and [25%; 75%]	985,902.5 [678,553.5; 1,556,431.8]	1,759,600.1 [1,052,798.0; 2,772,459.5]	
PC O-34:2 PC O-16:1_18:1__[M+H]__ 6.03			0.006
Mean ± Standard deviation	5,659,561.8 ± 2,454,512.1	9,413,917.9 ± 5,281,627.7	
Median and [25%; 75%]	4,855,674.3 [4,098,794.0; 6,561,596.0]	8,596,877.0 [4,745,787.8; 11,287,265.0]	
PC O-34:3 PC O-16:1_18:2__[M+H]__ 5.55			<0.001
Mean ± Standard deviation	12,273,881.8 ± 5,780,534.7	24,926,270.3 ± 19,114,610.3	
Median and [25%; 75%]	10,872,357.0 [8,142,126.8; 14,638,976.0]	15,804,905.4 [13,542,661.1; 31,042,744.5]	
PC O-35:0__[M+H]__ 5.67			0.001
Mean ± Standard deviation	3,742,179.1 ± 2,542,167.0	5,168,853.8 ± 2,243,739.6	
Median and [25%; 75%]	3,191,427.0 [2,215,281.3; 4,098,943.3]	4,797,468.8 [3,607,627.0; 5,682,585.8]	
PC O-35:0 PC O-17:0_18:0__[M+H]__ 6.12			<0.001
Mean ± Standard deviation	1,833,761.3 ± 935,212.9	3,138,921.1 ± 1,173,979.1	
Median and [25%; 75%]	1,443,756.0 [1,233,669.3; 2,307,449.8]	3,031,582.3 [2,216,726.3; 3,856,602.6]	
PC O-35:0 PC O-19:0_16:0__[M+H]__ 6.12			<0.001
Mean ± Standard deviation	1,833,761.3 ± 935,212.9	3,138,921.1 ± 1,173,979.1	
Median and [25%; 75%]	1,443,756.0 [1,233,669.3; 2,307,449.8]	3,031,582.3 [2,216,726.3; 3,856,602.6]	
PC O-35:1__[M+H]__ 5.67			<0.001
Mean ± Standard deviation	398,114,155.4 ± 100,400,563.2	537,432,887.5 ± 176,578,399.4	
Median and [25%; 75%]	397,847,792.0 [326,342,602.0; 439,680,000.0]	491,725,928.0 [435,508,096.0; 588,123,544.0]	
PC O-35:2__[M+H]__ 5.74			0.002
Mean ± Standard deviation	595,740,089.1 ± 133,704,423.3	767,507,147.5 ± 171,925,539.4	
Median and [25%; 75%]	611,402,912.0 [516,783,856.0; 679,934,000.0]	794,001,712.0 [593,857,368.0; 891,947,720.0]	
PC O-35:4 PC O-15:0_20:4__[M+H]__ 4.76			<0.001
Mean ± Standard deviation	431,583.2 ± 983,726.1	641,216.4 ± 333,784.7	
Median and [25%; 75%]	152,149.5 [70,428.8; 262,496.3]	501,346.3 [432,866.6; 836,325.0]	
PC O-36:1 OA1__[M+H]__ 5.92			<0.001
Mean ± Standard deviation	848,131.1 ± 479,016.7	1,616,985.0 ± 941,820.3	
Median and [25%; 75%]	757,673.5 [539,757.0; 1,054,300.3]	1,498,328.0 [1,119,661.4; 1,723,549.4]	
PC O-36:1__[M+H]__ 6.69			<0.001
Mean ± Standard deviation	3,786,106.4 ± 1,647,606.9	6,605,863.6 ± 2,950,352.5	
Median and [25%; 75%]	3,485,434.0 [2,521,574.3; 4,834,408.5]	5,797,526.3 [4,594,981.1; 8,487,831.0]	
PC O-36:1 PC O-18:0_18:1__[M+H]__ 5.93			<0.001
Mean ± Standard deviation	848,955.9 ± 478,559.6	1,617,327.7 ± 941,701.9	
Median and [25%; 75%]	757,673.5 [541,626.1; 1,055,598.3]	1,498,328.0 [1,119,661.4; 1,723,549.4]	
PC O-36:2__[M+H]__ 5.5			<0.001

Mean ± Standard deviation	5,117,535.0 ± 2,542,358.2	11,126,268.8 ± 6,343,137.0	
Median and [25%; 75%]	4,732,760.5 [3,504,939.6; 5,844,434.0]	9,367,344.5 [6,070,747.6; 14,903,774.4]	
PC O-36:2 PC O-18:1_18:1__[M+H]__ 6.65			0.052
Mean ± Standard deviation	306,422.5 ± 164,222.7	560,918.1 ± 429,826.4	
Median and [25%; 75%]	280,635.5 [193,098.1; 373,634.8]	403,088.6 [249,883.6; 757,196.6]	
PC O-36:3 PC O-18:1_18:2__[M+H]__ 5.7			0.306
Mean ± Standard deviation	813,279.8 ± 1,023,652.3	1,302,760.1 ± 1,332,774.8	
Median and [25%; 75%]	493,064.0 [273,543.9; 927,460.0]	783,364.3 [282,448.1; 2,029,892.9]	
PC O-36:4 PC O-16:1_20:3__[M+H]__ 5.7			0.033
Mean ± Standard deviation	35,520,010.5 ± 15,899,209.3	43,611,872.6 ± 15,268,233.2	
Median and [25%; 75%]	32,126,746.0 [25,833,157.5; 39,871,449]	41,528,005.0 [33,835,698.3; 53,872,419.5]	
PC O-36:5__[M+H]__ 5.4			<0.001
Mean ± Standard deviation	32,396,147.5 ± 10,073,466.7	46,994,633.1 ± 15,006,004.9	
Median and [25%; 75%]	29,982,879.0 [25,797,302.3; 37,713,654]	45,216,760.0 [40,055,929.3; 56,642,019.5]	
PC O-36:5 PC O-16:0_20:5__[M+H]__ 5.16			0.080
Mean ± Standard deviation	205,726.5 ± 523,202.9	419,252.1 ± 680,407.7	
Median and [25%; 75%]	97,497.5 [44,820.8; 190,052.9]	150,134.1 [107,465.6; 331,600.9]	
PC O-36:5 PC O-16:1_20:4__[M+H]__ 5.5			<0.001
Mean ± Standard deviation	32,423,393.5 ± 10,097,908.1	47,033,299.8 ± 15,023,469.8	
Median and [25%; 75%]	29,957,984.0 [25,798,597.8; 37,718,497]	45,254,052.0 [40,058,986.3; 56,640,551.5]	
PC O-36:7 OA1__[M+H]__ 6.13			0.027
Mean ± Standard deviation	622,433.9 ± 346,677.6	861,810.8 ± 350,467.7	
Median and [25%; 75%]	547,885.8 [372,263.0; 877,617.8]	735,819.9 [643,153.1; 999,955.1]	
PC O-36:7__[M+H]__ 5.67			0.031
Mean ± Standard deviation	630,074.5 ± 342,904.8	862,027.0 ± 350,472.1	
Median and [25%; 75%]	547,885.8 [388,757.9; 877,638.8]	735,819.9 [643,153.1; 1,000,148.4]	
PC O-37:0__[M+H]__ 6.26			<0.001
Mean ± Standard deviation	432,940.4 ± 372,263.8	1,192,205.4 ± 1,563,996.1	
Median and [25%; 75%]	364,847.0 [237,067.8; 472,005.1]	831,277.0 [387,443.6; 1,237,594.8]	
PC O-37:1 OA1__[M+H]__ 6.96			<0.001
Mean ± Standard deviation	16,111,333.0 ± 5,816,974.3	25,387,641.3 ± 8,318,291.9	
Median and [25%; 75%]	15,469,463.5 [12,129,478.6; 18,582,029]	22,688,954.0 [20,477,848.0; 31,568,561.1]	
PC O-37:1 OA2__[M+H]__ 6.27			<0.001
Mean ± Standard deviation	54,783,037.6 ± 28,387,562.2	127,684,269.3 ± 127,967,711.7	
Median and [25%; 75%]	50,210,815.0 [38,173,788.5; 60,917,530]	101,766,002.0 [64,393,505.0; 138,414,268.0]	
PC O-37:1__[M+H]__ 5.81			<0.001

Mean ± Standard deviation	4,014,426.4 ± 1,945,606.5	6,313,166.5 ± 2,461,119.1	
Median and [25%; 75%]	3,487,752.5 [2,785,270.5; 4,749,538.8]	5,910,743.8 [4,871,722.6; 7,352,212.3]	
PC O-37:2 OA1 [M+H] 6.41			<0.001
Mean ± Standard deviation	326,708,967.8 ± 168,891,320.8	585,899,843.9 ± 187,317,087.3	
Median and [25%; 75%]	360,870,416.0 [246,640,304.0; 443,517,	568,372,192.0 [400,149,268.0; 693,196,856.0]	
PC O-37:2 [M+H] 5.38			<0.001
Mean ± Standard deviation	2,081,963.3 ± 1,665,459.7	3,316,875.4 ± 1,268,843.7	
Median and [25%; 75%]	1,610,832.0 [1,256,044.0; 2,184,277.5]	3,189,905.0 [2,053,880.0; 4,009,051.8]	
PC O-37:3 [M+H] 5.38			<0.001
Mean ± Standard deviation	221,125,231.6 ± 93,001,259.6	348,191,377.5 ± 83,424,245.3	
Median and [25%; 75%]	213,307,196.0 [153,837,977.0; 262,149,	355,240,528.0 [282,287,386.0; 404,754,424.0]	
PC O-37:3 PC O-17:0_20:3 [M+H] 5.38			<0.001
Mean ± Standard deviation	220,896,139.8 ± 92,930,536.7	347,837,630.3 ± 83,676,002.7	
Median and [25%; 75%]	212,651,488.0 [153,632,362.0; 262,327,	354,454,816.0 [281,129,812.0; 404,779,276.0]	
PC O-37:8 OA1 [M+H] 5.94			0.093
Mean ± Standard deviation	198,336.0 ± 130,196.4	229,514.1 ± 90,913.0	
Median and [25%; 75%]	157,320.0 [114,135.6; 253,789.8]	236,537.0 [182,574.7; 279,916.6]	
PC O-37:8 PC O-18:4_19:4 [M+H] 4.75			0.036
Mean ± Standard deviation	136,826.2 ± 100,942.2	208,806.9 ± 121,665.1	
Median and [25%; 75%]	127,265.0 [59,445.5; 178,123.3]	158,432.3 [126,251.9; 252,059.4]	
PC O-38:1 [M+H] 7.34			<0.001
Mean ± Standard deviation	7,528,308.3 ± 2,816,461.3	12,343,155.9 ± 4,673,580.0	
Median and [25%; 75%]	7,619,393.0 [5,347,834.5; 9,000,176.4]	10,429,422.8 [9,101,962.5; 15,478,609.9]	
PC O-38:2 OA1 [M+H] 6.62			0.104
Mean ± Standard deviation	3,089,607.6 ± 1,657,965.1	3,688,412.7 ± 1,403,436.3	
Median and [25%; 75%]	2,923,690.5 [2,008,082.8; 3,750,036.5]	3,224,359.5 [2,831,842.3; 4,145,465.8]	
PC O-38:2 [M+H] 6.76			<0.001
Mean ± Standard deviation	4,240,982.1 ± 1,601,855.3	7,172,746.2 ± 2,943,162.2	
Median and [25%; 75%]	4,414,305.0 [3,212,538.3; 5,056,062.8]	6,295,250.8 [5,467,354.3; 7,642,679.6]	
PC O-38:2 PC O-20:0_18:2 [M+H] 6.09			<0.001
Mean ± Standard deviation	237,920.7 ± 127,130.5	707,430.4 ± 525,986.4	
Median and [25%; 75%]	220,569.0 [155,050.6; 296,722.5]	588,298.5 [287,910.3; 884,480.4]	
PC O-38:3 [M+H] 6.16			0.012
Mean ± Standard deviation	1,863,478.2 ± 597,521.2	2,520,404.7 ± 874,302.6	
Median and [25%; 75%]	1,764,185.3 [1,438,671.5; 2,276,344.4]	2,494,334.0 [1,962,669.1; 3,039,843.1]	
PC O-38:3 PC O-18:0_20:3 OA1 [M+H] 5.64			0.003

Mean ± Standard deviation	56,629.3 ± 45,436.2	86,555.6 ± 47,622.2	
Median and [25%; 75%]	40,530.0 [27,853.0; 73,050.3]	78,789.8 [61,865.5; 98,615.2]	
PC O-38:3 PC O-18:0_20:3__ [M+H]__ 6.35			0.132
Mean ± Standard deviation	207,702.6 ± 155,310.1	329,763.1 ± 314,005.3	
Median and [25%; 75%]	156,308.8 [112,090.3; 283,615.8]	233,184.5 [152,369.6; 379,850.1]	
PC O-38:4__ [M+H]__ 5.48			0.807
Mean ± Standard deviation	3,201,997.6 ± 2,845,913.6	3,001,145.7 ± 1,753,821.5	
Median and [25%; 75%]	2,244,997.0 [1,532,783.3; 3,798,516.5]	2,894,058.9 [1,466,026.4; 4,610,678.9]	
PC O-38:4 PC O-16:0_22:4__ [M+H]__ 5.91			0.899
Mean ± Standard deviation	2,297,681.9 ± 1,235,135.4	2,223,870.8 ± 1,015,578.7	
Median and [25%; 75%]	2,000,808.0 [1,300,783.5; 3,218,246.3]	2,308,522.5 [1,384,719.7; 2,981,740.5]	
PC O-38:5 OA1__ [M+H]__ 6.09			<0.001
Mean ± Standard deviation	8,121,001.7 ± 2,940,433.9	13,205,359.7 ± 5,233,232.8	
Median and [25%; 75%]	7,045,902.8 [6,379,813.9; 9,091,485.0]	12,976,402.4 [9,458,920.3; 17,202,732.9]	
PC O-38:5__ [M+H]__ 5.62			0.755
Mean ± Standard deviation	18,366,481.7 ± 9,890,684.4	17,749,514.1 ± 7,138,335.6	
Median and [25%; 75%]	15,830,477.5 [12,586,949.3; 20,848,235]	17,907,232.0 [13,636,791.4; 21,118,025.3]	
PC O-38:5 PC O-16:1_22:4__ [M+H]__ 5.9			0.679
Mean ± Standard deviation	18,373,715.4 ± 9,825,544.5	17,877,816.4 ± 7,096,277.7	
Median and [25%; 75%]	15,597,263.5 [12,547,506.0; 20,922,416]	17,940,038.8 [13,747,836.5; 21,261,931.9]	
PC O-38:5 PC O-18:4_20:1__ [M+H]__ 5.51			0.655
Mean ± Standard deviation	18,986,689.7 ± 9,843,875.2	18,728,240.1 ± 7,143,731.9	
Median and [25%; 75%]	16,545,390.5 [13,033,465.8; 21,538,000]	18,226,667.3 [14,588,576.6; 21,940,853.9]	
PC O-38:6 PC O-16:0_22:6 OA1__ [M+H]__ 4.82			0.306
Mean ± Standard deviation	212,974.0 ± 171,849.6	260,728.7 ± 188,029.4	
Median and [25%; 75%]	167,179.5 [71,802.3; 300,384.5]	237,929.5 [118,087.5; 358,181.3]	
PC O-38:6 PC O-16:0_22:6 OA2__ [M+H]__ 5.36			0.704
Mean ± Standard deviation	2,045,774.8 ± 1,241,345.7	2,383,199.3 ± 1,897,455.0	
Median and [25%; 75%]	1,599,872.8 [1,226,076.8; 2,803,147.3]	2,005,523.3 [1,284,480.9; 2,424,279.3]	
PC O-38:6 PC O-16:0_22:6__ [M+H]__ 5.35			0.692
Mean ± Standard deviation	2,031,361.2 ± 1,231,398.6	2,381,717.2 ± 1,897,901.0	
Median and [25%; 75%]	1,599,872.8 [1,218,381.5; 2,790,540.0]	1,993,666.6 [1,284,480.9; 2,424,279.3]	
PC O-38:7__ [M+H]__ 6.26			<0.001
Mean ± Standard deviation	108,773.1 ± 59,635.5	255,261.0 ± 228,844.9	
Median and [25%; 75%]	88,242.5 [64,190.5; 146,554.0]	186,252.5 [115,327.6; 281,734.8]	
PC O-38:7 PC O-16:1_22:6__ [M+H]__ 5.32			0.322

Mean ± Standard deviation	793,305.4 ± 582,825.3	1,048,183.7 ± 747,453.6	
Median and [25%; 75%]	712,973.5 [320,859.8; 1,081,337.3]	710,856.6 [562,448.3; 1,455,974.4]	
PC O-38:9 __[M+H]__ 5.39			<0.001
Mean ± Standard deviation	355,524.9 ± 218,403.2	628,675.3 ± 302,799.8	
Median and [25%; 75%]	333,074.5 [200,958.4; 486,441.5]	530,724.5 [448,685.6; 734,610.5]	
PC O-39:1 __[M+H]__ 7.73			<0.001
Mean ± Standard deviation	13,320,198.5 ± 5,269,707.2	20,204,882.3 ± 6,943,488.0	
Median and [25%; 75%]	13,149,171.0 [10,079,471.9; 16,819,077]	19,645,099.5 [14,858,568.0; 22,700,099.8]	
PC O-39:2 __[M+H]__ 7.14			<0.001
Mean ± Standard deviation	8,529,005.3 ± 3,649,036.7	12,193,227.9 ± 3,043,989.6	
Median and [25%; 75%]	8,829,649.0 [5,456,278.4; 10,931,365.5]	12,353,113.6 [9,655,628.4; 12,860,552.8]	
PC O-39:2 PC O-19:0_20:2 __[M+H]__ 6.31			0.001
Mean ± Standard deviation	1,299,329.2 ± 715,899.2	2,188,755.1 ± 862,518.7	
Median and [25%; 75%]	1,297,627.0 [871,656.0; 1,673,592.4]	1,850,226.3 [1,584,214.5; 2,781,903.0]	
PC O-39:3 __[M+H]__ 6.37			0.011
Mean ± Standard deviation	23,028,165.4 ± 7,783,608.6	28,866,846.0 ± 7,187,358.8	
Median and [25%; 75%]	21,646,140.0 [17,640,031.8; 28,241,160]	26,668,819.0 [24,195,987.3; 33,949,745.8]	
PC O-39:4 OA1 __[M+H]__ 5.51			0.794
Mean ± Standard deviation	234,788,294.1 ± 133,021,414.4	215,920,424.4 ± 113,474,093.0	
Median and [25%; 75%]	199,665,532.0 [133,874,351.0; 270,535,	209,212,382.0 [135,827,874.0; 326,355,288.0]	
PC O-39:4 __[M+H]__ 5.74			0.768
Mean ± Standard deviation	237,270,543.7 ± 133,179,089.3	216,056,180.9 ± 113,427,290.2	
Median and [25%; 75%]	201,074,420.0 [134,205,567.0; 270,482,	209,001,658.0 [138,771,160.0; 326,860,036.0]	
PC O-39:5 OA1 __[M+H]__ 5.34			0.005
Mean ± Standard deviation	8,678,977.6 ± 4,513,012.6	12,587,988.2 ± 4,865,265.5	
Median and [25%; 75%]	7,295,068.8 [5,807,144.8; 11,019,827.5]	11,609,148.3 [10,306,345.6; 14,923,030.1]	
PC O-39:5 OA2 __[M+H]__ 5.18			0.072
Mean ± Standard deviation	23,570,434.1 ± 22,266,051.0	26,353,579.4 ± 13,093,260.7	
Median and [25%; 75%]	14,105,400.0 [9,560,230.4; 25,201,123.0]	23,880,879.3 [14,808,519.0; 36,452,431.5]	
PC O-39:5 __[M+H]__ 5.05			0.374
Mean ± Standard deviation	3,796,621.6 ± 2,349,964.6	4,178,263.5 ± 1,807,192.9	
Median and [25%; 75%]	3,146,945.0 [2,066,697.4; 4,626,222.8]	4,353,074.8 [2,733,529.8; 5,539,495.8]	
PC O-39:6 __[M+H]__ 4.93			0.228
Mean ± Standard deviation	244,373,673.6 ± 90,001,280.7	287,246,897.0 ± 126,573,785.5	
Median and [25%; 75%]	232,479,724.0 [172,626,884.0; 316,531,	305,544,740.0 [200,781,136.0; 349,845,942.0]	
PC O-40:10 OA1 __[M+H]__ 5.75			0.322

Mean ± Standard deviation	385,605.4 ± 214,069.6	467,643.4 ± 270,470.0	
Median and [25%; 75%]	371,645.0 [236,737.3; 511,784.8]	421,534.0 [270,144.1; 600,017.0]	
PC O-40:2__[M+H]__ 7.21			0.030
Mean ± Standard deviation	728,968.0 ± 449,716.5	990,711.6 ± 452,237.1	
Median and [25%; 75%]	606,551.5 [391,604.0; 978,065.5]	902,845.0 [729,735.1; 1,272,952.9]	
PC O-40:4 PC O-18:0_22:4__[M+H]__ 6.55			0.013
Mean ± Standard deviation	599,964.2 ± 266,914.0	932,419.9 ± 602,498.0	
Median and [25%; 75%]	563,923.5 [418,192.9; 667,251.0]	773,828.0 [638,031.8; 1,227,134.6]	
PC O-40:4 PC O-20:0_20:4__[M+H]__ 6.83			<0.001
Mean ± Standard deviation	1,807,013.9 ± 677,210.0	2,963,139.2 ± 1,389,175.8	
Median and [25%; 75%]	1,836,995.5 [1,407,346.3; 2,251,911.0]	3,136,193.3 [2,412,772.5; 3,398,248.3]	
PC O-40:6 PC O-18:0_22:6 OA1__[M+H]__ 5.91			0.571
Mean ± Standard deviation	1,378,211.2 ± 782,532.0	1,612,227.5 ± 974,942.7	
Median and [25%; 75%]	1,250,906.0 [778,888.5; 1,701,349.3]	1,239,529.3 [871,329.5; 2,361,952.9]	
PC O-40:6 PC O-18:0_22:6__[M+H]__ 5.31			0.537
Mean ± Standard deviation	47,133.5 ± 35,756.5	51,379.9 ± 33,177.1	
Median and [25%; 75%]	37,218.5 [23,805.8; 63,143.3]	46,988.0 [28,760.9; 67,146.6]	
PC O-40:7 PC O-18:1_22:6__[M+H]__ 5.45			0.560
Mean ± Standard deviation	1,663,112.6 ± 1,049,135.7	1,498,422.3 ± 1,092,728.2	
Median and [25%; 75%]	1,473,208.0 [744,120.1; 2,458,410.9]	1,140,758.5 [944,359.1; 1,639,721.4]	
PC O-41:5__[M+H]__ 5.57			0.260
Mean ± Standard deviation	1,015,672.6 ± 808,737.1	1,311,889.3 ± 1,012,741.4	
Median and [25%; 75%]	748,769.5 [388,772.3; 1,270,767.6]	1,016,579.3 [606,145.3; 1,690,205.5]	
PC O-41:5 PC O-19:0_22:5__[M+H]__ 5.99			0.022
Mean ± Standard deviation	829,804.8 ± 1,045,979.3	1,723,787.9 ± 2,148,773.1	
Median and [25%; 75%]	525,358.0 [202,647.6; 825,143.5]	896,672.1 [458,140.6; 1,531,324.9]	
PC O-41:6__[M+H]__ 5.57			0.253
Mean ± Standard deviation	59,575,103.9 ± 35,421,838.4	77,645,414.7 ± 49,704,010.7	
Median and [25%; 75%]	51,150,176.0 [30,712,044.5; 79,108,151]	72,342,559.0 [45,690,011.0; 100,595,921.0]	
PC O-41:6 PC O-17:0_24:6__[M+H]__ 5.35			0.253
Mean ± Standard deviation	59,645,439.1 ± 35,483,005.0	77,688,324.1 ± 49,731,179.2	
Median and [25%; 75%]	51,183,486.0 [30,720,498.0; 79,170,965]	72,383,259.5 [45,704,589.0; 100,627,716.0]	
PC O-41:7__[M+H]__ 5.15			0.137
Mean ± Standard deviation	1,462,841.6 ± 1,442,744.6	1,857,625.7 ± 1,423,605.4	
Median and [25%; 75%]	984,762.5 [561,298.5; 1,709,766.0]	1,690,537.3 [941,674.4; 2,068,279.3]	
PC O-41:8 PC O-19:2_22:6__[M+H]__ 4.78			0.036

Mean ± Standard deviation	271,713.9 ± 236,948.3	399,019.4 ± 259,074.1	
Median and [25%; 75%]	217,319.0 [106,024.8; 323,532.4]	304,721.0 [183,939.9; 551,131.3]	
PC O-42:4 PC O-22:0_20:4__[M+H]__ 7.57			<0.001
Mean ± Standard deviation	1,302,159.0 ± 426,634.4	2,054,957.5 ± 871,335.3	
Median and [25%; 75%]	1,312,822.5 [1,098,697.9; 1,508,629.5]	2,086,828.8 [1,694,159.5; 2,448,877.5]	
PC O-42:5 PC O-22:1_20:4__[M+H]__ 6.81			0.018
Mean ± Standard deviation	2,828,463.3 ± 1,151,040.4	4,087,115.8 ± 2,237,961.1	
Median and [25%; 75%]	2,657,894.3 [2,125,169.1; 3,430,664.3]	3,968,943.8 [2,789,710.0; 4,867,102.3]	
PC O-44:6__[M+H]__ 6.89			0.583
Mean ± Standard deviation	1,507,140.0 ± 1,213,179.8	1,869,200.7 ± 1,875,413.1	
Median and [25%; 75%]	1,053,051.0 [676,947.3; 1,935,018.8]	1,238,216.0 [900,001.1; 1,948,146.8]	
PC O-44:6 PC O-24:2_20:4__[M+H]__ 6.87			0.980
Mean ± Standard deviation	1,667,222.4 ± 1,181,705.7	1,871,006.5 ± 1,875,808.1	
Median and [25%; 75%]	1,268,671.5 [782,171.5; 2,438,630.5]	1,166,371.0 [921,142.6; 1,962,220.6]	
PC O-44:7 PC O-22:1_22:6__[M+H]__ 6.55			0.156
Mean ± Standard deviation	289,139.4 ± 150,266.8	415,726.3 ± 315,643.6	
Median and [25%; 75%]	300,407.0 [167,489.5; 363,459.3]	335,215.8 [232,040.3; 482,422.0]	
PC O-46:7 PC O-24:1_22:6__[M+H]__ 7.24			0.084
Mean ± Standard deviation	359,526.3 ± 231,401.3	559,715.4 ± 444,188.7	
Median and [25%; 75%]	303,145.5 [185,694.0; 455,675.5]	413,444.3 [290,681.0; 560,556.1]	
PE 34:1 PE 16:0_18:1__[M+H]__ 5.83			0.057
Mean ± Standard deviation	142,931.6 ± 89,758.9	330,242.7 ± 576,733.2	
Median and [25%; 75%]	139,977.5 [70,458.8; 185,597.1]	160,549.0 [110,507.1; 285,733.6]	
PE 34:2 PE 16:0_18:2__[M+H]__ 5.37			0.026
Mean ± Standard deviation	91,840.6 ± 100,807.5	476,222.1 ± 1,130,090.7	
Median and [25%; 75%]	61,254.0 [29,188.3; 116,142.8]	123,141.0 [58,976.9; 304,820.8]	
PE 36:1__[M+H]__ 6.44			0.026
Mean ± Standard deviation	904,733.2 ± 497,305.9	1,279,443.1 ± 597,610.9	
Median and [25%; 75%]	809,743.0 [531,861.3; 1,227,278.4]	1,194,873.3 [826,726.9; 1,627,459.4]	
PE 36:2__[M+H]__ 5.92			<0.001
Mean ± Standard deviation	1,336,827.4 ± 913,710.5	4,838,632.9 ± 4,316,359.9	
Median and [25%; 75%]	1,136,781.5 [676,494.3; 1,849,399.3]	3,145,602.5 [1,707,046.8; 6,750,458.2]	
PE 36:2 PE 18:1_18:1__[M+H]__ 5.93			0.043
Mean ± Standard deviation	438,476.0 ± 539,206.9	850,418.9 ± 870,985.5	
Median and [25%; 75%]	310,596.5 [143,897.1; 537,207.3]	509,636.5 [220,557.8; 1,108,641.6]	
PE 36:4__[M+H]__ 5.34			0.452

Mean ± Standard deviation	220,694.8 ± 239,651.6	354,254.5 ± 478,125.3	
Median and [25%; 75%]	145,059.5 [61,175.0; 257,450.1]	190,248.0 [73,913.1; 305,980.3]	
PE 38:4 [M+H] 5.9			0.274
Mean ± Standard deviation	3,903,178.0 ± 2,348,135.9	6,374,614.5 ± 7,053,536.1	
Median and [25%; 75%]	3,713,450.5 [1,907,073.8; 5,174,304.6]	4,111,465.8 [2,390,956.7; 8,039,766.3]	
PE 38:6 PE 16:0_22:6 [M+H] 5.16			0.442
Mean ± Standard deviation	1,487,215.7 ± 1,305,406.6	1,858,739.5 ± 1,597,112.2	
Median and [25%; 75%]	1,025,848.5 [482,072.9; 1,946,021.3]	1,539,301.8 [458,424.7; 3,355,963.6]	
PE 40:6 [M+H] 5.7			0.314
Mean ± Standard deviation	211,499.5 ± 180,541.1	318,165.8 ± 315,797.2	
Median and [25%; 75%]	149,152.5 [78,199.5; 303,638.0]	166,844.0 [103,078.7; 423,519.4]	
PE O-40:6 [M+H] 6.06			0.025
Mean ± Standard deviation	92,284.3 ± 61,513.7	201,765.7 ± 205,259.1	
Median and [25%; 75%]	75,405.3 [48,596.5; 122,481.0]	115,719.8 [69,694.1; 213,861.0]	
PE P-36:2 PE P-18:0_18:2 [M+H] 6.33			0.100
Mean ± Standard deviation	295,858.6 ± 309,518.8	790,677.5 ± 1,118,274.6	
Median and [25%; 75%]	207,759.0 [119,125.8; 356,505.9]	269,502.0 [161,069.5; 836,745.9]	
PE P-36:4 PE P-16:0_20:4 [M+H] 5.65			0.093
Mean ± Standard deviation	465,359.0 ± 474,116.8	654,772.8 ± 526,636.3	
Median and [25%; 75%]	257,781.8 [148,305.8; 575,979.9]	463,931.4 [319,678.9; 910,931.0]	
PE P-38:6 PE P-16:0_22:6 [M+H] 5.46			0.084
Mean ± Standard deviation	722,205.7 ± 454,998.4	959,596.5 ± 467,533.6	
Median and [25%; 75%]	641,360.0 [330,958.5; 995,339.0]	918,516.8 [675,346.6; 1,217,450.1]	
PE P-40:7 PE P-18:1_22:6 [M+H] 5.52			0.097
Mean ± Standard deviation	197,739.4 ± 130,238.2	228,246.4 ± 90,388.9	
Median and [25%; 75%]	155,439.5 [113,854.0; 253,734.5]	235,323.3 [181,369.4; 278,315.6]	
PI 34:2 [M+NH4] 4.55			0.020
Mean ± Standard deviation	365,213.0 ± 254,676.2	540,191.9 ± 307,612.1	
Median and [25%; 75%]	318,749.8 [205,032.5; 459,391.3]	477,518.5 [315,001.2; 640,610.0]	
PI 34:2 [M+Na] 4.55			<0.001
Mean ± Standard deviation	118,052.2 ± 107,531.4	300,827.9 ± 146,745.7	
Median and [25%; 75%]	85,174.5 [41,660.5; 196,806.3]	281,918.5 [186,453.1; 386,882.8]	
PI 36:2 [M+NH4] 4.98			0.022
Mean ± Standard deviation	244,570.9 ± 158,066.6	338,553.2 ± 146,251.6	
Median and [25%; 75%]	226,930.0 [133,280.5; 319,833.5]	310,987.5 [271,024.9; 380,652.6]	
PI 36:4 [M+NH4] 4.53			0.001

Mean ± Standard deviation	665,851.9 ± 392,749.0	1,029,868.0 ± 366,784.5	
Median and [25%; 75%]	587,042.5 [402,097.0; 852,656.8]	965,500.0 [733,086.8; 1,199,188.6]	
PI 36:4 __[M+Na]__ 4.53			<0.001
Mean ± Standard deviation	163,943.1 ± 98,580.4	408,542.3 ± 124,937.0	
Median and [25%; 75%]	149,064.5 [107,025.5; 199,975.1]	372,613.5 [314,688.6; 490,804.5]	
PI 38:4 __[M+NH4]__ 4.96			0.135
Mean ± Standard deviation	5,704,427.9 ± 2,474,902.9	6,994,866.3 ± 2,972,312.1	
Median and [25%; 75%]	5,869,296.5 [3,946,990.5; 7,275,077.5]	6,002,529.8 [4,864,677.3; 8,903,142.9]	
SM 20:0;O3 __[M+H]__ 2.56			<0.001
Mean ± Standard deviation	1,213,476.3 ± 389,321.1	1,682,939.0 ± 528,551.5	
Median and [25%; 75%]	1,150,164.5 [946,696.8; 1,449,514.0]	1,625,740.0 [1,306,923.9; 1,949,980.9]	
SM 20:1;O3 __[M+H]__ 2.2			0.036
Mean ± Standard deviation	6,588,416.1 ± 1,903,396.2	8,523,206.0 ± 3,683,019.3	
Median and [25%; 75%]	6,206,391.0 [5,129,339.3; 7,694,551.4]	7,141,986.9 [6,006,808.0; 9,539,585.1]	
SM 20:2;O3 __[M+H]__ 1.78			0.022
Mean ± Standard deviation	8,394,454.7 ± 3,786,342.2	12,396,792.7 ± 6,880,223.5	
Median and [25%; 75%]	7,286,083.0 [6,274,615.8; 9,080,220.1]	11,044,484.5 [7,445,130.9; 14,359,761.3]	
SM 26:1;O3 __[M+H]__ 6.68			0.041
Mean ± Standard deviation	25,650.5 ± 41,853.0	40,405.6 ± 53,535.6	
Median and [25%; 75%]	6,813.5 [3,610.4; 21,267.5]	17,884.3 [9,639.1; 52,481.8]	
SM 30:1;O2 SM 18:1;O2/12:0 __[M+H]__ 4.2			<0.001
Mean ± Standard deviation	321,925.1 ± 281,148.1	756,592.6 ± 485,177.5	
Median and [25%; 75%]	254,295.0 [149,556.9; 376,978.8]	573,987.3 [406,351.6; 1,088,790.9]	
SM 30:3;O3 __[M+H]__ 6.85			0.926
Mean ± Standard deviation	73,556.8 ± 84,654.2	59,939.9 ± 52,106.6	
Median and [25%; 75%]	36,139.5 [19,841.9; 105,255.8]	49,761.3 [23,228.6; 76,047.8]	
SM 31:1;O2 SM 17:1;O2/14:0 __[M+H]__ 4.39			<0.001
Mean ± Standard deviation	195,792.0 ± 126,419.6	529,477.5 ± 344,740.8	
Median and [25%; 75%]	173,850.3 [103,271.3; 252,810.6]	449,131.5 [260,573.9; 839,414.2]	
SM 31:2;O3 __[M+H]__ 4.6			<0.001
Mean ± Standard deviation	1,165,707.7 ± 577,524.8	1,998,593.7 ± 610,730.0	
Median and [25%; 75%]	1,097,051.5 [684,237.5; 1,629,456.9]	1,804,351.0 [1,581,402.0; 2,522,302.6]	
SM 31:3;O3 __[M+H]__ 4.25			<0.001
Mean ± Standard deviation	57,247.1 ± 34,106.5	175,448.1 ± 254,305.6	
Median and [25%; 75%]	49,081.0 [35,137.8; 68,611.0]	116,185.8 [85,761.0; 143,127.1]	
SM 32:0;O2 __[M+H]__ 4.77			0.132

Mean ± Standard deviation	210,700.3 ± 185,159.5	312,782.5 ± 308,512.6	
Median and [25%; 75%]	150,845.0 [80,119.3; 283,195.5]	179,170.3 [140,048.9; 356,156.1]	
SM 32:1;O2__[M+Na]__4.63			0.442
Mean ± Standard deviation	927,123.6 ± 620,180.4	852,240.3 ± 375,002.8	
Median and [25%; 75%]	687,497.8 [469,018.4; 1,254,789.4]	739,650.0 [693,503.5; 1,004,731.5]	
SM 32:1;O2 SM 16:1;O2/16:0__[M+H]__4.6			<0.001
Mean ± Standard deviation	29,527,031.4 ± 8,546,009.4	50,909,124.9 ± 13,868,581.6	
Median and [25%; 75%]	29,844,793.0 [23,768,764.0; 33,146,093]	48,921,465.0 [43,190,066.0; 58,419,318.5]	
SM 32:2;O2__[M+H]__4.27			<0.001
Mean ± Standard deviation	1,179,716.5 ± 621,098.5	2,136,545.4 ± 764,568.7	
Median and [25%; 75%]	1,094,002.8 [722,862.3; 1,276,273.9]	1,918,730.8 [1,544,053.4; 2,826,460.8]	
SM 32:2;O2 SM 18:2;O2/14:0__[M+H]__4.26			<0.001
Mean ± Standard deviation	1,179,540.6 ± 620,816.0	2,136,473.1 ± 764,477.7	
Median and [25%; 75%]	1,094,002.8 [722,862.3; 1,276,273.9]	1,918,730.8 [1,544,053.4; 2,826,460.8]	
SM 33:1;O2__[M+Na]__4.82			0.387
Mean ± Standard deviation	746,119.0 ± 363,397.7	672,873.7 ± 250,964.9	
Median and [25%; 75%]	713,720.8 [516,107.8; 978,040.0]	591,080.0 [489,280.5; 875,613.8]	
SM 33:1;O2 SM 17:1;O2/16:0__[M+H]__4.83			<0.001
Mean ± Standard deviation	13,203,978.7 ± 4,711,851.6	21,257,462.0 ± 8,336,327.6	
Median and [25%; 75%]	13,128,103.0 [9,857,954.6; 15,409,181.3]	20,103,642.5 [14,032,910.8; 25,696,184.3]	
SM 33:1;O3__[M+H]__5.09			0.442
Mean ± Standard deviation	2,921,202.3 ± 1,327,234.5	3,427,557.4 ± 1,490,729.1	
Median and [25%; 75%]	2,935,515.0 [1,782,050.0; 3,404,163.5]	2,882,999.5 [2,361,029.9; 4,344,786.4]	
SM 33:2;O2 SM 17:2;O2/16:0__[M+H]__4.5			0.023
Mean ± Standard deviation	275,138.5 ± 185,976.7	403,342.8 ± 242,569.3	
Median and [25%; 75%]	229,193.0 [157,070.9; 366,243.9]	306,009.3 [241,661.9; 559,460.0]	
SM 34:0;O2__[M+H]__5.25			0.294
Mean ± Standard deviation	13,395,490.9 ± 3,507,697.6	14,750,288.0 ± 4,561,101.7	
Median and [25%; 75%]	13,514,143.5 [10,425,597.8; 15,193,250]	13,654,102.8 [12,281,574.5; 17,119,778.3]	
SM 34:1;O2__[M+Na]__5.12			<0.001
Mean ± Standard deviation	552,769.2 ± 296,598.0	314,863.3 ± 156,457.7	
Median and [25%; 75%]	505,967.0 [363,453.3; 632,657.3]	273,706.8 [183,621.4; 401,094.0]	
SM 34:1;O2 SM 18:1;O2/16:0__[M+H]__5.08			0.007
Mean ± Standard deviation	254,899,440.2 ± 43,171,854.7	293,122,135.8 ± 45,182,069.4	
Median and [25%; 75%]	257,879,208.0 [230,664,632.0; 285,147,	299,577,528.0 [262,759,978.0; 327,315,035.0]	
SM 34:1;O3__[M+H]__4.92			0.993

Mean ± Standard deviation	193,276.2 ± 119,978.6	190,455.5 ± 111,362.6	
Median and [25%; 75%]	159,244.0 [95,034.8; 262,003.6]	178,918.3 [98,737.8; 256,280.4]	
SM 34:2;O2__[M+Na]__4.67			0.212
Mean ± Standard deviation	3,036,625.1 ± 609,645.6	3,230,540.8 ± 626,718.9	
Median and [25%; 75%]	2,871,116.0 [2,596,332.6; 3,412,655.8]	3,247,696.0 [2,748,715.9; 3,683,136.4]	
SM 34:2;O2 SM 18:2;O2/16:0__[M+H]__4.68			<0.001
Mean ± Standard deviation	42,813,870.4 ± 9,127,894.4	56,794,874.2 ± 14,174,832.6	
Median and [25%; 75%]	42,728,190.0 [38,160,530.0; 50,230,569]	54,798,103.0 [46,198,820.0; 63,582,354.5]	
SM 34:2;O3__[M+H]__4.52			0.115
Mean ± Standard deviation	513,963.0 ± 190,629.3	646,013.8 ± 263,308.9	
Median and [25%; 75%]	474,177.0 [384,901.6; 614,532.0]	603,119.8 [396,156.4; 866,390.9]	
SM 35:1;O2__[M+H]__5.34			0.061
Mean ± Standard deviation	1,805,922.7 ± 934,096.2	2,201,718.6 ± 862,501.6	
Median and [25%; 75%]	1,617,690.5 [1,168,902.0; 2,007,778.0]	1,913,321.0 [1,657,056.6; 2,739,865.0]	
SM 35:1;O2 SM 18:1;O2/17:0__[M+H]__5.35			0.059
Mean ± Standard deviation	1,787,486.8 ± 948,675.3	2,201,420.6 ± 860,971.0	
Median and [25%; 75%]	1,607,250.5 [1,167,205.8; 2,002,431.8]	1,916,328.8 [1,656,038.1; 2,739,697.0]	
SM 35:1;O3__[M+H]__5.62			<0.001
Mean ± Standard deviation	1,179,925.8 ± 1,355,618.7	3,306,948.3 ± 1,986,883.6	
Median and [25%; 75%]	724,274.5 [281,885.0; 1,476,455.3]	2,575,595.0 [2,072,448.1; 4,149,105.0]	
SM 35:2;O3__[M+H]__5.62			0.169
Mean ± Standard deviation	2,590,027.6 ± 1,270,632.8	3,107,556.3 ± 1,242,608.6	
Median and [25%; 75%]	2,166,385.5 [1,734,092.8; 3,638,762.0]	2,894,598.4 [2,301,032.3; 4,289,368.6]	
SM 35:3;O3__[M+H]__5.17			0.022
Mean ± Standard deviation	930,072.6 ± 462,572.2	1,316,856.5 ± 604,074.1	
Median and [25%; 75%]	923,600.0 [568,192.3; 1,178,538.8]	1,143,325.8 [888,965.1; 1,564,954.4]	
SM 35:4;O3__[M+H]__4.82			0.348
Mean ± Standard deviation	109,089.9 ± 49,612.4	99,821.2 ± 39,833.3	
Median and [25%; 75%]	107,480.0 [73,317.8; 140,167.8]	90,407.0 [68,925.8; 113,179.8]	
SM 36:0;O2__[M+H]__5.84			0.442
Mean ± Standard deviation	317,912.7 ± 451,906.3	190,393.7 ± 206,737.8	
Median and [25%; 75%]	135,890.5 [65,623.0; 339,164.0]	118,763.0 [67,962.4; 203,499.9]	
SM 36:1;O2 SM 18:1;O2/18:0__[M+H]__5.62			0.084
Mean ± Standard deviation	42,399,680.8 ± 11,012,612.2	49,004,828.4 ± 13,027,019.8	
Median and [25%; 75%]	42,382,890.0 [35,171,925.3; 50,010,417]	49,014,129.5 [40,963,688.0; 58,344,570.5]	
SM 36:1;O3__[M+H]__6.04			0.078

Mean ± Standard deviation	3,480,453.5 ± 1,541,789.4	4,528,731.1 ± 2,001,870.7	
Median and [25%; 75%]	3,124,527.0 [2,517,314.3; 4,428,614.4]	4,476,704.5 [3,353,371.9; 4,867,891.4]	
SM 36:2;O2 SM 18:2;O2/18:0__[M+H]__ 5.17			0.060
Mean ± Standard deviation	15,750,092.5 ± 5,542,220.8	19,809,866.7 ± 7,434,680.2	
Median and [25%; 75%]	15,234,496.8 [12,267,756.3; 19,933,576]	18,634,690.8 [13,954,133.1; 23,638,223.5]	
SM 36:2;O3__[M+H]__ 5.93			0.002
Mean ± Standard deviation	1,713,542.5 ± 1,366,771.8	3,248,560.2 ± 2,038,438.6	
Median and [25%; 75%]	1,439,275.0 [990,383.6; 1,827,714.0]	2,555,484.0 [1,509,988.1; 4,128,210.8]	
SM 36:3;O3__[M+H]__ 5.55			0.002
Mean ± Standard deviation	3,167,428.4 ± 1,681,074.5	6,851,200.7 ± 5,859,524.4	
Median and [25%; 75%]	2,799,612.0 [2,169,123.8; 3,782,544.5]	4,245,316.6 [3,235,168.4; 8,853,465.3]	
SM 37:0;O3__[M+H]__ 5.66			<0.001
Mean ± Standard deviation	228,068.7 ± 213,472.6	320,875.8 ± 143,730.1	
Median and [25%; 75%]	164,511.5 [126,125.1; 233,143.3]	274,251.8 [215,016.5; 374,514.5]	
SM 37:1;O2 SM 21:1;O2/16:0__[M+H]__ 5.92			0.097
Mean ± Standard deviation	2,348,366.5 ± 1,229,103.3	3,145,874.3 ± 1,844,993.7	
Median and [25%; 75%]	2,063,504.3 [1,509,895.9; 2,935,839.0]	2,790,620.0 [2,098,211.9; 3,725,434.3]	
SM 37:1;O3__[M+H]__ 5.67			<0.001
Mean ± Standard deviation	185,943,716.4 ± 58,241,191.9	264,873,838.8 ± 99,954,592.7	
Median and [25%; 75%]	181,823,848.0 [151,007,448.0; 214,676,	245,256,144.0 [210,704,228.0; 300,642,120.0]	
SM 37:3;O3__[M+H]__ 5.75			0.537
Mean ± Standard deviation	232,589.5 ± 150,832.3	219,348.7 ± 173,845.4	
Median and [25%; 75%]	197,657.5 [133,891.3; 267,197.9]	183,855.5 [94,804.5; 256,031.6]	
SM 37:5;O3__[M+H]__ 5.41			0.055
Mean ± Standard deviation	996,422.8 ± 879,614.9	1,372,865.5 ± 958,561.0	
Median and [25%; 75%]	688,669.0 [419,525.8; 1,161,989.5]	1,062,157.3 [784,399.8; 1,689,779.9]	
SM 38:0;O2__[M+H]__ 6.33			0.059
Mean ± Standard deviation	406,830.5 ± 170,299.1	643,976.9 ± 425,460.7	
Median and [25%; 75%]	405,848.0 [292,313.5; 506,069.6]	496,195.0 [348,577.1; 793,763.4]	
SM 38:1;O3__[M+H]__ 6.0			0.013
Mean ± Standard deviation	457,596.2 ± 272,868.4	696,970.5 ± 446,158.6	
Median and [25%; 75%]	409,849.5 [295,549.6; 561,487.8]	633,947.0 [453,847.6; 832,508.3]	
SM 38:2;O2 SM 18:2;O2/20:0__[M+H]__ 5.74			0.087
Mean ± Standard deviation	4,057,195.9 ± 1,458,971.2	3,392,512.9 ± 1,388,475.8	
Median and [25%; 75%]	3,759,030.8 [2,966,097.8; 4,841,620.6]	3,216,870.5 [2,616,284.3; 4,055,330.9]	
SM 38:2;O3__[M+H]__ 5.5			<0.001

Mean ± Standard deviation	2,612,399.6 ± 1,192,420.5	5,373,971.5 ± 2,802,381.3	
Median and [25%; 75%]	2,411,006.5 [1,985,963.0; 3,055,418.5]	4,584,584.8 [3,044,967.0; 6,940,683.6]	
SM 38:3;O3__[M+H]__ 6.12			0.002
Mean ± Standard deviation	1,336,367.9 ± 638,608.2	2,636,731.6 ± 1,759,504.6	
Median and [25%; 75%]	1,196,930.0 [802,219.5; 1,892,752.3]	1,861,613.8 [1,525,036.5; 3,367,404.3]	
SM 38:4;O2__[M+H]__ 5.4			0.041
Mean ± Standard deviation	2,068,743.5 ± 825,913.9	1,708,613.1 ± 465,644.1	
Median and [25%; 75%]	2,179,987.8 [1,466,355.3; 2,596,172.6]	1,693,685.0 [1,417,140.7; 1,998,214.5]	
SM 38:4;O3__[M+H]__ 5.55			0.033
Mean ± Standard deviation	9,810,209.0 ± 4,787,322.9	11,919,226.0 ± 4,328,202.9	
Median and [25%; 75%]	8,532,309.0 [6,813,504.3; 11,720,988.0]	11,545,382.8 [9,233,654.9; 14,441,460.1]	
SM 38:5;O3__[M+H]__ 5.16			0.742
Mean ± Standard deviation	3,290,916.2 ± 5,608,441.5	843,215.8 ± 3,012,238.9	
Median and [25%; 75%]	38,617.0 [19,137.1; 7,416,856.0]	40,924.8 [29,402.8; 91,322.8]	
SM 38:6;O3__[M+H]__ 5.16			0.041
Mean ± Standard deviation	109,604.2 ± 104,255.8	190,910.4 ± 170,059.3	
Median and [25%; 75%]	80,391.0 [40,193.4; 150,242.8]	133,077.3 [77,467.8; 230,467.1]	
SM 38:7;O3__[M+H]__ 6.12			<0.001
Mean ± Standard deviation	1,637.0 ± 1,147.2	3,070.0 ± 1,371.9	
Median and [25%; 75%]	1,467.5 [826.5; 1,906.8]	2,693.0 [1,993.6; 3,986.3]	
SM 39:0;O2__[M+H]__ 6.69			<0.001
Mean ± Standard deviation	634,512.2 ± 262,584.2	1,266,582.3 ± 596,824.9	
Median and [25%; 75%]	588,854.0 [440,486.9; 756,226.8]	1,136,786.3 [798,205.1; 1,638,541.1]	
SM 39:1;O2__[M+H]__ 6.17			0.080
Mean ± Standard deviation	314,501.6 ± 228,839.0	566,141.8 ± 509,587.2	
Median and [25%; 75%]	249,531.0 [170,115.3; 384,187.9]	470,766.3 [213,305.0; 653,939.1]	
SM 39:1;O2 SM 16:1;O2/23:0__[M+H]__ 6.67			<0.001
Mean ± Standard deviation	12,967,136.9 ± 4,616,928.7	22,412,221.3 ± 9,690,495.2	
Median and [25%; 75%]	12,804,240.0 [9,003,652.5; 15,303,149.9]	20,021,757.0 [15,520,733.4; 28,645,105.9]	
SM 39:1;O3 OA1__[M+H]__ 5.81			<0.001
Mean ± Standard deviation	238,403.0 ± 113,805.3	426,866.1 ± 193,946.0	
Median and [25%; 75%]	221,370.0 [161,257.6; 299,231.1]	426,793.5 [284,501.2; 530,466.0]	
SM 39:1;O3 OA2__[M+H]__ 6.96			<0.001
Mean ± Standard deviation	24,964,175.1 ± 11,371,725.8	63,659,198.4 ± 68,301,256.2	
Median and [25%; 75%]	23,293,443.0 [17,047,558.8; 27,906,448.0]	52,371,159.0 [28,963,229.8; 64,018,176.3]	
SM 39:1;O3__[M+H]__ 6.26			<0.001

Mean ± Standard deviation	26,203,221.4 ± 11,034,976.3	63,627,143.9 ± 68,268,449.2	
Median and [25%; 75%]	24,407,255.0 [17,812,025.0; 29,335,594]	52,336,158.0 [28,946,188.6; 63,989,758.0]	
SM 39:2;O2__[M+H]__ 6.1			0.009
Mean ± Standard deviation	1,611,926.4 ± 625,346.2	2,658,567.9 ± 1,559,162.9	
Median and [25%; 75%]	1,619,947.0 [1,196,789.8; 2,018,823.4]	2,202,130.8 [1,611,420.6; 3,683,188.4]	
SM 39:3;O3__[M+H]__ 5.38			<0.001
Mean ± Standard deviation	99,805,332.5 ± 39,353,041.5	166,734,285.1 ± 46,025,263.7	
Median and [25%; 75%]	95,015,412.0 [71,572,352.0; 125,841,72]	165,268,656.0 [131,531,882.0; 192,977,300.0]	
SM 39:6;O2__[M+H]__ 5.67			<0.001
Mean ± Standard deviation	1,444,027.5 ± 564,979.5	2,466,766.5 ± 914,584.3	
Median and [25%; 75%]	1,491,969.5 [986,138.9; 1,838,014.8]	2,196,490.3 [1,736,842.1; 3,035,784.0]	
SM 39:8;O3__[M+H]__ 5.91			0.504
Mean ± Standard deviation	30,004.5 ± 18,269.9	31,545.4 ± 15,622.1	
Median and [25%; 75%]	26,833.5 [17,206.0; 38,670.0]	28,710.8 [23,146.8; 39,956.9]	
SM 39:9;O2__[M+H]__ 4.89			<0.001
Mean ± Standard deviation	990,728.2 ± 712,664.2	2,601,205.3 ± 1,427,069.9	
Median and [25%; 75%]	813,566.0 [477,366.5; 1,400,817.0]	2,305,304.8 [1,619,174.3; 3,091,284.3]	
SM 40:0;O2__[M+H]__ 6.96			<0.001
Mean ± Standard deviation	3,253,629.2 ± 1,287,333.0	5,569,803.3 ± 2,456,901.9	
Median and [25%; 75%]	2,905,528.5 [2,320,932.0; 3,884,317.0]	4,906,514.0 [4,057,608.0; 6,728,057.3]	
SM 40:1;O2__[M+H]__ 6.34			<0.001
Mean ± Standard deviation	2,819,796.7 ± 1,035,941.1	4,283,689.5 ± 1,438,942.0	
Median and [25%; 75%]	2,997,664.3 [1,984,348.0; 3,289,041.0]	4,251,268.5 [3,432,844.7; 5,047,426.8]	
SM 40:2;O2 SM 18:2;O2/22:0__[M+H]__ 6.4			<0.001
Mean ± Standard deviation	66,747,270.9 ± 14,997,889.8	93,249,803.1 ± 21,071,097.1	
Median and [25%; 75%]	66,993,604.0 [57,498,148.0; 76,036,844]	94,327,244.0 [79,595,968.0; 102,953,107.0]	
SM 40:2;O3 OA1__[M+H]__ 6.76			<0.001
Mean ± Standard deviation	439,603.7 ± 204,967.5	758,028.8 ± 258,063.4	
Median and [25%; 75%]	433,069.5 [297,657.5; 560,964.0]	715,777.3 [590,066.2; 846,084.9]	
SM 40:2;O3__[M+H]__ 6.09			<0.001
Mean ± Standard deviation	110,716.7 ± 69,740.4	345,062.9 ± 266,953.3	
Median and [25%; 75%]	98,700.5 [69,025.3; 128,627.1]	260,532.5 [140,351.1; 450,523.0]	
SM 40:4;O3 OA1__[M+H]__ 5.48			0.886
Mean ± Standard deviation	1,437,008.2 ± 1,395,142.5	1,313,937.9 ± 832,692.1	
Median and [25%; 75%]	956,143.0 [607,045.5; 1,592,722.6]	1,211,963.1 [580,145.4; 2,068,931.1]	
SM 40:4;O3__[M+H]__ 6.15			0.003

Mean ± Standard deviation	7,435,303.8 ± 2,666,046.7	10,521,647.8 ± 4,166,671.1	
Median and [25%; 75%]	7,217,689.0 [5,463,035.0; 8,835,245.4]	10,959,332.5 [8,858,403.4; 11,745,094.0]	
SM 40:5;O3__[M+H]__ 5.63			0.630
Mean ± Standard deviation	5,412,951.9 ± 3,175,064.6	5,129,037.6 ± 1,981,388.9	
Median and [25%; 75%]	4,488,478.5 [3,346,343.1; 5,992,375.3]	4,991,955.9 [3,996,555.4; 6,472,451.5]	
SM 40:6;O3__[M+H]__ 5.36			0.606
Mean ± Standard deviation	392,923.3 ± 277,971.1	470,414.0 ± 459,152.6	
Median and [25%; 75%]	326,768.0 [167,722.3; 575,434.8]	364,439.0 [221,687.4; 442,406.7]	
SM 40:8;O2__[M+H]__ 5.5			<0.001
Mean ± Standard deviation	1,571,789.7 ± 735,496.5	3,183,508.9 ± 1,902,087.2	
Median and [25%; 75%]	1,532,538.3 [1,058,440.3; 2,101,902.1]	2,644,514.5 [2,106,184.3; 3,624,388.4]	
SM 40:8;O3__[M+H]__ 6.28			0.001
Mean ± Standard deviation	19,078.5 ± 13,009.0	33,744.9 ± 19,642.9	
Median and [25%; 75%]	14,478.5 [8,974.3; 26,967.8]	28,790.0 [20,257.6; 44,684.4]	
SM 41:0;O2__[M+H]__ 7.34			<0.001
Mean ± Standard deviation	1,524,932.8 ± 444,466.9	2,584,468.8 ± 887,497.9	
Median and [25%; 75%]	1,543,226.5 [1,169,030.5; 1,893,248.0]	2,542,146.0 [1,921,745.1; 3,092,534.8]	
SM 41:1;O2 SM 18:1;O2/23:0__[M+H]__ 7.34			<0.001
Mean ± Standard deviation	36,088,916.8 ± 10,579,995.8	58,788,414.2 ± 20,672,869.5	
Median and [25%; 75%]	36,981,248.0 [26,899,687.3; 42,790,673.0]	51,388,561.0 [42,130,418.8; 78,611,765.0]	
SM 41:1;O3__[M+H]__ 7.72			<0.001
Mean ± Standard deviation	812,284.1 ± 424,317.5	1,400,696.9 ± 728,263.5	
Median and [25%; 75%]	752,421.0 [562,668.0; 1,038,718.1]	1,287,506.3 [831,918.3; 1,527,538.1]	
SM 41:2;O2 SM 17:1;O2/24:1__[M+H]__ 6.61			0.002
Mean ± Standard deviation	12,496,994.0 ± 4,222,508.8	16,797,244.6 ± 4,440,465.2	
Median and [25%; 75%]	11,676,689.0 [9,225,322.0; 15,283,602.0]	16,643,813.5 [13,067,464.6; 18,519,346.3]	
SM 41:2;O2 SM 18:2;O2/23:0__[M+H]__ 6.77			<0.001
Mean ± Standard deviation	19,331,495.4 ± 5,986,233.8	31,895,597.2 ± 11,320,133.9	
Median and [25%; 75%]	19,420,010.0 [15,269,673.0; 22,451,566.0]	28,812,158.0 [25,754,829.8; 36,169,190.8]	
SM 41:2;O3 OA1__[M+H]__ 6.96			0.021
Mean ± Standard deviation	3,110,836.9 ± 1,402,066.6	3,968,818.6 ± 1,130,925.9	
Median and [25%; 75%]	2,643,095.5 [2,069,404.8; 4,239,589.3]	3,682,500.0 [3,305,969.8; 4,315,310.1]	
SM 41:2;O3__[M+H]__ 7.73			0.001
Mean ± Standard deviation	6,156,327.4 ± 3,229,917.4	9,316,157.9 ± 3,272,875.9	
Median and [25%; 75%]	5,641,391.0 [4,588,905.8; 7,871,738.9]	8,907,130.0 [6,947,565.9; 11,442,655.6]	
SM 41:3;O2__[M+H]__ 6.06			0.001

Mean ± Standard deviation	5,588,870.1 ± 2,621,872.0	8,671,137.7 ± 3,027,772.1	
Median and [25%; 75%]	5,221,976.0 [3,680,448.0; 6,876,836.5]	8,459,090.3 [6,817,264.9; 10,635,317.9]	
SM 41:3;O3__[M+H]__ 5.94			0.003
Mean ± Standard deviation	34,509,757.6 ± 20,536,195.3	53,043,014.4 ± 26,613,245.0	
Median and [25%; 75%]	30,248,035.0 [18,994,939.0; 41,870,688]	46,006,211.0 [36,189,727.3; 61,923,946.5]	
SM 41:4;O3__[M+H]__ 5.75			0.846
Mean ± Standard deviation	112,326,016.1 ± 64,161,217.9	105,434,250.4 ± 55,852,641.7	
Median and [25%; 75%]	92,515,120.0 [65,698,995.0; 130,992,42]	100,958,244.0 [65,459,433.0; 157,746,856.0]	
SM 41:5;O3 OA1__[M+H]__ 5.34			0.080
Mean ± Standard deviation	11,679,298.3 ± 10,535,929.4	14,176,579.6 ± 7,268,311.8	
Median and [25%; 75%]	7,645,484.5 [4,794,393.3; 13,257,742.8]	14,101,207.5 [6,850,930.3; 21,381,241.3]	
SM 41:5;O3__[M+H]__ 5.18			0.002
Mean ± Standard deviation	4,537,074.4 ± 2,209,963.6	6,935,188.7 ± 2,979,076.6	
Median and [25%; 75%]	3,887,931.0 [2,890,689.8; 5,534,522.0]	6,189,574.0 [4,820,524.8; 8,469,103.5]	
SM 41:7;O2__[M+H]__ 5.81			<0.001
Mean ± Standard deviation	1,507,471.8 ± 712,543.0	2,721,702.9 ± 1,450,998.1	
Median and [25%; 75%]	1,451,955.0 [1,037,510.3; 1,838,995.8]	2,227,919.3 [1,675,118.1; 3,401,881.5]	
SM 41:8;O2__[M+H]__ 5.38			<0.001
Mean ± Standard deviation	675,392.7 ± 350,616.3	1,465,905.7 ± 513,831.1	
Median and [25%; 75%]	635,558.0 [359,894.4; 877,588.8]	1,269,715.6 [1,093,716.6; 1,899,640.4]	
SM 42:0;O2 SM 18:0;O2/24:0__[M+H]__ 7.72			<0.001
Mean ± Standard deviation	2,999,515.7 ± 972,608.5	4,566,128.2 ± 1,819,957.2	
Median and [25%; 75%]	2,897,405.5 [2,309,715.5; 3,561,107.3]	3,813,389.8 [3,278,080.3; 5,393,125.1]	
SM 42:1;O2__[M+H]__ 7.72			<0.001
Mean ± Standard deviation	63,825,763.3 ± 19,506,178.0	95,242,261.7 ± 32,895,236.0	
Median and [25%; 75%]	64,807,442.0 [48,170,230.0; 75,409,876]	93,296,114.0 [69,519,622.0; 110,559,075.0]	
SM 42:2;O2 SM 18:2;O2/24:0__[M+H]__ 7.15			<0.001
Mean ± Standard deviation	41,685,869.7 ± 13,744,955.4	56,321,874.1 ± 13,067,482.4	
Median and [25%; 75%]	42,333,530.0 [33,653,995.0; 50,345,720]	61,479,424.0 [47,073,022.5; 62,883,622.5]	
SM 42:3;O2 SM 18:2;O2/24:1__[M+H]__ 6.38			0.027
Mean ± Standard deviation	108,226,340.5 ± 24,617,319.5	127,872,871.9 ± 29,646,068.6	
Median and [25%; 75%]	108,011,176.0 [87,499,782.0; 123,680,0]	119,899,500.0 [105,077,593.5; 145,767,586.0]	
SM 42:4;O2__[M+H]__ 5.86			0.043
Mean ± Standard deviation	4,952,965.2 ± 2,271,716.4	3,951,488.1 ± 2,504,004.9	
Median and [25%; 75%]	4,591,045.0 [3,342,167.0; 6,422,705.3]	3,246,642.4 [2,778,269.8; 4,147,813.3]	
SM 42:4;O2 SM 18:2;O2/24:2__[M+H]__ 5.86			0.044

Mean ± Standard deviation	4,957,913.0 ± 2,284,479.9	3,953,501.1 ± 2,510,482.3	
Median and [25%; 75%]	4,591,045.0 [3,342,167.0; 6,422,705.3]	3,246,642.4 [2,778,269.8; 4,147,813.3]	
SM 42:4;O3__[M+H]__ 6.83			<0.001
Mean ± Standard deviation	612,247.5 ± 256,567.7	1,016,161.3 ± 526,344.5	
Median and [25%; 75%]	582,628.5 [449,926.0; 790,128.8]	973,645.8 [808,417.1; 1,175,092.6]	
SM 42:6;O3__[M+H]__ 5.91			0.899
Mean ± Standard deviation	377,739.0 ± 253,614.9	374,331.1 ± 229,408.9	
Median and [25%; 75%]	346,387.3 [165,511.0; 478,876.8]	284,513.6 [233,937.4; 474,944.6]	
SM 42:7;O3__[M+H]__ 5.45			0.899
Mean ± Standard deviation	354,137.0 ± 275,376.7	314,342.5 ± 237,963.0	
Median and [25%; 75%]	260,091.5 [137,302.3; 538,765.1]	229,091.8 [189,542.4; 325,443.1]	
SM 43:2;O2__[M+H]__ 7.2			0.015
Mean ± Standard deviation	3,469,205.5 ± 2,244,829.4	4,931,015.8 ± 1,934,465.2	
Median and [25%; 75%]	2,935,702.0 [1,738,134.8; 4,831,590.5]	4,965,501.5 [4,106,246.4; 6,314,240.1]	
SM 43:2;O2 SM 19:1;O2/24:1__[M+H]__ 7.2			0.015
Mean ± Standard deviation	3,496,423.1 ± 2,241,529.5	4,938,354.3 ± 1,941,839.1	
Median and [25%; 75%]	2,935,702.0 [1,738,134.8; 4,831,590.5]	4,965,501.5 [4,106,246.4; 6,314,240.1]	
SM 43:4;O3__[M+H]__ 6.12			0.034
Mean ± Standard deviation	1,476,185.4 ± 1,228,139.2	2,385,137.7 ± 1,757,967.6	
Median and [25%; 75%]	996,806.5 [655,686.5; 1,779,172.0]	2,305,679.5 [1,081,744.4; 2,829,143.3]	
SM 43:5;O3__[M+H]__ 5.71			0.006
Mean ± Standard deviation	403,036.0 ± 319,963.8	652,248.4 ± 395,451.1	
Median and [25%; 75%]	303,094.0 [207,804.0; 437,299.0]	485,957.3 [400,772.8; 994,116.5]	
SM 43:6;O3__[M+H]__ 5.57			0.188
Mean ± Standard deviation	31,675,051.7 ± 17,752,761.4	40,048,801.8 ± 22,315,708.5	
Median and [25%; 75%]	25,601,867.0 [18,106,586.5; 40,329,791]	36,386,294.0 [29,208,173.8; 49,808,975.0]	
SM 43:7;O3__[M+H]__ 5.15			0.219
Mean ± Standard deviation	735,381.3 ± 689,899.2	1,017,835.0 ± 1,017,205.3	
Median and [25%; 75%]	520,806.0 [284,414.8; 923,726.0]	864,583.5 [370,279.4; 1,192,425.6]	
SM 43:9;O2__[M+H]__ 5.95			<0.001
Mean ± Standard deviation	11,346,577.6 ± 5,401,544.7	18,396,034.6 ± 6,306,888.9	
Median and [25%; 75%]	10,099,151.0 [7,772,762.1; 15,541,908.3]	16,096,055.5 [13,817,598.9; 23,156,500.3]	
SM 44:5;O3__[M+H]__ 6.85			0.024
Mean ± Standard deviation	1,134,218.2 ± 506,699.5	1,644,382.2 ± 878,306.5	
Median and [25%; 75%]	1,083,841.5 [768,411.4; 1,391,336.4]	1,646,145.0 [1,024,636.0; 1,995,097.4]	
SM 44:6;O3__[M+H]__ 6.23			0.717

Mean ± Standard deviation	152,352.9 ± 109,119.6	161,303.9 ± 161,075.5	
Median and [25%; 75%]	137,300.3 [66,732.5; 202,573.0]	115,710.3 [61,208.6; 177,028.5]	
SM 46:6;O3__[M+H]__ 6.87			0.781
Mean ± Standard deviation	534,706.7 ± 494,392.6	571,081.0 ± 645,714.0	
Median and [25%; 75%]	316,192.0 [191,502.3; 757,084.5]	375,832.0 [250,894.3; 451,761.6]	
SM 47:4;O2__[M+H]__ 7.53			0.008
Mean ± Standard deviation	1,247,163.4 ± 621,454.8	1,919,282.5 ± 1,020,436.3	
Median and [25%; 75%]	1,145,900.5 [855,714.0; 1,391,484.6]	1,945,502.0 [1,217,252.9; 2,262,809.1]	
ST 27:1;O OA1__[M+H-H2O]__ 4.56			0.643
Mean ± Standard deviation	40,338,699.8 ± 12,610,448.2	38,660,908.5 ± 12,101,228.2	
Median and [25%; 75%]	39,059,964.0 [32,439,022.5; 49,002,896]	35,923,528.8 [32,273,526.8; 42,131,238.0]	
ST 27:1;O OA2__[M+H-H2O]__ 12.61			0.210
Mean ± Standard deviation	99,333,354.5 ± 17,645,064.5	90,323,254.9 ± 25,652,265.6	
Median and [25%; 75%]	95,629,716.0 [85,648,106.0; 114,371,130]	90,972,342.0 [76,327,897.5; 108,277,588.0]	
ST 27:1;O OA3__[M+H-H2O]__ 10.65			0.166
Mean ± Standard deviation	8,318,982.0 ± 13,729,367.7	7,988,797.2 ± 9,183,698.9	
Median and [25%; 75%]	3,075,249.0 [1,198,700.3; 7,697,709.8]	4,823,692.6 [3,174,148.4; 8,630,186.4]	
TG 40:0 TG 10:0_14:0_16:0__[M+NH4]__ 9.27			<0.001
Mean ± Standard deviation	47,601.1 ± 214,018.8	2,110,813.5 ± 5,714,322.0	
Median and [25%; 75%]	886.5 [394.5; 1,473.5]	55,376.3 [3,017.3; 1,023,338.1]	
TG 40:0 TG 12:0_12:0_16:0__[M+NH4]__ 9.25			<0.001
Mean ± Standard deviation	47,319.3 ± 208,135.7	2,113,103.7 ± 5,718,055.1	
Median and [25%; 75%]	1,610.0 [1,281.9; 2,395.5]	56,130.3 [3,743.3; 1,025,392.3]	
TG 40:0 TG 12:0_12:0_16:0__[M+Na]__ 9.25			<0.001
Mean ± Standard deviation	14,207.3 ± 58,860.0	350,453.2 ± 812,264.4	
Median and [25%; 75%]	1,169.0 [931.8; 2,106.5]	10,329.5 [2,472.1; 270,165.6]	
TG 40:1 TG 10:0_12:0_18:1__[M+NH4]__ 8.66			<0.001
Mean ± Standard deviation	3,435.6 ± 11,643.6	443,359.7 ± 826,152.9	
Median and [25%; 75%]	166.0 [62.3; 468.5]	18,033.1 [1,760.4; 377,607.1]	
TG 42:0 TG 12:0_14:0_16:0__[M+NH4]__ 9.99			<0.001
Mean ± Standard deviation	156,751.5 ± 699,439.0	3,319,925.2 ± 7,031,062.7	
Median and [25%; 75%]	6,198.0 [4,359.0; 8,087.5]	261,276.3 [26,511.9; 2,897,545.5]	
TG 42:0 TG 14:0_14:0_14:0__[M+Na]__ 10.0			<0.001
Mean ± Standard deviation	22,677.3 ± 107,593.3	333,446.9 ± 612,098.1	
Median and [25%; 75%]	464.0 [304.0; 891.8]	12,493.8 [1,480.9; 549,564.8]	
TG 42:1 TG 10:0_14:0_18:1__[M+NH4]__ 9.39			<0.001

Mean ± Standard deviation	67,453.9 ± 296,708.8	1,942,710.1 ± 3,750,306.4	
Median and [25%; 75%]	2,781.0 [1,203.0; 3,977.3]	255,936.3 [28,963.9; 1,608,085.9]	
TG 42:1 TG 12:0_12:0_18:1__[M+Na]__ 9.39			<0.001
Mean ± Standard deviation	17,695.5 ± 76,997.2	359,386.6 ± 641,245.1	
Median and [25%; 75%]	1,065.0 [401.0; 1,431.5]	42,912.3 [3,129.4; 423,319.6]	
TG 42:2 TG 10:0_14:0_18:2__[M+NH4]__ 8.74			<0.001
Mean ± Standard deviation	14,969.1 ± 53,029.7	621,042.3 ± 1,152,393.5	
Median and [25%; 75%]	332.5 [108.1; 711.5]	64,719.4 [9,308.4; 582,012.5]	
TG 44:2 TG 10:0_16:0_18:2__[M+NH4]__ 9.48			<0.001
Mean ± Standard deviation	5,161.5 ± 10,694.9	2,349,599.7 ± 3,782,790.8	
Median and [25%; 75%]	1,221.5 [272.8; 4,749.0]	441,881.4 [137,658.4; 2,908,338.8]	
TG 44:2 TG 10:0_16:0_18:2__[M+Na]__ 9.48			<0.001
Mean ± Standard deviation	1,755.1 ± 6,880.4	470,253.8 ± 685,285.1	
Median and [25%; 75%]	352.0 [96.4; 1,181.6]	116,456.0 [18,404.0; 817,690.4]	
TG 46:2 TG 12:0_16:0_18:2__[M+NH4]__ 10.21			<0.001
Mean ± Standard deviation	636,464.0 ± 1,951,756.0	11,259,240.0 ± 13,009,611.5	
Median and [25%; 75%]	113,588.0 [24,151.3; 443,400.5]	7,376,581.6 [3,681,563.3; 11,073,923.0]	
TG 46:3 TG 10:0_18:1_18:2__[M+NH4]__ 9.59			<0.001
Mean ± Standard deviation	83,203.9 ± 334,290.6	1,911,847.6 ± 2,631,227.5	
Median and [25%; 75%]	5,653.5 [937.0; 15,341.8]	750,397.5 [426,484.1; 2,301,025.0]	
TG 48:0 TG 16:0_16:0_16:0__[M+NH4]__ 11.56			<0.001
Mean ± Standard deviation	602,384.6 ± 740,166.0	4,700,214.0 ± 2,816,941.1	
Median and [25%; 75%]	402,585.0 [162,245.8; 674,660.8]	4,353,638.5 [2,880,972.6; 6,319,378.3]	
TG 48:1 TG 14:0_16:0_18:1__[M+NH4]__ 10.95			<0.001
Mean ± Standard deviation	419,891.2 ± 544,540.7	4,225,207.1 ± 3,100,244.1	
Median and [25%; 75%]	256,664.0 [87,586.5; 489,064.3]	3,591,902.5 [2,225,167.7; 4,966,081.6]	
TG 48:2 TG 12:0_18:1_18:1__[M+NH4]__ 10.31			<0.001
Mean ± Standard deviation	100,357.5 ± 192,576.1	1,315,667.3 ± 1,244,797.2	
Median and [25%; 75%]	49,715.5 [12,450.5; 106,674.0]	1,039,848.5 [625,142.3; 1,352,213.3]	
TG 48:2 TG 14:0_16:0_18:2__[M+NH4]__ 10.94			<0.001
Mean ± Standard deviation	9,137,310.4 ± 9,354,442.3	63,451,657.0 ± 38,463,027.2	
Median and [25%; 75%]	6,659,605.0 [2,889,618.0; 10,943,868.5]	60,207,725.0 [39,478,040.8; 73,837,799.0]	
TG 48:2 TG 16:0_16:1_16:1__[M+Na]__ 10.94			<0.001
Mean ± Standard deviation	202,247.4 ± 217,779.2	991,045.1 ± 642,196.4	
Median and [25%; 75%]	109,252.5 [71,033.3; 235,833.0]	725,240.8 [548,684.6; 1,423,504.1]	
TG 48:3 TG 12:0_18:1_18:2__[M+NH4]__ 10.3			<0.001

Mean ± Standard deviation	2,192,765.6 ± 3,266,143.1	19,517,042.3 ± 15,753,089.0	
Median and [25%; 75%]	1,202,668.5 [502,684.4; 2,719,719.3]	15,164,249.8 [11,054,203.7; 23,065,251.8]	
TG 48:3 TG 16:1_16:1_16:1__[M+Na]__10.29			<0.001
Mean ± Standard deviation	194,148.3 ± 269,567.6	1,249,793.4 ± 755,884.6	
Median and [25%; 75%]	92,776.0 [30,167.0; 255,851.0]	1,274,181.5 [759,977.7; 1,505,193.6]	
TG 48:4 TG 12:0_18:2_18:2__[M+NH4]__9.67			<0.001
Mean ± Standard deviation	197,705.6 ± 628,320.1	2,507,098.6 ± 3,427,578.2	
Median and [25%; 75%]	52,363.0 [8,672.5; 119,310.8]	1,229,213.0 [877,313.6; 1,885,097.1]	
TG 48:4 TG 12:0_18:2_18:2__[M+Na]__9.67			<0.001
Mean ± Standard deviation	43,557.8 ± 153,133.9	488,307.4 ± 582,043.7	
Median and [25%; 75%]	6,612.5 [2,124.0; 20,964.6]	295,266.0 [200,158.1; 419,646.6]	
TG 49:2 TG 15:0_16:0_18:2__[M+NH4]__11.27			<0.001
Mean ± Standard deviation	285,841.1 ± 314,036.7	3,292,605.8 ± 2,656,947.1	
Median and [25%; 75%]	155,409.0 [42,035.4; 456,427.8]	2,773,459.8 [1,498,373.5; 4,200,139.9]	
Mean ± Standard deviation			<0.001
Mean ± Standard deviation	80,012.9 ± 107,647.8	974,850.4 ± 838,843.2	
Median and [25%; 75%]	40,978.0 [11,442.4; 101,519.8]	720,563.5 [424,439.5; 1,216,000.6]	
TG 50:0 TG 16:0_16:0_18:0__[M+NH4]__12.6			0.075
Mean ± Standard deviation	2,668,716.7 ± 2,652,973.9	6,966,045.5 ± 6,727,723.7	
Median and [25%; 75%]	1,747,219.0 [1,122,597.8; 2,812,301.3]	6,406,088.0 [1,071,474.9; 9,764,162.6]	
TG 50:1 TG 16:0_16:0_18:1__[M+NH4]__11.66			<0.001
Mean ± Standard deviation	8,063,979.0 ± 5,218,346.6	26,652,084.3 ± 12,479,401.3	
Median and [25%; 75%]	6,673,906.5 [3,880,691.5; 11,990,288.0]	22,971,780.5 [18,688,192.2; 36,686,367.5]	
TG 50:2;O3 TG 16:0_18:2_16:0;O3__[M+NH4]__10.98			0.010
Mean ± Standard deviation	13,150,555.6 ± 6,818,423.5	51,977,750.0 ± 108,822,140.0	
Median and [25%; 75%]	12,536,113.0 [7,413,747.0; 17,228,955.5]	23,434,093.8 [12,546,171.9; 42,872,115.5]	
TG 50:2 TG 16:0_16:0_18:2__[M+NH4]__11.63			<0.001
Mean ± Standard deviation	104,622,081.1 ± 58,486,713.4	271,581,554.3 ± 79,977,139.6	
Median and [25%; 75%]	99,768,740.0 [53,270,043.0; 146,277,690.0]	276,440,726.0 [239,516,394.0; 334,922,528.0]	
TG 50:2 TG 16:0_16:0_18:2__[M+Na]__11.63			0.002
Mean ± Standard deviation	1,400,615.6 ± 601,980.7	2,068,854.3 ± 763,327.7	
Median and [25%; 75%]	1,275,177.5 [886,497.3; 1,820,555.8]	2,087,132.3 [1,336,829.6; 2,691,861.9]	
TG 50:2 TG 16:0_16:1_18:1__[M+NH4]__11.66			<0.001
Mean ± Standard deviation	105,015,733.7 ± 58,138,675.3	271,581,554.3 ± 79,977,139.6	
Median and [25%; 75%]	99,768,740.0 [54,794,914.0; 146,277,690.0]	276,440,726.0 [239,516,394.0; 334,922,528.0]	
TG 50:3 TG 16:0_16:1_18:2__[M+NH4]__11.04			<0.001

Mean ± Standard deviation	50,151,913.1 ± 32,784,701.6	168,537,749.9 ± 84,487,261.7	
Median and [25%; 75%]	40,419,409.0 [23,255,581.0; 64,944,815]	178,018,856.0 [100,680,353.0; 233,129,142.0]	
TG 50:3 TG 16:0_16:1_18:2__[M+Na]__ 11.04			<0.001
Mean ± Standard deviation	1,101,668.4 ± 342,482.2	1,821,644.6 ± 607,465.5	
Median and [25%; 75%]	1,129,501.5 [799,853.5; 1,359,560.0]	1,935,285.0 [1,353,396.4; 2,279,013.1]	
TG 50:4 TG 14:0_16:0_20:4__[M+NH4]__ 10.74			<0.001
Mean ± Standard deviation	10,895,642.8 ± 9,002,470.3	43,120,084.4 ± 21,464,564.9	
Median and [25%; 75%]	10,283,163.0 [4,180,598.5; 13,001,313.5]	43,504,275.0 [22,880,626.0; 61,362,113.5]	
TG 50:4 TG 14:0_18:2_18:2__[M+NH4]__ 10.4			<0.001
Mean ± Standard deviation	10,836,094.2 ± 8,943,467.3	43,136,844.0 ± 21,520,309.2	
Median and [25%; 75%]	10,202,310.0 [4,109,710.4; 13,002,587.9]	43,527,262.5 [22,885,139.8; 61,145,743.3]	
TG 50:4 TG 14:0_18:2_18:2__[M+Na]__ 10.4			<0.001
Mean ± Standard deviation	537,633.0 ± 458,854.8	1,758,972.1 ± 606,343.3	
Median and [25%; 75%]	402,129.5 [223,895.3; 684,037.0]	1,738,304.0 [1,507,971.0; 2,246,269.6]	
TG 50:4 TG 16:0_16:1_18:3__[M+NH4]__ 10.58			<0.001
Mean ± Standard deviation	10,734,477.7 ± 8,858,051.4	42,997,806.0 ± 21,358,726.9	
Median and [25%; 75%]	9,760,825.5 [4,183,686.3; 12,975,473.1]	43,560,652.5 [22,909,627.5; 58,709,091.5]	
TG 50:4 TG 16:1_16:1_18:2__[M+NH4]__ 10.25			<0.001
Mean ± Standard deviation	10,904,136.7 ± 9,005,946.9	43,228,175.9 ± 21,551,047.7	
Median and [25%; 75%]	10,283,375.5 [4,182,773.8; 13,006,725.5]	43,547,051.0 [22,903,207.3; 61,419,589.0]	
TG 50:5 TG 14:0_18:2_18:3__[M+NH4]__ 9.79			<0.001
Mean ± Standard deviation	180,886.4 ± 255,846.1	1,388,581.0 ± 927,431.7	
Median and [25%; 75%]	126,088.5 [22,504.3; 204,729.0]	1,018,093.8 [742,542.3; 1,766,277.0]	
TG 50:5 TG 14:1_18:2_18:2__[M+NH4]__ 9.95			<0.001
Mean ± Standard deviation	187,766.5 ± 232,707.2	1,475,847.0 ± 1,167,951.2	
Median and [25%; 75%]	127,149.0 [46,217.9; 195,455.5]	947,608.0 [566,517.4; 2,270,248.8]	
TG 50:5 TG 16:0_18:2_16:3__[M+NH4]__ 10.15			<0.001
Mean ± Standard deviation	99,318.5 ± 185,265.8	797,516.9 ± 962,423.4	
Median and [25%; 75%]	43,886.5 [14,884.3; 80,865.3]	487,875.8 [297,381.4; 900,540.1]	
TG 51:0 TG 17:0_17:0_17:0__[M+Na]__ 10.53			<0.001
Mean ± Standard deviation	10,602,979.6 ± 7,556,989.5	35,932,240.9 ± 40,517,603.3	
Median and [25%; 75%]	9,604,514.5 [5,009,672.3; 14,159,581.8]	24,641,843.3 [15,374,781.5; 37,380,385.8]	
TG 51:1 TG 16:0_17:0_18:1__[M+NH4]__ 12.49			<0.001
Mean ± Standard deviation	2,010,060.4 ± 1,042,466.9	7,930,386.4 ± 4,143,102.3	
Median and [25%; 75%]	2,001,133.8 [1,126,569.9; 2,492,371.3]	7,918,516.1 [4,659,777.3; 10,723,364.5]	
TG 51:3;O TG 18:1_18:1_15:1;O__[M+NH4]__ 11.76			<0.001

Mean ± Standard deviation	17,448,433.4 ± 9,445,512.2	29,821,247.5 ± 10,721,031.1	
Median and [25%; 75%]	14,851,895.0 [10,449,118.0; 23,313,742]	32,054,568.3 [23,075,374.0; 38,199,739.3]	
TG 51:3 TG 15:0_18:1_18:2__[M+NH4]__ 11.4			<0.001
Mean ± Standard deviation	3,654,737.9 ± 3,560,172.3	14,838,237.6 ± 8,913,024.4	
Median and [25%; 75%]	2,652,515.5 [556,766.0; 4,920,208.5]	13,179,344.5 [7,819,827.8; 19,760,559.1]	
TG 51:4 TG 15:0_18:2_18:2__[M+NH4]__ 10.75			<0.001
Mean ± Standard deviation	1,084,120.9 ± 1,197,779.1	3,246,155.9 ± 2,633,804.8	
Median and [25%; 75%]	758,488.5 [117,680.6; 1,707,077.5]	2,194,654.4 [1,432,006.8; 3,656,787.5]	
TG 51:5;O TG 16:1_18:2_17:2;O__[M+NH4]__ 10.52			<0.001
Mean ± Standard deviation	793,138.2 ± 619,176.1	2,714,915.7 ± 2,283,116.1	
Median and [25%; 75%]	669,049.5 [312,726.5; 1,082,370.1]	2,251,638.0 [1,928,289.9; 2,839,812.8]	
TG 51:5 TG 15:1_18:2_18:2__[M+NH4]__ 10.33			0.005
Mean ± Standard deviation	69,664.5 ± 151,139.7	281,500.7 ± 654,708.3	
Median and [25%; 75%]	29,192.0 [7,749.4; 77,747.3]	82,140.1 [50,325.6; 172,906.5]	
TG 52:1 TG 16:0_18:0_18:1__[M+NH4]__ 12.63			<0.001
Mean ± Standard deviation	20,535,367.6 ± 14,019,551.1	57,601,926.8 ± 16,480,149.1	
Median and [25%; 75%]	17,597,778.3 [8,475,424.3; 25,085,939.8]	59,995,019.0 [44,686,789.5; 70,654,839.5]	
TG 52:1 TG 17:0_17:0_18:1__[M+Na]__ 12.62			0.002
Mean ± Standard deviation	677,288.4 ± 313,702.5	1,002,508.4 ± 324,233.0	
Median and [25%; 75%]	650,492.0 [485,191.0; 811,220.3]	981,939.5 [800,537.4; 1,187,308.9]	
TG 52:2 TG 16:0_18:1_18:1__[M+NH4]__ 11.76			<0.001
Mean ± Standard deviation	57,697,961.1 ± 34,680,863.3	107,437,307.7 ± 49,268,773.2	
Median and [25%; 75%]	51,685,812.0 [28,768,385.3; 78,684,420]	107,951,953.0 [79,669,645.3; 134,807,551.0]	
TG 52:3;O2 TG 16:0_18:2_18:1;O2__[M+NH4]__ 7.97			<0.001
Mean ± Standard deviation	3,597.4 ± 7,524.9	353,191.7 ± 1,386,335.4	
Median and [25%; 75%]	1,572.0 [244.3; 3,225.6]	6,021.8 [3,723.9; 8,511.4]	
TG 52:3;O TG 16:0_18:1_18:2;O OA1__[M+NH4]__ 9.61			<0.001
Mean ± Standard deviation	4,269.2 ± 7,129.5	259,169.6 ± 712,012.2	
Median and [25%; 75%]	2,607.3 [907.3; 4,757.3]	65,350.8 [22,369.6; 156,848.1]	
TG 52:3;O TG 16:0_18:2_18:1;O__[M+NH4]__ 8.98			<0.001
Mean ± Standard deviation	4,727.6 ± 13,229.4	543,838.2 ± 2,142,038.4	
Median and [25%; 75%]	332.5 [163.8; 733.0]	4,019.0 [1,735.9; 14,024.8]	
TG 52:3 TG 16:0_18:1_18:2__[M+NH4]__ 11.81			<0.001
Mean ± Standard deviation	379,748,975.4 ± 138,864,551.5	570,476,725.0 ± 141,319,285.4	
Median and [25%; 75%]	352,559,632.0 [283,082,184.0; 482,591,000.0]	598,648,416.0 [488,812,536.0; 665,778,108.0]	
TG 52:4;O TG 16:0_18:1_18:3;O__[M+NH4]__ 9.19			<0.001

Mean ± Standard deviation	5,627.3 ± 8,406.7	862,422.9 ± 3,027,087.5	
Median and [25%; 75%]	2,901.5 [1,285.0; 6,151.3]	117,928.8 [12,152.4; 178,736.6]	
TG 52:4;O TG 16:0_18:2_18:2;O__[M+NH4]__ 9.0			<0.001
Mean ± Standard deviation	6,007.2 ± 8,840.8	860,864.2 ± 3,019,154.9	
Median and [25%; 75%]	2,993.3 [1,297.8; 6,573.4]	117,959.5 [12,176.1; 182,339.5]	
TG 52:4;O TG 18:2_18:2_16:0;O__[M+NH4]__ 8.61			<0.001
Mean ± Standard deviation	1,844.2 ± 7,317.0	1,030,114.1 ± 4,100,220.1	
Median and [25%; 75%]	122.3 [38.1; 336.5]	2,016.0 [903.5; 6,555.0]	
TG 52:4 TG 16:0_16:0_20:4__[M+NH4]__ 11.49			<0.001
Mean ± Standard deviation	292,713,270.2 ± 151,777,976.7	450,644,436.3 ± 169,971,782.6	
Median and [25%; 75%]	301,848,144.0 [171,073,560.0; 422,347,	478,282,052.0 [397,461,544.0; 574,022,534.0]	
TG 52:4 TG 16:0_18:2_18:2__[M+NH4]__ 11.04			0.001
Mean ± Standard deviation	287,887,712.0 ± 154,294,226.5	439,176,095.8 ± 170,177,274.3	
Median and [25%; 75%]	297,898,464.0 [144,981,873.5; 419,208,	469,748,544.0 [360,833,500.0; 573,245,838.0]	
TG 52:4 TG 16:0_18:2_18:2__[M+Na]__ 11.04			0.455
Mean ± Standard deviation	4,303,255.2 ± 1,171,396.5	4,589,640.2 ± 1,330,263.8	
Median and [25%; 75%]	3,957,645.0 [3,460,925.3; 5,015,977.0]	4,709,954.5 [3,417,601.3; 5,688,397.4]	
TG 52:4 TG 16:1_18:1_18:2__[M+NH4]__ 10.52			<0.001
Mean ± Standard deviation	2,169,387.4 ± 1,542,327.8	6,903,791.8 ± 7,588,125.9	
Median and [25%; 75%]	1,765,396.0 [962,797.3; 3,012,827.6]	4,755,021.5 [2,803,593.6; 7,670,846.3]	
TG 52:5 TG 16:0_16:1_20:4__[M+NH4]__ 10.88			<0.001
Mean ± Standard deviation	32,224,758.1 ± 20,251,943.0	88,271,504.2 ± 69,433,551.6	
Median and [25%; 75%]	29,787,649.0 [16,794,656.5; 41,744,048	72,780,000.0 [55,064,416.0; 109,746,787.0]	
TG 52:5 TG 16:0_18:1_18:4__[M+Na]__ 10.71			<0.001
Mean ± Standard deviation	1,651,156.0 ± 690,116.4	2,188,159.3 ± 437,136.9	
Median and [25%; 75%]	1,547,675.5 [1,279,698.9; 2,027,577.3]	2,194,851.3 [1,866,561.5; 2,504,496.8]	
TG 52:5 TG 16:0_18:2_18:3__[M+NH4]__ 10.7			0.014
Mean ± Standard deviation	20,092,993.6 ± 17,777,240.7	49,245,736.0 ± 70,973,884.4	
Median and [25%; 75%]	11,826,964.5 [6,606,855.6; 32,008,879.0]	25,007,414.5 [15,071,221.7; 43,908,448.0]	
TG 52:5 TG 16:1_18:2_18:2__[M+NH4]__ 10.52			<0.001
Mean ± Standard deviation	24,833,327.1 ± 16,758,700.1	70,550,136.5 ± 71,210,543.0	
Median and [25%; 75%]	23,352,363.0 [10,127,764.4; 37,620,905	48,370,638.0 [33,264,852.8; 70,678,864.5]	
TG 52:5 TG 16:1_18:2_18:2__[M+Na]__ 10.52			0.001
Mean ± Standard deviation	1,605,634.5 ± 655,140.5	2,146,885.5 ± 461,765.3	
Median and [25%; 75%]	1,569,508.5 [1,342,561.8; 2,074,370.3]	2,239,427.3 [1,735,612.6; 2,501,633.9]	
TG 52:6 TG 16:1_16:1_20:4__[M+NH4]__ 10.25			<0.001

Mean ± Standard deviation	952,703.7 ± 1,369,622.9	4,574,605.3 ± 6,112,530.7	
Median and [25%; 75%]	631,326.5 [298,729.9; 961,607.0]	2,234,880.3 [1,515,006.6; 3,628,273.6]	
TG 52:6 TG 16:1_18:2_18:3 OA1__[M+NH4]__ 9.94			0.001
Mean ± Standard deviation	965,605.7 ± 1,082,679.2	4,623,287.6 ± 6,185,194.5	
Median and [25%; 75%]	637,585.5 [208,753.8; 1,199,695.3]	2,376,195.3 [832,326.6; 4,737,778.6]	
TG 52:6 TG 16:1_18:2_18:3__[M+NH4]__ 10.11			0.002
Mean ± Standard deviation	1,090,327.3 ± 1,459,221.0	4,445,013.8 ± 6,199,989.6	
Median and [25%; 75%]	662,566.0 [267,069.8; 1,254,079.4]	2,208,151.8 [904,147.1; 3,737,039.8]	
TG 53:2;O2 TG 16:0_18:1_19:1;O2__[M+NH4]__ 11.25			0.260
Mean ± Standard deviation	7,313,450.5 ± 8,954,234.5	8,884,204.4 ± 7,066,261.8	
Median and [25%; 75%]	4,280,727.5 [2,309,915.5; 8,602,669.5]	8,519,609.5 [3,374,617.0; 13,016,363.6]	
TG 53:2;O2 TG 16:0_18:2_19:0;O2__[M+NH4]__ 10.92			0.606
Mean ± Standard deviation	4,915,774.9 ± 5,275,571.5	5,792,353.7 ± 5,151,661.4	
Median and [25%; 75%]	3,014,978.5 [1,832,532.5; 5,917,396.8]	4,427,265.4 [888,506.0; 8,539,943.9]	
TG 53:2 TG 17:0_18:1_18:1__[M+NH4]__ 12.53			<0.001
Mean ± Standard deviation	5,460,753.3 ± 2,599,758.7	13,757,084.5 ± 5,007,321.4	
Median and [25%; 75%]	5,552,870.0 [3,759,244.8; 7,043,978.0]	13,378,921.4 [10,778,266.3; 17,999,478.0]	
TG 53:2 TG 17:0_18:1_18:1__[M+Na]__ 12.53			<0.001
Mean ± Standard deviation	375,746.8 ± 240,918.2	624,228.6 ± 240,654.3	
Median and [25%; 75%]	374,768.3 [164,343.3; 523,992.1]	689,346.8 [543,483.9; 781,090.6]	
TG 53:3;O2 TG 16:0_18:2_19:1;O2__[M+NH4]__ 10.65			0.365
Mean ± Standard deviation	14,924,399.5 ± 16,562,165.3	16,498,451.5 ± 12,567,641.8	
Median and [25%; 75%]	8,615,775.0 [5,040,806.8; 17,974,544.6]	14,951,992.8 [8,003,321.4; 24,475,328.5]	
TG 53:3 TG 17:0_18:1_18:2__[M+NH4]__ 12.11			<0.001
Mean ± Standard deviation	6,790,275.0 ± 4,932,455.5	18,711,989.9 ± 10,077,071.1	
Median and [25%; 75%]	6,469,220.8 [2,335,852.8; 9,773,615.3]	17,783,424.5 [12,350,926.8; 22,784,404.3]	
TG 53:4 TG 17:1_18:1_18:2__[M+NH4]__ 11.5			<0.001
Mean ± Standard deviation	3,167,920.2 ± 2,374,703.1	7,346,134.7 ± 4,171,942.0	
Median and [25%; 75%]	2,898,263.5 [1,401,293.4; 4,164,538.3]	6,294,728.3 [4,405,961.4; 10,113,568.6]	
TG 53:5 TG 17:1_18:2_18:2__[M+NH4]__ 10.91			<0.001
Mean ± Standard deviation	139,547.8 ± 163,008.0	886,636.8 ± 1,814,024.1	
Median and [25%; 75%]	78,788.0 [26,697.0; 203,654.3]	337,345.9 [212,191.5; 647,558.6]	
TG 53:6;O TG 18:2_18:2_17:2;O__[M+NH4]__ 10.62			0.066
Mean ± Standard deviation	1,365,351.2 ± 1,463,099.2	6,046,211.5 ± 13,105,320.9	
Median and [25%; 75%]	1,251,166.8 [361,837.4; 1,797,806.0]	1,479,063.3 [903,949.6; 4,090,744.4]	
TG 54:1 TG 18:0_18:0_18:1 OA1__[M+NH4]__ 12.81			<0.001

Mean ± Standard deviation	2,632,743.6 ± 3,509,241.8	7,738,614.0 ± 4,028,666.0	
Median and [25%; 75%]	2,092,431.8 [1,138,968.4; 2,781,201.5]	6,856,151.3 [4,887,805.2; 8,975,457.9]	
TG 54:1 TG 18:0_18:0_18:1__[M+NH4]__12.81			<0.001
Mean ± Standard deviation	2,725,289.2 ± 1,637,178.1	5,704,722.0 ± 2,088,827.7	
Median and [25%; 75%]	2,607,383.5 [1,818,350.3; 3,191,748.8]	5,633,564.6 [4,059,037.8; 7,451,934.8]	
TG 54:2 TG 18:0_18:1_18:1__[M+NH4]__12.66			<0.001
Mean ± Standard deviation	26,085,693.3 ± 16,186,328.5	60,422,733.0 ± 21,043,845.9	
Median and [25%; 75%]	25,156,769.0 [15,486,529.3; 31,493,137]	58,463,538.5 [42,804,322.8; 79,756,708.0]	
TG 54:2 TG 18:0_18:1_18:1__[M+Na]__12.66			0.248
Mean ± Standard deviation	772,113.5 ± 323,748.4	869,027.3 ± 264,162.0	
Median and [25%; 75%]	799,856.0 [501,886.5; 945,405.9]	871,463.8 [759,065.6; 1,038,218.6]	
TG 54:3 TG 18:0_18:1_18:2_OA1__[M+NH4]__11.88			<0.001
Mean ± Standard deviation	13,546,590.1 ± 9,501,022.8	34,308,379.8 ± 32,427,568.9	
Median and [25%; 75%]	10,427,878.0 [6,988,038.1; 17,079,294.3]	23,681,981.0 [17,520,735.1; 39,202,550.5]	
TG 54:3 TG 18:0_18:1_18:2__[M+NH4]__12.41			<0.001
Mean ± Standard deviation	88,553,338.9 ± 40,014,098.2	172,556,439.0 ± 59,742,922.1	
Median and [25%; 75%]	79,885,284.0 [62,720,728.5; 109,577,54]	163,067,340.0 [136,626,014.0; 203,247,150.0]	
TG 54:3 TG 18:1_18:1_18:1__[M+Na]__12.43			0.003
Mean ± Standard deviation	1,076,564.7 ± 597,062.1	1,646,399.5 ± 695,589.2	
Median and [25%; 75%]	1,065,683.5 [612,739.6; 1,366,035.5]	1,579,812.8 [1,263,435.7; 1,863,628.4]	
TG 54:4 TG 16:0_18:1_20:3__[M+NH4]__12.17			<0.001
Mean ± Standard deviation	134,466,530.1 ± 69,980,702.5	260,157,207.8 ± 128,336,551.8	
Median and [25%; 75%]	127,212,406.0 [86,084,002.0; 183,808,7]	242,396,912.0 [192,909,196.0; 316,844,036.0]	
TG 54:4 TG 18:1_18:1_18:2__[M+NH4]__11.86			<0.001
Mean ± Standard deviation	130,603,463.5 ± 71,782,131.3	261,279,858.5 ± 132,885,173.3	
Median and [25%; 75%]	120,999,348.0 [83,407,435.0; 180,667,2]	242,401,058.0 [193,486,039.0; 319,209,304.0]	
TG 54:4 TG 18:1_18:1_18:2__[M+Na]__11.86			0.298
Mean ± Standard deviation	2,130,258.7 ± 939,705.7	2,548,665.8 ± 1,277,261.2	
Median and [25%; 75%]	2,291,313.0 [1,229,559.5; 2,714,202.0]	2,470,889.9 [1,656,924.8; 2,947,887.9]	
TG 54:5;O3 TG 18:1_20:4_16:0;O3__[M+NH4]__10.92			0.873
Mean ± Standard deviation	3,177,434.8 ± 3,206,135.4	2,766,020.9 ± 2,362,079.9	
Median and [25%; 75%]	2,070,537.0 [875,811.0; 4,058,836.3]	2,432,761.0 [1,034,910.1; 4,673,274.8]	
TG 54:5 TG 16:0_18:1_20:4__[M+NH4]__11.6			0.041
Mean ± Standard deviation	26,734,101.8 ± 14,841,848.4	89,491,281.3 ± 202,264,824.0	
Median and [25%; 75%]	23,486,579.0 [17,718,747.8; 30,737,531]	40,270,238.5 [25,120,346.0; 56,597,392.0]	
TG 54:5 TG 18:1_18:2_18:2__[M+NH4]__11.25			<0.001

Mean ± Standard deviation	64,963,595.6 ± 56,986,179.0	182,502,703.0 ± 202,590,590.0	
Median and [25%; 75%]	44,273,513.0 [22,483,293.5; 87,602,888	112,809,392.0 [73,535,326.5; 207,316,254.0]	
TG 54:5 TG 18:1_18:2_18:2__[M+Na]__11.25			0.232
Mean ± Standard deviation	634,815.7 ± 425,629.2	1,294,936.0 ± 1,920,558.0	
Median and [25%; 75%]	534,986.8 [384,774.8; 823,943.0]	673,052.3 [462,610.9; 921,443.5]	
TG 54:6 TG 16:0_18:2_20:4__[M+NH4]__10.85			0.024
Mean ± Standard deviation	25,444,586.4 ± 16,332,245.1	124,280,731.3 ± 261,989,963.4	
Median and [25%; 75%]	21,891,373.0 [12,283,444.6; 37,662,292	39,632,000.3 [22,551,933.0; 77,370,983.0]	
TG 54:6 TG 18:2_18:2_18:2__[M+NH4]__10.62			0.005
Mean ± Standard deviation	27,142,872.0 ± 26,649,450.3	135,286,315.2 ± 266,121,297.9	
Median and [25%; 75%]	16,514,663.0 [8,766,022.0; 40,975,994.0]	42,177,726.0 [26,312,433.9; 79,211,799.0]	
TG 54:7;O2 TG 18:2_18:3_18:2;O2__[M+NH4]__6.64			0.014
Mean ± Standard deviation	2,506.5 ± 10,404.1	134,580.8 ± 513,773.9	
Median and [25%; 75%]	18.0 [0.0; 60.0]	146.3 [22.9; 516.0]	
TG 54:7;O TG 18:2_18:2_18:3;O__[M+NH4]__7.96			0.007
Mean ± Standard deviation	2,458.0 ± 9,788.5	1,758,157.9 ± 6,969,907.2	
Median and [25%; 75%]	77.8 [30.0; 198.0]	222.0 [82.8; 16,046.5]	
TG 54:7;O TG 18:3_18:3_18:1;O__[M+NH4]__7.62			0.096
Mean ± Standard deviation	1,330.5 ± 7,455.3	669,078.0 ± 2,576,368.6	
Median and [25%; 75%]	61.0 [31.0; 112.0]	96.0 [57.4; 1,878.0]	
TG 54:7 TG 18:2_18:2_18:3__[M+NH4]__10.17			0.339
Mean ± Standard deviation	7,404,546.8 ± 12,087,890.1	50,296,565.3 ± 145,836,347.7	
Median and [25%; 75%]	1,457,783.0 [698,080.5; 9,114,838.1]	2,817,490.3 [766,150.6; 17,089,182.8]	
TG 54:8 TG 14:0_18:2_22:6__[M+NH4]__9.9			<0.001
Mean ± Standard deviation	217,507.0 ± 324,761.1	958,226.7 ± 604,981.9	
Median and [25%; 75%]	52,652.3 [2,476.8; 279,696.3]	906,713.0 [653,333.5; 1,158,371.6]	
TG 55:2 TG 18:0_18:1_19:1__[M+NH4]__12.76			<0.001
Mean ± Standard deviation	113,660.7 ± 60,571.5	378,342.4 ± 168,178.8	
Median and [25%; 75%]	111,244.5 [68,200.9; 153,785.4]	353,866.5 [272,989.9; 511,074.9]	
TG 55:3 TG 18:1_18:1_19:1__[M+NH4]__12.57			<0.001
Mean ± Standard deviation	206,100.9 ± 109,920.3	475,632.4 ± 140,025.6	
Median and [25%; 75%]	199,622.5 [121,722.4; 283,483.3]	459,935.0 [382,511.3; 577,861.0]	
TG 55:4;O2 TG 18:1_18:2_19:1;O2__[M+NH4]__10.73			0.537
Mean ± Standard deviation	3,359,430.3 ± 4,136,436.0	2,434,303.6 ± 2,418,446.7	
Median and [25%; 75%]	1,802,112.5 [748,419.8; 4,945,564.4]	1,949,191.9 [701,033.5; 3,582,210.8]	
TG 55:5;O2 TG 18:2_18:2_19:1;O2__[M+NH4]__10.27			0.087

Mean ± Standard deviation	739,978.0 ± 890,433.2	578,189.6 ± 906,972.4	
Median and [25%; 75%]	396,975.5 [211,095.0; 755,523.0]	199,540.6 [49,745.4; 643,174.4]	
TG 56:2 TG 20:0_18:1_18:1__[M+NH4]__12.83			<0.001
Mean ± Standard deviation	997,177.5 ± 1,244,907.5	2,763,471.4 ± 2,061,221.3	
Median and [25%; 75%]	731,327.0 [343,037.8; 1,123,669.8]	2,535,350.0 [1,570,092.9; 3,463,429.0]	
TG 56:3 TG 18:1_18:1_20:1__[M+NH4]__12.69			<0.001
Mean ± Standard deviation	1,272,720.6 ± 677,102.3	2,889,868.0 ± 1,988,221.9	
Median and [25%; 75%]	1,198,383.0 [771,373.0; 1,716,876.0]	2,184,950.0 [1,652,340.3; 3,346,815.3]	
TG 56:3 TG 20:0_18:1_18:2__[M+NH4]__12.7			<0.001
Mean ± Standard deviation	1,261,963.7 ± 667,654.4	2,889,727.0 ± 1,988,219.3	
Median and [25%; 75%]	1,204,047.5 [771,373.0; 1,625,785.8]	2,184,950.0 [1,652,340.3; 3,346,815.3]	
TG 56:4 TG 18:1_20:1_18:2__[M+NH4]__12.46			0.011
Mean ± Standard deviation	2,027,963.3 ± 1,140,789.6	3,844,168.3 ± 2,964,131.9	
Median and [25%; 75%]	1,874,486.0 [1,077,443.5; 2,751,958.3]	3,154,658.0 [1,979,677.3; 4,530,169.4]	
TG 56:5 TG 16:0_18:1_22:4__[M+NH4]__12.02			0.008
Mean ± Standard deviation	4,943,970.7 ± 4,386,993.7	9,469,883.1 ± 5,773,493.4	
Median and [25%; 75%]	3,544,709.5 [987,596.9; 8,272,559.3]	10,238,061.6 [5,645,889.4; 12,265,191.4]	
TG 56:5 TG 18:0_18:1_20:4__[M+NH4]__12.29			0.075
Mean ± Standard deviation	5,537,766.8 ± 3,792,784.5	3,808,438.0 ± 3,658,793.6	
Median and [25%; 75%]	4,285,719.0 [2,940,232.1; 8,502,774.8]	2,831,719.8 [1,082,574.3; 5,170,916.4]	
TG 56:6 TG 16:0_18:1_22:5__[M+NH4]__11.51			0.246
Mean ± Standard deviation	15,032,544.9 ± 10,809,977.6	20,080,231.0 ± 13,523,720.7	
Median and [25%; 75%]	12,814,504.5 [7,300,117.6; 19,559,451.5]	18,510,922.0 [10,249,000.0; 33,471,281.9]	
TG 56:6 TG 18:1_18:1_20:4__[M+NH4]__11.7			0.194
Mean ± Standard deviation	9,164,760.5 ± 5,283,913.5	6,997,164.9 ± 4,675,244.0	
Median and [25%; 75%]	8,040,809.5 [5,664,382.4; 11,330,730.5]	6,752,443.4 [4,238,154.1; 8,935,721.8]	
TG 56:7 TG 16:0_18:1_22:6__[M+NH4]__11.25			0.084
Mean ± Standard deviation	9,252,090.7 ± 12,187,929.1	13,947,827.9 ± 10,992,697.1	
Median and [25%; 75%]	5,798,930.0 [2,696,194.3; 9,891,152.6]	12,546,824.3 [4,389,708.8; 20,485,361.5]	
TG 56:7 TG 16:0_18:2_22:5__[M+NH4]__10.94			0.679
Mean ± Standard deviation	7,172,164.5 ± 4,631,592.2	8,664,835.4 ± 7,359,797.8	
Median and [25%; 75%]	5,867,862.5 [4,138,766.3; 10,042,375.8]	6,645,319.8 [2,017,420.5; 13,576,497.8]	
TG 56:8 TG 16:0_18:2_22:6__[M+NH4]__10.64			0.267
Mean ± Standard deviation	18,219,125.7 ± 17,783,240.3	22,301,239.8 ± 16,713,012.9	
Median and [25%; 75%]	13,055,680.5 [5,719,488.8; 21,379,836.0]	20,212,052.5 [11,339,740.1; 28,948,365.9]	
TG 56:8 TG 16:0_18:2_22:6__[M+Na]__10.64			0.161

Mean ± Standard deviation	568,980.4 ± 466,616.4	405,582.1 ± 394,541.3	
Median and [25%; 75%]	453,222.0 [237,186.8; 721,458.4]	323,422.0 [96,772.2; 574,803.9]	
TG 56:8 TG 18:2_18:2_20:4__[M+NH4]__10.27			0.432
Mean ± Standard deviation	5,917,459.3 ± 3,883,223.8	4,873,638.7 ± 3,522,256.8	
Median and [25%; 75%]	4,911,318.5 [3,148,626.3; 7,942,472.0]	4,704,921.6 [2,712,887.8; 6,365,470.6]	
TG 56:9 TG 16:1_18:2_22:6__[M+NH4]__10.03			0.704
Mean ± Standard deviation	1,224,215.7 ± 1,288,567.4	1,289,998.5 ± 992,564.4	
Median and [25%; 75%]	1,032,223.5 [396,269.9; 1,498,489.3]	1,152,958.5 [578,098.0; 2,056,771.1]	
TG 56:9 TG 18:2_18:2_20:5__[M+NH4]__9.85			0.717
Mean ± Standard deviation	489,032.0 ± 558,350.8	538,615.3 ± 495,606.1	
Median and [25%; 75%]	329,968.5 [130,924.5; 603,297.0]	396,269.0 [170,750.6; 796,654.6]	
TG 57:6;O2 TG 18:1_20:4_19:1;O2__[M+NH4]__10.55			0.059
Mean ± Standard deviation	134,634.9 ± 233,361.8	55,423.9 ± 82,200.7	
Median and [25%; 75%]	43,916.0 [17,055.3; 138,103.8]	17,942.0 [10,839.9; 64,093.0]	
TG 58:1 TG 16:0_24:0_18:1__[M+NH4]__13.03			0.001
Mean ± Standard deviation	307,059.6 ± 698,130.2	366,751.5 ± 218,248.9	
Median and [25%; 75%]	162,269.0 [125,996.9; 242,834.3]	290,967.8 [228,925.5; 463,515.3]	
TG 58:2 TG 22:0_18:1_18:1__[M+NH4]__12.95			<0.001
Mean ± Standard deviation	352,948.3 ± 692,256.2	887,212.9 ± 1,092,822.6	
Median and [25%; 75%]	152,332.5 [88,297.3; 375,586.1]	648,201.3 [414,479.8; 874,109.9]	
TG 58:3 TG 22:0_18:1_18:2__[M+NH4]__12.86			<0.001
Mean ± Standard deviation	220,963.9 ± 262,461.6	872,957.1 ± 1,507,867.7	
Median and [25%; 75%]	137,977.5 [55,030.4; 231,540.3]	301,004.0 [203,540.3; 732,936.5]	
TG 58:4 TG 22:0_18:2_18:2__[M+NH4]__12.74			0.030
Mean ± Standard deviation	139,224.6 ± 188,740.6	870,681.3 ± 2,192,411.8	
Median and [25%; 75%]	71,164.0 [30,794.1; 152,169.9]	133,802.0 [80,905.6; 426,835.1]	
TG 58:5 TG 18:0_18:1_22:4__[M+NH4]__12.53			0.050
Mean ± Standard deviation	128,961.6 ± 76,542.3	317,818.4 ± 417,270.9	
Median and [25%; 75%]	115,918.8 [80,005.8; 180,434.3]	254,280.1 [79,618.6; 340,386.9]	
TG 58:6 TG 18:1_18:1_22:4__[M+NH4]__12.18			0.141
Mean ± Standard deviation	250,069.1 ± 190,578.5	380,321.2 ± 279,541.8	
Median and [25%; 75%]	205,572.5 [132,543.3; 299,996.0]	374,541.8 [177,246.0; 591,977.9]	
TG 58:7 TG 18:1_18:1_22:5 OA1__[M+NH4]__11.59			0.595
Mean ± Standard deviation	457,618.0 ± 428,592.0	356,412.3 ± 283,778.8	
Median and [25%; 75%]	334,642.0 [176,260.8; 600,239.8]	381,184.3 [87,468.1; 564,546.6]	
TG 58:7 TG 18:1_18:1_22:5__[M+NH4]__11.97			0.606

Mean ± Standard deviation	511,161.1 ± 434,735.3	599,746.2 ± 493,943.8	
Median and [25%; 75%]	385,339.0 [220,618.4; 654,978.8]	443,778.3 [184,293.0; 988,481.8]	
TG 58:8 TG 18:1_18:1_22:6__ [M+NH4]__ 11.38			0.232
Mean ± Standard deviation	993,567.7 ± 1,496,138.7	1,508,655.9 ± 1,671,915.8	
Median and [25%; 75%]	263,784.8 [151,979.3; 928,712.0]	891,157.0 [272,169.5; 2,500,454.6]	
TG 58:9 TG 18:1_18:2_22:6__ [M+NH4]__ 10.74			0.873
Mean ± Standard deviation	3,522,416.2 ± 4,138,343.1	3,742,127.3 ± 3,693,521.6	
Median and [25%; 75%]	2,192,622.5 [1,030,765.4; 4,145,719.4]	2,498,354.6 [1,359,370.9; 5,961,210.4]	
TG 58:9 TG 18:1_20:4_20:4__ [M+NH4]__ 10.55			0.667
Mean ± Standard deviation	4,574,859.5 ± 4,939,444.4	3,898,425.3 ± 3,643,116.4	
Median and [25%; 75%]	3,265,457.0 [1,216,134.3; 5,982,235.0]	3,532,659.5 [1,441,657.8; 6,019,797.7]	
TG 60:12 TG 16:0_22:6_22:6__ [M+NH4]__ 10.14			0.374
Mean ± Standard deviation	360,742.4 ± 1,009,779.0	132,867.5 ± 190,689.2	
Median and [25%; 75%]	63,122.5 [9,757.3; 269,853.4]	27,117.8 [4,289.4; 172,722.6]	
TG 60:3 TG 24:0_18:1_18:2__ [M+NH4]__ 12.96			<0.001
Mean ± Standard deviation	58,230.5 ± 65,615.0	158,134.7 ± 180,070.7	
Median and [25%; 75%]	34,038.5 [12,863.5; 82,766.8]	119,003.0 [74,107.1; 147,457.8]	
TG O-34:1 TG O-14:1_10:0_10:0__ [M+Na]__ 5.89			0.913
Mean ± Standard deviation	498,192.3 ± 904,797.6	1,020,132.0 ± 2,886,736.7	
Median and [25%; 75%]	68,657.0 [10,285.9; 521,794.3]	59,253.3 [12,416.8; 210,558.6]	
TG O-43:1 TG O-19:1_12:0_12:0__ [M+NH4]__ 9.35			<0.001
Mean ± Standard deviation	8,548.5 ± 37,580.8	406,065.9 ± 880,700.4	
Median and [25%; 75%]	289.8 [80.5; 552.1]	22,439.3 [2,961.4; 252,493.3]	
TG O-50:2 TG O-19:2_15:0_16:0__ [M+NH4]__ 11.28			<0.001
Mean ± Standard deviation	33,584.1 ± 28,589.6	392,580.6 ± 427,370.4	
Median and [25%; 75%]	26,529.5 [13,019.0; 46,434.6]	255,635.3 [134,698.9; 366,608.3]	
TG O-51:0 TG O-19:0_16:0_16:0__ [M+NH4]__ 12.59			0.119
Mean ± Standard deviation	768,301.7 ± 741,567.4	1,963,408.2 ± 1,813,946.2	
Median and [25%; 75%]	590,488.5 [346,224.3; 832,511.4]	1,674,022.0 [341,598.1; 3,443,710.8]	
TG O-51:1 TG O-19:1_16:0_16:0__ [M+NH4]__ 12.26			<0.001
Mean ± Standard deviation	26,461,247.9 ± 19,603,844.0	82,406,104.8 ± 38,998,797.8	
Median and [25%; 75%]	24,278,224.0 [10,228,277.0; 37,368,818]	83,563,842.0 [51,699,272.3; 109,180,751.0]	
TG O-51:2 TG O-17:1_16:0_18:1__ [M+NH4]__ 11.65			<0.001
Mean ± Standard deviation	42,126,072.7 ± 33,506,005.8	149,225,598.1 ± 80,711,941.8	
Median and [25%; 75%]	36,292,528.0 [14,874,917.3; 59,210,706]	134,798,852.0 [99,479,061.0; 215,144,272.0]	
TG O-51:4 TG O-15:0_18:2_18:2__ [M+NH4]__ 10.21			<0.001

Mean ± Standard deviation	3,159,354.9 ± 3,538,363.2	14,683,834.1 ± 9,470,464.0	
Median and [25%; 75%]	2,469,556.0 [826,736.1; 3,248,265.0]	12,482,353.9 [7,733,416.0; 20,190,252.4]	
TG O-53:1 TG O-19:1_16:0_18:0__[M+NH4]__12.63			<0.001
Mean ± Standard deviation	10,235,301.1 ± 7,380,474.2	25,107,438.6 ± 9,550,435.7	
Median and [25%; 75%]	8,701,994.0 [5,533,780.0; 12,400,527.3]	24,946,453.5 [20,129,973.0; 27,015,453.0]	
TG O-53:3 TG O-17:1_18:1_18:1__[M+NH4]__11.75			0.003
Mean ± Standard deviation	327,836,939.9 ± 199,693,221.2	552,488,671.5 ± 263,620,830.1	
Median and [25%; 75%]	296,585,896.0 [172,105,166.0; 459,895,000.0]	514,180,968.0 [460,861,108.0; 697,452,416.0]	
TG O-53:3 TG O-17:1_18:1_18:1__[M+Na]__11.75			0.080
Mean ± Standard deviation	877,720.0 ± 478,789.3	630,350.4 ± 282,229.4	
Median and [25%; 75%]	717,287.0 [543,740.8; 1,081,101.0]	538,033.8 [433,114.1; 797,261.0]	
TG O-53:4 TG O-17:0_18:2_18:2__[M+NH4]__11.12			0.008
Mean ± Standard deviation	179,202,407.3 ± 135,134,006.9	347,683,262.6 ± 233,177,881.6	
Median and [25%; 75%]	162,887,792.0 [69,589,211.0; 259,877,100.0]	258,760,412.0 [195,189,934.0; 534,315,838.0]	
TG O-53:5 TG O-17:0_18:2_18:3__[M+NH4]__10.53			<0.001
Mean ± Standard deviation	8,328,007.8 ± 7,899,507.5	34,170,718.0 ± 41,004,866.5	
Median and [25%; 75%]	7,201,537.0 [2,933,767.8; 11,985,159.8]	22,603,069.9 [12,334,353.3; 35,791,854.3]	
TG O-53:5 TG O-19:3_16:0_18:2__[M+NH4]__10.53			<0.001
Mean ± Standard deviation	8,323,866.6 ± 7,892,980.8	33,475,570.3 ± 41,251,900.0	
Median and [25%; 75%]	7,202,087.5 [2,612,604.3; 11,985,517.8]	21,684,194.3 [12,334,353.3; 35,791,854.3]	
TG O-54:2 TG O-18:0_18:1_18:1__[M+NH4]__12.52			<0.001
Mean ± Standard deviation	2,290,043.1 ± 1,443,520.2	5,393,476.3 ± 2,892,638.2	
Median and [25%; 75%]	2,056,417.5 [1,301,912.1; 3,030,866.5]	5,437,356.6 [3,211,784.0; 6,507,616.2]	
TG O-55:1 TG O-19:1_18:0_18:0__[M+NH4]__12.81			<0.001
Mean ± Standard deviation	1,353,300.2 ± 2,868,162.5	3,088,067.3 ± 1,798,578.3	
Median and [25%; 75%]	739,863.5 [527,298.5; 1,126,945.0]	2,710,457.5 [1,816,945.5; 3,854,510.6]	
TG O-55:4 TG O-19:2_18:1_18:1__[M+NH4]__11.87			0.001
Mean ± Standard deviation	65,799,975.9 ± 58,838,672.9	175,483,674.4 ± 193,272,540.2	
Median and [25%; 75%]	50,121,814.0 [25,982,969.5; 91,912,742.0]	103,534,268.0 [65,668,657.3; 184,338,451.0]	
TG O-55:5 TG O-19:1_16:0_20:4__[M+NH4]__11.58			0.504
Mean ± Standard deviation	11,177,892.6 ± 10,537,283.4	10,128,076.2 ± 9,344,633.0	
Median and [25%; 75%]	7,777,768.5 [4,993,681.8; 14,253,314.0]	6,873,192.4 [3,223,772.4; 16,316,717.6]	
TG O-55:6 TG O-19:2_18:2_18:2__[M+NH4]__10.62			0.061
Mean ± Standard deviation	18,582,545.8 ± 29,754,007.6	129,584,755.7 ± 349,937,106.6	
Median and [25%; 75%]	13,596,438.0 [4,345,170.3; 20,116,516.5]	20,979,394.9 [10,376,160.1; 68,923,795.0]	
TG O-57:2 TG O-19:1_18:0_20:1__[M+NH4]__12.83			<0.001

Mean ± Standard deviation	342,672.4 ± 400,637.8	953,850.5 ± 923,867.1	
Median and [25%; 75%]	235,587.0 [142,538.0; 364,559.5]	719,157.0 [415,482.0; 1,097,306.1]	
VAE 18:0__[M+Na]__4.55			<0.001
Mean ± Standard deviation	221,140.3 ± 163,321.3	382,292.8 ± 161,225.9	
Median and [25%; 75%]	198,973.0 [96,396.5; 296,413.0]	349,204.5 [245,348.5; 453,839.4]	
VAE 20:2__[M+Na]__4.53			<0.001
Mean ± Standard deviation	324,940.2 ± 168,661.6	552,242.1 ± 158,162.3	
Median and [25%; 75%]	317,522.5 [217,820.8; 404,969.0]	586,323.0 [456,010.0; 638,502.9]	
VAE 22:2__[M+Na]__4.96			0.002
Mean ± Standard deviation	1,160,756.4 ± 530,800.9	1,804,577.0 ± 787,013.6	
Median and [25%; 75%]	1,167,999.5 [888,934.3; 1,390,874.5]	1,697,701.3 [1,251,236.0; 2,226,920.0]	