

Time-Dependent Effect of Sciatic Nerve Injury on Rat Plasma Lipidome

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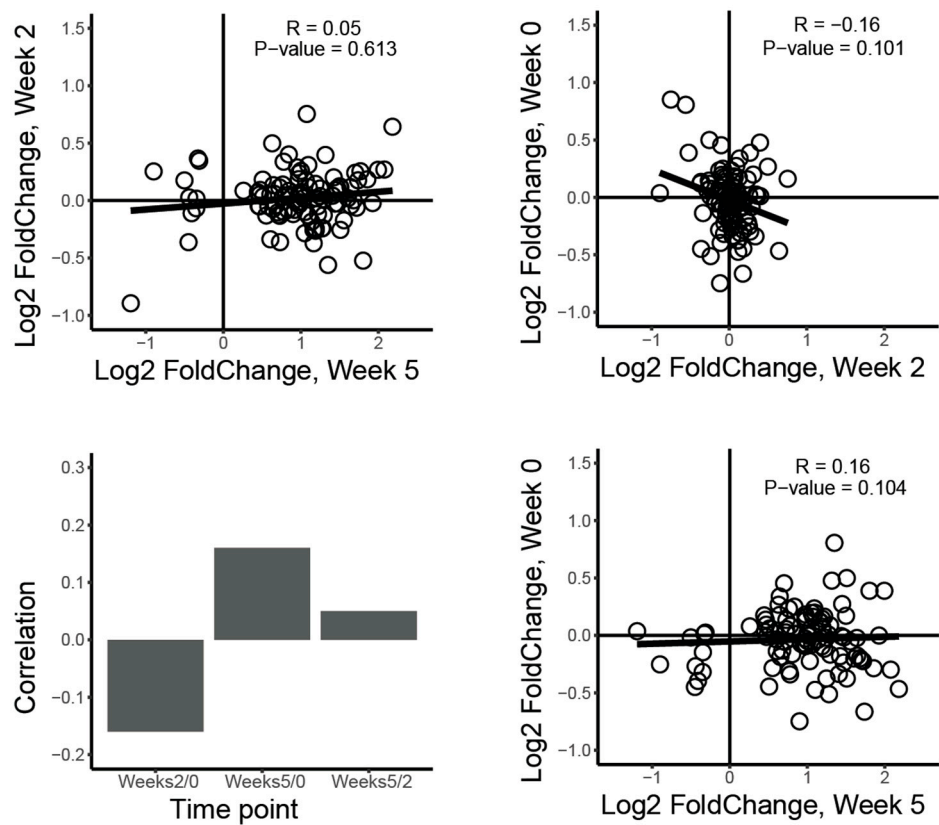


Figure S1. Analysis of 106 NI-associated lipids at the w0 and w2 time points. Here are shown the scatter plots of log2 fold changes between NI and CL at the different time points. The Pearson correlation coefficients and corresponding p -values are included on the plots. No evident alteration trend correlated with w5 alterations was found at w0 and w2.

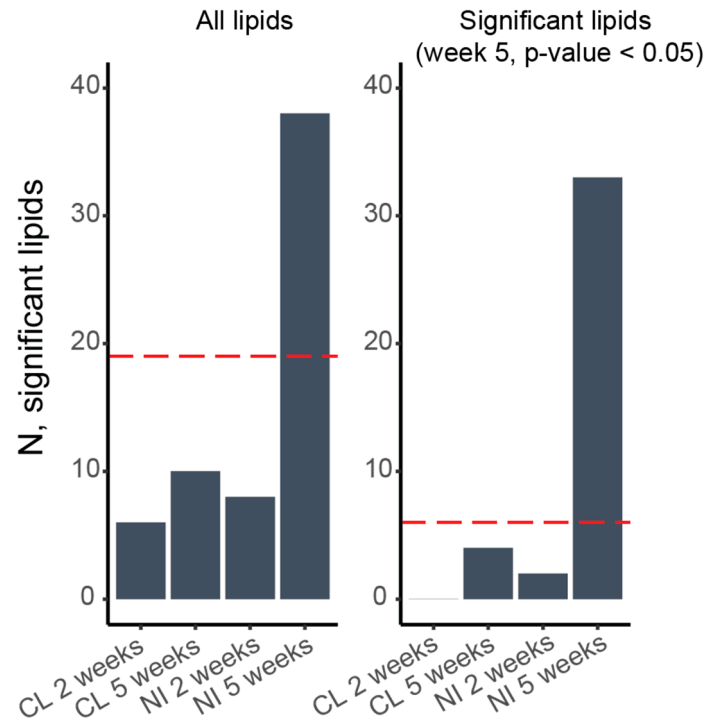


Figure S2. Changes in lipid abundances from the first time point to the later ones for the NI and CL groups, separately. Here are shown the number of lipids with significant (paired t-test, nominal p -value < 0.05) changes in abundance between weeks 0/2 or 0/5 for CL and NI groups. The analysis was performed for all lipids (left) and only NI-associated lipids (right). The red line indicates the expected number of significant lipids under a uniform p -value distribution (total number of lipids \times 0.05). Changes in the NI group between week 0 and 5 were most pronounced among all other comparisons.

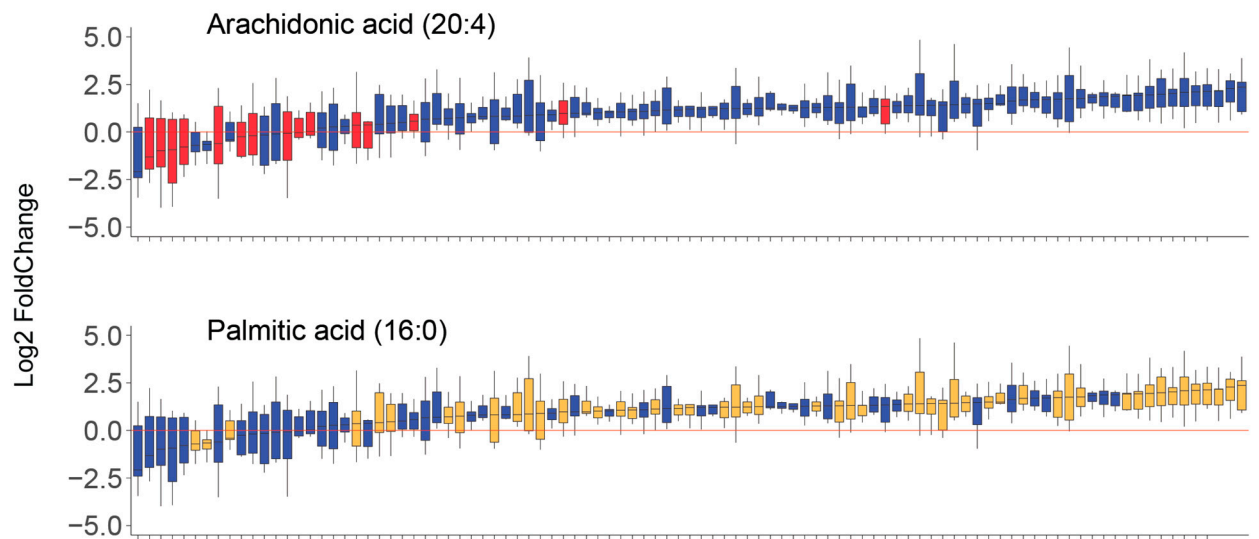


Figure S3. Effect of fatty acid composition on triglyceride abundances in NI at w5. For each triglyceride, the boxplot indicates the distribution of the differences between log2 abundances in NI and the mean log2 abundance in CL. TG features are ordered by boxplot medians. Top: TG containing arachidonic acid are colored in red. Bottom: TG containing palmitic acid are colored in yellow.

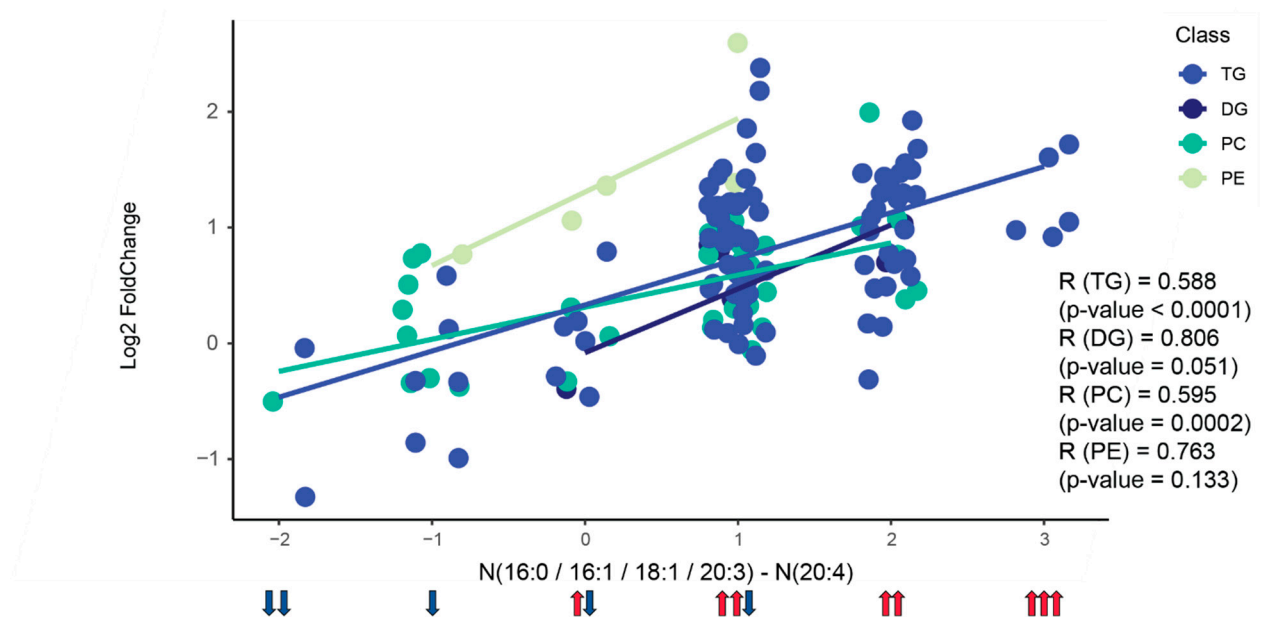


Figure S4. Additive effect of fatty acid residues, shown separately by lipid class. For a particular lipid, the number of fatty acids with negative direction of effect in NI (20:4) is subtracted from the number of fatty acids with positive direction (16:0, 16:1, 18:1, or 20:3), which is indicated on the x -axis, while its log2 fold changes between NI and CL is indicated on the y -axis. All lipid classes with 2 or 3 fatty acid residues (excluding PI, $n = 2$), were considered in this analysis: PC, PE, DG, TG. Moreover, only lipids including at least one of the affected fatty acids (16:0, 16:1, 18:1, 20:3, 20:4) are included in the plot. For each lipid class separately, a linear regression was used to visualize the relationship, with correlation coefficient and corresponding p -value marked on the plot.

Table S1. MS-DIAL parameters of data processing.

MS-DIAL ver. 4.70		
#Project		
MS1 Data type	Profile	
MS2 Data type	Profile	
Ion mode	Positive/Negative	
Target	Lipidomics	
Mode	ddMSMS	
#Data collection parameters		
Retention time begin		1
Retention time end		17
Mass range begin		200
Mass range end		1200
MS2 mass range begin		50
MS2 mass range end		1200
#Centroid parameters		
MS1 tolerance		0.01
MS2 tolerance		0.025
#Isotope recognition		
Maximum charged number		2
#Data processing		
Number of threads		5
#Peak detection parameters		
Smoothing method	LinearWeightedMovingAverage	
Smoothing level		3
Minimum peak width		5
Minimum peak height	10000 (positive) / 20000 (negative)	
#Peak spotting parameters		
Mass slice width		0.1
#Deconvolution parameters		
Sigma window value		0.5
MS2Dec amplitude cut off		0
Exclude after precursor	True	
Keep isotope until		0.5
Keep original precursor isotopes	False	
#MSP file and MS/MS identification setting		
MSP file	LipidMsmsBinaryDB-VS68-FiehnO	
Retention time tolerance	-	
Accurate mass tolerance (MS1)		0.01
Accurate mass tolerance (MS2)		0.05
Identification score cut off		80
Using retention time for scoring	False	
Using retention time for filtering	False	
#Selected lipid types		
All		
#Advanced setting for identification		
Relative abundance cut off		0

Top candidate report	False
#Adduct ion setting [M+H] ⁺	
#Alignment parameters setting	
Retention time tolerance	0.1
MS1 tolerance	0.015
Retention time factor	0.5
MS1 factor	0.5
Peak count filter	75
N% detected in at least one group	0
Remove feature based on peak height fold-change	False
Sample max / blank average	5
Sample average / blank average	5
Keep identified and annotated metabolites	True
Keep removable features and assign the tag for checking	True
Gap filling by compulsion	True
#Tracking of isotope labels	
Tracking of isotopic labels	FALSE
#Ion mobility	
Ion mobility data	FALSE

Table S2. Full list annotated lipids. RT indicates retention time in minutes, m/z indicates mass-to-charge ratio. Lipid nomenclature was kept as reported by MS-DIAL.

Lipid	Class	Category	Adduct	RT	m/z
CAR 16:0	CAR	Fatty acyls	[M+H] ⁺	2.874	400.34119
CAR 16:1	CAR	Fatty acyls	[M+H] ⁺	2.352	398.3259
CAR 18:0	CAR	Fatty acyls	[M+H] ⁺	3.583	428.37402
CAR 18:1	CAR	Fatty acyls	[M+H] ⁺	3.098	426.35651
CE 18:1	CE	Sterol lipids	[M+NH ₄] ⁺	15.564	668.63318
CE 18:2	CE	Sterol lipids	[M+NH ₄] ⁺	15.268	666.61816
CE 18:3	CE	Sterol lipids	[M+NH ₄] ⁺	14.949	664.60156
CE 20:4	CE	Sterol lipids	[M+NH ₄] ⁺	15.061	690.61951
CE 22:5	CE	Sterol lipids	[M+NH ₄] ⁺	15.083	716.63367
CE 22:6	CE	Sterol lipids	[M+NH ₄] ⁺	14.842	714.61835
Cer 34:1;2O Cer 18:1;2O/16:0	Cer	Sphingolipids	[M+H-H ₂ O] ⁺	7.323	520.50739
Cer 40:1;2O Cer 18:1;2O/22:0	Cer	Sphingolipids	[M+H-H ₂ O] ⁺	11.354	604.60071
Cer 41:1;2O Cer 18:1;2O/23:0	Cer	Sphingolipids	[M+CH ₃ COO] ⁻	13.713	618.61993
Cer 42:1;2O Cer 18:1;2O/24:0	Cer	Sphingolipids	[M+H-H ₂ O] ⁺	13.099	632.63452
Cer 42:2;2O Cer 18:1;2O/24:1	Cer	Sphingolipids	[M+H-H ₂ O] ⁺	11.407	630.61908
Cer 42:3;2O Cer 18:1;2O/24:2	Cer	Sphingolipids	[M+H] ⁺	10.149	646.61139
Cer 43:1;2O Cer 18:1;2O/25:0	Cer	Sphingolipids	[M+H-H ₂ O] ⁺	13.72	646.65045
Cer 44:1;2O Cer 18:1;2O/26:0	Cer	Sphingolipids	[M+H] ⁺	14.161	678.67511
CoQ9	Other	Other	[M+H] ⁺	14.194	795.62512
DG 32:1	DG	Glycerolipids	[M+Na] ⁺	8.514	589.48102
DG 32:3	DG	Glycerolipids	[M+Na] ⁺	7.67	585.44458
DG 34:0	DG	Glycerolipids	[M+Na] ⁺	10.888	619.52692
DG 34:0	DG	Glycerolipids	[M+Na] ⁺	11.029	619.52704
DG 34:1 DG 16:0_18:1	DG	Glycerolipids	[M+NH ₄] ⁺	9.811	612.55798
DG 34:2 DG 16:0_18:2	DG	Glycerolipids	[M+NH ₄] ⁺	8.754	610.54199
DG 34:3 DG 16:1_18:2	DG	Glycerolipids	[M+NH ₄] ⁺	7.845	608.52588
DG 36:2 DG 18:1_18:1	DG	Glycerolipids	[M+NH ₄] ⁺	10.076	638.57361
DG 36:3 DG 18:1_18:2	DG	Glycerolipids	[M+NH ₄] ⁺	8.998	636.5578
DG 36:4	DG	Glycerolipids	[M+Na] ⁺	8.503	639.49689
DG 36:4 DG 18:2_18:2	DG	Glycerolipids	[M+NH ₄] ⁺	8.055	634.54053
DG 36:5 DG 18:2_18:3	DG	Glycerolipids	[M+NH ₄] ⁺	7.467	632.52588
DG 37:6	DG	Glycerolipids	[M+Na] ⁺	7.764	649.47607
DG 37:7	DG	Glycerolipids	[M+Na] ⁺	12.363	647.45929
DG 37:7	DG	Glycerolipids	[M+Na] ⁺	5.359	647.46216
DG 38:2	DG	Glycerolipids	[M+Na] ⁺	15.268	671.57373
DG 38:4	DG	Glycerolipids	[M+Na] ⁺	9.717	667.52722
DG 38:5 DG 18:1_20:4	DG	Glycerolipids	[M+NH ₄] ⁺	8.774	660.55737
DG 38:6	DG	Glycerolipids	[M+Na] ⁺	7.861	663.49683
DG 40:2	DG	Glycerolipids	[M+Na] ⁺	13.247	699.59332
DG 40:4	DG	Glycerolipids	[M+Na] ⁺	15.062	695.57367
DG 40:5	DG	Glycerolipids	[M+Na] ⁺	9.735	693.54358
DG 40:5	DG	Glycerolipids	[M+Na] ⁺	14.708	693.55902

DG 40:6	DG	Glycerolipids	[M+Na] ⁺	9.266	691.52759
DG 40:8	DG	Glycerolipids	[M+Na] ⁺	11.449	687.49689
DG 42:4	DG	Glycerolipids	[M+Na] ⁺	15.401	723.60431
DG 42:5	DG	Glycerolipids	[M+Na] ⁺	15.156	721.58972
DG 42:6	DG	Glycerolipids	[M+Na] ⁺	14.842	719.57404
DG 43:6	DG	Glycerolipids	[M+Na] ⁺	14.333	733.57483
DG 44:9	DG	Glycerolipids	[M+Na] ⁺	6.174	741.52887
DG 49:6	DG	Glycerolipids	[M+Na] ⁺	15.461	817.66711
DG 49:8	DG	Glycerolipids	[M+Na] ⁺	14.94	813.63739
DG 51:10	DG	Glycerolipids	[M+Na] ⁺	14.669	837.63556
DG 51:6	DG	Glycerolipids	[M+Na] ⁺	15.7	845.69781
DG 51:7	DG	Glycerolipids	[M+Na] ⁺	15.497	843.68414
DG 51:8	DG	Glycerolipids	[M+Na] ⁺	15.263	841.66589
DG 51:9	DG	Glycerolipids	[M+Na] ⁺	14.995	839.65198
DG 52:7	DG	Glycerolipids	[M+Na] ⁺	15.621	857.69855
FA 14:0	FA	Fatty acyls	[M-H] ⁻	3.475	227.2014
FA 14:1	FA	Fatty acyls	[M-H] ⁻	2.924	225.18555
FA 15:0	FA	Fatty acyls	[M-H] ⁻	3.849	241.2168
FA 16:0	FA	Fatty acyls	[M-H] ⁻	4.192	255.23264
FA 16:1	FA	Fatty acyls	[M-H] ⁻	3.693	253.21706
FA 17:0	FA	Fatty acyls	[M-H] ⁻	4.512	269.2486
FA 17:1	FA	Fatty acyls	[M-H] ⁻	4.039	267.23315
FA 18:0	FA	Fatty acyls	[M-H] ⁻	4.812	283.26382
FA 18:1	FA	Fatty acyls	[M-H] ⁻	4.364	281.24863
FA 18:2	FA	Fatty acyls	[M-H] ⁻	3.907	279.23309
FA 18:3	FA	Fatty acyls	[M-H] ⁻	3.469	277.21722
FA 18:3	FA	Fatty acyls	[M-H] ⁻	3.547	277.21722
FA 19:1	FA	Fatty acyls	[M-H] ⁻	4.653	295.26395
FA 20:0	FA	Fatty acyls	[M-H] ⁻	5.44	311.29605
FA 20:1	FA	Fatty acyls	[M-H] ⁻	4.912	309.27969
FA 20:2	FA	Fatty acyls	[M-H] ⁻	4.506	307.26425
FA 20:3	FA	Fatty acyls	[M-H] ⁻	4.28	305.24866
FA 20:4	FA	Fatty acyls	[M-H] ⁻	3.867	303.23257
FA 20:4;O	FA	Fatty acyls	[M-H] ⁻	2.508	319.22797
FA 20:5	FA	Fatty acyls	[M-H] ⁻	3.44	301.21756
FA 21:0	FA	Fatty acyls	[M-H] ⁻	5.812	325.31146
FA 22:0	FA	Fatty acyls	[M-H] ⁻	6.248	339.3269
FA 22:4	FA	Fatty acyls	[M-H] ⁻	4.365	331.26465
FA 22:5	FA	Fatty acyls	[M-H] ⁻	3.995	329.24844
FA 22:5	FA	Fatty acyls	[M-H] ⁻	4.128	329.24893
FA 22:6	FA	Fatty acyls	[M-H] ⁻	3.743	327.23297
FA 24:0	FA	Fatty acyls	[M-H] ⁻	7.275	367.35779
FA 24:1	FA	Fatty acyls	[M-H] ⁻	6.332	365.3428
FA 26:0	FA	Fatty acyls	[M-H] ⁻	8.57	395.38977
FA 26:1	FA	Fatty acyls	[M-H] ⁻	7.388	393.37387
FA 28:0	FA	Fatty acyls	[M-H] ⁻	10.15	423.4213

FA 28:7	FA	Fatty acyls	[M-H]-	5.865	409.31354
FA 30:0	FA	Fatty acyls	[M-H]-	11.98	451.45239
HexCer 34:1;2O	HexCer	Sphingolipids	[M+CH3COO]-	7.061	758.57947
HexCer 40:1;2O	HexCer	Sphingolipids	[M+CH3COO]-	11.224	842.67322
HexCer 41:1;2O	HexCer	Sphingolipids	[M+CH3COO]-	12.147	856.68927
HexCer 42:1;2O	HexCer	Sphingolipids	[M+CH3COO]-	13.096	870.70569
HexCer 42:2;2O	HexCer	Sphingolipids	[M+CH3COO]-	11.278	868.6889
LPC 14:0	LPC	Glycerophospholipids	[M+H]+	1.801	468.3089
LPC 14:0	LPC	Glycerophospholipids	[M+H]+	1.955	468.30844
LPC 15:0	LPC	Glycerophospholipids	[M+H]+	2.353	482.32294
LPC 16:0	LPC	Glycerophospholipids	[M+H]+	2.579	496.34076
LPC 16:0	LPC	Glycerophospholipids	[M+H]+	2.738	496.34061
LPC 16:1	LPC	Glycerophospholipids	[M+H]+	2.204	494.32266
LPC 17:0	LPC	Glycerophospholipids	[M+H]+	3.113	510.35495
LPC 17:1	LPC	Glycerophospholipids	[M+H]+	2.59	508.34061
LPC 18:0	LPC	Glycerophospholipids	[M+H]+	3.325	524.36993
LPC 18:0	LPC	Glycerophospholipids	[M+H]+	3.471	524.36969
LPC 18:1	LPC	Glycerophospholipids	[M+H]+	2.816	522.35394
LPC 18:1	LPC	Glycerophospholipids	[M+H]+	2.96	522.35406
LPC 18:2	LPC	Glycerophospholipids	[M+H]+	2.316	520.33856
LPC 18:2	LPC	Glycerophospholipids	[M+H]+	2.462	520.33856
LPC 18:3	LPC	Glycerophospholipids	[M+H]+	2.114	518.32361
LPC 19:0	LPC	Glycerophospholipids	[M+H]+	3.802	538.38593
LPC 20:0	LPC	Glycerophospholipids	[M+H]+	4.12	552.40149
LPC 20:1	LPC	Glycerophospholipids	[M+H]+	3.607	550.38739
LPC 20:2	LPC	Glycerophospholipids	[M+H]+	3.142	548.37201
LPC 20:3	LPC	Glycerophospholipids	[M+H]+	2.753	546.35583
LPC 20:4	LPC	Glycerophospholipids	[M+H]+	2.357	544.33862
LPC 20:4	LPC	Glycerophospholipids	[M+H]+	2.475	544.33856
LPC 22:0	LPC	Glycerophospholipids	[M+H]+	4.705	580.43445
LPC 22:1	LPC	Glycerophospholipids	[M+H]+	4.212	578.41687
LPC 22:4	LPC	Glycerophospholipids	[M+H]+	3.043	572.37189
LPC 22:5	LPC	Glycerophospholipids	[M+H]+	2.624	570.35437
LPC 22:5	LPC	Glycerophospholipids	[M+H]+	2.842	570.35437
LPC 22:6	LPC	Glycerophospholipids	[M+H]+	2.286	568.34088
LPC 22:6	LPC	Glycerophospholipids	[M+H]+	2.408	568.34094
LPC 24:0	LPC	Glycerophospholipids	[M+H]+	5.211	608.46533
LPC 24:1	LPC	Glycerophospholipids	[M+H]+	4.733	606.44891
LPE 16:0	LPE	Glycerophospholipids	[M-H]-	2.937	452.27856
LPE 18:0	LPE	Glycerophospholipids	[M-H]-	4.184	480.30939
LPE 18:1	LPE	Glycerophospholipids	[M-H]-	3.601	478.29391
LPE 18:2	LPE	Glycerophospholipids	[M-H]-	2.678	476.2789
PC 30:0 PC 14:0_16:0	PC	Glycerophospholipids	[M+CH3COO]-	6.842	764.54523
PC 31:0 PC 15:0_16:0	PC	Glycerophospholipids	[M+CH3COO]-	7.33	778.5614
PC 32:0	PC	Glycerophospholipids	[M+H]+	6.361	734.56897
PC 32:0 PC 16:0_16:0	PC	Glycerophospholipids	[M+CH3COO]-	7.863	792.57556

PC 32:1 PC 16:0_16:1	PC	Glycerophospholipids	[M+CH3COO]-	7.071	790.56122
PC 32:2 PC 14:0_18:2	PC	Glycerophospholipids	[M+CH3COO]-	6.374	788.54724
PC 33:0	PC	Glycerophospholipids	[M+H]+	7.623	748.58331
PC 33:1 PC 15:0_18:1	PC	Glycerophospholipids	[M+CH3COO]-	7.578	804.57672
PC 33:2 PC 15:0_18:2	PC	Glycerophospholipids	[M+CH3COO]-	6.802	802.56323
PC 34:0 PC 16:0_18:0	PC	Glycerophospholipids	[M+CH3COO]-	9.147	820.60693
PC 34:1 PC 16:0_18:1	PC	Glycerophospholipids	[M+CH3COO]-	8.147	818.59143
PC 34:2 PC 16:0_18:2	PC	Glycerophospholipids	[M+CH3COO]-	7.288	816.57648
PC 34:3	PC	Glycerophospholipids	[M+H]+	6.295	756.5542
PC 34:3 PC 16:1_18:2	PC	Glycerophospholipids	[M+CH3COO]-	6.549	814.56073
PC 34:4 PC 14:0_20:4	PC	Glycerophospholipids	[M+CH3COO]-	6.34	812.54675
PC 35:0	PC	Glycerophospholipids	[M+H]+	8.725	776.61792
PC 35:1	PC	Glycerophospholipids	[M+H]+	7.87	774.59985
PC 35:2 PC 17:0_18:2	PC	Glycerophospholipids	[M+CH3COO]-	7.832	830.59357
PC 35:3	PC	Glycerophospholipids	[M+H]+	6.441	770.56824
PC 35:4	PC	Glycerophospholipids	[M+H]+	6.234	768.55249
PC 36:0 PC 18:0_18:0	PC	Glycerophospholipids	[M+CH3COO]-	10.636	848.6402
PC 36:1 PC 18:0_18:1	PC	Glycerophospholipids	[M+CH3COO]-	9.482	846.62549
PC 36:2 PC 18:0_18:2	PC	Glycerophospholipids	[M+CH3COO]-	8.451	844.60828
PC 36:2 PC 18:1_18:1	PC	Glycerophospholipids	[M+H]+	7.589	786.59766
PC 36:3 PC 16:0_20:3	PC	Glycerophospholipids	[M+CH3COO]-	7.596	842.59229
PC 36:3 PC 16:0_20:3	PC	Glycerophospholipids	[M+CH3COO]-	8.03	842.59235
PC 36:3 PC 16:0_20:3	PC	Glycerophospholipids	[M+CH3COO]-	7.793	842.59265
PC 36:3 PC 18:1_18:2	PC	Glycerophospholipids	[M+CH3COO]-	7.497	842.59235
PC 36:4	PC	Glycerophospholipids	[M+H]+	6.618	782.56964
PC 36:4	PC	Glycerophospholipids	[M+H]+	6.22	782.56964
PC 36:4 PC 16:0_20:4	PC	Glycerophospholipids	[M+CH3COO]-	7.241	840.57556
PC 36:4 PC 18:2_18:2	PC	Glycerophospholipids	[M+CH3COO]-	6.744	840.57776
PC 36:5 PC 16:1_20:4	PC	Glycerophospholipids	[M+CH3COO]-	6.506	838.56226
PC 36:6 PC 14:0_22:6	PC	Glycerophospholipids	[M+CH3COO]-	6.127	836.54596
PC 37:1	PC	Glycerophospholipids	[M+H]+	9.057	802.63239
PC 37:2 PC 19:0_18:2	PC	Glycerophospholipids	[M+CH3COO]-	9.125	858.62518
PC 37:2 PC 19:0_18:2	PC	Glycerophospholipids	[M+CH3COO]-	8.969	858.62585
PC 37:4	PC	Glycerophospholipids	[M+CH3COO]-	8.387	854.59253
PC 37:4 PC 17:0_20:4	PC	Glycerophospholipids	[M+CH3COO]-	7.785	854.59308
PC 37:5	PC	Glycerophospholipids	[M+H]+	6.529	794.56714
PC 37:6 PC 15:0_22:6	PC	Glycerophospholipids	[M+CH3COO]-	6.522	850.5603
PC 38:1	PC	Glycerophospholipids	[M+H]+	9.525	816.64935
PC 38:2 PC 18:0_20:2	PC	Glycerophospholipids	[M+CH3COO]-	9.63	872.64038
PC 38:2 PC 20:0_18:2	PC	Glycerophospholipids	[M+CH3COO]-	9.869	872.64026
PC 38:3 PC 18:0_20:3	PC	Glycerophospholipids	[M+CH3COO]-	8.82	870.625
PC 38:3 PC 18:0_20:3	PC	Glycerophospholipids	[M+CH3COO]-	9.07	870.62732
PC 38:4 PC 16:0_22:4	PC	Glycerophospholipids	[M+CH3COO]-	7.99	868.60889
PC 38:4 PC 18:0_20:4	PC	Glycerophospholipids	[M+CH3COO]-	8.389	868.60724
PC 38:5 PC 16:0_22:5	PC	Glycerophospholipids	[M+CH3COO]-	7.231	866.59143
PC 38:5 PC 16:0_22:5	PC	Glycerophospholipids	[M+CH3COO]-	7.663	866.59155

PC 38:5 PC 18:1_20:4	PC	Glycerophospholipids	[M+CH3COO]-	7.432	866.59174
PC 38:6 PC 16:0_22:6	PC	Glycerophospholipids	[M+CH3COO]-	6.965	864.57776
PC 38:6 PC 18:2_20:4	PC	Glycerophospholipids	[M+CH3COO]-	6.698	864.57715
PC 38:7	PC	Glycerophospholipids	[M+H]+	5.847	804.54456
PC 39:5 PC 17:0_22:5	PC	Glycerophospholipids	[M+CH3COO]-	8.238	880.60712
PC 39:6 PC 17:0_22:6	PC	Glycerophospholipids	[M+CH3COO]-	7.464	878.59351
PC 39:7	PC	Glycerophospholipids	[M+H]+	7.057	818.56659
PC 40:2	PC	Glycerophospholipids	[M+H]+	10.146	842.66113
PC 40:3	PC	Glycerophospholipids	[M+H]+	9.135	840.64905
PC 40:4	PC	Glycerophospholipids	[M+H]+	8.663	838.63239
PC 40:4 PC 18:0_22:4	PC	Glycerophospholipids	[M+CH3COO]-	9.282	896.64136
PC 40:4 PC 20:0_20:4	PC	Glycerophospholipids	[M+CH3COO]-	9.815	896.63989
PC 40:5	PC	Glycerophospholipids	[M+H]+	7.63	836.61499
PC 40:5 PC 18:0_22:5	PC	Glycerophospholipids	[M+CH3COO]-	8.901	894.62378
PC 40:5 PC 18:0_22:5	PC	Glycerophospholipids	[M+CH3COO]-	8.364	894.62335
PC 40:6 PC 18:0_22:6	PC	Glycerophospholipids	[M+CH3COO]-	8.036	892.60651
PC 40:6 PC 20:2_20:4	PC	Glycerophospholipids	[M+CH3COO]-	7.603	892.60919
PC 40:7 PC 18:1_22:6	PC	Glycerophospholipids	[M+CH3COO]-	7.136	890.59186
PC 40:8 PC 18:2_22:6	PC	Glycerophospholipids	[M+CH3COO]-	6.463	888.57587
PC 40:8 PC 20:4_20:4	PC	Glycerophospholipids	[M+CH3COO]-	6.602	888.57648
PC 40:9	PC	Glycerophospholipids	[M+H]+	5.663	828.55707
PC 41:5	PC	Glycerophospholipids	[M+H]+	8.45	850.6286
PC 42:10 PC 20:4_22:6	PC	Glycerophospholipids	[M+CH3COO]-	6.384	912.57672
PC 42:5	PC	Glycerophospholipids	[M+H]+	8.745	864.64746
PC 42:6 PC 18:0_24:6	PC	Glycerophospholipids	[M+CH3COO]-	8.822	920.63959
PC 42:8	PC	Glycerophospholipids	[M+H]+	6.635	858.59662
PC 42:9 PC 20:4_22:5	PC	Glycerophospholipids	[M+CH3COO]-	6.99	914.59381
PC O-32:0 PC O-16:0_16:0	PC-O	Glycerophospholipids	[M+CH3COO]-	8.57	778.59814
PC O-32:1	PC-O	Glycerophospholipids	[M+H]+	7.666	718.57568
PC O-32:1	PC-O	Glycerophospholipids	[M+H]+	6.979	718.57562
PC O-34:0	PC-O	Glycerophospholipids	[M+H]+	8.904	748.62408
PC O-34:1 PC O-18:1_16:0	PC-O	Glycerophospholipids	[M+CH3COO]-	8.8	804.61407
PC O-34:2	PC-O	Glycerophospholipids	[M+H]+	7.17	744.58868
PC O-34:3 PC O-16:1_18:2	PC-O	Glycerophospholipids	[M+CH3COO]-	7.838	800.58124
PC O-36:3	PC-O	Glycerophospholipids	[M+H]+	7.317	770.60413
PC O-36:3	PC-O	Glycerophospholipids	[M+H]+	7.448	770.60333
PC O-36:4 PC O-16:0_20:4	PC-O	Glycerophospholipids	[M+CH3COO]-	7.85	826.59863
PC O-36:5 PC O-16:1_20:4	PC-O	Glycerophospholipids	[M+CH3COO]-	7.751	824.58234
PC O-38:4 PC O-16:0_22:4	PC-O	Glycerophospholipids	[M+CH3COO]-	8.687	854.63074
PC O-38:4 PC O-18:0_20:4	PC-O	Glycerophospholipids	[M+CH3COO]-	9.153	854.62836
PC O-38:5 PC O-16:1_22:4	PC-O	Glycerophospholipids	[M+CH3COO]-	8.343	852.61426
PC O-38:5 PC O-18:1_20:4	PC-O	Glycerophospholipids	[M+CH3COO]-	8.051	852.61243
PC O-38:6 PC O-16:0_22:6	PC-O	Glycerophospholipids	[M+CH3COO]-	7.511	850.59717
PC O-38:6 PC O-18:2_20:4	PC-O	Glycerophospholipids	[M+CH3COO]-	7.948	850.5976
PC O-38:7 PC O-16:1_22:6	PC-O	Glycerophospholipids	[M+CH3COO]-	7.426	848.5827
PC O-39:10	PC-O	Glycerophospholipids	[M+H]+	7.358	798.53906

PC O-40:4 PC O-20:0_20:4	PC-O	Glycerophospholipids	[M+CH3COO]-	10.725	882.66107
PC O-40:7 PC O-18:1_22:6	PC-O	Glycerophospholipids	[M+CH3COO]-	7.692	876.61249
PC O-40:8	PC-O	Glycerophospholipids	[M+H]+	7.266	816.59113
PC O-41:10	PC-O	Glycerophospholipids	[M+H]+	8.438	826.57202
PC O-41:11	PC-O	Glycerophospholipids	[M+H]+	7.58	824.55493
PE 34:2 PE 16:0_18:2	PE	Glycerophospholipids	[M-H]-	7.468	714.5105
PE 36:2 PE 18:0_18:2	PE	Glycerophospholipids	[M-H]-	8.669	742.53906
PE 36:4 PE 16:0_20:4	PE	Glycerophospholipids	[M-H]-	7.412	738.51044
PE 38:4 PE 18:0_20:4	PE	Glycerophospholipids	[M-H]-	8.601	766.53998
PE 38:5 PE 18:1_20:4	PE	Glycerophospholipids	[M-H]-	7.658	764.52545
PE 38:6 PE 16:0_22:6	PE	Glycerophospholipids	[M-H]-	7.12	762.51025
PE 40:6 PE 18:0_22:6	PE	Glycerophospholipids	[M-H]-	6.968	790.53973
PE O-36:5 PE O-16:1_20:4	PE-O	Glycerophospholipids	[M-H]-	7.988	722.51453
PE O-38:5 PE O-18:1_20:4	PE-O	Glycerophospholipids	[M-H]-	9.304	750.5459
PE O-38:6 PE O-18:2_20:4	PE-O	Glycerophospholipids	[M-H]-	8.192	748.5293
PE P-36:4 PE P-16:0_20:4	PE-P	Glycerophospholipids	[M+H]+	7.245	724.52771
PE P-38:5 PE P-18:1_20:4	PE-P	Glycerophospholipids	[M+H]+	7.403	750.54468
PI 36:4	PI	Glycerophospholipids	[M-H]-	6.046	857.52344
PI 38:4 PI 18:0_20:4	PI	Glycerophospholipids	[M-H]-	6.862	885.55011
SE 28:1/20:4	Other	Other	[M+NH4]+	15.236	704.63147
SE 29:1/20:4	Other	Other	[M+NH4]+	15.402	718.64874
SE 29:2/20:4	Other	Other	[M+NH4]+	15.158	716.63367
SM 32:1;2O	SM	Sphingolipids	[M+H]+	5.516	675.54181
SM 33:1;2O	SM	Sphingolipids	[M+H]+	5.834	689.55804
SM 34:0;2O	SM	Sphingolipids	[M+H]+	6.41	705.591
SM 34:1;2O	SM	Sphingolipids	[M+H]+	6.172	703.57684
SM 34:1;3O	SM	Sphingolipids	[M+H]+	5.939	719.5686
SM 34:2;2O	SM	Sphingolipids	[M+H]+	5.639	701.55902
SM 34:2;3O	SM	Sphingolipids	[M+H]+	5.454	717.55292
SM 35:1;2O	SM	Sphingolipids	[M+H]+	6.568	717.59039
SM 36:1;2O	SM	Sphingolipids	[M+H]+	6.996	731.60822
SM 36:2;2O	SM	Sphingolipids	[M+H]+	6.343	729.58997
SM 38:1;2O	SM	Sphingolipids	[M+H]+	8.051	759.63727
SM 39:1;2O	SM	Sphingolipids	[M+H]+	8.682	773.65027
SM 40:1;2O	SM	Sphingolipids	[M+H]+	9.336	787.66608
SM 40:2;2O	SM	Sphingolipids	[M+H]+	8.332	785.65222
SM 40:2;2O	SM	Sphingolipids	[M+H]+	8.141	785.6521
SM 41:1;2O	SM	Sphingolipids	[M+H]+	10.072	801.68402
SM 41:2;2O	SM	Sphingolipids	[M+H]+	8.989	799.66962
SM 41:2;2O	SM	Sphingolipids	[M+H]+	8.739	799.66931
SM 42:1;2O	SM	Sphingolipids	[M+H]+	10.831	815.7002
SM 42:2;2O	SM	Sphingolipids	[M+H]+	9.346	813.68555
SM 42:2;2O	SM	Sphingolipids	[M+H]+	9.686	813.68085
SM 42:3;2O	SM	Sphingolipids	[M+H]+	8.339	811.66962
SM 43:1;2O	SM	Sphingolipids	[M+H]+	11.494	829.71619
SM 43:1;2O	SM	Sphingolipids	[M+H]+	11.672	829.71478

SM 43:2;2O	SM	Sphingolipids	[M+H] ⁺	10.244	827.70178
ST 24:1;O4	ST	Sterol lipids	[M-H] ⁻	1.197	391.28586
ST 24:1;O4	ST	Sterol lipids	[M-H] ⁻	1.825	391.28589
ST 24:1;O4	ST	Sterol lipids	[M-H] ⁻	1.972	391.28595
ST 27:1;O	ST	Sterol lipids	[M+H-H ₂ O] ⁺	5.498	369.3512
ST 27:1;O	ST	Sterol lipids	[M+H-H ₂ O] ⁺	3.886	369.35114
ST 27:1;O;S	ST	Sterol lipids	[M-H] ⁻	3.996	465.30414
ST 28:1;O;S	ST	Sterol lipids	[M-H] ⁻	4.178	479.3201
TG 42:1 TG 12:0_12:0_18:1	TG	Glycerolipids	[M+NH ₄] ⁺	14.468	738.65985
TG 44:0 TG 14:0_14:0_16:0	TG	Glycerolipids	[M+NH ₄] ⁺	15.176	768.70807
TG 44:1 TG 12:0_16:0_16:1	TG	Glycerolipids	[M+NH ₄] ⁺	15.061	766.69147
TG 44:1 TG 14:0_16:0_14:1	TG	Glycerolipids	[M+NH ₄] ⁺	14.911	766.69116
TG 45:0 TG 14:0_15:0_16:0	TG	Glycerolipids	[M+NH ₄] ⁺	15.325	782.71918
TG 45:1 TG 14:0_15:0_16:1	TG	Glycerolipids	[M+NH ₄] ⁺	15.083	780.70911
TG 46:0 TG 14:0_16:0_16:0	TG	Glycerolipids	[M+NH ₄] ⁺	15.467	796.73883
TG 46:1 TG 14:0_16:0_16:1	TG	Glycerolipids	[M+NH ₄] ⁺	15.248	794.72321
TG 46:2 TG 12:0_16:0_18:2	TG	Glycerolipids	[M+NH ₄] ⁺	15.032	792.70605
TG 46:3 TG 12:0_16:1_18:2	TG	Glycerolipids	[M+NH ₄] ⁺	14.595	790.69354
TG 47:0 TG 15:0_16:0_16:0	TG	Glycerolipids	[M+NH ₄] ⁺	15.583	810.75439
TG 47:1 TG 15:0_16:0_16:1	TG	Glycerolipids	[M+NH ₄] ⁺	15.39	808.73889
TG 48:0 TG 16:0_16:0_16:0	TG	Glycerolipids	[M+NH ₄] ⁺	15.709	824.77197
TG 48:1 TG 14:0_16:0_18:1	TG	Glycerolipids	[M+NH ₄] ⁺	15.502	822.75281
TG 48:2 TG 14:0_16:0_18:2	TG	Glycerolipids	[M+NH ₄] ⁺	15.265	820.73914
TG 48:4 TG 12:0_18:2_18:2	TG	Glycerolipids	[M+NH ₄] ⁺	14.681	816.70428
TG 49:0 TG 15:0_16:0_18:0	TG	Glycerolipids	[M+NH ₄] ⁺	15.815	838.7876
TG 49:1 TG 15:0_16:0_18:1	TG	Glycerolipids	[M+NH ₄] ⁺	15.62	836.76892
TG 49:2 TG 16:0_16:1_17:1	TG	Glycerolipids	[M+NH ₄] ⁺	15.406	834.75317
TG 49:3 TG 15:0_16:1_18:2	TG	Glycerolipids	[M+NH ₄] ⁺	15.145	832.73785
TG 50:0 TG 16:0_16:0_18:0	TG	Glycerolipids	[M+NH ₄] ⁺	15.923	852.80359
TG 50:1 TG 16:0_16:0_18:1	TG	Glycerolipids	[M+NH ₄] ⁺	15.731	850.78589
TG 50:2 TG 16:0_16:1_18:1	TG	Glycerolipids	[M+NH ₄] ⁺	15.528	848.76862
TG 50:3 TG 16:0_16:1_18:2	TG	Glycerolipids	[M+NH ₄] ⁺	15.295	846.75311
TG 50:4 TG 16:1_16:1_18:2	TG	Glycerolipids	[M+NH ₄] ⁺	15.054	844.74091
TG 50:5 TG 16:0_16:1_18:4	TG	Glycerolipids	[M+NH ₄] ⁺	14.888	842.72449
TG 51:0 TG 16:0_17:0_18:0	TG	Glycerolipids	[M+NH ₄] ⁺	16.021	866.81622
TG 51:1 TG 16:0_17:0_18:1	TG	Glycerolipids	[M+NH ₄] ⁺	15.835	864.79895
TG 51:2 TG 16:0_17:1_18:1	TG	Glycerolipids	[M+NH ₄] ⁺	15.643	862.78784
TG 51:3 TG 15:0_18:1_18:2	TG	Glycerolipids	[M+NH ₄] ⁺	15.431	860.77222
TG 51:4 TG 15:0_18:2_18:2	TG	Glycerolipids	[M+NH ₄] ⁺	15.272	858.75171
TG 52:0 TG 16:0_18:0_18:0	TG	Glycerolipids	[M+NH ₄] ⁺	16.12	880.8299
TG 52:1 TG 16:0_18:0_18:1	TG	Glycerolipids	[M+NH ₄] ⁺	15.938	878.815
TG 52:2 TG 16:0_18:1_18:1	TG	Glycerolipids	[M+NH ₄] ⁺	15.751	876.80127
TG 52:3 TG 16:0_18:1_18:2	TG	Glycerolipids	[M+NH ₄] ⁺	15.547	874.7865
TG 52:4 TG 16:0_18:2_18:2	TG	Glycerolipids	[M+NH ₄] ⁺	15.322	872.7713
TG 52:5 TG 16:0_18:2_18:3	TG	Glycerolipids	[M+NH ₄] ⁺	15.063	870.75128
TG 52:6 TG 16:1_18:2_18:3	TG	Glycerolipids	[M+NH ₄] ⁺	14.934	868.73798

TG 53:1 TG 17:0_18:0_18:1	TG	Glycerolipids	[M+NH4] ⁺	16.035	892.83533
TG 53:2 TG 17:0_18:1_18:1	TG	Glycerolipids	[M+NH4] ⁺	15.851	890.81409
TG 53:3 TG 17:0_18:1_18:2	TG	Glycerolipids	[M+NH4] ⁺	15.661	888.79974
TG 53:4 TG 17:1_18:1_18:2	TG	Glycerolipids	[M+NH4] ⁺	15.547	886.78619
TG 53:5 TG 16:0_18:2_19:3	TG	Glycerolipids	[M+NH4] ⁺	15.338	884.76849
TG 53:6 TG 15:0_18:2_20:4	TG	Glycerolipids	[M+NH4] ⁺	15.09	882.75458
TG 54:0 TG 16:0_18:0_20:0	TG	Glycerolipids	[M+NH4] ⁺	16.32	908.86292
TG 54:2 TG 18:0_18:1_18:1	TG	Glycerolipids	[M+NH4] ⁺	15.951	904.83105
TG 54:3 TG 18:0_18:1_18:2	TG	Glycerolipids	[M+NH4] ⁺	15.768	902.81812
TG 54:4 TG 16:0_18:1_20:3	TG	Glycerolipids	[M+NH4] ⁺	15.569	900.80103
TG 54:4 TG 18:1_18:1_18:2	TG	Glycerolipids	[M+NH4] ⁺	15.659	900.80206
TG 54:5 TG 16:0_18:1_20:4	TG	Glycerolipids	[M+NH4] ⁺	15.359	898.78558
TG 54:6 TG 16:0_18:2_20:4	TG	Glycerolipids	[M+NH4] ⁺	15.233	896.77039
TG 54:7 TG 16:0_18:2_20:5	TG	Glycerolipids	[M+NH4] ⁺	15.053	894.75494
TG 54:7 TG 18:2_18:2_18:3	TG	Glycerolipids	[M+NH4] ⁺	14.987	894.75415
TG 55:0 TG 15:0_16:0_24:0	TG	Glycerolipids	[M+NH4] ⁺	16.433	922.88165
TG 55:2 TG 17:0_18:1_20:1	TG	Glycerolipids	[M+NH4] ⁺	16.045	918.84735
TG 55:3 TG 19:0_18:1_18:2	TG	Glycerolipids	[M+NH4] ⁺	15.868	916.83527
TG 55:4 TG 17:0_18:1_20:3	TG	Glycerolipids	[M+NH4] ⁺	15.691	914.8222
TG 55:5 TG 17:0_18:1_20:4	TG	Glycerolipids	[M+NH4] ⁺	15.581	912.79901
TG 55:6 TG 16:0_17:0_22:6	TG	Glycerolipids	[M+NH4] ⁺	15.365	910.78284
TG 56:0 TG 16:0_16:0_24:0	TG	Glycerolipids	[M+NH4] ⁺	16.529	936.8949
TG 56:1 TG 16:0_18:0_22:1	TG	Glycerolipids	[M+NH4] ⁺	16.327	934.87781
TG 56:2 TG 16:0_22:0_18:2	TG	Glycerolipids	[M+NH4] ⁺	16.127	932.86102
TG 56:3 TG 16:0_22:1_18:2	TG	Glycerolipids	[M+NH4] ⁺	15.938	930.85071
TG 56:4 TG 16:0_18:1_22:3	TG	Glycerolipids	[M+NH4] ⁺	15.78	928.83405
TG 56:5 TG 16:0_18:1_22:4	TG	Glycerolipids	[M+NH4] ⁺	15.684	926.81653
TG 56:6 TG 16:0_18:2_22:4	TG	Glycerolipids	[M+NH4] ⁺	15.533	924.79901
TG 56:7 TG 18:1_18:2_20:4	TG	Glycerolipids	[M+NH4] ⁺	15.284	922.78149
TG 56:8 TG 18:2_18:2_20:4	TG	Glycerolipids	[M+NH4] ⁺	15.098	920.77075
TG 56:9 TG 18:2_18:2_20:5	TG	Glycerolipids	[M+NH4] ⁺	14.821	918.75299
TG 56:9 TG 18:2_18:3_20:4	TG	Glycerolipids	[M+NH4] ⁺	14.899	918.7536
TG 57:0 TG 16:0_17:0_24:0	TG	Glycerolipids	[M+NH4] ⁺	16.635	950.90869
TG 57:1 TG 16:0_23:0_18:1	TG	Glycerolipids	[M+NH4] ⁺	16.446	948.89398
TG 57:3 TG 18:1_18:1_21:1	TG	Glycerolipids	[M+NH4] ⁺	16.064	944.86707
TG 57:5 TG 17:0_18:1_22:4	TG	Glycerolipids	[M+NH4] ⁺	15.781	940.83081
TG 57:7 TG 17:0_18:1_22:6	TG	Glycerolipids	[M+NH4] ⁺	15.469	936.80084
TG 58:0 TG 16:0_18:0_24:0	TG	Glycerolipids	[M+NH4] ⁺	16.742	964.92609
TG 58:1 TG 16:0_24:0_18:1	TG	Glycerolipids	[M+NH4] ⁺	16.526	962.91064
TG 58:10 TG 18:2_18:2_22:6	TG	Glycerolipids	[M+NH4] ⁺	14.94	944.76941
TG 58:2 TG 16:0_18:1_24:1	TG	Glycerolipids	[M+NH4] ⁺	16.335	960.89417
TG 58:3 TG 22:0_18:1_18:2	TG	Glycerolipids	[M+NH4] ⁺	16.149	958.87799
TG 58:4 TG 18:1_22:1_18:2	TG	Glycerolipids	[M+NH4] ⁺	15.951	956.85974
TG 58:6 TG 18:0_18:1_22:5	TG	Glycerolipids	[M+NH4] ⁺	15.75	952.8316
TG 58:7 TG 18:1_18:1_22:5	TG	Glycerolipids	[M+NH4] ⁺	15.564	950.81598
TG 58:8 TG 18:1_18:2_22:5	TG	Glycerolipids	[M+NH4] ⁺	15.399	948.79791

TG 58:9 TG 18:2_20:3_20:4	TG	Glycerolipids	[M+NH4] ⁺	15.203	946.78644
TG 60:10 TG 18:1_20:4_22:5	TG	Glycerolipids	[M+NH4] ⁺	15.291	972.80188
TG 60:11 TG 18:2_20:4_22:5	TG	Glycerolipids	[M+NH4] ⁺	15.056	970.7832
TG 60:12 TG 18:2_20:4_22:6	TG	Glycerolipids	[M+NH4] ⁺	14.846	968.76764
TG 60:2 TG 16:0_20:1_24:1	TG	Glycerolipids	[M+NH4] ⁺	16.527	988.92578
TG 60:3 TG 16:0_26:1_18:2	TG	Glycerolipids	[M+NH4] ⁺	16.335	986.90851
TG 60:5 TG 24:1_18:2_18:2	TG	Glycerolipids	[M+NH4] ⁺	16.042	982.87842
TG 60:9 TG 18:0_20:4_22:5	TG	Glycerolipids	[M+NH4] ⁺	15.456	974.81641
TG 60:9 TG 18:1_20:4_22:4	TG	Glycerolipids	[M+NH4] ⁺	15.219	974.81567
TG 62:13 TG 20:4_20:4_22:5	TG	Glycerolipids	[M+NH4] ⁺	14.954	994.78546
TG 62:14 TG 20:4_20:4_22:6	TG	Glycerolipids	[M+NH4] ⁺	14.701	992.77051
TG 62:2 TG 18:0_18:1_26:1	TG	Glycerolipids	[M+NH4] ⁺	16.727	1016.95728
TG 62:4 TG 18:1_26:1_18:2	TG	Glycerolipids	[M+NH4] ⁺	16.344	1012.9231

Table S3. List of *p*-values and log2 fold changes at the three time points for 377 lipids.

Lipid	<i>p</i> -Value			log2 FoldChange			NI Associated
	Week 5	Week 2	Week 0	Week 5	Week 2	Week 0	
CAR 16:0	0.507	0.317	0.252	0.228	-0.329	-0.366	No
CAR 16:1	0.522	0.661	0.455	0.719	-0.281	-0.550	No
CAR 18:0	0.266	0.223	0.524	0.450	-0.334	-0.183	No
CAR 18:1	0.827	0.193	0.455	0.085	-0.442	-0.262	No
CE 18:1	0.292	0.515	0.135	0.394	0.196	0.408	No
CE 18:2	0.572	0.674	0.578	0.192	0.100	0.133	No
CE 18:3	0.355	0.117	0.875	0.563	0.584	0.085	No
CE 20:4	0.016	0.862	0.016	-0.441	0.027	-0.268	Yes
CE 22:5	0.044	0.452	0.249	-0.900	0.254	-0.252	Yes
CE 22:6	0.609	0.404	0.714	-0.201	-0.252	0.084	No
Cer 34:1;2O Cer 18:1;2O/16:0	0.278	0.492	0.521	0.546	0.328	0.206	No
Cer 40:1;2O Cer 18:1;2O/22:0	0.079	0.282	0.190	0.776	0.405	0.548	No
Cer 41:1;2O Cer 18:1;2O/23:0	0.007	0.467	0.185	0.644	0.134	0.339	Yes
Cer 42:1;2O Cer 18:1;2O/24:0	0.057	0.170	0.274	0.581	0.337	0.307	No
Cer 42:2;2O Cer 18:1;2O/24:1	0.096	0.322	0.408	0.878	0.365	0.282	No
Cer 42:3;2O Cer 18:1;2O/24:2	0.293	0.507	0.850	0.846	0.513	0.094	No
Cer 43:1;2O Cer 18:1;2O/25:0	0.185	0.345	0.930	0.950	0.693	0.035	No
Cer 44:1;2O Cer 18:1;2O/26:0	0.254	0.671	0.087	0.587	-0.161	0.930	No
CoQ9	0.084	0.031	0.994	0.591	0.620	0.003	No
DG 32:1	0.007	0.710	0.109	1.101	0.116	-0.474	Yes
DG 32:3	0.011	0.408	0.786	-0.130	-0.047	-0.013	No
DG 34:0	0.492	0.795	0.090	0.068	-0.028	-0.208	No
DG 34:0	0.033	0.830	0.795	0.605	0.051	-0.035	Yes
DG 34:1 DG 16:0_18:1	0.008	0.949	0.542	1.032	0.021	-0.224	Yes
DG 34:2 DG 16:0_18:2	0.031	0.879	0.685	0.805	0.046	-0.163	Yes
DG 34:3 DG 16:1_18:2	0.048	0.854	0.191	0.849	0.085	-1.258	Yes
DG 36:2 DG 18:1_18:1	0.049	0.797	0.504	0.700	-0.103	0.454	Yes
DG 36:3 DG 18:1_18:2	0.307	0.606	0.752	0.381	-0.159	-0.122	No
DG 36:4	0.287	0.716	0.149	0.457	-0.119	-0.489	No
DG 36:4 DG 18:2_18:2	0.525	0.508	0.438	0.257	-0.206	-0.341	No
DG 36:5 DG 18:2_18:3	0.558	0.754	0.132	-0.497	-0.180	-1.039	No
DG 37:6	0.131	0.110	0.598	-2.019	-1.672	0.548	No
DG 37:7	0.397	0.982	0.965	-0.360	-0.004	-0.005	No
DG 37:7	0.230	0.127	0.537	-2.507	-2.007	-1.100	No
DG 38:2	0.688	0.440	0.396	-0.107	0.136	0.118	No
DG 38:4	0.197	0.177	0.795	0.533	0.403	-0.066	No
DG 38:5 DG 18:1_20:4	0.526	0.486	0.194	-0.393	-0.119	-0.291	No
DG 38:6	0.277	0.323	0.191	-0.640	-0.189	-0.422	No
DG 40:2	0.335	0.924	0.734	0.194	0.006	0.039	No
DG 40:4	0.011	0.887	0.045	-0.347	0.016	-0.147	Yes
DG 40:5	0.547	0.484	0.960	0.333	0.116	-0.014	No
DG 40:5	0.630	0.470	0.901	-0.363	0.233	0.092	No
DG 40:6	0.790	0.908	0.551	-0.277	-0.022	-0.231	No

DG 40:8	0.046	0.715	0.050	-0.188	0.032	-0.148	No
DG 42:4	0.026	0.997	0.849	-1.719	-0.002	-0.070	Yes
DG 42:5	0.441	0.816	0.622	0.246	0.100	-0.146	No
DG 42:6	0.539	0.790	0.838	-0.183	-0.056	0.032	No
DG 43:6	0.916	0.406	0.138	0.017	0.098	0.162	No
DG 44:9	0.797	0.686	0.523	-0.181	0.118	0.182	No
DG 49:6	0.962	0.046	0.582	0.019	0.261	-0.114	No
DG 49:8	0.016	0.814	0.965	1.639	0.117	-0.022	Yes
DG 51:10	0.155	0.489	0.685	1.154	0.370	-0.326	No
DG 51:6	0.135	0.629	0.237	0.289	-0.059	-0.168	No
DG 51:7	0.010	0.690	0.153	1.247	0.105	-0.375	Yes
DG 51:8	0.014	0.713	0.466	1.737	0.176	-0.664	Yes
DG 51:9	0.015	0.766	0.457	1.509	0.116	-0.375	Yes
DG 52:7	0.140	0.444	0.968	0.429	0.096	-0.006	No
FA 14:0	0.770	0.780	0.451	-0.045	0.055	-0.270	No
FA 14:1	0.726	0.570	0.256	-0.176	0.205	-0.738	No
FA 15:0	0.382	0.616	0.563	0.074	-0.062	0.087	No
FA 16:0	0.988	0.474	0.381	0.003	-0.103	-0.191	No
FA 16:1	0.677	0.791	0.421	-0.156	0.108	-0.454	No
FA 17:0	0.168	0.003	0.632	0.264	-0.378	-0.123	No
FA 17:1	0.999	0.394	0.346	0.000	-0.322	-0.399	No
FA 18:0	0.094	0.932	0.453	-0.197	-0.011	-0.079	No
FA 18:1	0.499	0.425	0.547	-0.237	-0.280	-0.270	No
FA 18:2	0.186	0.285	0.266	-0.377	-0.259	-0.473	No
FA 18:3	0.782	0.510	0.318	-0.102	-0.259	-0.512	No
FA 18:3	0.322	0.940	0.145	-0.295	-0.020	-0.579	No
FA 19:1	0.564	0.130	0.232	-0.330	-0.875	-0.618	No
FA 20:0	0.029	0.016	0.825	0.159	-0.148	-0.022	No
FA 20:1	0.917	0.093	0.208	0.030	-0.495	-0.405	No
FA 20:2	0.994	0.604	0.035	-0.001	-0.115	-0.667	No
FA 20:3	0.842	0.852	0.337	0.074	0.051	-0.339	No
FA 20:4	0.050	0.375	0.019	-0.410	-0.110	-0.397	Yes
FA 20:4;O	0.617	0.384	0.780	0.800	-0.815	0.240	No
FA 20:5	0.957	0.349	0.010	0.018	-0.272	-1.002	No
FA 21:0	0.058	0.718	0.129	0.225	0.092	0.195	No
FA 22:0	0.163	0.700	0.732	0.165	0.040	-0.039	No
FA 22:4	0.089	0.876	0.018	-0.655	-0.032	-0.701	No
FA 22:5	0.303	0.252	0.014	-0.490	-0.260	-0.750	No
FA 22:5	0.724	0.557	0.057	-0.169	-0.100	-0.574	No
FA 22:6	0.238	0.278	0.148	-0.380	-0.230	-0.292	No
FA 24:0	0.303	0.777	0.775	0.112	-0.027	0.031	No
FA 24:1	0.237	0.076	0.813	0.384	-0.352	-0.069	No
FA 26:0	0.726	0.587	0.928	0.041	0.060	0.011	No
FA 26:1	0.194	0.240	0.787	0.680	-0.759	0.146	No
FA 28:0	0.879	0.553	0.994	0.020	0.090	-0.001	No
FA 28:7	0.143	0.624	0.608	-0.303	-0.132	-0.170	No

FA 30:0	0.786	0.549	0.728	-0.034	0.095	-0.059	No
HexCer 34:1;2O	0.225	0.633	0.373	0.490	0.146	0.316	No
HexCer 40:1;2O	0.109	0.118	0.123	0.424	0.357	0.462	No
HexCer 41:1;2O	0.686	0.800	0.143	0.146	-0.077	0.521	No
HexCer 42:1;2O	0.455	0.895	0.503	0.153	-0.026	0.158	No
HexCer 42:2;2O	0.370	0.344	0.177	0.348	0.373	0.447	No
LPC 14:0	0.217	0.298	0.270	1.440	-1.324	-0.397	No
LPC 14:0	0.057	0.101	0.145	0.578	0.436	-0.267	No
LPC 15:0	0.478	0.418	0.938	0.203	0.142	-0.019	No
LPC 16:0	0.506	0.199	0.424	0.105	0.197	-0.064	No
LPC 16:0	0.597	0.156	0.313	0.084	0.212	-0.082	No
LPC 16:1	0.084	0.254	0.581	0.326	0.214	-0.101	No
LPC 17:0	0.482	0.935	0.248	-0.187	0.011	-0.218	No
LPC 17:1	0.497	0.621	0.950	0.395	-0.238	0.024	No
LPC 18:0	0.090	0.752	0.045	-0.313	0.040	-0.328	No
LPC 18:0	0.078	0.913	0.028	-0.314	0.011	-0.308	No
LPC 18:1	0.518	0.157	0.410	0.102	0.178	0.105	No
LPC 18:1	0.458	0.175	0.995	0.114	0.160	-0.001	No
LPC 18:2	0.505	0.125	0.972	0.171	0.197	0.005	No
LPC 18:2	0.610	0.113	0.858	0.136	0.238	0.026	No
LPC 18:3	0.371	0.025	0.573	0.353	0.704	0.178	No
LPC 19:0	0.182	0.149	0.106	-0.550	-0.288	-0.391	No
LPC 20:0	0.449	0.463	0.181	-0.277	0.114	-0.270	No
LPC 20:1	0.288	0.061	0.266	-0.345	-0.249	-0.227	No
LPC 20:2	0.941	0.262	0.299	0.026	0.310	-0.249	No
LPC 20:3	0.031	0.129	0.237	0.629	0.498	0.267	Yes
LPC 20:4	0.012	0.016	0.742	-0.313	0.347	0.025	Yes
LPC 20:4	0.010	0.015	0.880	-0.328	0.366	0.014	Yes
LPC 22:0	0.682	0.784	0.068	0.148	-0.216	-0.596	No
LPC 22:1	0.643	0.733	0.202	-0.202	0.123	-0.353	No
LPC 22:4	0.381	0.190	0.827	0.282	0.822	-0.088	No
LPC 22:5	0.122	0.336	0.547	0.584	0.490	-0.189	No
LPC 22:5	0.761	0.163	0.435	0.075	0.493	-0.197	No
LPC 22:6	0.099	0.134	0.735	-0.667	0.310	0.065	No
LPC 22:6	0.333	0.422	0.711	-0.227	0.155	0.070	No
LPC 24:0	0.933	0.041	0.694	0.021	-0.448	-0.074	No
LPC 24:1	0.534	0.623	0.137	0.359	-0.869	-1.673	No
LPE 16:0	0.191	0.119	0.898	0.857	0.815	-0.136	No
LPE 18:0	0.779	0.938	0.144	-0.144	-0.072	0.759	No
LPE 18:1	0.655	0.122	0.246	0.585	1.939	0.988	No
LPE 18:2	0.110	0.368	0.837	1.827	-1.602	0.350	No
PC 30:0 PC 14:0_16:0	0.117	0.692	0.548	0.674	0.148	-0.174	No
PC 31:0 PC 15:0_16:0	0.705	0.815	0.532	0.203	0.100	-0.366	No
PC 32:0	0.291	0.063	0.027	-0.711	-1.197	-1.505	No
PC 32:0 PC 16:0_16:0	0.323	0.957	0.862	0.380	0.019	-0.041	No
PC 32:1 PC 16:0_16:1	0.019	0.821	0.995	1.012	0.048	-0.002	Yes

PC 32:2 PC 14:0_18:2	0.008	0.343	0.947	1.000	0.258	0.016	Yes
PC 33:0	0.061	0.965	0.967	0.418	-0.012	-0.012	No
PC 33:1 PC 15:0_18:1	0.006	0.590	0.505	1.056	-0.099	0.196	Yes
PC 33:2 PC 15:0_18:2	0.096	0.789	0.355	0.585	-0.058	0.299	No
PC 34:0 PC 16:0_18:0	0.500	0.790	0.306	0.136	0.042	0.136	No
PC 34:1 PC 16:0_18:1	0.004	0.830	0.238	0.763	0.028	0.233	Yes
PC 34:2 PC 16:0_18:2	0.015	0.578	0.359	0.444	0.072	0.174	Yes
PC 34:3	0.215	0.424	0.813	0.487	0.161	-0.091	No
PC 34:3 PC 16:1_18:2	0.001	0.735	0.956	0.849	0.052	0.014	Yes
PC 34:4 PC 14:0_20:4	0.029	0.345	0.305	0.777	0.338	-0.339	Yes
PC 35:0	0.856	0.509	0.992	-0.120	-0.378	0.006	No
PC 35:1	0.001	0.641	0.261	0.835	-0.081	0.250	Yes
PC 35:2 PC 17:0_18:2	0.140	0.251	0.320	0.458	-0.183	0.309	No
PC 35:3	0.198	0.201	0.836	0.628	-0.394	0.097	No
PC 35:4	0.646	0.956	0.738	0.128	-0.009	-0.089	No
PC 36:0 PC 18:0_18:0	0.091	0.591	0.587	-0.357	0.091	-0.096	No
PC 36:1 PC 18:0_18:1	0.001	0.683	0.303	0.641	-0.075	0.177	Yes
PC 36:2 PC 18:0_18:2	0.019	0.663	0.393	0.463	-0.050	0.137	Yes
PC 36:2 PC 18:1_18:1	0.036	0.718	0.856	0.455	-0.046	0.030	Yes
PC 36:3 PC 16:0_20:3	0.000	0.083	0.575	1.075	0.754	0.162	Yes
PC 36:3 PC 16:0_20:3	0.001	0.454	0.360	1.993	0.267	0.389	Yes
PC 36:3 PC 16:0_20:3	0.011	0.153	0.792	0.950	0.289	-0.084	Yes
PC 36:3 PC 18:1_18:2	0.365	0.231	0.499	0.302	-0.222	0.160	No
PC 36:4	0.751	0.731	0.397	0.065	0.056	-0.187	No
PC 36:4	0.396	0.406	0.334	0.452	-0.138	0.320	No
PC 36:4 PC 16:0_20:4	0.730	0.911	0.571	0.061	-0.015	-0.091	No
PC 36:4 PC 18:2_18:2	0.281	0.343	0.232	0.592	-0.182	0.422	No
PC 36:5 PC 16:1_20:4	0.494	0.406	0.420	0.309	0.192	-0.276	No
PC 36:6 PC 14:0_22:6	0.070	0.196	0.961	1.132	0.509	-0.021	No
PC 37:1	0.163	0.318	0.909	0.636	-0.555	0.050	No
PC 37:2 PC 19:0_18:2	0.579	0.122	0.392	0.199	-0.405	0.239	No
PC 37:2 PC 19:0_18:2	0.866	0.183	0.182	0.100	-0.838	-0.442	No
PC 37:4	0.044	0.544	0.015	-0.350	-0.067	-0.319	Yes
PC 37:4 PC 17:0_20:4	0.357	0.123	0.330	-0.300	-0.243	-0.198	No
PC 37:5	0.007	0.733	0.934	0.971	0.187	-0.027	Yes
PC 37:6 PC 15:0_22:6	0.232	0.525	0.187	0.433	-0.199	0.381	No
PC 38:1	0.091	0.224	0.702	0.537	-0.482	-0.162	No
PC 38:2 PC 18:0_20:2	0.025	0.160	0.584	0.730	-0.362	0.135	Yes
PC 38:2 PC 20:0_18:2	0.038	0.480	0.756	0.975	0.238	0.157	Yes
PC 38:3 PC 18:0_20:3	0.007	0.566	0.900	0.722	0.114	0.027	Yes
PC 38:3 PC 18:0_20:3	0.047	0.480	0.198	0.765	0.139	-0.311	Yes
PC 38:4 PC 16:0_22:4	0.042	0.418	0.978	0.843	0.401	0.010	Yes
PC 38:4 PC 18:0_20:4	0.072	0.131	0.076	-0.342	-0.173	-0.263	No
PC 38:5 PC 16:0_22:5	0.429	0.752	0.503	0.325	0.093	-0.175	No
PC 38:5 PC 16:0_22:5	0.043	0.694	0.809	1.063	0.174	-0.078	Yes
PC 38:5 PC 18:1_20:4	0.169	0.292	0.533	-0.329	-0.136	-0.139	No

PC 38:6 PC 16:0_22:6	0.611	0.586	0.502	0.136	-0.107	0.136	No
PC 38:6 PC 18:2_20:4	0.753	0.538	0.501	0.066	0.104	0.173	No
PC 38:7	0.551	0.504	0.716	0.149	0.167	-0.119	No
PC 39:5 PC 17:0_22:5	0.028	0.425	0.705	0.606	-0.337	-0.137	Yes
PC 39:6 PC 17:0_22:6	0.911	0.072	0.963	-0.038	-0.342	-0.011	No
PC 39:7	0.139	0.200	0.118	-0.462	-0.283	-0.333	No
PC 40:2	0.125	0.123	0.491	0.809	-0.928	-0.312	No
PC 40:3	0.002	0.538	0.473	2.076	0.270	-0.298	Yes
PC 40:4	0.307	0.635	0.083	-0.284	-0.076	-0.320	No
PC 40:4 PC 18:0_22:4	0.187	0.754	0.420	0.457	0.105	-0.194	No
PC 40:4 PC 20:0_20:4	0.643	0.831	0.332	0.290	-0.092	-0.675	No
PC 40:5	0.024	0.035	0.048	-0.450	-0.363	-0.449	Yes
PC 40:5 PC 18:0_22:5	0.102	0.525	0.054	0.774	-0.182	-0.411	No
PC 40:5 PC 18:0_22:5	0.553	0.267	0.046	0.147	-0.159	-0.357	No
PC 40:6 PC 18:0_22:6	0.652	0.083	0.156	-0.122	-0.384	-0.147	No
PC 40:6 PC 20:2_20:4	0.017	0.691	0.234	0.507	0.182	-0.445	Yes
PC 40:7 PC 18:1_22:6	0.804	0.337	0.382	-0.060	-0.192	0.292	No
PC 40:8 PC 18:2_22:6	0.364	0.666	0.611	0.357	-0.153	0.217	No
PC 40:8 PC 20:4_20:4	0.009	0.291	0.934	-0.502	0.175	-0.017	Yes
PC 40:9	0.453	0.010	0.850	0.954	2.252	-0.291	No
PC 41:5	0.375	0.083	0.099	0.699	-0.621	-0.748	No
PC 42:10 PC 20:4_22:6	0.183	0.930	0.640	-0.374	-0.027	0.154	No
PC 42:5	0.928	0.270	0.442	0.031	-0.512	-0.292	No
PC 42:6 PC 18:0_24:6	0.075	0.795	0.402	1.272	0.190	-0.390	No
PC 42:8	0.180	0.530	0.856	-0.575	0.312	-0.089	No
PC 42:9 PC 20:4_22:5	0.207	0.631	0.767	0.734	-0.315	-0.106	No
PC O-32:0 PC O-16:0_16:0	0.603	0.596	0.972	0.144	-0.141	-0.008	No
PC O-32:1	0.712	0.221	0.285	0.080	-0.235	0.247	No
PC O-32:1	0.884	0.812	0.438	-0.080	0.095	-0.401	No
PC O-34:0	0.362	0.993	0.595	0.442	0.005	-0.308	No
PC O-34:1 PC O-18:1_16:0	0.296	0.772	0.597	0.240	-0.054	0.100	No
PC O-34:2	0.160	0.914	0.712	0.379	0.026	-0.068	No
PC O-34:3 PC O-16:1_18:2	0.780	0.233	0.790	0.130	-1.478	0.116	No
PC O-36:3	0.248	0.739	0.504	0.335	0.116	-0.196	No
PC O-36:3	0.121	0.691	0.753	1.159	0.197	-0.162	No
PC O-36:4 PC O-16:0_20:4	0.346	0.935	0.726	0.202	-0.012	-0.074	No
PC O-36:5 PC O-16:1_20:4	0.779	0.203	0.539	-0.055	-0.253	0.130	No
PC O-38:4 PC O-16:0_22:4	0.194	0.640	0.245	0.296	-0.060	0.204	No
PC O-38:4 PC O-18:0_20:4	0.217	0.724	0.582	0.267	-0.052	-0.117	No
PC O-38:5 PC O-16:1_22:4	0.444	0.378	0.679	0.473	0.382	-0.249	No
PC O-38:5 PC O-18:1_20:4	0.427	0.437	0.806	0.167	-0.113	-0.054	No
PC O-38:6 PC O-16:0_22:6	0.437	0.596	0.488	0.325	0.098	0.206	No
PC O-38:6 PC O-18:2_20:4	0.340	0.169	0.777	-0.450	-0.562	-0.115	No
PC O-38:7 PC O-16:1_22:6	0.081	0.554	0.399	-0.936	-0.280	0.304	No
PC O-39:10	0.004	0.772	0.497	0.975	0.063	0.182	Yes
PC O-40:4 PC O-20:0_20:4	0.263	0.377	0.008	0.446	-0.251	-0.929	No

PC O-40:7 PC O-18:1_22:6	0.658	0.530	0.904	0.351	-0.165	0.067	No
PC O-40:8	0.806	0.236	0.615	0.071	-0.196	-0.148	No
PC O-41:10	0.002	0.664	0.828	0.711	-0.125	-0.056	Yes
PC O-41:11	0.077	0.713	0.480	0.552	-0.089	-0.168	No
PE 34:2 PE 16:0_18:2	0.041	0.478	0.169	2.594	-0.752	0.851	Yes
PE 36:2 PE 18:0_18:2	0.011	0.512	0.455	1.802	-0.523	0.389	Yes
PE 36:4 PE 16:0_20:4	0.066	0.758	0.907	1.059	-0.125	0.046	No
PE 38:4 PE 18:0_20:4	0.085	0.782	0.703	0.768	-0.136	-0.109	No
PE 38:5 PE 18:1_20:4	0.258	0.652	0.279	1.362	-0.303	-0.655	No
PE 38:6 PE 16:0_22:6	0.131	0.449	0.632	1.385	-0.468	0.276	No
PE 40:6 PE 18:0_22:6	0.586	0.227	0.952	0.162	-0.412	0.016	No
PE O-36:5 PE O-16:1_20:4	0.668	0.569	0.365	0.261	-0.232	-0.340	No
PE O-38:5 PE O-18:1_20:4	0.287	0.591	0.104	0.541	-0.204	-0.499	No
PE O-38:6 PE O-18:2_20:4	0.266	0.398	0.361	1.106	-0.529	-0.518	No
PE P-36:4 PE P-16:0_20:4	0.855	0.820	0.128	0.141	-0.105	-0.882	No
PE P-38:5 PE P-18:1_20:4	0.757	0.749	0.301	0.281	-0.166	-0.716	No
PI 36:4	0.456	0.418	0.380	0.219	-0.214	-0.255	No
PI 38:4 PI 18:0_20:4	0.470	0.025	0.009	-0.228	-0.421	-0.667	No
SE 28:1/20:4	0.127	0.951	0.625	-1.148	-0.024	-0.155	No
SE 29:1/20:4	0.082	0.945	0.506	-0.859	0.028	-0.264	No
SE 29:2/20:4	0.177	0.291	0.274	1.082	-0.901	-0.398	No
SM 32:1;2O	0.382	0.455	0.350	0.375	0.186	-0.276	No
SM 33:1;2O	0.627	0.274	0.855	0.103	-0.144	-0.026	No
SM 34:0;2O	0.354	0.488	0.666	0.322	0.144	-0.086	No
SM 34:1;2O	0.877	0.624	0.511	0.041	0.078	0.104	No
SM 34:1;3O	0.760	0.238	0.769	-0.128	-0.674	-0.119	No
SM 34:2;2O	0.342	0.033	0.569	-0.262	-0.380	-0.105	No
SM 34:2;3O	0.638	0.139	0.126	0.337	-0.754	-0.973	No
SM 35:1;2O	0.125	0.870	0.963	0.234	-0.028	0.007	No
SM 36:1;2O	0.218	0.266	0.853	0.435	0.282	0.040	No
SM 36:2;2O	0.725	0.327	0.091	0.072	-0.180	-0.260	No
SM 38:1;2O	0.079	0.149	0.124	0.478	0.307	0.268	No
SM 39:1;2O	0.166	0.948	0.870	0.697	-0.041	-0.087	No
SM 40:1;2O	0.182	0.109	0.112	0.232	0.257	0.202	No
SM 40:2;2O	0.859	0.225	0.679	0.049	-0.265	0.083	No
SM 40:2;2O	0.633	0.989	0.635	0.111	-0.002	0.104	No
SM 41:1;2O	0.972	0.299	0.364	-0.006	-0.183	0.100	No
SM 41:2;2O	0.347	0.037	0.621	-0.520	-0.801	-0.128	No
SM 41:2;2O	0.130	0.565	0.850	0.391	0.085	-0.042	No
SM 42:1;2O	0.693	0.772	0.717	-0.057	-0.037	0.037	No
SM 42:2;2O	0.295	0.200	0.374	0.256	0.234	0.134	No
SM 42:2;2O	0.390	0.048	0.562	-0.340	-0.454	-0.115	No
SM 42:3;2O	0.462	0.508	0.920	0.162	0.141	0.015	No
SM 43:1;2O	0.048	0.052	0.900	-1.195	-0.895	0.037	Yes
SM 43:1;2O	0.832	0.330	0.495	-0.059	-0.270	-0.222	No
SM 43:2;2O	0.691	0.009	0.857	-0.285	-1.840	-0.166	No

ST 24:1;O4	0.042	0.589	0.016	1.768	0.255	1.536	No
ST 24:1;O4	0.318	0.430	0.583	0.792	-0.611	0.446	No
ST 24:1;O4	0.556	0.149	0.142	0.667	0.598	1.455	Yes
ST 27:1;O	0.150	0.665	0.935	0.346	-0.094	0.020	No
ST 27:1;O	0.940	0.439	0.424	-0.023	-0.258	-0.286	No
ST 27:1;O;S	0.651	0.226	0.516	0.112	-0.334	-0.167	No
ST 28:1;O;S	0.468	0.043	0.332	-0.415	-0.643	-0.248	No
TG 42:1 TG 12:0_12:0_18:1	0.087	0.007	0.710	0.628	0.348	0.087	No
TG 44:0 TG 14:0_14:0_16:0	0.052	0.320	0.948	0.440	-0.124	0.008	No
TG 44:1 TG 12:0_16:0_16:1	0.518	0.515	0.455	-0.312	0.206	-0.296	No
TG 44:1 TG 14:0_16:0_14:1	0.014	0.617	0.041	0.652	0.060	-0.187	Yes
TG 45:0 TG 14:0_15:0_16:0	0.377	0.900	0.686	0.089	0.008	-0.044	No
TG 45:1 TG 14:0_15:0_16:1	0.328	0.600	0.778	0.119	0.070	0.023	No
TG 46:0 TG 14:0_16:0_16:0	0.018	0.761	0.578	0.677	-0.042	-0.131	Yes
TG 46:1 TG 14:0_16:0_16:1	0.013	0.718	0.428	0.983	0.054	-0.079	Yes
TG 46:2 TG 12:0_16:0_18:2	0.005	0.410	0.194	0.553	-0.130	-0.284	Yes
TG 46:3 TG 12:0_16:1_18:2	0.025	0.322	0.599	2.181	0.643	-0.466	Yes
TG 47:0 TG 15:0_16:0_16:0	0.003	0.273	0.917	0.474	0.092	-0.013	Yes
TG 47:1 TG 15:0_16:0_16:1	0.015	0.575	0.859	0.579	-0.049	0.016	Yes
TG 48:0 TG 16:0_16:0_16:0	0.002	0.857	0.678	0.977	-0.035	-0.094	Yes
TG 48:1 TG 14:0_16:0_18:1	0.003	0.993	0.402	1.680	0.002	-0.200	Yes
TG 48:2 TG 14:0_16:0_18:2	0.006	0.601	0.411	1.856	0.184	-0.286	Yes
TG 48:4 TG 12:0_18:2_18:2	0.153	0.592	0.144	1.037	0.399	-1.272	No
TG 49:0 TG 15:0_16:0_18:0	0.045	0.695	0.537	0.470	0.053	0.093	Yes
TG 49:1 TG 15:0_16:0_18:1	0.003	0.842	0.929	1.245	0.039	-0.020	Yes
TG 49:2 TG 16:0_16:1_17:1	0.010	0.760	0.604	1.499	0.124	0.171	Yes
TG 49:3 TG 15:0_16:1_18:2	0.022	0.651	0.606	1.423	0.202	-0.181	Yes
TG 50:0 TG 16:0_16:0_18:0	0.003	0.957	0.717	0.970	-0.013	-0.083	Yes
TG 50:1 TG 16:0_16:0_18:1	0.002	0.871	0.574	1.718	-0.062	-0.224	Yes
TG 50:2 TG 16:0_16:1_18:1	0.004	0.957	0.580	1.606	0.021	-0.202	Yes
TG 50:3 TG 16:0_16:1_18:2	0.009	0.908	0.362	1.408	0.042	-0.336	Yes
TG 50:4 TG 16:1_16:1_18:2	0.030	0.834	0.725	1.469	0.108	-0.237	Yes
TG 50:5 TG 16:0_16:1_18:4	0.043	0.425	0.199	1.280	-0.240	-0.512	Yes
TG 51:0 TG 16:0_17:0_18:0	0.053	0.408	0.412	0.428	0.126	0.127	No
TG 51:1 TG 16:0_17:0_18:1	0.002	0.921	0.953	1.471	-0.026	-0.018	Yes
TG 51:2 TG 16:0_17:1_18:1	0.006	0.924	0.985	1.438	-0.027	-0.006	Yes
TG 51:3 TG 15:0_18:1_18:2	0.027	0.753	0.798	1.220	-0.116	-0.116	Yes
TG 51:4 TG 15:0_18:2_18:2	0.039	0.880	0.937	1.002	0.076	-0.049	Yes
TG 52:0 TG 16:0_18:0_18:0	0.037	0.850	0.726	0.512	0.036	0.060	Yes
TG 52:1 TG 16:0_18:0_18:1	0.002	0.949	0.998	1.925	-0.022	-0.001	Yes
TG 52:2 TG 16:0_18:1_18:1	0.008	0.453	0.882	1.049	-0.284	0.062	Yes
TG 52:3 TG 16:0_18:1_18:2	0.059	0.561	0.835	0.686	-0.183	-0.078	No
TG 52:4 TG 16:0_18:2_18:2	0.078	0.591	0.731	0.868	-0.207	-0.156	No
TG 52:5 TG 16:0_18:2_18:3	0.062	0.851	0.559	0.908	-0.072	-0.253	No
TG 52:6 TG 16:1_18:2_18:3	0.046	0.672	0.101	0.900	-0.118	-0.748	Yes
TG 53:1 TG 17:0_18:0_18:1	0.004	0.873	0.577	1.218	-0.049	0.163	Yes

TG 53:2 TG 17:0_18:1_18:1	0.007	0.658	0.817	1.294	-0.127	0.087	Yes
TG 53:3 TG 17:0_18:1_18:2	0.011	0.497	0.983	1.269	-0.243	0.009	Yes
TG 53:4 TG 17:1_18:1_18:2	0.005	0.947	0.888	1.199	0.021	0.055	Yes
TG 53:5 TG 16:0_18:2_19:3	0.095	0.918	0.477	0.872	-0.038	-0.282	No
TG 53:6 TG 15:0_18:2_20:4	0.298	0.247	0.726	0.584	-0.619	-0.222	No
TG 54:0 TG 16:0_18:0_20:0	0.041	0.398	0.460	0.259	0.085	0.079	No
TG 54:2 TG 18:0_18:1_18:1	0.007	0.673	0.893	1.555	-0.172	-0.052	Yes
TG 54:3 TG 18:0_18:1_18:2	0.016	0.685	0.931	1.136	-0.185	-0.038	Yes
TG 54:4 TG 16:0_18:1_20:3	0.048	0.826	0.865	0.920	-0.081	-0.072	Yes
TG 54:4 TG 18:1_18:1_18:2	0.006	0.585	0.777	1.187	0.145	-0.095	Yes
TG 54:5 TG 16:0_18:1_20:4	0.115	0.901	0.651	0.940	-0.045	-0.220	No
TG 54:6 TG 16:0_18:2_20:4	0.665	0.244	0.284	0.192	-0.216	-0.338	No
TG 54:7 TG 16:0_18:2_20:5	0.340	0.790	0.023	0.391	-0.058	-0.493	No
TG 54:7 TG 18:2_18:2_18:3	0.803	0.811	0.060	0.119	-0.067	-0.594	No
TG 55:0 TG 15:0_16:0_24:0	0.902	0.522	0.559	-0.007	0.050	0.066	No
TG 55:2 TG 17:0_18:1_20:1	0.113	0.912	0.609	0.919	0.047	0.211	No
TG 55:3 TG 19:0_18:1_18:2	0.019	0.531	0.742	1.189	-0.263	0.145	Yes
TG 55:4 TG 17:0_18:1_20:3	0.029	0.598	0.747	1.095	0.309	0.198	Yes
TG 55:5 TG 17:0_18:1_20:4	0.051	0.875	0.899	0.792	0.033	0.059	No
TG 55:6 TG 16:0_17:0_22:6	0.175	0.471	0.871	0.678	-0.167	-0.069	No
TG 56:0 TG 16:0_16:0_24:0	0.054	0.687	0.436	0.144	0.048	0.080	No
TG 56:1 TG 16:0_18:0_22:1	0.014	0.889	0.775	0.979	0.054	0.132	Yes
TG 56:2 TG 16:0_22:0_18:2	0.005	0.935	0.725	1.644	-0.043	-0.177	Yes
TG 56:3 TG 16:0_22:1_18:2	0.014	0.849	0.548	1.449	0.091	0.273	Yes
TG 56:4 TG 16:0_18:1_22:3	0.014	0.989	0.725	1.295	0.006	-0.167	Yes
TG 56:5 TG 16:0_18:1_22:4	0.185	0.905	0.297	0.491	-0.031	-0.414	No
TG 56:6 TG 16:0_18:2_22:4	0.306	0.657	0.439	0.428	-0.071	-0.254	No
TG 56:7 TG 18:1_18:2_20:4	0.758	0.660	0.668	0.145	0.093	-0.168	No
TG 56:8 TG 18:2_18:2_20:4	0.375	0.186	0.441	-0.333	-0.290	-0.222	No
TG 56:9 TG 18:2_18:2_20:5	0.540	0.856	0.272	-0.217	-0.040	-0.326	No
TG 56:9 TG 18:2_18:3_20:4	0.804	0.439	0.002	0.123	-0.207	-0.764	No
TG 57:0 TG 16:0_17:0_24:0	0.024	0.149	0.254	-0.107	0.133	0.094	No
TG 57:1 TG 16:0_23:0_18:1	0.020	0.577	0.889	0.726	-0.133	0.055	Yes
TG 57:3 TG 18:1_18:1_21:1	0.023	0.622	0.510	1.316	0.397	0.477	Yes
TG 57:5 TG 17:0_18:1_22:4	0.398	0.448	0.301	0.598	-0.275	-0.512	No
TG 57:7 TG 17:0_18:1_22:6	0.210	0.380	0.631	1.110	-0.270	-0.223	No
TG 58:0 TG 16:0_18:0_24:0	0.241	0.769	0.834	0.158	0.038	-0.016	No
TG 58:1 TG 16:0_24:0_18:1	0.012	0.837	0.814	0.777	-0.099	0.084	Yes
TG 58:10 TG 18:2_18:2_22:6	0.123	0.360	0.060	-1.091	-0.337	-0.566	No
TG 58:2 TG 16:0_18:1_24:1	0.026	0.657	0.831	1.161	-0.256	0.118	Yes
TG 58:3 TG 22:0_18:1_18:2	0.035	0.699	0.903	1.192	-0.244	0.076	Yes
TG 58:4 TG 18:1_22:1_18:2	0.098	0.714	0.827	1.083	-0.227	0.168	No
TG 58:6 TG 18:0_18:1_22:5	0.096	0.745	0.753	2.379	0.119	-0.168	No
TG 58:7 TG 18:1_18:1_22:5	0.702	0.101	0.990	0.171	0.385	0.004	No
TG 58:8 TG 18:1_18:2_22:5	0.842	0.496	0.299	0.094	-0.188	-0.258	No
TG 58:9 TG 18:2_20:3_20:4	0.439	0.669	0.058	-0.462	-0.151	-0.463	No

TG 60:10 TG 18:1_20:4_22:5	0.664	0.923	0.695	-0.285	-0.025	-0.120	No
TG 60:11 TG 18:2_20:4_22:5	0.185	0.508	0.406	-0.991	-0.155	-0.225	No
TG 60:12 TG 18:2_20:4_22:6	0.343	0.247	0.013	-0.858	-0.456	-0.649	No
TG 60:2 TG 16:0_20:1_24:1	0.030	0.848	0.705	1.090	-0.129	0.235	Yes
TG 60:3 TG 16:0_26:1_18:2	0.038	0.587	0.851	1.164	-0.372	0.121	Yes
TG 60:5 TG 24:1_18:2_18:2	0.026	0.802	0.685	1.700	0.242	-0.217	Yes
TG 60:9 TG 18:0_20:4_22:5	0.693	0.200	0.870	-0.325	0.334	-0.038	No
TG 60:9 TG 18:1_20:4_22:4	0.975	0.234	0.182	0.019	-0.416	-0.387	No
TG 62:13 TG 20:4_20:4_22:5	0.392	0.335	0.151	-1.326	-0.666	-0.512	No
TG 62:14 TG 20:4_20:4_22:6	0.987	0.569	0.408	-0.041	-0.271	-0.363	No
TG 62:2 TG 18:0_18:1_26:1	0.026	0.818	0.535	1.509	-0.255	0.499	Yes
TG 62:4 TG 18:1_26:1_18:2	0.046	0.615	0.464	1.349	-0.561	0.806	Yes

Table S4. Enrichment analysis results for lipid classes and fatty acid residues.

Class / Residue	Number of Features			<i>p</i> -Value		Enrichment Score	
	Total	Increased	Decreased	Increase	Decrease	Increase	Decrease
FA 12:0	6	0	0	-	-	-	-
FA 14:0	16	7	0	0.634461	1	0.973536	0
FA 15:0	17	8	0	0.524319	1	1.047165	0
FA 16:0	82	50	0	0.001069	1	1.356845	0
FA 16:1	20	14	0	0.019074	1	1.557658	0
FA 17:0	18	6	0	0.895631	1	0.741742	0
FA 17:1	5	0	0	-	-	-	-
FA 18:0	39	17	0	0.632847	1	0.96997	0
FA 18:1	69	40	0	0.013514	1	1.289986	0
FA 18:2	76	31	0	0.819999	1	0.907658	0
FA 18:3	9	1	0	0.995622	1	0.247247	0
FA 20:0	5	0	0	-	-	-	-
FA 20:3	9	7	0	0.047855	1	1.730731	0
FA 20:4	51	8	6	0.999999	5.93E-06	0.349055	8.302521
FA 22:0	5	0	0	-	-	-	-
FA 22:4	10	1	0	0.997626	1	0.222523	0
FA 22:5	18	3	1	0.997807	0.230062	0.370871	3.920635
FA 22:6	22	0	0	1	1	0	0
FA 24:0	8	0	0	-	-	-	-
FA 24:1	9	0	0	-	-	-	-
CAR	4	0	0	-	-	-	-
CE	6	0	2	1	0.011026	0	11.36364
Cer	8	1	0	0.903087	1	0.49867	0
DG	38	10	3	0.493366	0.308382	1.049832	1.794258
FA	33	0	1	1	0.642172	0	1.033058
HexCer	5	0	0	-	-	-	-
LPC	31	1	2	0.999916	0.228206	0.128689	2.199413
LPE	4	0	0	-	-	-	-
PC	77	24	3	0.108964	0.400539	1.243437	1.328217
PC-O	24	2	0	0.992612	1	0.332447	0
PE	7	2	0	0.558402	1	1.139818	0
PE-O	3	0	0	-	-	-	-
PE-P	2	0	0	-	-	-	-
PI	2	0	0	-	-	-	-
SM	25	0	1	1	0.536804	0	1.363636
ST	7	1	0	0.86984	1	0.569909	0
TG	97	53	0	8.87e-14	1	2.179754	0