Supplementary Information

Unmasking the Lipid Landscape: Carbamazepine's Induces Alterations in Leydig Cells Lipidome

Inês Nobre [a,b,c], Ana D. Martins [b,d], Inês M. S. Guerra [a,b], Marisa Pinho [a], Laura Goracci [e], Stefano Bonciarelli [e], Tânia Melo [a,b], Pedro Domingues [b], Artur Paiva [f,g,h], Pedro F. Oliveira [b,d], and M. Rosário Domingues *[a,b]

[a] CESAM-Centre for Environmental and Marine Studies, Department of Chemistry, University of Aveiro, Santiago University Campus, 3810-193 Aveiro, Portugal

[b] Mass Spectrometry Centre, LAQV-REQUIMTE, Department of Chemistry, University of Aveiro, Santiago University Campus, 3810-193 Aveiro, Portugal

[c] Serviço Patologia Clínica, ULS Coimbra, 3004-561 Coimbra, Portugal

[d] LAQV-REQUIMTE and Department of Chemistry, University of Aveiro, 3810-193 Aveiro, Portugal

[e] Department of Chemistry, Biology and Biotechnology, University of Perugia, 06123 Perugia, Italy

[f] Unidade de Gestão Operacional em Citometria, Centro Hospitalar e Universitário de Coimbra (CHUC), 3004-561 Coimbra, Portugal

[g] Faculty of Medicine, Coimbra Institute for Clinical and Biomedical Research (iCBR), University of Coimbra, 3000-370 Coimbra, Portugal

[h] Ciências Biomédicas Laboratoriais, ESTESC - Coimbra Health School, Instituto Politécnico de Coimbra, 3046-854 Coimbra, Portugal

Corresponding author: Rosário Domingues*

Address reprint requests to: Rosário Domingues, Lipidomic laboratory, Departamento de Química, Universidade de Aveiro, Campus Universitário de Santiago, 3810-193 Aveiro (PORTUGAL)
Phone: +351 234 370698
Fax: +351 234 370084
E-mail: mrd@ua.pt

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Supplementary Table S1. Significant variations between the FA identified by GC-MS from Leydig cells treated with 25 µM or 200 µM CBZ and CTR groups, sorted by increasing number of carbon atoms and double bonds. Significant differences (*p*-values<0.05) between the groups revealed by Two-way ANOVA and Tukey's multiple comparisons test are marked with * if *p*<0.05 and ns-not significant.

Tukey's multiple comparisons test	*p*-value	Statistical significance level
FA 14:0		
CTR vs. 25 µM	0.9598	ns
CTR vs. 200 µM	0.6971	ns
25 µM vs. 200 µM	0.8531	ns
FA 16:0		
CTR vs. 25 µM	0.9998	ns
CTR vs. 200 µM	0.9998	ns
25 µM vs. 200 µM	>0.9999	ns
FA 16:1 *n*-9		
CTR vs. 25 µM	0.9219	ns
CTR vs. 200 µM	0.2251	ns
25 µM vs. 200 µM	0.1052	ns
FA 16:1 *n*-7		
CTR vs. 25 µM	0.9458	ns
CTR vs. 200 µM	0.8457	ns
25 µM vs. 200 µM	0.9704	ns
FA 18:0		
CTR vs. 25 µM	0.9996	ns
CTR vs. 200 µM	0.9939	ns
25 µM vs. 200 µM	0.9906	ns
FA 18:1 *n*-9		
CTR vs. 25 µM	0.9956	ns
CTR vs. 200 µM	0.9973	ns
25 µM vs. 200 µM	0.9998	ns
FA 18:1 *n*-7		
CTR vs. 25 µM	0.9998	ns
CTR vs. 200 µM	0.9985	ns
25 µM vs. 200 µM	0.9995	ns
FA 18:2 *n*-6		
CTR vs. 25 µM	0.9099	ns
CTR vs. 200 µM	0.8682	ns
25 µM vs. 200 µM	0.6278	ns
FA 20:4 *n*-6		
CTR vs. 25 µM	0.604	ns
CTR vs. 200 µM	0.9991	ns
25 µM vs. 200 µM	0.5779	ns
FA 22:4 *n*-6		

CTR vs. 25 µM	0.8648	ns
CTR vs. 200 µM	0.9509	ns
25 µM vs. 200 µM	0.9757	ns
FA 22:5 *n*-3		
CTR vs. 25 µM	0.9371	ns
CTR vs. 200 µM	0.9998	ns
25 µM vs. 200 µM	0.93	ns
FA 22:6 *n*-3		
CTR vs. 25 µM	0.965	ns
CTR vs. 200 µM	0.0538	ns
25 µM vs. 200 µM	0.0278	*

Supplementary Table S2. Significant variations between the Σ FA identified by GC-MS from Leydig cells treated with 25 µM or 200 µM CBZ and CTR groups, sorted by increasing number of carbon atoms and double bonds. Significant differences (*p*-values<0.05) between the groups revealed by Two-way ANOVA and Tukey's multiple comparisons test are marked with *** if *p*<0.001. ns-not significant.

Tukey's multiple comparisons test	*p*-value	Statistical significance level
Σ *n*-3		
CTR vs. 25 µM	0.9981	ns
CTR vs. 200 µM	0.1346	ns
25 µM vs. 200 µM	0.1518	ns
Σ *n*-6		
CTR vs. 25 µM	0.1576	ns
CTR vs. 200 µM	0.9936	ns
25 µM vs. 200 µM	0.1265	ns
***n*-6/*n*-3**		
CTR vs. 25 µM	0.1769	ns
CTR vs. 200 µM	0.1071	ns
25 µM vs. 200 µM	0.0005	***
Σ SFA		
CTR vs. 25 µM	>0.9999	ns
CTR vs. 200 µM	0.996	ns
25 µM vs. 200 µM	0.995	ns
Σ MUFA		
CTR vs. 25 µM	>0.9999	ns
CTR vs. 200 µM	>0.9999	ns
25 µM vs. 200 µM	0.9999	ns
Σ PUFA		
CTR vs. 25 µM	0.7285	ns
CTR vs. 200 µM	0.9001	ns
25 µM vs. 200 µM	0.9445	ns

Supplementary Table S3. Lipid molecular species identified by LC-MS and MS/MS in Leydig cells treated with 25 µM or 200 µM CBZ and in control group. The 'O-' prefix is used for plasmanyl species to indicate the presence of an alkyl ether substituent, whereas the 'P-' prefix is used for plasmenyl species to indicate the alk-1-enyl ether substituent. Lipid class **Abbreviations:** Cer, ceramide; PC, phosphatidylcholine; LPC, lysophosphatidylcholine; SM, sphingomyelin; PE, phosphatidylethanolamine; LPE, lysophosphatidylethanolamine; PG, phosphatidylglycerol; LPG, lysophosphatidylglycerol; PI, phosphatidylinositol; PS, phosphatidylserine. C-total of carbon atoms in fatty acids; N-number of double bonds; *identified based on exact mass measurements and retention time, no loss of the polar head group and FA acyl-chain fragments observed.

Lipid specie (C:N)	Observed *m/z*	Theoretical *m/z*	Error (ppm)	Fatty acyl chain(s) C:N	Formula
Cer and HexCer identified as $[M+H]^+$					
Cer 34:0;O2	540.5343	540.5350	1.4	16:0;O2_18:0	C34H69NO3
Cer 34:1;O2	538.5186	538.5194	1.5	16:0;O2_18:1	C34H67NO3
Cer 34:2;O2	536.5029	536.5037	1.5	16:0;O2_18:2	C34H65NO3
Cer 40:1;O2	622.6134	622.6133	0.2	18:1;O2_22:0	C40H79NO3
Cer 40:2;O2	620.5977	620.5976	0.1	18:1;O2_22:1	C40H77NO3
Cer 41:1;O2	636.6292	636.6289	0.4	18:1;O2_23:0	C41H81NO3
Cer 41:2;O2	634.6133	634.6133	0	18:1;O2_23:1	C41H79NO3
Cer 42:1;O2	650.6444	650.6446	0.2	18:1;O2_24:0	C42H83NO3
Cer 42:2;O2	648.6290	648.6289	0.2	18:1;O2_24:1	C42H81NO3
Cer 43:1;O2	664.6606	664.6602	0.6	18:1;O2_25:0	C43H85NO3
Cer 43:2;O2	662.6453	662.6446	1.2	18:1;O2_25:1	C43H83NO3
Cer 44:2;O2	676.6610	676.6602	1.1	18:1;O2_26:1	C44H85NO3
HexCer 34:1;O2	700.5706	700.5722	2.2	16:0;O2_18:1	C40H77NO8
HexCer 42:2;O2	810.6812	810.6817	0.7	18:1;O2_24:1	C48H91NO8
HexCer 40:1;O2	784.6652	784.6661	1.2	18:1;O2_22:0	C46H89NO8
HexCer 42:1;O2	812.6969	812.6974	0.7	18:1;O2_24:0	C48H93NO8
Coenzyme identified as $[M+H]^+$					
Coenzyme Q10	863.6899	863.6912	1.4	*	C59H90O4
DG identified as $[M+NH_4]^+$					
DG 34:1	612.5560	612.5562	0.3	16:0_18:1	C37H70O5
DG 36:2	638.5715	638.5718	0.4	18:1_18:1	C39H72O5

DG 36:4	634.5392	634.5405	2.1	16:0_20:4	C39H68O5
DG 38:4	662.5717	662.5718	0.1	18:0_20:4	C41H72O5
DG 38:5	660.5551	660.5562	1.6	16:0_22:5	C41H70O5
DG 38:6	658.5394	658.5405	1.7	16:0_22:6	C41H68O5
DG 40:5	688.5861	688.5875	1.9	18:0_22:5	C43H74O5
DG 40:6	686.5708	686.5718	1.5	18:0_22:6	C43H72O5
LPC identified as $[M+H]^+$ (determination of fatty acyl chains by MS/MS of $[M+HCOO]^-$)					
LPC 16:0	496.3393	496.3398	1	16:0	C24H50NO7P
LPC 16:1	494.3236	494.3241	1.1	*	C24H48NO7P
LPC 18:0	524.3709	524.3711	0.3	18:0	C26H54NO7P
LPC 18:1	522.3551	522.3554	0.5	*	C26H52NO7P
PC identified as $[M+H]^+$ (determination of fatty acyl chains by MS/MS of $[M+HCOO]^-$)					
PC 28:1	676.4916	676.4912	0.6	*	C36H70NO8P
PC 30:0	706.5369	706.5381	1.7	14:0_16:0	C38H76NO8P
PC 30:1	704.5218	704.5225	1	14:0_16:1	C38H74NO8P
PC 31:0_A	720.5528	720.5538	1.4	*	C39H78NO8P
PC 31:0_B	720.5526	720.5538	1.6	15:0_16:0	C39H78NO8P
PC 31:1	718.5374	718.5381	1	*	C39H76NO8P
PC 32:0	734.5682	734.5694	1.7	16:0_16:0	C40H80NO8P
PC 32:1	732.5527	732.5538	1.4	*	C40H78NO8P
PC 32:2_A	730.5375	730.5381	0.8	16:1_16:1	C40H76NO8P
PC 32:2_B	730.5356	730.5381	3.4	*	C40H76NO8P
PC 33:0	748.5838	748.5851	1.7	*	C41H82NO8P
PC 33:1	746.5685	746.5694	1.2	15:0_18:1 and 16:0_17:1	C41H80NO8P
PC 33:2_A	744.5530	744.5538	1.1	16:1_17:1	C41H78NO8P
PC 33:2_B	744.5517	744.5538	2.9	*	C41H78NO8P
PC 34:0	762.5983	762.6007	3.1	*	C42H84NO8P

PC 34:1	760.5839	760.5851	1.6	16:0_18:1	C42H82NO8P
PC 34:2_A	758.5672	758.5694	2.9	16:1_18:1	C42H80NO8P
PC 34:2_B	758.5678	758.5694	2.2	*	C42H80NO8P
PC 34:3_A	756.5533	756.5538	0.7	12:0_22:3	C42H78NO8P
PC 34:3_B	756.5532	756.5538	0.8	*	C42H78NO8P
PC 34:3_C	756.5530	756.5538	1.1	*	C42H78NO8P
PC 34:3_D	756.5521	756.5538	2.2	*	C42H78NO8P
PC 34:4	754.5365	754.5381	2.2	*	C42H76NO8P
PC 35:0	776.6134	776.6164	3.8	*	C43H86NO8P
PC 35:1_A	774.5991	774.6007	2.1	*	C43H84NO8P
PC 35:1_B	774.5996	774.6007	1.4	*	C43H84NO8P
PC 35:2_A	772.5836	772.5851	1.9	16:1_19:1 and 17:1_18:1	C43H82NO8P
PC 35:2_B	772.5823	772.5851	3.6	*	C43H82NO8P
PC 35:3	770.5658	770.5694	4.8	*	C43H80NO8P
PC 35:4	768.5524	768.5538	1.8	*	C43H78NO8P
PC 36:1	788.6160	788.6164	0.5	*	C44H86NO8P
PC 36:2	786.5984	786.6007	2.9	18:1_18:1	C44H84NO8P
PC 36:3_A	784.5819	784.5851	4	*	C44H82NO8P
PC 36:3_B	784.5833	784.5851	2.3	*	C44H82NO8P
PC 36:3_C	784.5812	784.5851	4.9	*	C44H82NO8P
PC 36:4	782.5667	782.5694	3.5	*	C44H80NO8P
PC 36:5_A	780.5524	780.5538	1.8	16:1_20:4 and 14:0_22:5	C44H78NO8P
PC 36:5_B	780.5528	780.5538	1.3	*	C44H78NO8P
PC 36:6_A	778.5379	778.5381	0.3	*	C44H76NO8P
PC 36:6_B	778.5375	778.5381	0.8	*	C44H76NO8P
PC 36:7	776.5188	776.5225	4.7	*	C44H74NO8P
PC 37:1	802.6310	802.632	1.3	*	C45H88NO8P
PC 37:2_A	800.6147	800.6164	2.1	18:1_19:1	C45H86NO8P

PC 37:2_B	800.6149	800.6164	1.9	*	C45H86NO8P
PC 37:2_C	800.6140	800.6164	2.9	*	C45H86NO8P
PC 37:5	794.5685	794.5694	1.2	*	C45H80NO8P
PC 37:6	792.5528	792.5538	1.2	*	C45H78NO8P
PC 38:1	816.6464	816.6477	1.6	18:0_20:1	C46H90NO8P
PC 38:2_A	814.6297	814.632	2.9	18:1_20:1	C46H88NO8P
PC 38:2_B	814.6302	814.632	2.3	*	C46H88NO8P
PC 38:3_A	812.6128	812.6164	4.4	16:1_22:2 and 18:1_20:2 and 18:2_20:1 and 18:3_20:0	C46H86NO8P
PC 38:3_B	812.6149	812.6164	1.9	18:0_20:3	C46H86NO8P
PC 38:4_A	810.5988	810.6007	2.4	16:0_22:4 and 18:1_20:3	C46H84NO8P
PC 38:4_B	810.5972	810.6007	4.4	18:0_20:4	C46H84NO8P
PC 38:5_A	808.5822	808.5851	3.5	18:1_20:4 and 16:0_22:5	C46H82NO8P
PC 38:5_B	808.5824	808.5851	3.3	16:0_22:5 and 18:0_20:5 and 18:1_20:4	C46H82NO8P
PC 38:6_A	806.5690	806.5694	0.6	*	C46H80NO8P
PC 38:6_B	806.5681	806.5694	1.6	16:0_22:6	C46H80NO8P
PC 38:7	804.5524	804.5538	1.7	16:1_22:6	C46H78NO8P
PC 39:2	828.6465	828.6477	1.4	*	C47H90NO8P
PC 39:3	826.6300	826.632	2.5	*	C47H88NO8P
PC 39:4_A	824.6126	824.6164	4.6	*	C47H86NO8P
PC 39:4_B	824.6128	824.6164	4.4	*	C47H86NO8P
PC 39:5	822.5980	822.6007	3.3	*	C47H84NO8P
PC 40:1	844.6779	844.679	1.2	*	C48H94NO8P
PC 40:2	842.6617	842.6633	1.9	16:1_24:1 and 18:1_22:1 and 20:1/20:1	C48H92NO8P
PC 40:3_A	840.6455	840.6477	2.7	18:1_22:2 and 20:1_20:2	C48H90NO8P
PC 40:3_B	840.6467	840.6477	1.2	*	C48H90NO8P
PC 40:4_A	838.6297	838.632	2.7	*	C48H88NO8P

PC 40:4_B	838.6297	838.632	2.8	*	C48H88NO8P
PC 40:5_A	836.6133	836.6164	3.7	18:0_22:5	C48H86NO8P
PC 40:5_B	836.6141	836.6164	2.7	18:0_22:5	C48H86NO8P
PC 40:6_A	834.5976	834.6007	3.7	18:1_22:5	C48H84NO8P
PC 40:6_B	834.5981	834.6007	3.2	18:0_22:6 and 18:2_22:4 and 18:4_22:2 and 20:1_20:5 and 20:2_20:4 and 20:3/20:3	C48H84NO8P
PC 40:7_A	832.5824	832.5851	3.3	18:1_22:6	C48H82NO8P
PC 40:7_B	832.5811	832.5851	4.8	*	C48H82NO8P
PC 40:8	830.5676	830.5694	2.2	*	C48H80NO8P
PC 41:2	856.6778	856.679	1.4	*	C49H94NO8P
PC 41:6	848.6153	848.6164	1.3	*	C49H86NO8P
PC 41:7	846.5977	846.6007	3.5	*	C49H84NO8P
PC 42:1	872.7084	872.7103	2.1	*	C50H98NO8P
PC 42:10	854.5683	854.5694	1.3	*	C50H80NO8P
PC 42:2	870.6933	870.6946	1.6	*	C50H96NO8P
PC 42:3	868.6779	868.679	1.2	*	C50H94NO8P
PC 42:4_A	866.6625	866.6633	1	*	C50H92NO8P
PC 42:4_B	866.6627	866.6633	0.7	*	C50H92NO8P
PC 42:5_A	864.6484	864.6477	0.8	*	C50H90NO8P
PC 42:5_B	864.6482	864.6477	0.5	*	C50H90NO8P
PC 42:6	862.6295	862.632	2.9	*	C50H88NO8P
PC 42:7_A	860.6134	860.6164	3.4	*	C50H86NO8P
PC 42:7_B	860.6133	860.6164	3.6	*	C50H86NO8P
PC 42:8	858.5993	858.6007	1.6	*	C50H84NO8P
PC 44:2	898.7243	898.7259	1.8	*	C52H100NO8P
PC 44:3	896.7087	896.7103	1.8	*	C52H98NO8P
PC 44:5	892.6782	892.679	0.9	*	C52H94NO8P
PC 44:6	890.6637	890.6633	0.4	*	C52H92NO8P

PC O-30:0	692.5576	692.5589	1.9	O-14:0_16:0	C38H78NO7P
PC O-30:1/PC P-30:0_A	690.5421	690.5432	1.7	*	C38H76NO7P
PC O-30:1/PC P-30:0_B	690.5410	690.5432	3.3	*	C38H76NO7P
PC O-31:0	706.5716	706.5745	4.1	*	C39H80NO7P
PC O-32:0	720.5892	720.5902	1.4	O-16:0_16:0	C40H82NO7P
PC O-32:1_A	718.5726	718.5745	2.7	*	C40H80NO7P
PC O-32:1_B	718.5736	718.5745	1.3	O-16:0_16:1	C40H80NO7P
PC O-33:1/PC P-33:0_A	732.5887	732.5902	2	*	C41H82NO7P
PC O-33:1/PC P-33:0_B	732.5879	732.5902	3	*	C41H82NO7P
PC O-33:2/PC P-33:1	730.5731	730.5745	2	*	C41H80NO7P
PC O-34:0	748.6197	748.6215	2.4	*	C42H86NO7P
PC O-34:1/PC P-34:0_A	746.6044	746.6058	2	O-18:1_16:0 and P-18:0_16:0	C42H84NO7P
PC O-34:1/PC P-34:0_B	746.6042	746.6058	2.1	*	C42H84NO7P
PC O-34:2/PC P-34:1_A	744.5887	744.5902	2	*	C42H82NO7P
PC O-34:2/PC P-34:1_B	744.5887	744.5902	2	*	C42H82NO7P
PC O-34:3/PC P-34:2_A	742.5728	742.5745	2.3	*	C42H80NO7P
PC O-34:3/PC P-34:2_B	742.5722	742.5745	3.1	*	C42H80NO7P
PC O-35:2/PC P-35:1	758.6051	758.6058	0.9	*	C43H84NO7P
PC O-36:1/PC P-36:0	774.6359	774.6371	1.5	*	C44H88NO7P
PC O-36:2/PC P-36:1	772.6198	772.6215	2.1	*	C44H86NO7P
PC O-36:3/PC P-36:2_A	770.6035	770.6058	3	*	C44H84NO7P
PC O-36:3/PC P-36:2_B	770.6043	770.6058	2	*	C44H84NO7P
PC O-36:4/PC P-36:3	768.5887	768.5902	2	*	C44H82NO7P
PC O-36:5/ PC P-36:4	766.5722	766.5745	3	*	C44H80NO7P
PC O-35:1/PC P-35:0	782.6049	782.6058	1.2	*	C45H84NO7P
PC O-38:2	800.6506	800.6528	2.8	O-16:0_22:2	C46H90NO7P
PC O-38:3/PC P-38:2_A	798.6339	798.6371	4.1	*	C46H88NO7P
PC O-38:3/PC P-38:2_B	798.6351	798.6371	2.5	*	C46H88NO7P

PC O-38:4/PC P-38:3_A	796.6198	796.6215	2.1	*	C46H86NO7P
PC O-38:4/PC P-38:3_B	796.6193	796.6215	2.8	*	C46H86NO7P
PC O-38:5/PC P-38:4_A	794.6034	794.6058	3	*	C46H84NO7P
PC O-38:5/PC P-38:4_B	794.6035	794.6058	2.9	*	C46H84NO7P
PC O-38:5/PC P-38:4_C	794.6024	794.6058	4.3	*	C46H84NO7P
PC O-38:6/PC P-38:5	792.5881	792.5902	2.6	*	C46H82NO7P
PC O-40:2/PC P-40:1	828.6826	828.6841	1.7	*	C48H94NO7P
PC O-40:5/PC P-40:4_A	822.6351	822.6371	2.5	*	C48H88NO7P
PC O-40:5/PC P-40:4_B	822.6355	822.6371	2	*	C48H88NO7P
PC O-40:6/PC P-40:5	820.6189	820.6215	3.1	*	C48H86NO7P
PC O-32:2/PC P-32:1	716.5572	716.5589	2.4	*	C40H78NO7P
PC P-34:1	744.5889	744.5902	1.7	P-16:0_18:1	C42H82NO7P
PC P-36:5_A	764.5580	764.5589	1.1	*	C44H78NO7P
PC P-36:5_B	764.5587	764.5589	0.2	*	C44H78NO7P
PC P-37:2	784.6207	784.6215	1	*	C45H86NO7P
PC P-38:6	790.5723	790.5745	2.8	*	C46H80NO7P
PC P-39:1	814.6685	814.6684	0	*	C47H92NO7P
PC P-40:6	818.6034	818.6058	2.9	*	C48H84NO7P
SM identified as $[M+H]^+$					
SM 32:1;O2	675.5444	675.5436	1.2	*	C37H75N2O6P
SM 33:1;O2	689.5581	689.5592	1.5	*	C38H77N2O6P
SM 34:0;O2	705.5888	705.5905	2.4	16:0;O2_18:0	C39H81N2O6P
SM 34:1;O3	719.5692	719.5698	0.8	*	C39H79N2O7P
SM 34:1;O2_A	703.5742	703.5749	0.9	18:1;O2_16:0	C39H79N2O6P
SM 34:1;O2_B	703.5734	703.5749	2	*	C39H79N2O6P
SM 34:2;O2	701.5575	701.5592	2.4	*	C39H77N2O6P
SM 35:1;O2	717.5893	717.5905	1.7	*	C40H81N2O6P
SM 36:1;O2	731.6032	731.6062	4	*	C41H83N2O6P

SM 38:1;O2	759.6362	759.6375	1.7	*	C43H87N2O6P
SM 40:0;O2	789.6824	789.6844	2.5	*	C45H93N2O6P
SM 40:1;O2_A	787.6675	787.6688	1.6	*	C45H91N2O6P
SM 40:1;O2_B	787.6680	787.6688	1	16:1;O2_24:0 and 18:1;O2_22:0	C45H91N2O6P
SM 40:2;O2	785.6526	785.6531	0.7	*	C45H89N2O6P
SM 41:1;O2	801.6840	801.6844	0.5	*	C46H93N2O6P
SM 41:2;O2	799.6681	799.6688	0.8	*	C46H91N2O6P
SM 42:1;O2	815.6994	815.7001	0.8	*	C47H95N2O6P
SM 42:2;O2	813.6838	813.6844	0.7	*	C47H93N2O6P
SM 43:1;O2	829.7162	829.7157	0.6	*	C48H97N2O6P
SM 43:2;O2	827.7000	827.7001	0	*	C48H95N2O6P
SM 44:2;O2	841.7148	841.7157	1.1	*	C49H97N2O6P
SPB identified as $[M+H]^+$					
SPB 16:0;O2	274.2736	274.2741	1.7	16:0;O2	C16H35NO2
SPB 16:1;O2	272.2579	272.2584	2	16:1;O2	C16H33NO2
SPB 18:0;O2_A	302.3049	302.3054	1.5	18:0;O2	C18H39NO2
SPB 18:0;O2_B	302.3049	302.3054	1.5	18:0;O2	C18H39NO2
SPB 18:0;O2_C	302.3048	302.3054	1.7	18:0;O2	C18H39NO2
SPB 18:1;O2	300.2891	300.2897	2	18:1;O2	C18H37NO2
SPB 20:0;O2	330.3359	330.3367	2.4	20:0;O2	C20H43NO2
TG identified as $[M+NH_4]^+$					
TG 40:0	712.6446	712.645	0.5	12:0_12:0_16:0 and 12:0_14:0_14:0	C43H82O6
TG 42:0	740.6755	740.6763	1.1	12:0_14:0_16:0	C45H86O6
TG 44:1	766.6910	766.6919	1.1	12:0_14:0_18:1 and 14:1_15:0_15:0	C47H88O6
TG 45:0	782.7222	782.7232	1.3	13:0_15:0_17:0 and 14:0_15:0_16:0	C48H92O6
TG 46:0	796.7376	796.7389	1.6	14:0_16:0_16:0 and 15:0_15:0_16:0	C49H94O6
TG 46:1	794.7222	794.7232	1.2	14:0_14:0_18:1 and 14:1_16:0_16:0	C49H92O6
TG 46:2	792.7068	792.7076	1	12:0_16:1_18:1 and 14:0_16:1_16:1	C49H90O6

TG 47:0	810.7534	810.7545	1.4	15:0_16:0_16:0 and 14:0_16:0_17:0 and 15:0_15:0_17:0	C50H96O6
TG 47:1	808.7378	808.7389	1.4	14:0_15:0_18:1 and 14:0_16:0_17:1 and 14:0_16:1_17:0	C50H94O6
TG 48:0	824.7690	824.7702	1.4	16:0_16:0_16:0	C51H98O6
TG 48:1	822.7534	822.7545	1.4	16:0_16:0_16:1 and 14:0_16:0_18:1	C51H96O6
TG 48:2	820.7378	820.7389	1.2	14:0_16:1_18:1 and 14:1_16:0_18:1 and 14:0_16:0_18:2	C51H94O6
TG 48:3	818.7226	818.7232	0.8	14:1_16:1_18:1 and 14:0_16:1_18:2	C51H92O6
TG 49:0	838.7844	838.7858	1.7	16:0_16:0_17:0 and 15:0_16:0_18:0 and 15:0_17:0_17:0 and 14:0_17:0_18:0	C52H100O6
TG 49:1	836.7692	836.7702	1.2	15:0_16:0_18:1 and 16:0_16:0_17:1 and 16:0_16:1_17:0 and 14:0_16:0_19:1 and 14:0_17:0_18:1 and 15:0_15:0_19:1 and 15:0_16:1_18:0	C52H98O6
TG 49:2	834.7537	834.7545	1	15:0/16:1/18:1 and 16:0/16:1/17:1 and 14:0/17:1/18:1	C52H96O6
TG 50:0	852.8004	852.8015	1.3	16:0_16:0_18:0 and 14:0_18:0_18:0	C53H102O6
TG 50:1	850.7846	850.7858	1.4	16:0_16:0_18:1	C53H100O6
TG 50:2	848.7688	848.7702	1.6	16:0_16:1_18:1 and 16:0_16:0_18:2 and 14:0_18:1_18:1	C53H98O6
TG 50:3	846.7531	846.7545	1.7	16:0_16:1_18:2 and 14:0_18:1_18:2 and 14:0_16:0_20:3 and 14:1_16:0_20:2	C53H96O6
TG 51:0	866.8152	866.8171	2.2	16:0_17:0_18:0 and 15:0_16:0_20:0 and 15:0_18:0_18:0 and 14:0_17:0_20:0	C54H104O6
TG 51:1	864.7997	864.8015	2	16:0_17:0_18:1 and 15:0_16:0_20:1 and 16:0_17:1_18:0 and 17:0_17:0_17:1 and 14:0_17:0_20:1 and 15:0_18:0_18:1	C54H102O6
TG 51:2	862.7846	862.7858	1.5	16:0_17:1_18:1 and 15:0_18:1_18:1 and 16:1_17:0_18:1	C54H100O6

TG 51:3	860.7686	860.7702	1.8	16:1_17:1_18:1 and 15:0_18:1_18:2 and 16:0_17:1_18:2	C54H98O6
TG 52:0	880.8316	880.8328	1.3	16:0_18:0_18:0 and 16:0_16:0_20:0 and 14:0_18:0_20:0	C55H106O6
TG 52:2	876.7999	876.8015	1.8	16:0/18:1/18:1 and 16:0/16:0/20:2 and 16:1/18:0/18:1	C55H102O6
TG 52:3	874.7840	874.7858	2.1	16:0_18:1_18:2 and 16:1_18:1_18:1 and 16:0_16:1_20:2 and 14:0_18:1_20:2 and 16:0_16:0_20:3	C55H100O6
TG 52:4	872.7688	872.7702	1.6	16:1_18:1_18:2 and 16:0_18:1_18:3 and 14:0_18:1_20:3 and 16:1_16:1_20:2 and 16:0_18:2_18:2	C55H98O6
TG 53:1_A	892.8302	892.8328	2.8	17:0_18:0_18:1	C56H106O6
TG 53:1_B	892.8296	892.8328	3.5	17:0_18:0_18:1	C56H106O6
TG 53:2	890.8154	890.8171	2	17:0_18:1_18:1 and 15:0_18:1_20:1 and 16:0_17:1_20:1	C56H104O6
TG 53:3	888.7999	888.8015	1.8	17:1/18:1/18:1 and 16:1/18:1/19:1	C56H102O6
TG 54:0	908.8628	908.8641	1.4	16:0_16:0_22:0	C57H110O6
TG 54:1	906.8469	906.8484	1.7	16:0_16:0_22:1 and 16:0_18:0_20:1 and 16:0_18:1_20:0 and 14:0_18:0_22:1	C57H108O6
TG 54:2	904.8316	904.8328	1.3	18:0_18:1_18:1 and 16:0_18:1_20:1 and 16:0_18:0_20:2	C57H106O6
TG 54:3	902.8150	902.8171	2.4	16:0_18:1_20:2 and 16:1_18:1_20:1 and 16:1_18:0_20:2 and 16:0_18:2_20:1	C57H104O6
TG 54:4	900.7993	900.8015	2.5	18:1_18:1_18:2 and 16:0_18:1_20:3 and 16:0_18:2_20:2 and 18:0_18:2_18:2	C57H102O6
TG 54:5	898.7843	898.7858	1.7	16:0_18:1_20:4 and 18:1_18:1_18:3 and 16:0_16:0_22:5 and 16:1_18:1_20:3 and16:0_16:1_22:4 and 18:1_18:2_18:2 and 16:0_18:2_20:3	C57H100O6
TG 54:7	894.7537	894.7545	1	18:1_18:3_18:3	C57H96O6

TG 55:2	918.8464	918.8484	2.2	17:0_18:1_20:1	C58H108O6
TG 55:3	916.8310	916.8328	2	18:1_18:1_19:1	C58H106O6
TG 56:1	934.8779	934.8797	1.9	16:0_18:1_22:0 and 16:0_18:0_22:1	C59H112O6
TG 56:3	930.8465	930.8484	2.1	18:1/18:1/20:1 and 18:0/18:1/20:2 and 16:0/18:1/22:2 and 16:0/20:1/20:2 and	C59H108O6
TG 56:4	928.8298	928.8328	3.2	16:0_18:1_22:3 and 18:1_18:1_20:2 and 16:1_18:1_22:2 and 16:0_20:2_20:2 and 18:0_18:2_20:2 and 16:1_20:1_20:2	C59H106O6
TG 56:6	924.7990	924.8015	2.7	16:0_18:1_22:5 and 18:1_18:1_20:4	C59H102O6
TG 56:7	922.7844	922.7858	1.5	16:1/18:1/22:5	C59H100O6
TG 57:3	944.8620	944.8641	2.2	18:1_19:1_20:1	C60H110O6
TG 58:0	964.9250	964.9267	1.7	16:0_20:0_22:0	C61H118O6
TG 58:2	960.8936	960.8954	1.8	16:0_20:1_22:1	C61H114O6
TG 58:3	958.8776	958.8797	2.2	18:1_18:1_22:1 and 18:1_20:1_20:1 and 16:1_20:1_22:1 and 18:0_18:2_22:1	C61H112O6
TG 58:4	956.8613	956.8641	2.9	18:0_18:1_22:3 and 18:1_20:1_20:2	C61H110O6
TG 58:5	954.8450	954.8484	3.6	18:0_20:1_20:4	C61H108O6
TG 58:6	952.8303	952.8328	2.5	18:1_18:1_22:4	C61H106O6
TG 58:8	948.7998	948.8015	1.8	18:1_18:1_22:6	C61H102O6
TG 60:4	984.8926	984.8954	2.8	18:1_20:1_22:2	C63H114O6
TG 62:0	1020.9875	1020.9893	1.7	18:0_22:0_22:0	C65H126O6
TG 62:4	1012.9242	1012.9267	2.5	18:1_22:1_22:2	C65H118O6
CL identified as $[M-H]^-$					
CL 70:5	1425.9769	1425.9806	2.6	16:1_18:1_18:1_18:2	C79H144O17P2
CL 70:6	1423.9614	1423.965	2.5	16:1_18:2_18:1_18:2	C79H142O17P2
CL 72:2	1460.0649	1460.0589	4.1	16:0_18:1_18:1_20:0	C81H154O17P2
CL 72:8	1447.9588	1447.965	4.3	16:1_18:2_18:1_20:4	C81H142O17P2

CL 74:3	1486.0785	1486.0745	2.7	18:1_18:1_18:1_20:0	C83H156O17P2
CL 76:5	1510.0772	1510.0745	1.8	18:0_18:1_20:0_20:4	C85H156O17P2
LPE identified as $[M-H]^-$ (confirmation of polar head group by MS/MS of $[M+H]^+$)					
LPE 16:0	452.2778	452.2783	1	16:0	C21H44NO7P
LPE 18:0	480.3090	480.3096	1.2	18:0	C23H48NO7P
LPE 18:1	478.2934	478.2939	1.1	*	C23H46NO7P
PE identified as $[M-H]^-$ (confirmation of polar head group by MS/MS of $[M+H]^+$)					
PE 30:1	660.4595	660.461	2.2	14:0_16:1	C35H68NO8P
PE 32:0	690.5066	690.5079	1.9	16:0/16:0	C37H74NO8P
PE 32:1	688.4905	688.4923	2.6	16:0_16:1 and 14:0_18:1	C37H72NO8P
PE 32:2	686.4751	686.4766	2.3	16:1_16:1	C37H70NO8P
PE 33:1	702.5065	702.5079	2	16:0_17:1 and 15:0_18:1	C38H74NO8P
PE 34:1	716.5218	716.5236	2.5	16:0_18:1	C39H76NO8P
PE 34:2	714.5056	714.5079	3.2	16:1_18:1	C39H74NO8P
PE 34:3	712.4904	712.4923	2.6	16:0_18:3	C39H72NO8P
PE 34:4	710.4751	710.4766	2.1	*	C39H70NO8P
PE 35:1	730.5372	730.5392	2.7	*	C40H78NO8P
PE 35:2	728.5215	728.5236	2.8	17:1_18:1 and 16:1_19:1	C40H76NO8P
PE 36:1	744.5536	744.5549	1.7	*	C41H80NO8P
PE 36:2	742.5374	742.5392	2.4	18:1/18:1	C41H78NO8P
PE 36:3_A	740.5218	740.5236	2.4	18:1_18:2	C41H76NO8P
PE 36:3_B	740.5219	740.5236	2.2	*	C41H76NO8P
PE 36:4	738.5058	738.5079	2.8	*	C41H74NO8P
PE 36:5	736.4892	736.4923	4.1	16:1_20:4	C41H72NO8P
PE 37:4	752.5214	752.5236	2.9	*	C42H76NO8P
PE 38:1	772.5854	772.5862	1	18:0_20:1	C43H84NO8P
PE 38:2_A	770.5686	770.5705	2.5	*	C43H82NO8P

PE 38:2_B	770.5697	770.5705	1.1	18:0_20:2	C43H82NO8P
PE 38:3_A	768.5529	768.5549	2.5	*	C43H80NO8P
PE 38:3_B	768.5530	768.5549	2.4	18:0_20:3 and 18:1_20:2	C43H80NO8P
PE 38:4_A	766.5370	766.5392	2.9	18:1_20:3	C43H78NO8P
PE 38:4_B	766.5369	766.5392	3	18:0_20:4	C43H78NO8P
PE 38:5	764.5199	764.5236	4.8	*	C43H76NO8P
PE 38:6	762.5070	762.5079	1.2	16:0_22:6	C43H74NO8P
PE 38:7	760.4897	760.4923	3.4	16:1_22:6	C43H72NO8P
PE 40:1	800.6166	800.6175	1.1	*	C45H88NO8P
PE 40:2	798.6013	798.6018	0.6	*	C45H86NO8P
PE 40:3_A	796.5851	796.5862	1.3	18:1_22:2	C45H84NO8P
PE 40:3_B	796.5858	796.5862	0.5	*	C45H84NO8P
PE 40:3_C	796.5855	796.5862	0.9	20:1_20:2 and 18:1_22:2	C45H84NO8P
PE 40:4	794.5687	794.5705	2.4	18:0_22:4	C45H82NO8P
PE 40:5	792.5527	792.5549	2.7	*	C45H80NO8P
PE 40:6_A	790.5359	790.5392	4.3	*	C45H78NO8P
PE 40:6_B	790.5382	790.5392	1.4	*	C45H78NO8P
PE 40:7	788.5206	788.5236	3.7	18:1_22:6	C45H76NO8P
PE 42:1	828.6484	828.6488	0.4	24:0_18:1	C47H92NO8P
PE 42:5	820.5849	820.5862	1.5	20:2_22:3	C47H84NO8P
PE O-32:0	676.5277	676.5287	1.4	O-16:0_16:0	C37H76NO7P
PE O-36:1	730.5729	730.5756	3.8	*	C41H82NO7P
PE O-36:3	726.5425	726.5443	2.5	*	C41H78NO7P
PE O-36:4	724.5277	724.5287	1.3	O-16:0_20:4	C41H76NO7P
PE O-38:3/PE P38:2	754.5746	754.5756	1.3	*	C43H82NO7P
PE O-38:4/PE P-38:3	752.5577	752.56	3	*	C43H80NO7P
PE O-38:6	748.5264	748.5287	3	*	C43H76NO7P
PE P-32:0	674.5119	674.513	1.7	P-16:0_16:0	C37H74NO7P

PE P-33:1	686.5114	686.513	2.3	P-16:0_17:1	C38H74NO7P
PE O-34:1/PE P-34:0	702.5428	702.5443	2.2	O-16:0_18:1 and P-18:0_16:0	C39H78NO7P
PE P-34:1	700.5277	700.5287	1.3	*	C39H76NO7P
PE P-34:2_A	698.5116	698.513	2	P-16:0_18:2	C39H74NO7P
PE P-34:2_B	698.5115	698.513	2.2	*	C39H74NO7P
PE P-36:1	728.5590	728.56	1.4	P-16:0_20:1	C41H80NO7P
PE P-36:2	726.5424	726.5443	2.6	P-16:0_20:2	C41H78NO7P
PE P-36:4	722.5111	722.513	2.6	P-16:0_20:4	C41H74NO7P
PE P-36:5	720.4956	720.4974	2.4	P-16:0_20:5	C41H72NO7P
PE P-38:1	756.5905	756.5913	1	*	C43H84NO7P
PE P-38:2	754.5742	754.5756	1.9	*	C43H82NO7P
PE P-38:4_A	750.5415	750.5443	3.7	*	C43H78NO7P
PE P-38:4_B	750.5424	750.5443	2.5	P-16:0_22:4	C43H78NO7P
PE P-38:4_C	750.5425	750.5443	2.5	*	C43H78NO7P
PE P-38:6	746.5111	746.513	2.6	*	C43H74NO7P
PE P-40:4	778.5756	778.5756	0	*	C45H82NO7P
PE P-40:7	772.5265	772.5287	2.8	P-18:1_22:6	C45H76NO7P
PG identified as $[M-H]^-$					
PG 34:1_A	747.5165	747.5182	2.2	16:0_18:1	C40H77O10P
PG 34:1_B	747.5161	747.5182	2.8	16:0_18:1	C40H77O10P
PG 34:2_A	745.5013	745.5025	1.7	16:1_18:1	C40H75O10P
PG 34:2_B	745.5005	745.5025	2.6	16:1_18:1	C40H75O10P
PG 36:2_A	773.5318	773.5338	2.6	18:1_18:1	C42H79O10P
PG 36:2_B	773.5316	773.5338	2.9	18:1_18:1	C42H79O10P
PG 36:3	771.5163	771.5182	2.5	16:1_20:2 and 18:1_18:2	C42H77O10P
PG 38:2	801.5634	801.5651	2.2	18:1_20:1	C44H83O10P
PG 38:3	799.5476	799.5495	2.3	18:1_20:2	C44H81O10P
PG 40:4	825.5626	825.5651	3	20:2_20:2	C46H83O10P

PG 40:7	819.5168	819.5182	1.7	18:1_22:6 and 18:2_22:5	C46H77O10P
PG 40:8	817.5006	817.5025	2.3	18:2_22:6	C46H75O10P
PG 42:8	845.5321	845.5338	2	20:2_22:6	C48H79O10P
PG 44:12	865.5010	865.5025	1.7	22:6_22:6	C50H75O10P
PI identified as $[M-H]^-$					
PI 32:1	807.5009	807.5029	2.4	16:0_16:1	C41H77O13P
PI 34:1	835.5315	835.5342	3.3	16:0_18:1	C43H81O13P
PI 34:2	833.5154	833.5186	3.7	16:1_18:1	C43H79O13P
PI 36:1	863.5630	863.5655	2.8	18:0_18:1	C45H85O13P
PI 36:2_A	861.5469	861.5499	3.4	18:1_18:1	C45H83O13P
PI 36:2_B	861.5476	861.5499	2.6	18:0_18:2 and 16:0_20:2	C45H83O13P
PI 36:4	857.5163	857.5186	2.6	16:0_20:4	C45H79O13P
PI 37:2	875.5636	875.5655	2.2	*	C46H85O13P
PI 37:4	871.5318	871.5342	2.8	17:0_20:4	C46H81O13P
PI 38:2	889.5785	889.5812	3	18:0_20:2	C47H87O13P
PI 38:4_A	885.5477	885.5499	2.4	16:0_22:4	C47H83O13P
PI 38:4_B	885.5470	885.5499	3.2	18:0_20:4	C47H83O13P
PI 38:5	883.5318	883.5342	2.7	18:1_20:4	C47H81O13P
PI 40:4	913.5784	913.5812	3	18:0_22:4	C49H87O13P
PI 40:6	909.5476	909.5499	2.5	18:0_22:6	C49H83O13P
PS identified as $[M-H]^-$					
PS 34:1	760.5112	760.5134	2.9	16:0_18:1 and 16:1_18:0	C40H76NO10P
PS 36:1_A	788.5429	788.5447	2.3	18:0_18:1	C42H80NO10P
PS 36:1_B	788.5429	788.5447	2.2	18:0_18:1	C42H80NO10P
PS 36:2	786.5266	786.5291	3.1	18:1/18:1	C42H78NO10P
PS 38:2	814.5584	814.5604	2.4	18:0_20:2 and 18:1_20:1	C44H82NO10P
PS 40:4	838.5575	838.5604	3.4	18:0:22:4	C46H82NO10P
PS 40:5	836.5411	836.5447	4.4	18:0_22:5	C46H80NO10P

PS 40:6	834.5267	834.5291	2.8	18:0_22:6	C46H78NO10P

Supplementary Table S4. Univariate analysis of the LC-MS data from of the three groups. Homogeneity of variances was tested using the Levine test. Normality was assessed using Shapiro-Wilk normality test. *P*-values were calculated using the ANOVA test (in green). In cases where non-normality was suspected, *p*-values were calculated using the Kruskal-Wallis test (in orange). *P*-values were adjusted using Benjamin- Hochberg correction (*p*.adj). Adjusted p-value significance symbols (p.adj.signif): **** $p<0.0001$, *** $p<0.001$, ** $p<0.01$, * $p<0.05$.

Lipid species	*p*.adj	*p*.adj.signif
PG.40.4	5.58E-06	****
PG.34.1_B	1.79E-05	****
PC.O.32.1_B	5.37E-05	****
PC.32.2_A	5.37E-05	****
PE.P.38.6	6.55E-05	****
PG.36.2_B	0.000239	***
PC.30.1	0.000265	***
SM.34.1.O2_A	0.000265	***
PC.34.3_A	0.000360	***
PE.32.0	0.000672	***
SM.34.2.O2	0.000974	***
PC.P.32.1	0.000974	***
HexCer.42.1.O2	0.000986	***
PS.40.6	0.000986	***
PC.34.3_B	0.000989	***
PC.36.5_B	0.001134	**
PC.O.32.0	0.001163	**
PC.36.1	0.001182	**
PE.P.36.4	0.001400	**
Cer.40.2.O2	0.001483	**
PC.36.6_A	0.001803	**
PC.34.2_A	0.001927	**
PC.O.35.2	0.002173	**
PC.O.40.6	0.002593	**
CL.70.6	0.002593	**
PC.38.2_B	0.002593	**
PE.38.2_A	0.003014	**
PI.36.2_B	0.003014	**
PE.O.32.0	0.003014	**
PC.O.31.0	0.003389	**
PG.38.3	0.003408	**
TG.46.1	0.003976	**
PS.36.2	0.004027	**
PC.O.30.0	0.004539	**
Cer.34.1.O2	0.005204	**
PC.40.3_A	0.005477	**
LPC.18.1	0.006519	**
TG.44.1	0.006519	**
TG.56.1	0.006871	**
PE.P.40.7	0.006915	**

PC.33.2_B	0.007058	**
PC.34.1	0.007058	**
PI.38.2	0.007058	**
PE.P.38.4_C	0.007058	**
PC.42.1	0.007058	**
TG.48.2	0.007058	**
SPB.18.0.O2_B	0.007058	**
PS.40.4	0.007058	**
PC.34.4	0.011651	*
PC.28.1	0.011651	*
LPC.16.0	0.011651	*
SPB.20.0.O2	0.011651	*
PE.P.40.4	0.011651	*
PE.38.7	0.011651	*
PC.30.0	0.011651	*
PE.40.3_C	0.011651	*
PE.30.1	0.011651	*
PS.40.5	0.011651	*
TG.46.2	0.011651	*
TG.48.1	0.016938	*
PC.44.2	0.020110	*
PE.38.4_B	0.020110	*
PC.36.6_B	0.020110	*
PI.37.2	0.020110	*
Cer.44.2.O2	0.020110	*
PC.40.3_B	0.020110	*
PE.P.38.1	0.020110	*
PE.40.4	0.023526	*
PC.O.30.1_B	0.023526	*
PC.O.38.3_A	0.023526	*
PC.42.8	0.023526	*
SPB.16.0.O2	0.023526	*
PC.P.37.2	0.026530	*
PE.40.3_B	0.026530	*
PC.34.3_D	0.026530	*
PC.P.36.5_A	0.029872	*
SM.34.1.O2_B	0.029872	*
PC.44.3	0.033747	*
TG.46.0	0.035138	*
PE.32.2	0.035138	*
PE.O.36.1	0.035138	*
HexCer.42.2.O2	0.035138	*
PC.36.5_A	0.035138	*
SPB.18.0.O2_C	0.035138	*
PC.36.3_A	0.035138	*
PE.P.36.5	0.037835	*
SM.32.1.O2	0.037835	*

PC.O.40.2	0.037835	*
PC.O.38.5	0.039194	*
PC.33.2_A	0.039194	*
PC.O.33.1_B	0.039194	*
PC.42.10	0.039194	*
PE.O.36.4	0.039194	*
PC.32.0	0.039194	*
PC.40.1	0.039304	*
PG.42.8	0.039304	*
PC.42.2	0.039860	*
SM.43.1.O2	0.041547	*
Cer.34.2.O2	0.041547	*
PC.31.0_A	0.041547	*
SM.44.2.O2	0.044176	*
PC.32.1	0.044176	*
PE.P.34.0	0.046709	*
PC.31.1	0.046709	*
PE.P.32.0	0.048717	*
PC.31.0_B	0.048717	*
PS.36.1_A	0.050797	ns
PE.P.34.2_A	0.051061	ns
PE.P.34.1	0.051061	ns
PE.36.5	0.053784	ns
PE.P.38.4_A	0.055513	ns
PC.34.2_B	0.055513	ns
PI.40.6	0.055513	ns
PS.38.2	0.056273	ns
SM.40.2.O2	0.057628	ns
PC.O.32.1_A	0.057628	ns
PC.P.40.6	0.059354	ns
PG.40.8	0.062659	ns
PE.40.2	0.064592	ns
TG.54.1	0.065945	ns
PE.38.2_B	0.065945	ns
PE.40.7	0.065945	ns
HexCer.40.1.O2	0.070577	ns
TG.58.2	0.070856	ns
PE.P.33.1	0.070856	ns
PE.36.3_B	0.075641	ns
PE.40.3_A	0.077263	ns
PC.42.4_B	0.078837	ns
TG.53.1_A	0.078837	ns
PC.40.2	0.080956	ns
PE.O.38.4	0.081849	ns
TG.52.2	0.081849	ns
TG.54.3	0.081849	ns
TG.50.1	0.086507	ns

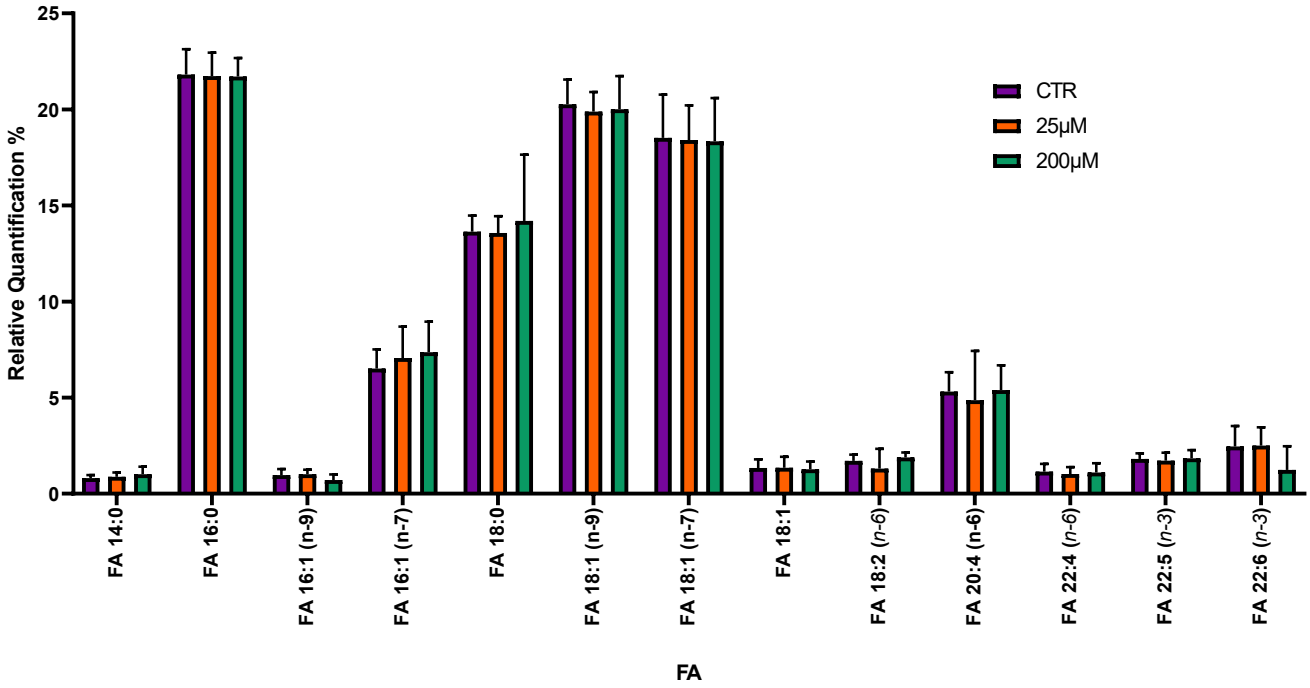
SM.43.2.O2	0.087259	ns
PE.38.4_A	0.087259	ns
PE.40.6_B	0.089201	ns
PC.39.2	0.091117	ns
PI.38.4_B	0.092374	ns
PC.O.38.4_B	0.092374	ns
TG.50.2	0.093824	ns
TG.50.3	0.099214	ns
PI.40.4	0.104240	ns
TG.52.3	0.106628	ns
SPB.16.1.O2	0.108376	ns
PC.P.34.1	0.113382	ns
TG.58.0	0.113382	ns
PE.38.1	0.113480	ns
TG.48.0	0.118838	ns
PC.O.34.3_B	0.127131	ns
PC.38.7	0.137329	ns
TG.48.3	0.138801	ns
PC.39.4_B	0.139244	ns
PC.O.36.2	0.142592	ns
Cer.42.1.O2	0.146335	ns
PC.32.2_B	0.147723	ns
CL.76.5	0.149094	ns
PC.O.38.6	0.157607	ns
PC.40.8	0.160145	ns
PE.O.38.6	0.160145	ns
PC.38.3_B	0.165398	ns
Cer.43.1.O2	0.170235	ns
PE.40.5	0.173611	ns
PC.O.38.5_B	0.174762	ns
PC.35.2_A	0.181409	ns
PC.41.2	0.182414	ns
PC.38.6_A	0.188865	ns
PC.37.2_B	0.188865	ns
Cer.34.O.O2	0.189963	ns
TG.62.4	0.196302	ns
PE.36.1	0.197772	ns
PC.35.3	0.201532	ns
PE.O.38.3	0.203423	ns
PC.O.37.4	0.203423	ns
PE.40.1	0.203518	ns
PC.P.38.6	0.213565	ns
TG.52.4	0.213565	ns
PS.36.1_B	0.216590	ns
PC.O.33.1_A	0.216590	ns
SM.42.1.O2	0.216590	ns
PE.P.36.1	0.216590	ns

LPE.16.0	0.216590	ns
PC.34.0	0.216590	ns
PC.O.33.2	0.219402	ns
TG.54.2	0.224168	ns
PC.42.4_A	0.235508	ns
TG.47.1	0.235508	ns
Coenzyme.Q10	0.236207	ns
PC.35.1_A	0.251712	ns
DG.34.1	0.251712	ns
PE.36.2	0.251712	ns
PC.36.7	0.259958	ns
CL.70.5	0.260513	ns
PI.38.4_A	0.266737	ns
PE.38.3_A	0.267251	ns
PC.39.3	0.268264	ns
PC.36.3_C	0.276177	ns
PG.36.3	0.276633	ns
PG.34.2_A	0.277085	ns
SM.34.0.O2	0.281184	ns
PS.34.1	0.283426	ns
PC.36.2	0.291069	ns
SM.41.1.O2	0.291441	ns
PC.40.4_A	0.309712	ns
PC.44.5	0.317117	ns
PC.37.1	0.322889	ns
SM.40.0.O2	0.324856	ns
PC.O.36.4	0.325057	ns
CL.72.8	0.325256	ns
PE.38.6	0.327184	ns
PC.O.34.2_B	0.329094	ns
PE.34.2	0.330663	ns
PE.P.34.2_B	0.330986	ns
TG.51.3	0.333019	ns
TG.49.1	0.333019	ns
CL.74.3	0.333484	ns
PG.44.12	0.333484	ns
TG.62.0	0.338641	ns
PC.42.5_B	0.343613	ns
LPC.18.0	0.363709	ns
Cer.40.1.O2	0.370277	ns
PE.32.1	0.383758	ns
DG.40.6	0.384784	ns
PC.O.36.3_A	0.384784	ns
TG.49.2	0.387925	ns
TG.51.2	0.400655	ns
PC.O.34.1_B	0.402412	ns
PC.O.36.3_B	0.403700	ns

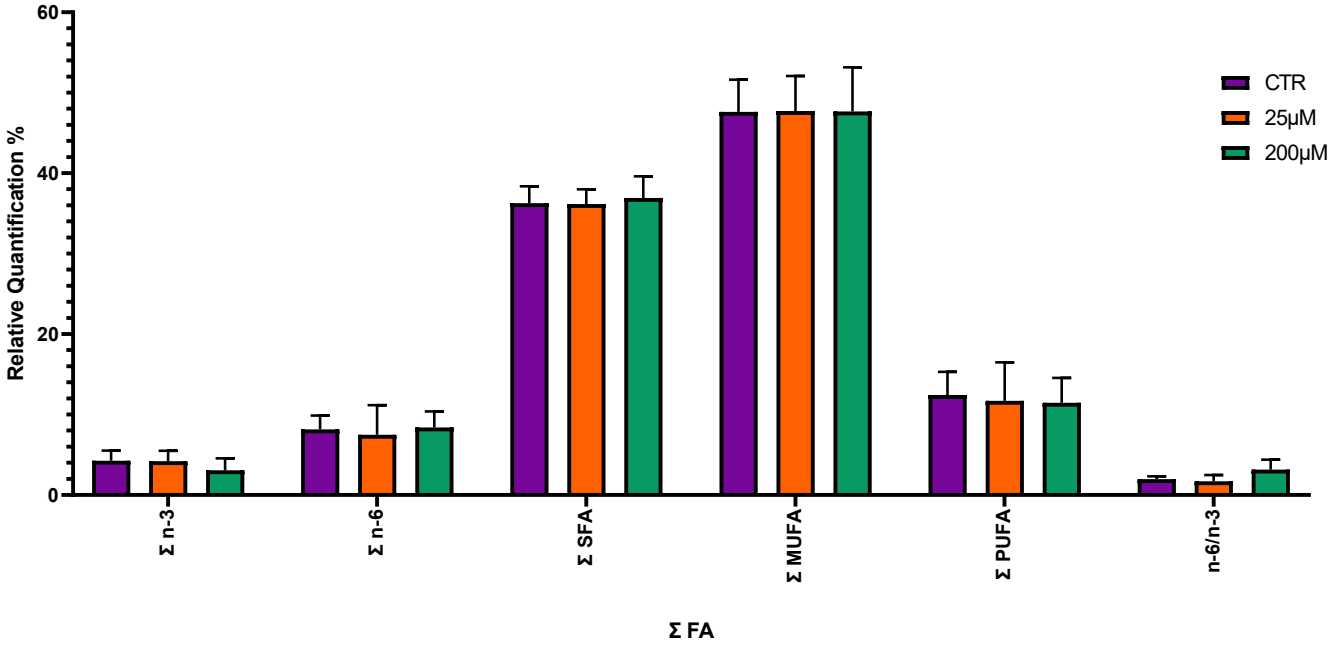
LPE.18.0	0.406719	ns
PE.38.5	0.414051	ns
PI.34.1	0.414051	ns
TG.51.1	0.414051	ns
TG.54.4	0.417621	ns
CL.72.2	0.424295	ns
PC.39.4_A	0.427913	ns
PC.35.2_B	0.428681	ns
LPE.18.1	0.435813	ns
PE.34.3	0.435813	ns
SM.38.1.O2	0.441618	ns
PC.37.5	0.450409	ns
PE.P.38.4_B	0.453086	ns
TG.56.3	0.456191	ns
PE.38.3_B	0.462869	ns
TG.58.4	0.464867	ns
PC.39.5	0.472673	ns
TG.56.4	0.486867	ns
PC.36.3_B	0.487376	ns
PC.38.3_A	0.488359	ns
TG.53.1_B	0.492705	ns
PI.37.4	0.492705	ns
SPB.18.0.O2_A	0.492705	ns
SM.36.1.O2	0.493651	ns
TG.50.0	0.496949	ns
PC.38.4_A	0.496949	ns
LPC.16.1	0.503558	ns
PE.35.2	0.507729	ns
PC.35.4	0.532788	ns
PC.37.6	0.534973	ns
PC.O.36.5	0.541360	ns
TG.58.5	0.552502	ns
PG.40.7	0.554702	ns
DG.40.5	0.555384	ns
TG.54.0	0.557451	ns
PC.O.40.5_B	0.558060	ns
DG.38.4	0.558060	ns
PC.O.38.5_A	0.558060	ns
PC.41.6	0.562467	ns
SM.34.1.O3	0.564194	ns
PC.O.40.5_A	0.566190	ns
PC.40.7_A	0.569530	ns
TG.52.0	0.571036	ns
PC.35.0	0.574199	ns
PC.38.6_B	0.575370	ns
PC.36.4	0.575370	ns
TG.53.2	0.586664	ns

TG.58.8	0.592538	ns
PE.37.4	0.605018	ns
TG.53.3	0.609482	ns
PI.36.2_A	0.609482	ns
PC.38.5_A	0.609482	ns
TG.56.7	0.609482	ns
PG.34.1_A	0.610365	ns
SM.40.1.O2_A	0.610365	ns
TG.54.7	0.616764	ns
PC.O.30.1_A	0.631912	ns
PI.36.1	0.649308	ns
TG.55.2	0.655181	ns
SPB.18.1.O2	0.655181	ns
PC.37.2_A	0.671559	ns
Cer.41.1.O2	0.680029	ns
TG.60.4	0.680029	ns
PC.42.3	0.681934	ns
DG.36.2	0.682469	ns
PC.O.34.0	0.682469	ns
PE.40.6_A	0.682469	ns
TG.42.0	0.683898	ns
TG.54.5	0.684068	ns
PC.40.5_A	0.696678	ns
PC.40.4_B	0.711682	ns
PE.42.5	0.719271	ns
TG.58.3	0.722199	ns
HexCer.34.1.O2	0.729123	ns
PC.44.6	0.729139	ns
PC.P.39.1	0.730378	ns
PC.28.0	0.741196	ns
DG.38.6	0.742053	ns
PE.34.1	0.750736	ns
Cer.41.2.O2	0.759023	ns
SM.41.2.O2	0.760129	ns
PC.38.2_A	0.774252	ns
PC.38.4_B	0.779875	ns
PE.P.38.2	0.779875	ns
PC.42.7_A	0.783246	ns
PI.36.4	0.787594	ns
PC.40.7_B	0.787594	ns
PI.34.2	0.792587	ns
PG.34.2_B	0.803684	ns
PE.33.1	0.811324	ns
PE.36.3_A	0.811324	ns
PG.36.2_A	0.813351	ns
PE.34.4	0.814956	ns
PC.O.34.3_A	0.818869	ns

PE.O.36.3	0.827460	ns
PC.38.1	0.827460	ns
PE.36.4	0.849537	ns
Cer.43.2.O2	0.850366	ns
DG.38.5	0.850366	ns
PI.32.1	0.850366	ns
TG.49.0	0.854187	ns
TG.58.6	0.860052	ns
PC.37.2_C	0.861327	ns
SM.40.1.O2_B	0.865230	ns
TG.55.3	0.868160	ns
PC.40.6_B	0.879477	ns
PC.42.7_B	0.879477	ns
TG.51.0	0.884536	ns
Cer.42.2.O2	0.885374	ns
DG.36.4	0.885374	ns
PC.O.34.2_A	0.891441	ns
PC.O.38.2	0.896991	ns
TG.57.3	0.896991	ns
PC.34.3_C	0.897589	ns
PC.33.0	0.917500	ns
PC.P.36.5_B	0.921670	ns
PC.35.1_B	0.926542	ns
PE.35.1	0.926542	ns
PC.O.36.1	0.926542	ns
PC.42.6	0.927046	ns
PC.33.1	0.938592	ns
TG.47.0	0.945651	ns
PC.40.5_B	0.945651	ns
TG.45.0	0.945651	ns
PC.41.7	0.949210	ns
SM.33.1.O2	0.952749	ns
PC.42.5_A	0.956674	ns
PC.40.6_A	0.956674	ns
TG.56.6	0.960162	ns
PI.38.5	0.967081	ns
PE.42.1	0.968472	ns
PE.P.36.2	0.976986	ns
PC.O.38.4_A	0.976986	ns
SM.42.2.O2	0.976986	ns
PG.38.2	0.976986	ns
PC.O.34.1_A	0.977326	ns
PC.O.38.3_B	0.989697	ns
PC.38.5_B	0.994000	ns
TG.40.0	0.997000	ns



Supplementary Figure S1. Fatty acid profile of Leydig cells treated with CBZ (25 μM and 200 μM) and control (CTR) obtained by GC-MS.



Supplementary Figure S2. Sum and ratio of fatty acid profile of Leydig cells treated with CBZ (25 μM and 200 μM) and control (CTR) obtained by GC-MS.

A)

B)

Supplementary Figure S3. PC identification. **A)** LC-MS/MS spectrum of the $[M+H]^+$ ion of PC 30:1 at *m/z* 704.50. Confirmation of PC class was achieved by identification of the typical product ions at *m/z* 184.07, corresponding to the phosphocholine polar head group. **B)** LC-MS/MS spectrum of the $[M+HCOO]^-$ ion of PC 30:1 at *m/z* 748.53. Fragment ions characteristic of demethylated phosphocholine polar head at *m/z* 168.04 and the typical neutral loss of 60 Da ($HCOOCH_3$) were observed. The PC molecular species composition was confirmed by the identification of the carboxylate anions of the fatty acyl chains ($[RCOO]^-$) identified at *m/z* 227.20 and *m/z* 253.22 corresponding to 14:0 and 16:1, respectively forming the PC 14:0_16:1. This fragmentation pattern was also used to identify LPC class, with only one fatty acyl chain observed in negative ion mode.

A)

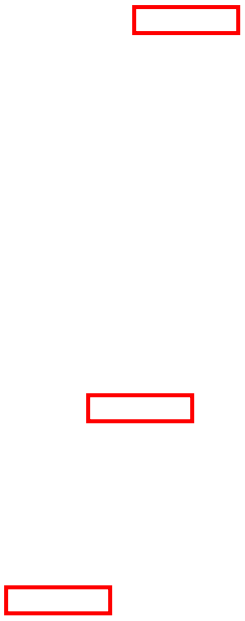
B)

Supplementary Figure S4. SM identification. **A)** LC-MS/MS spectrum of the $[M+H]^+$ ion of SM 34:0;O2 at *m/z* 705.49. Confirmation of SM class was achieved by the identification of the product ion at *m/z* 184.07, corresponding to the phosphocholine polar head. **B)** LC-MS/MS spectrum of the $[M+HCOO]^-$ ion of SM 34:0;O2 at *m/z* 749.52. Confirmation of SM class was achieved by the identification of the product ion at *m/z* 168.04, corresponding to the demethylated phosphocholine polar, and the typical neutral loss of 60 Da ($HCOOCH_3$).

A)

B)

Supplementary Figure S5. PE identification. **A)** LC-MS/MS spectrum of the $[M+H]^+$ ion of PE 34:2 at *m/z* 716.46. Confirmation of PE class was achieved by the identification of the neutral loss of 141 Da, corresponding to phosphoethanolamine polar head (*m/z* 575.50). **B)** LC-MS/MS spectrum of the $[M-H]^-$ ion of PE 34:2 at *m/z* 714.48. The carboxylate anions of the fatty acyl chains ($[RCOO]^-$) were identified at *m/z* 253.22 and 281.25, corresponding to 16:1 and 18:1, forming the PE 16:1_18:1. This fragmentation pattern was also used to identify LPE class, with only one fatty acyl chain observed in negative ion mode.



Supplementary Figure S6. PG identification. LC-MS/MS spectrum of the $[M-H]^-$ ion of PG 34:1 at *m/z* 747.52. Confirmation of PG class was achieved by the identification of the product ion at *m/z* 171.00, corresponding to the glycerol phosphate anion. The carboxylate anions of the fatty acyl chains ($[RCOO]^-$) were observed at *m/z* 255.23 and 281.25, corresponding to 16:0 and 18:1, forming PG 16:0_18:1.

Supplementary Figure S7. PI identification. LC-MS/MS spectrum of $[M-H]^-$ ion of PI 38:2 at *m/z* 889.58. Confirmation of PI class was achieved by the identification of the product ion at *m/z* 241.01 corresponding to the phosphoinositol head group. The carboxylate anions of the fatty acyl chains ($[RCOO]^-$) were observed at *m/z* 283.26 and 307.26, corresponding to 18:0 and 20:2, forming PI 18:0_20:2.

Supplementary Figure S8. PS identification. LC-MS/MS spectrum of $[M-H]^-$ ion of PS 36:2 at *m/z* 786.52. Confirmation of PS class was achieved by the identification of the typical neutral loss of 87 Da (*m/z* 699.49) and the product ion at *m/z* 152.99, corresponding to glycerol-3-phosphate with loss of one molecule of water. The carboxylate anions of the fatty acyl chains ($[RCOO]^-$) were observed at *m/z* 281.25, corresponding to 18:1, forming PS 18:1_18:1.

Supplementary Figure S9. Cer identification. LC-MS/MS spectrum of the $[M+H]^+$ ion of Cer 34:0;O2 at *m/z* 540.53. Confirmation of Cer class was achieved by the identification of the abundant product ions of the sphingoid base at *m/z* 256.26 and 284.29, corresponding to 16:0;O2 and 18:0;O2, respectively (Cer 16:0;O2_18:0).

Supplementary Figure S10. CL identification. LC-MS/MS spectrum of the $[M-H]^-$ ion of CL 70:5 at *m/z* 1425.98. Confirmation of CL class was achieved by the product ion at *m/z* 152.99, corresponding to glycerol-3-phosphate backbone with loss of one molecule of water. The *m/z* 671.47 and 697.48 correspond to PA 34:2 and PA 36:3, respectively. The fatty acyl chains were observed at *m/z* 253.22, 279.23 and 281.25, corresponding to the FA 16:1, 18:2 and 18:1, forming CL 16:1_18:1_18:1_18:2.