

Supplementary Information

Table S1. Plaque cholesteryl esters.

Metabolite	Formula	<i>m/z</i> Found	mDa	PPM	Time	Area %
CE 18:2	C ₄₅ H ₇₉ NO ₂	666.6204	1.5	2.3	9.17	33.34
CE 18:3	C ₄₅ H ₇₇ NO ₂	664.6039	0.7	1	8.94	15.13
CE 22:4	C ₄₉ H ₈₃ NO ₂	718.6522	2	2.8	9.28	12.45
CE 20:3	C ₄₇ H ₈₁ NO ₂	692.6372	2.7	3.9	9.27	10.35
CE 24:2	C ₅₁ H ₉₁ NO ₂	750.713	0.2	0.3	9.96	7.12
CE 20:1	C ₄₇ H ₈₅ NO ₂	696.6668	1	1.4	9.68	4.39
CE 18:1	C ₄₅ H ₈₁ NO ₂	668.6354	0.9	1.3	9.4	3.76
CE 24:1	C ₅₁ H ₉₃ NO ₂	752.7309	2.5	3.3	10.15	3.48
CE 22:2	C ₄₉ H ₈₇ NO ₂	722.6819	0.4	0.6	9.7	2.65
CE 22:1	C ₄₉ H ₈₉ NO ₂	724.6968	-0.3	-0.5	9.94	1.50
CE 22:5	C ₄₉ H ₈₁ NO ₂	716.6349	0.4	0.5	9.12	0.97
CE 24:4	C ₅₁ H ₈₇ NO ₂	746.6808	-0.7	-0.9	9.53	0.89
CE 16:1	C ₄₃ H ₇₇ NO ₂	640.6038	0.6	0.9	9.13	0.82
CE 26:2	C ₅₃ H ₉₅ NO ₂	778.7448	0.7	0.9	10.17	0.77
CE 18:0	C ₄₅ H ₈₃ NO ₂	670.6501	-0.1	-0.1	9.57	0.54
CE 24:5	C ₅₁ H ₈₅ NO ₂	744.666	0.2	0.2	9.33	0.52
CE 24:3	C ₅₁ H ₈₉ NO ₂	748.6974	0.3	0.4	9.78	0.44
CE 26:1	C ₅₃ H ₉₇ NO ₂	780.7601	0.4	0.5	10.36	0.36
CE 26:3	C ₅₃ H ₉₃ NO ₂	776.7288	0.4	0.5	9.99	0.14
CE 26:4	C ₅₃ H ₉₁ NO ₂	774.7115	-1.3	-1.7	9.79	0.14
CE 20:2	C ₄₇ H ₈₃ NO ₂	694.6499	-0.3	-0.4	9.37	0.10

Table S2. Plaque triacylglycerols.

Metabolite	Formula	<i>m/z</i> Found	mDa	PPM	Time	Area %
TG 52:4	C ₅₅ H ₁₀₁ NO ₆	872.7699	-0.8	-0.9	8.56	10.17
TG 54:6	C ₅₇ H ₁₀₁ NO ₆	896.7709	0.2	0.2	8.38	8.89
TG 52:3	C ₅₅ H ₁₀₃ NO ₆	874.7882	1.9	2.1	8.8	7.40
TG 54:5	C ₅₇ H ₁₀₃ NO ₆	898.7861	-0.2	-0.3	8.62	7.32
TG 52:5	C ₅₅ H ₉₉ NO ₆	870.7543	-0.7	-0.9	8.35	7.23
TG 52:2	C ₅₅ H ₁₀₅ NO ₆	876.8045	2.5	2.9	9.03	6.13
TG 54:7	C ₅₇ H ₉₉ NO ₆	894.7551	0.1	0.1	8.14	5.82
TG 54:4	C ₅₇ H ₁₀₅ NO ₆	900.8044	2.4	2.7	8.84	5.67
TG 50:2	C ₅₃ H ₁₀₁ NO ₆	848.7718	1.1	1.3	8.76	5.45
TG 50:1	C ₅₃ H ₁₀₃ NO ₆	850.7883	2	2.3	8.96	4.97
TG 50:3	C ₅₃ H ₉₉ NO ₆	846.7545	-0.5	-0.6	8.52	4.38
TG 54:3	C ₅₇ H ₁₀₇ NO ₆	902.8206	3	3.3	9.06	3.99
TG 50:4	C ₅₃ H ₉₇ NO ₆	844.7394	0	0	8.31	3.06
TG 54:2	C ₅₇ H ₁₀₉ NO ₆	904.8304	-2.9	-3.2	9.26	2.89
TG 52:6	C ₅₅ H ₉₇ NO ₆	868.7403	0.9	1	8.1	2.50
TG 48:0	C ₅₁ H ₁₀₁ NO ₆	824.7731	2.4	2.9	8.95	2.32

Table S2. Cont.

Metabolite	Formula	<i>m/z</i> Found	mDa	PPM	Time	Area %
TG 48:2	C ₅₁ H ₉₇ NO ₆	820.738	-1.4	-1.7	8.5	2.28
TG 48:1	C ₅₁ H ₉₉ NO ₆	822.7538	-1.2	-1.5	8.73	1.64
TG 48:3	C ₅₁ H ₉₅ NO ₆	818.7233	-0.4	-0.5	8.26	1.34
TG 54:8	C ₅₇ H ₉₇ NO ₆	892.7384	-1	-1.1	7.91	1.13
TG 50:5	C ₅₃ H ₉₅ NO ₆	842.7247	1	1.1	8.07	1.05
TG 46:0	C ₄₉ H ₉₇ NO ₆	796.7384	-1	-1.2	8.72	0.47
TG 56:6	C ₅₉ H ₁₀₅ NO ₆	924.8013	-0.7	-0.7	8.69	0.46
TG 56:7	C ₅₉ H ₁₀₃ NO ₆	922.7852	-1.1	-1.2	8.49	0.40
TG 46:1	C ₄₉ H ₉₅ NO ₆	794.7227	-1	-1.3	8.48	0.39
TG 46:2	C ₄₉ H ₉₃ NO ₆	792.7072	-0.9	-1.1	8.24	0.38
TG 56:5	C ₅₉ H ₁₀₇ NO ₆	926.8188	1.2	1.3	8.89	0.30
TG 56:8	C ₅₉ H ₁₀₁ NO ₆	920.77	-0.7	-0.8	8.28	0.26
TG 48:4	C ₅₁ H ₉₃ NO ₆	816.7067	-1.4	-1.7	8.02	0.25
TG 56:4	C ₅₉ H ₁₀₉ NO ₆	928.8317	-1.6	-1.7	9.09	0.19
TG 56:3	C ₅₉ H ₁₁₁ NO ₆	930.8468	-2.1	-2.3	9.28	0.18
TG 52:7	C ₅₅ H ₉₅ NO ₆	866.7227	-1	-1.2	7.87	0.15

Table S3. Plaque phosphatidylcholines.

Metabolite	Formula	<i>m/z</i> Found	mDa	PPM	Time	Area %
PC 34:2	C ₄₂ H ₈₀ NO ₈ P	758.5709	0.9	1.2	4.83	21.34
PC 36:2	C ₄₄ H ₈₄ NO ₈ P	786.6002	-1.1	-1.3	5.41	16.69
PC 34:1	C ₄₂ H ₈₂ NO ₈ P	760.5865	0.9	1.2	5.28	12.96
PC 36:3	C ₄₄ H ₈₂ NO ₈ P	784.586	0.4	0.5	4.91	12.09
PC 36:4	C ₄₄ H ₈₀ NO ₈ P	782.5703	0.3	0.4	4.74	10.89
PC 36:4	C ₄₄ H ₈₀ NO ₈ P	782.5684	-1.6	-2	4.44	5.22
PC 38:4	C ₄₆ H ₈₄ NO ₈ P	810.6002	-1.1	-1.3	5.35	3.74
PC 36:1	C ₄₄ H ₈₆ NO ₈ P	788.6161	-0.8	-1	5.83	3.53
PC 32:1	C ₄₀ H ₇₈ NO ₈ P	732.5553	1	1.4	4.68	3.35
PC 34:3	C ₄₂ H ₇₈ NO ₈ P	756.5541	-0.2	-0.3	4.39	2.21
PC 38:6	C ₄₆ H ₈₀ NO ₈ P	806.5701	0.1	0.2	4.34	1.80
PC 34:3	C ₄₂ H ₇₈ NO ₈ P	756.5545	0.2	0.3	4.31	1.36
PC 32:2	C ₄₀ H ₇₆ NO ₈ P	730.5395	0.8	1.2	4.2	0.77
PC 38:4	C ₄₆ H ₈₄ NO ₈ P	810.5999	-1.4	-1.7	4.98	0.64
PC 38:5	C ₄₆ H ₈₂ NO ₈ P	808.5854	-0.2	-0.3	4.77	0.60
PC 38:5	C ₄₆ H ₈₂ NO ₈ P	808.5854	-0.2	-0.3	4.97	0.57
PC 38:4	C ₄₆ H ₈₄ NO ₈ P	810.6024	1.1	1.4	5.15	0.38
PC 36:5	C ₄₄ H ₇₈ NO ₈ P	780.555	0.7	0.9	4.34	0.36
PC 38:2	C ₄₆ H ₈₈ NO ₈ P	814.6329	0.3	0.4	5.9	0.27
PC 38:3	C ₄₆ H ₈₆ NO ₈ P	812.6171	0.2	0.2	5.56	0.25
PC 36:5	C ₄₄ H ₇₈ NO ₈ P	780.5558	1.5	1.9	4.01	0.23
PC 38:3	C ₄₆ H ₈₆ NO ₈ P	812.6154	-1.5	-1.9	5.45	0.23
PC 36:5	C ₄₄ H ₇₈ NO ₈ P	780.5543	0	0	4.21	0.18
PC 40:4	C ₄₈ H ₈₈ NO ₈ P	838.6312	-1.4	-1.6	5.72	0.13
PC 34:4	C ₄₂ H ₇₆ NO ₈ P	754.5413	2.6	3.5	4.13	0.11

Table S4. Plaque sphingomyelins.

Metabolite	Formula	<i>m/z</i> Found	mDa	PPM	Time	Area %
SM 16:0	C ₃₉ H ₇₉ N ₂ O ₆ P	703.5763	0.9	1.3	4.59	30.27
SM 24:0	C ₄₇ H ₉₅ N ₂ O ₆ P	815.699	-1.6	-1.9	6.8	18.49
SM 24:1	C ₄₇ H ₉₃ N ₂ O ₆ P	813.683	-1.9	-2.4	6.28	12.05
SM 16:1	C ₃₉ H ₇₇ N ₂ O ₆ P	701.5619	2.2	3.1	4.05	8.66
SM 22:0	C ₄₅ H ₉₁ N ₂ O ₆ P	787.6685	-0.8	-1	6.34	8.55
SM 24:1	C ₄₇ H ₉₃ N ₂ O ₆ P	813.6852	0.3	0.3	6.42	7.68
SM 24:2	C ₄₇ H ₉₁ N ₂ O ₆ P	811.6678	-1.5	-1.8	5.88	5.46
SM 20:0	C ₄₃ H ₈₇ N ₂ O ₆ P	759.6374	-0.6	-0.8	5.78	4.47
SM 22:1	C ₄₅ H ₈₉ N ₂ O ₆ P	785.653	-0.6	-0.8	5.92	2.49
SM 18:1	C ₄₁ H ₈₁ N ₂ O ₆ P	729.5923	1.3	1.7	4.69	0.68
SM 14:0	C ₃₇ H ₇₅ N ₂ O ₆ P	675.5459	1.8	2.7	3.94	0.67
SM 20:1	C ₄₃ H ₈₅ N ₂ O ₆ P	757.6223	0	0	5.34	0.28
SM 26:0	C ₄₉ H ₉₉ N ₂ O ₆ P	843.7312	-0.7	-0.8	7.24	0.14

Table S5. Plaque diacylglycerols.

Metabolite	Formula	<i>m/z</i> Found	mDa	PPM	Time	Area %
DG 46:11	C ₄₉ H ₇₇ NO ₅	760.5865	-1.5	-1.9	5.28	51.32
DG 44:10	C ₄₇ H ₇₅ NO ₅	734.573	0.7	0.9	5.19	28.13
DG 38:4	C ₄₁ H ₇₅ NO ₅	662.5737	1.4	2.1	6.52	8.04
DG 46:10	C ₄₉ H ₇₉ NO ₅	762.601	-2.6	-3.4	5.75	5.83
DG 36:2	C ₃₉ H ₇₅ NO ₅	638.5737	1.4	2.2	6.62	2.66
DG 34:2	C ₃₇ H ₇₁ NO ₅	610.5426	1.6	2.6	6.12	1.95
DG 36:3	C ₃₉ H ₇₃ NO ₅	636.5576	0.9	1.5	6.17	0.63
DG 36:4	C ₃₉ H ₇₁ NO ₅	634.5419	0.9	1.4	6.01	0.46
DG 34:1	C ₃₇ H ₇₃ NO ₅	612.5568	0.1	0.2	6.5	0.41
DG 36:1	C ₃₉ H ₇₇ NO ₅	640.5883	0.3	0.5	6.97	0.31

Table S6. Plaque PE-plas.

Metabolite	Formula	<i>m/z</i> Found	mDa	PPM	Time	Area %
PE_plas 38:4	C ₄₃ H ₇₈ NO ₇ P	752.5596	0.2	0.3	5.82	49.86
PE_plas 40:4	C ₄₅ H ₈₂ NO ₇ P	780.5913	0.6	0.8	6.17	13.92
PE_plas 38:5	C ₄₃ H ₇₆ NO ₇ P	750.5443	0.6	0.7	5.31	7.30
PE_plas 36:1	C ₄₁ H ₈₀ NO ₇ P	730.5765	1.5	2	6.28	6.56
PE_plas 36:4	C ₄₁ H ₇₄ NO ₇ P	724.5288	0.7	1	5.23	6.48
PE_plas 40:5	C ₄₅ H ₈₀ NO ₇ P	778.5758	0.8	1	5.99	4.08
PE_plas 38:4	C ₄₃ H ₇₈ NO ₇ P	752.5593	-0.1	-0.1	5.65	2.89
PE_plas 40:6	C ₄₅ H ₇₈ NO ₇ P	776.5585	-0.9	-1.2	5.66	2.54
PE_plas 40:5	C ₄₅ H ₈₀ NO ₇ P	778.575	0	-0.1	5.84	2.07
PE_plas 34:1	C ₃₉ H ₇₆ NO ₇ P	702.5452	1.5	2.1	5.75	1.97
PE_plas 36:2	C ₄₁ H ₇₈ NO ₇ P	728.5615	2.1	2.9	5.91	1.45
PE_plas 38:3	C ₄₃ H ₈₀ NO ₇ P	754.5743	-0.7	-1	6.08	0.63
PE_plas 32:4	C ₃₇ H ₆₆ NO ₇ P	668.4722	6.7	10	7.05	0.16

Table S7. Plaque PC-plas.

Metabolite	Formula	<i>m/z</i> Found	mDa	PPM	Time	Area %
PC-plas 36:4	C ₄₄ H ₈₀ NO ₇ P	766.5742	−0.8	−1.1	5.03	33.06
PC-plas 34:0	C ₄₂ H ₈₄ NO ₇ P	746.6058	−0.5	−0.7	5.64	21.89
PC-plas 38:4	C ₄₆ H ₈₄ NO ₇ P	794.6055	−0.8	−1.1	5.61	13.61
PC-plas 36:3	C ₄₄ H ₈₂ NO ₇ P	768.5907	0	0	5.11	10.66
PC-plas 38:4	C ₄₆ H ₈₄ NO ₇ P	794.6052	−1.1	−1.4	5.15	6.24
PC-plas 38:5	C ₄₆ H ₈₂ NO ₇ P	792.5909	0.2	0.3	5.07	4.65
PC-plas 38:3	C ₄₆ H ₈₆ NO ₇ P	796.6212	−0.8	−1	5.7	2.62
PC-plas 32:0	C ₄₀ H ₈₀ NO ₇ P	718.576	1	1.3	5.5	2.53
PC-plas 34:1	C ₄₂ H ₈₂ NO ₇ P	744.5905	−0.2	−0.3	5.19	1.65
PC-plas 36:1	C ₄₄ H ₈₆ NO ₇ P	772.6226	0.6	0.8	5.7	1.52
PC-plas 34:4	C ₄₂ H ₇₆ NO ₇ P	738.5445	0.8	1	5.54	0.56
PC-plas 36:2	C ₄₄ H ₈₄ NO ₇ P	770.6043	−2	−2.7	5.69	0.38
PC-plas 36:1	C ₄₄ H ₈₆ NO ₇ P	772.6212	−0.8	−1	6.11	0.36
PC-plas 40:3	C ₄₈ H ₉₀ NO ₇ P	824.6522	−1.1	−1.3	6.22	0.12

Table S8. Plaque fatty acids.

Metabolite	Formula	<i>m/z</i> Found	mDa	PPM	Time	Area %
FA 20:3	C ₂₀ H ₃₂ O ₂	303.2341	1.7	5.5	2.05	45.41
FA 18:0	C ₁₈ H ₃₄ O ₂	281.2485	0.4	1.5	2.62	22.95
FA 18:1	C ₁₈ H ₃₂ O ₂	279.2339	1.5	5.2	2.14	12.11
FA 22:3	C ₂₂ H ₃₆ O ₂	331.2642	0.5	1.4	2.52	5.96
FA 20:4	C ₂₀ H ₃₀ O ₂	301.2178	1	3.4	2.13	5.72
FA 22:4	C ₂₂ H ₃₄ O ₂	329.2487	0.6	1.9	2.12	2.88
FA 20:2	C ₂₀ H ₃₄ O ₂	305.2492	1.1	3.7	2.33	2.06
FA 20:1	C ₂₀ H ₃₆ O ₂	307.2643	0.6	1.8	2.76	0.76
FA 20:0	C ₂₀ H ₃₈ O ₂	309.2802	0.8	2.6	3.32	0.78
FA 22:2	C ₂₂ H ₃₈ O ₂	333.2789	−0.5	−1.4	3.02	0.64
FA 20:5	C ₂₀ H ₂₈ O ₂	299.2022	1.1	3.6	1.66	0.49
FA 22:5	C ₂₂ H ₃₂ O ₂	327.2331	0.7	2	1.88	0.12

Table S9. Plaque phosphatidylserines.

Metabolite	Formula	<i>m/z</i> Found	mDa	PPM	Time	Area %
PS 36:2	C ₄₂ H ₇₈ NO ₁₀ P	786.5281	−0.4	−0.6	4.91	77.41
PS 38:4	C ₄₄ H ₇₈ NO ₁₀ P	810.5272	−1.3	−1.6	4.91	9.14
PS 36:1	C ₄₂ H ₈₀ NO ₁₀ P	788.5422	−2	−2.5	5.36	5.84
PS 40:5	C ₄₆ H ₈₀ NO ₁₀ P	836.5426	−1.6	−1.9	4.91	4.66
PS 38:1	C ₄₄ H ₈₄ NO ₁₀ P	816.5726	−2.9	−3.5	5.14	1.25
PS 38:0	C ₄₄ H ₈₆ NO ₁₀ P	818.5909	−0.2	−0.3	5.56	0.87
PS 40:1	C ₄₆ H ₈₈ NO ₁₀ P	844.6029	−3.9	−4.6	5.7	0.32
PS 40:3	C ₄₆ H ₈₄ NO ₁₀ P	840.5715	−4	−4.7	5.05	0.22
PS 46:3	C ₅₂ H ₉₆ NO ₁₀ P	924.6756	6.2	6.7	6.97	0.18
PS 44:3	C ₅₀ H ₉₂ NO ₁₀ P	896.645	6.9	7.7	6.52	0.11

Table S10. Plaque lyso-phosphatidylcholines.

Metabolite	Formula	<i>m/z</i> Found	mDa	PPM	Time	Area %
LPC 18:0	C ₂₆ H ₅₄ NO ₇ P	524.3723	0.7	1.4	1.94	53.57
LPC 16:0	C ₂₄ H ₅₀ NO ₇ P	496.3405	0.2	0.4	1.49	38.20
LPC 18:1	C ₂₆ H ₅₂ NO ₇ P	522.3562	0.3	0.5	1.56	4.68
LPC 18:2	C ₂₆ H ₅₀ NO ₇ P	520.3405	0.2	0.4	1.31	3.56

Table S11. Plaque ceramides.

Metabolite	Formula	<i>m/z</i> Found	mDa	PPM	Time	Area %
Cer 24:0	C ₄₃ H ₈₅ NO ₅	694.6354	0.4	0.6	7.46	30.80
Cer 24:1	C ₄₃ H ₈₃ NO ₅	692.6192	-0.1	-0.2	7.03	20.79
Cer 22:0	C ₄₁ H ₈₁ NO ₅	666.6036	-0.1	-0.1	7.05	12.31
Cer 20:0	C ₃₉ H ₇₇ NO ₅	638.5743	1.9	3	6.58	8.22
Cer 24:1	C ₄₃ H ₈₃ NO ₅	692.6201	0.8	1.1	7.12	6.58
Cer 16:0	C ₃₅ H ₆₉ NO ₅	582.5099	0.1	0.2	5.5	6.55
Cer 24:2	C ₄₃ H ₈₁ NO ₅	690.6045	0.8	1.2	6.64	6.51
Cer 18:0	C ₃₇ H ₇₃ NO ₅	610.5396	-1.5	-2.4	6.09	3.65
Cer 22:1	C ₄₁ H ₇₉ NO ₅	664.5893	1.3	1.9	6.67	2.65
Cer 20:1	C ₃₉ H ₇₅ NO ₅	636.5552	-1.5	-2.4	6.16	1.17
Cer 24:3	C ₄₃ H ₇₉ NO ₅	688.5886	0.6	0.8	6.25	0.26
Cer 26:0	C ₄₅ H ₈₉ NO ₅	722.6662	-0.1	-0.1	7.84	0.25
Cer 16:4	C ₃₅ H ₆₁ NO ₅	574.4483	1.1	2	3.06	0.24

Table S12. Plaque phosphatidylglycerols.

Metabolite	Formula	<i>m/z</i> Found	mDa	PPM	Time	Area %
PG 36:3	C ₄₂ H ₇₇ O ₁₀ P	771.5178	0.2	0.2	4.03	19.62
PG 36:2	C ₄₂ H ₇₉ O ₁₀ P	773.5335	0.2	0.3	4.48	19.41
PG 36:1	C ₄₂ H ₈₁ O ₁₀ P	775.5472	-1.7	-2.2	4.97	11.26
PG 36:4	C ₄₂ H ₇₅ O ₁₀ P	769.5003	-1.7	-2.2	3.27	10.80
PG 36:3	C ₄₂ H ₇₇ O ₁₀ P	771.5144	-3.2	-4.2	3.66	7.12
PG 38:2	C ₄₄ H ₈₃ O ₁₀ P	801.5627	-1.9	-2.4	4.99	6.51
PG 36:2	C ₄₂ H ₇₉ O ₁₀ P	773.5325	-0.8	-1	4.19	3.58
PG 36:2	C ₄₂ H ₇₉ O ₁₀ P	773.5319	-1.4	-1.8	4.97	3.48
PG 36:2	C ₄₂ H ₇₉ O ₁₀ P	773.5331	-0.2	-0.2	4.91	3.23
PG 36:4	C ₄₂ H ₇₅ O ₁₀ P	769.5	-2	-2.6	3.6	2.39
PG 34:1	C ₄₀ H ₇₇ O ₁₀ P	747.5172	-0.4	-0.6	4.38	2.21
PG 36:3	C ₄₂ H ₇₇ O ₁₀ P	771.5154	-2.2	-2.9	3.82	2.19
PG 36:2	C ₄₂ H ₇₉ O ₁₀ P	773.5317	-1.6	-2	4.32	1.53
PG 34:2	C ₄₀ H ₇₅ O ₁₀ P	745.5021	0.1	0.2	3.94	1.47
PG 34:2	C ₄₀ H ₇₅ O ₁₀ P	745.5005	-1.5	-2	3.47	1.09
PG 34:3	C ₄₀ H ₇₃ O ₁₀ P	743.4861	-0.2	-0.3	3.04	0.60
PG 36:4	C ₄₂ H ₇₅ O ₁₀ P	769.5016	-0.4	-0.5	3.46	0.56
PG 38:1	C ₄₄ H ₈₅ O ₁₀ P	803.576	-4.2	-5.3	5.05	0.44

Table S12. *Cont.*

Metabolite	Formula	<i>m/z</i> Found	mDa	PPM	Time	Area %
PG 36:4	C ₄₂ H ₇₅ O ₁₀ P	769.5003	−1.7	−2.2	3.06	0.40
PG 34:1	C ₄₀ H ₇₇ O ₁₀ P	747.5153	−2.3	−3.1	4.21	0.37
PG 34:3	C ₄₀ H ₇₃ O ₁₀ P	743.4866	0.3	0.4	3.44	0.30
PG 38:4	C ₄₄ H ₇₉ O ₁₀ P	797.5336	0.3	0.4	4.07	0.25
PG 38:6	C ₄₄ H ₇₅ O ₁₀ P	793.5034	1.4	1.8	3.05	0.22
PG 34:2	C ₄₀ H ₇₅ O ₁₀ P	745.4987	−3.3	−4.4	3.58	0.19
PG 34:2	C ₄₀ H ₇₅ O ₁₀ P	745.5016	−0.4	−0.5	3.63	0.18
PG 34:2	C ₄₀ H ₇₅ O ₁₀ P	745.4984	−3.6	−4.8	3.69	0.17
PG 36:3	C ₄₂ H ₇₇ O ₁₀ P	771.5158	−1.8	−2.4	4.2	0.15
PG 36:5	C ₄₂ H ₇₃ O ₁₀ P	767.4822	−4.1	−5.4	3.02	0.14
PG 38:4	C ₄₄ H ₇₉ O ₁₀ P	797.5334	0.1	0.1	4.21	0.14

Table S13. Plaque phosphatidylinositols.

Metabolite	Formula	<i>m/z</i> Found	mDa	PPM	Time	Area %
PI 38:4	C ₄₇ H ₈₃ O ₁₃ P	885.5511	1.8	2	4.72	55.41
PI 38:3	C ₄₇ H ₈₅ O ₁₃ P	887.5631	−1.9	−2.1	4.95	32.95
PI 36:1	C ₄₅ H ₈₅ O ₁₃ P	863.5639	−1.1	−1.3	4.95	4.96
PI 36:2	C ₄₅ H ₈₃ O ₁₃ P	861.5517	2.4	2.7	4.79	1.77
PI 38:5	C ₄₇ H ₈₁ O ₁₃ P	883.5317	−2	−2.2	4.2	1.40
PI 36:4	C ₄₅ H ₇₉ O ₁₃ P	857.5182	0.2	0.2	4.13	1.18
PI 34:1	C ₄₃ H ₈₁ O ₁₃ P	835.5361	2.4	2.9	4.65	0.89
PI 36:3	C ₄₅ H ₈₁ O ₁₃ P	859.532	−1.7	−2	4.28	0.75
PI 34:2	C ₄₃ H ₇₉ O ₁₃ P	833.5151	−2.9	−3.5	4.19	0.71

Table S14. Plaque phosphatidylethanolamines.

Metabolite	Formula	<i>m/z</i> Found	mDa	PPM	Time	Area %
PE 36:4	C ₄₁ H ₇₄ NO ₈ P	738.5074	0	0	4.95	36.80
PE 38:4	C ₄₃ H ₇₈ NO ₈ P	766.5383	−0.4	−0.5	5.53	24.49
PE 38:5	C ₄₃ H ₇₆ NO ₈ P	764.5226	−0.5	−0.6	4.99	18.22
PE 36:2	C ₄₁ H ₇₈ NO ₈ P	742.5384	−0.3	−0.4	5.61	10.57
PE 36:1	C ₄₁ H ₈₀ NO ₈ P	744.5533	−1.1	−1.4	6.01	3.85
PE 34:2	C ₃₉ H ₇₄ NO ₈ P	714.5077	0.3	0.4	4.99	3.13
PE 36:3	C ₄₁ H ₇₆ NO ₈ P	740.5206	−2.5	−3.3	5.1	1.95
PE 34:1	C ₃₉ H ₇₆ NO ₈ P	716.5231	0	0.1	5.49	0.54
PE 40:5	C ₄₅ H ₈₀ NO ₈ P	792.5518	−2.6	−3.2	5.73	0.22
PE 42:1	C ₄₇ H ₉₂ NO ₈ P	828.647	−1.3	−1.5	7.34	0.12
PE 38:2	C ₄₃ H ₈₂ NO ₈ P	770.5706	0.6	0.8	6.05	0.10