Electronic Supplementary Material (ESI) for Chemical Science.

Supplementary Information

Visible-Light Activated [2+2] Cycloaddition Reaction Enables Pinpointing Carbon-Carbon Double Bonds in Lipids

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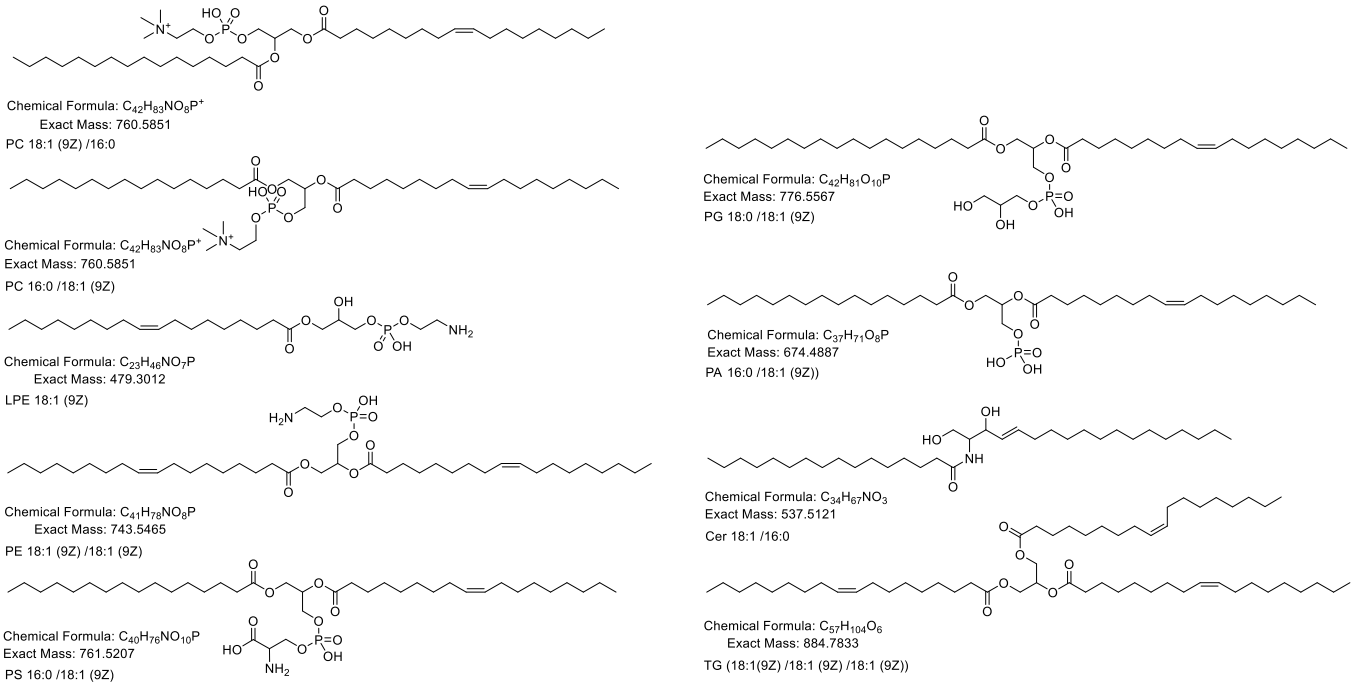

Fig. S1. Chemical structures of the phospholipid standards.

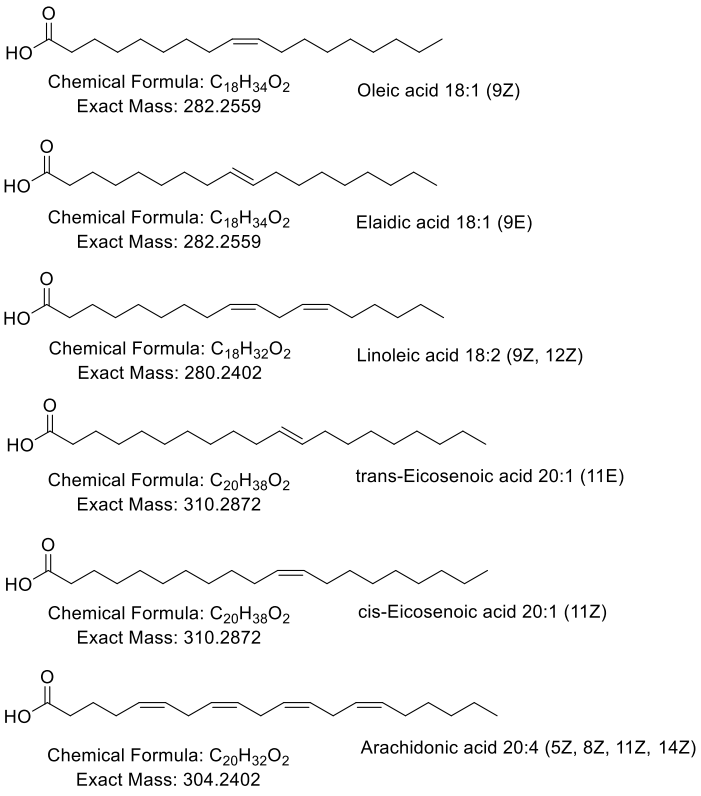

Fig. S2. Chemical structures of the fatty acid standards.

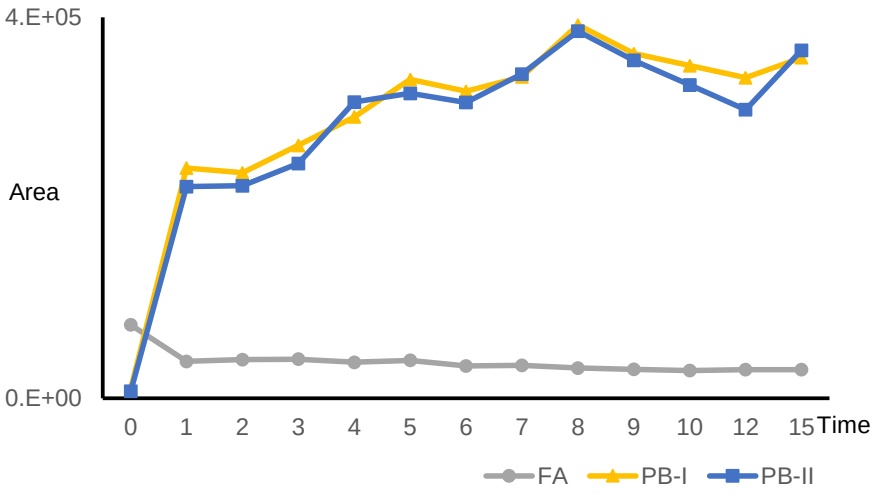

Fig. S3. Optimization of the reaction time of anthraquinone with fatty acid FA 20:1 (11*Z*).

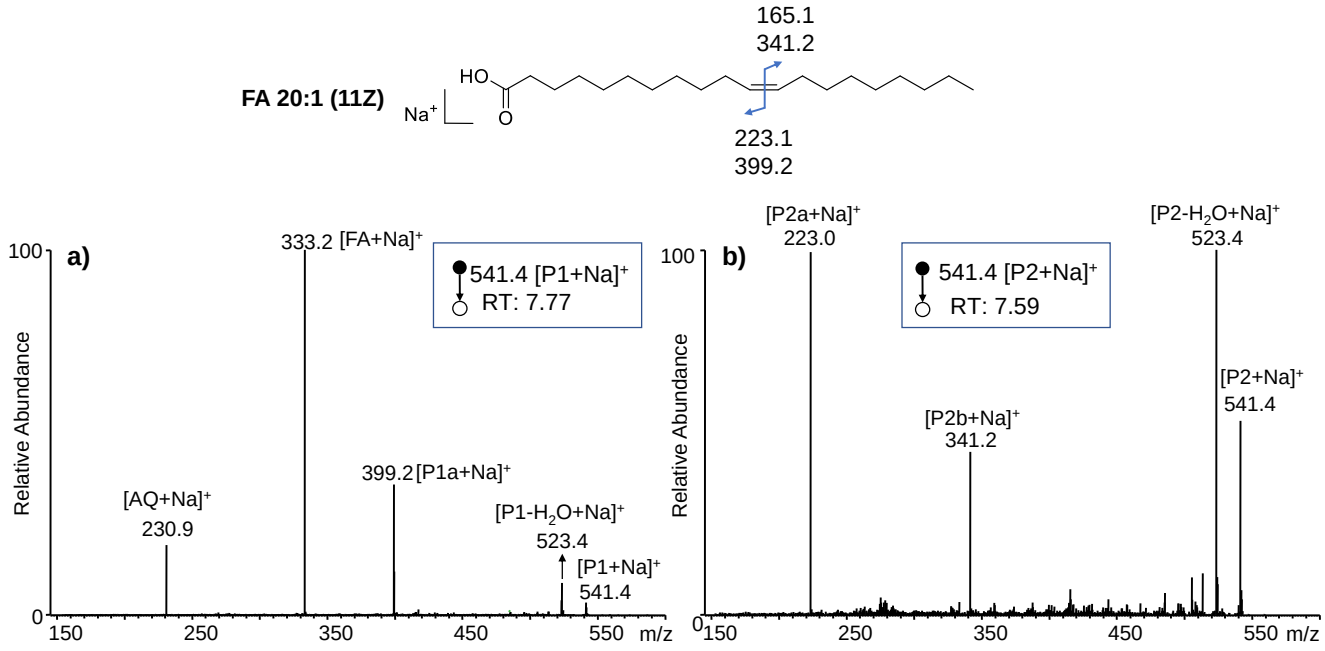

Fig. S4. MS/MS spectra of the VACA reaction products of FA 20:1 (11*Z*) with anthraquinone in the positive ion mode correspond to the EIC peaks at a) 7.77 and b) 7.59 min in liquid chromatography, respectively. The chemical structures on the top shows the positions of C=C bonds and the *m/z* values of the possible diagnostic fragment ions of VACA reaction products via CID.

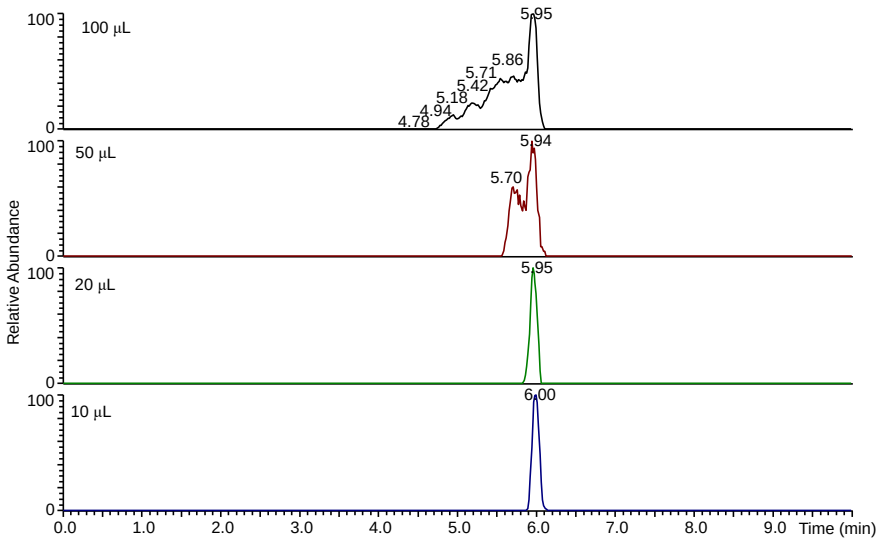

Fig. S5. Comparison of different inject volumes (10, 20, 50 and 100 *µ*L) of VACA reaction products of FA 20:1 (11*Z*) acquired by LC-MS in the positive ion mode by extracted ion chromatogram (EIC) at *m/z* 519.3.

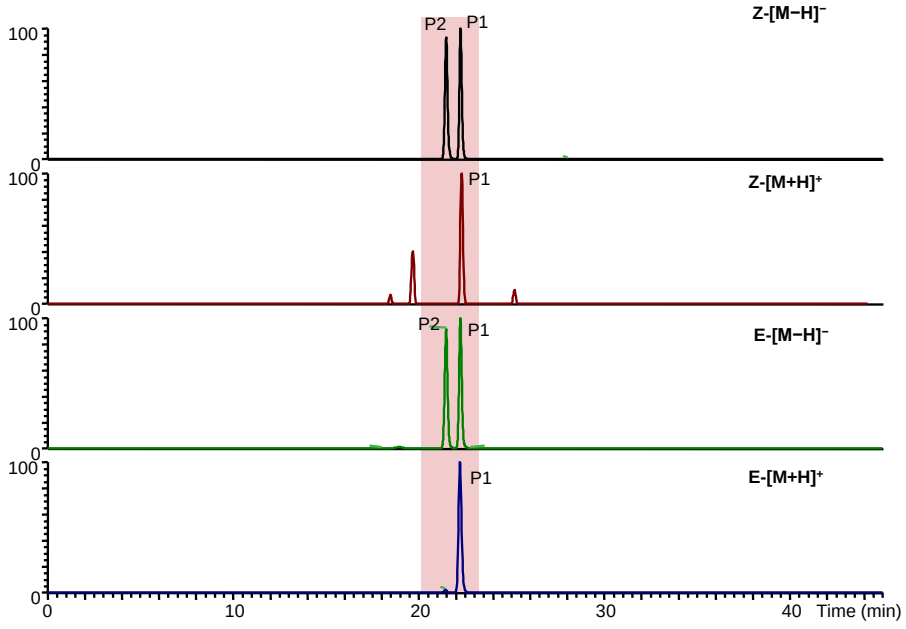

Fig. S6. Comparison of the VACA reaction products between *cis*-FA and *trans*-FA 20:1 (11*Z* and 11*E*) in both positive (*m/z* 519.3) and negative ion (*m/z* 517.3) modes by EICs.

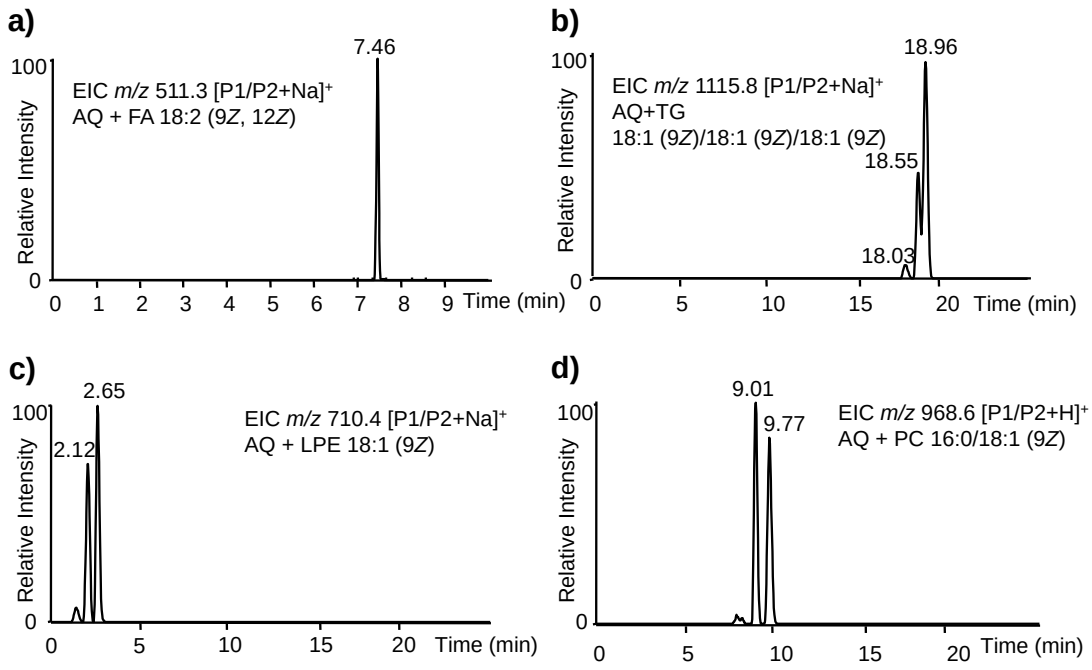

Fig. S7. EIC of the VACA reaction products between AQ and a) FA 18:2 (9*Z*, 12*Z*), b) TG 18:1 (9*Z*)/18:1 (9*Z*) /18:1 (9*Z*), c) LPE 18:1 (9*Z*), and d) PC 16:0/18:1 (9*Z*).

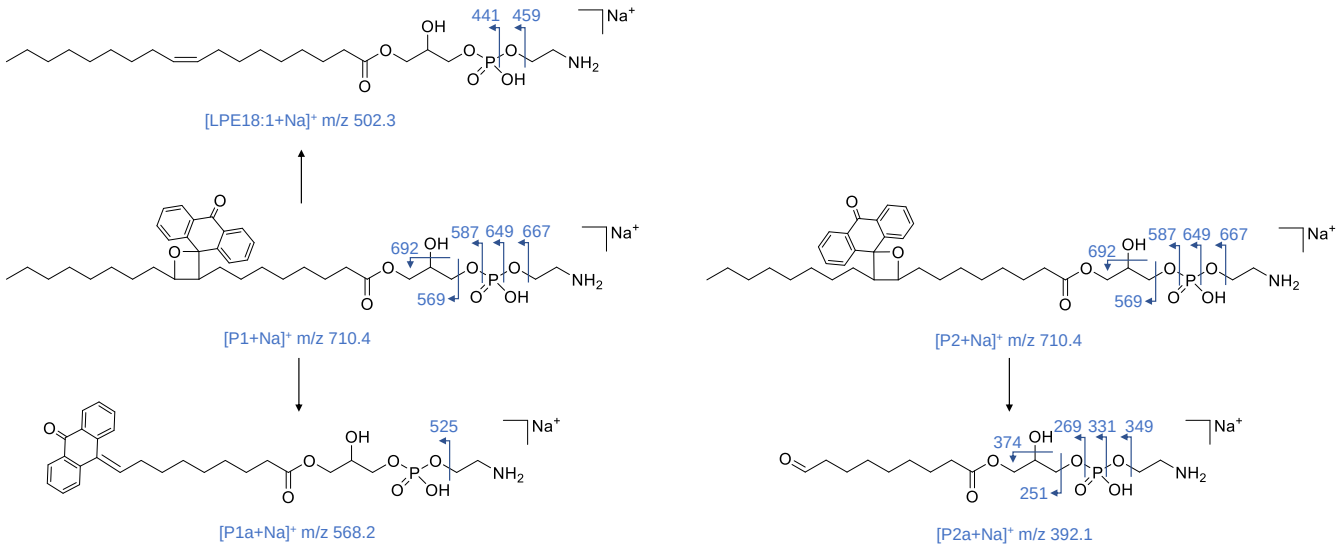

Fig. S8. Structures and fragmentation pathways of sodiated photocycloaddition products (P1/P2) ions of LPE 18:1 (9*Z*) in CID. The figures on each structure correspond to the *m/z* values of the formed fragment ions, and the arrows denote the possible positions of fragmentation.

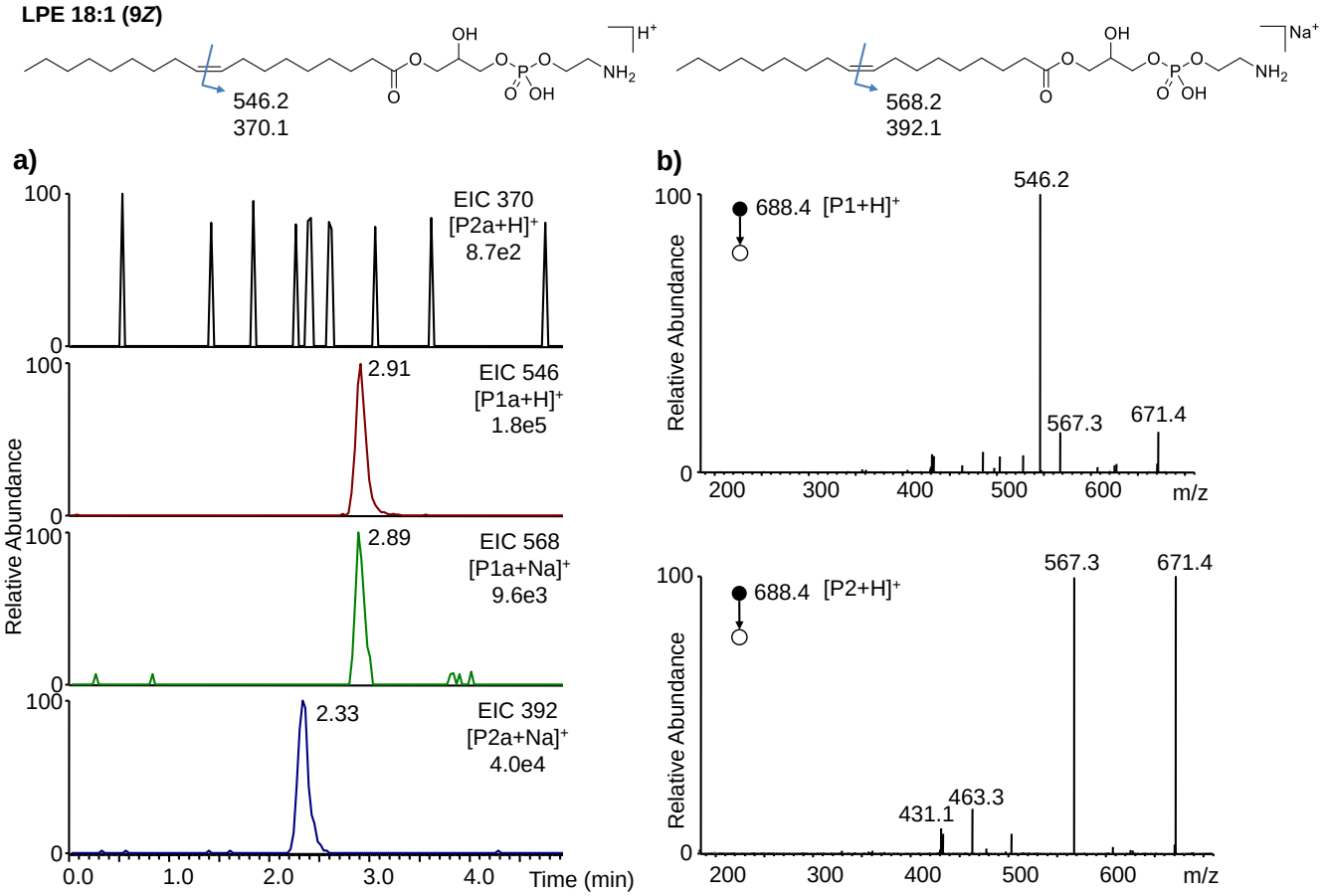

Fig. S9. Analysis of VACA reaction products of LPE 18:1 (9*Z*) with anthraquinone by LC-MS/MS. a) EICs of the ions at *m/z* 370.1 (corresponds to $[P2a+H]^+$) and *m/z* 546.2 (corresponds to $[P1a+H]^+$) extracted from the MS/MS spectra of protonated products (*m/z* 688.4), and EICs of the ions at *m/z* 568.2 (corresponds to $[P1a+Na]^+$) and *m/z* 392.1 (corresponds to $[P2a+Na]^+$) from the MS/MS spectra of sodiated products (*m/z* 710.4) of LPE 18:1 (9*Z*). b) CID spectra of protonated products P1 (2.91 min) and P2 (2.33 min) of LPE 18:1 (9*Z*). The chemical structures on the top shows the positions of C=C bonds and the *m/z* values of the possible diagnostic fragment ions of VACA reaction products via CID.

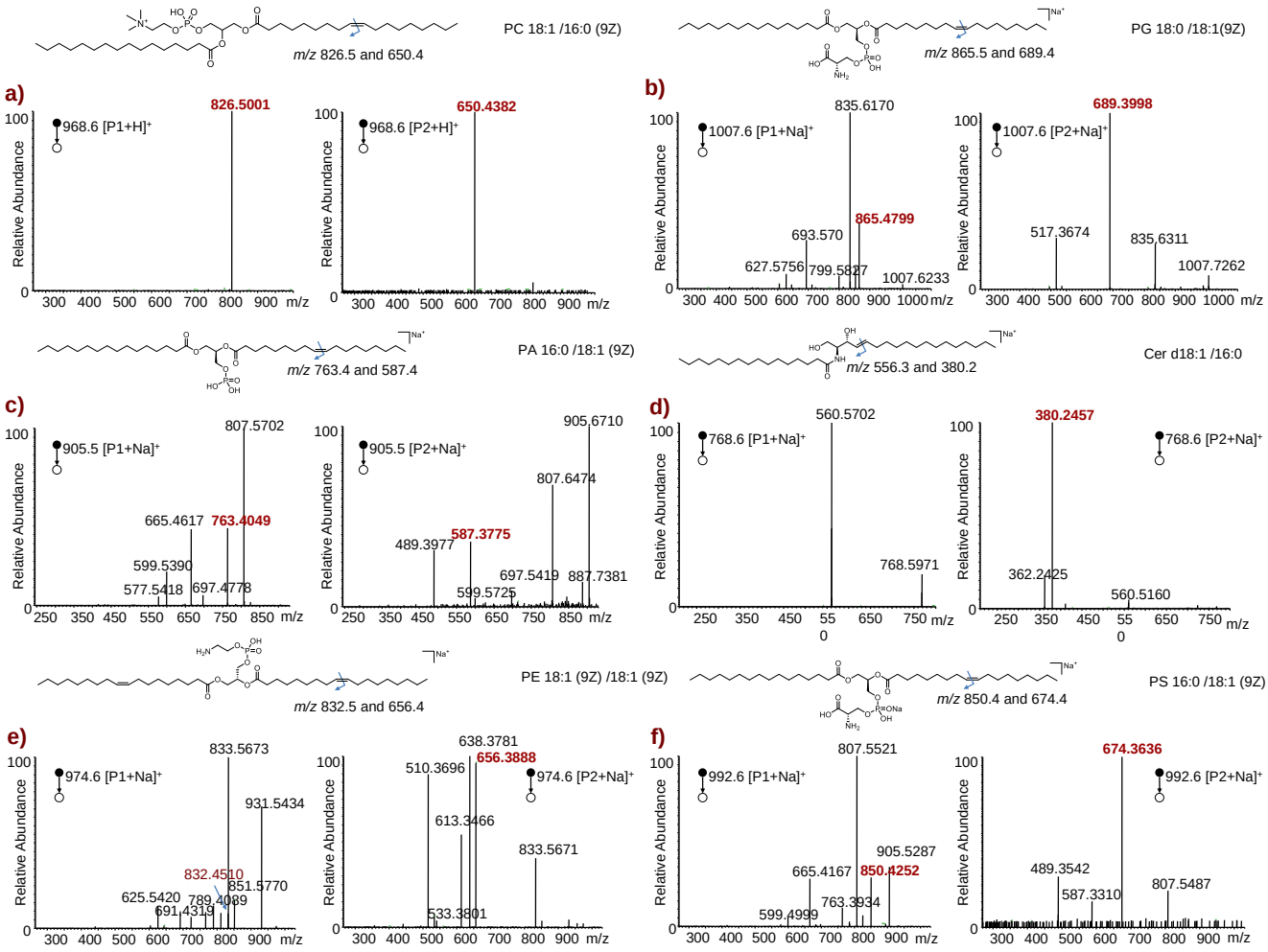

Fig. S10. VACA reaction of anthraquinone with different unsaturated lipids. a-f) The MS/MS spectra of the VACA product ions produced from the reaction of anthraquinone with a) 18:1/16:0 (9*Z*), b) PG 18:0 /18:1 (9*Z*), c) PA 16:0/18:1 (9*Z*), d) Cer d18:1 /16:0, e) 18:1 (9*Z*)/18:1 (9*Z*) and f) 16:0 /18:1 (9*Z*). The chemical structures on the top of each MS/MS spectrum shows the positions of C=C bonds and the *m/z* values of the possible diagnostic fragment ions of VACA reaction products via CID.

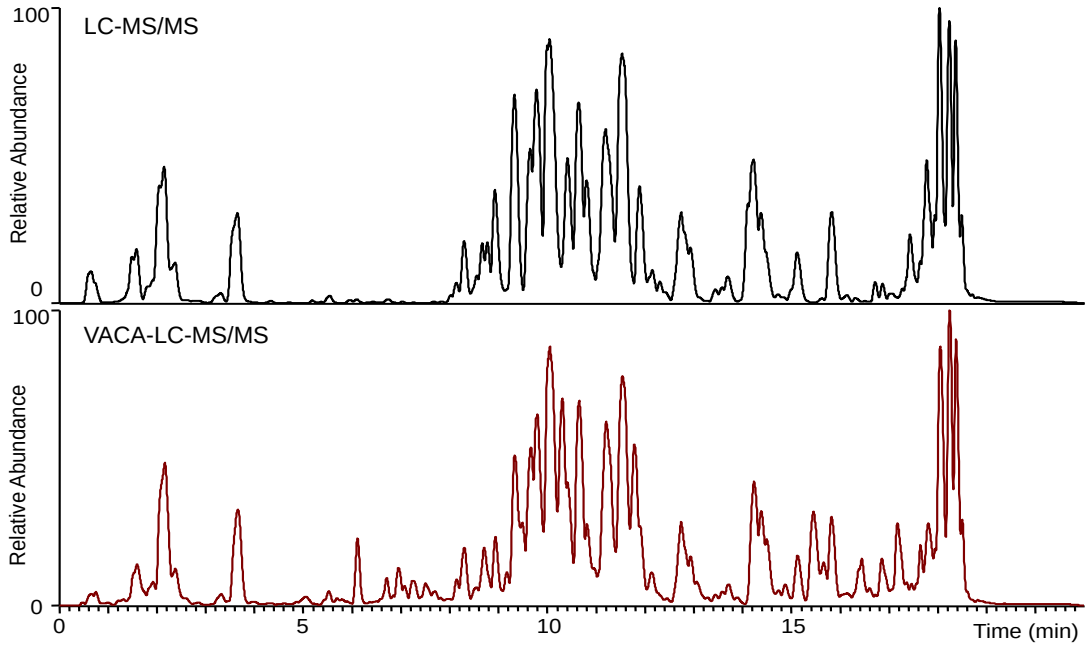

Fig. S11. Base peak ion chromatograms of serum extract in positive ion mode before and after VACA reaction.

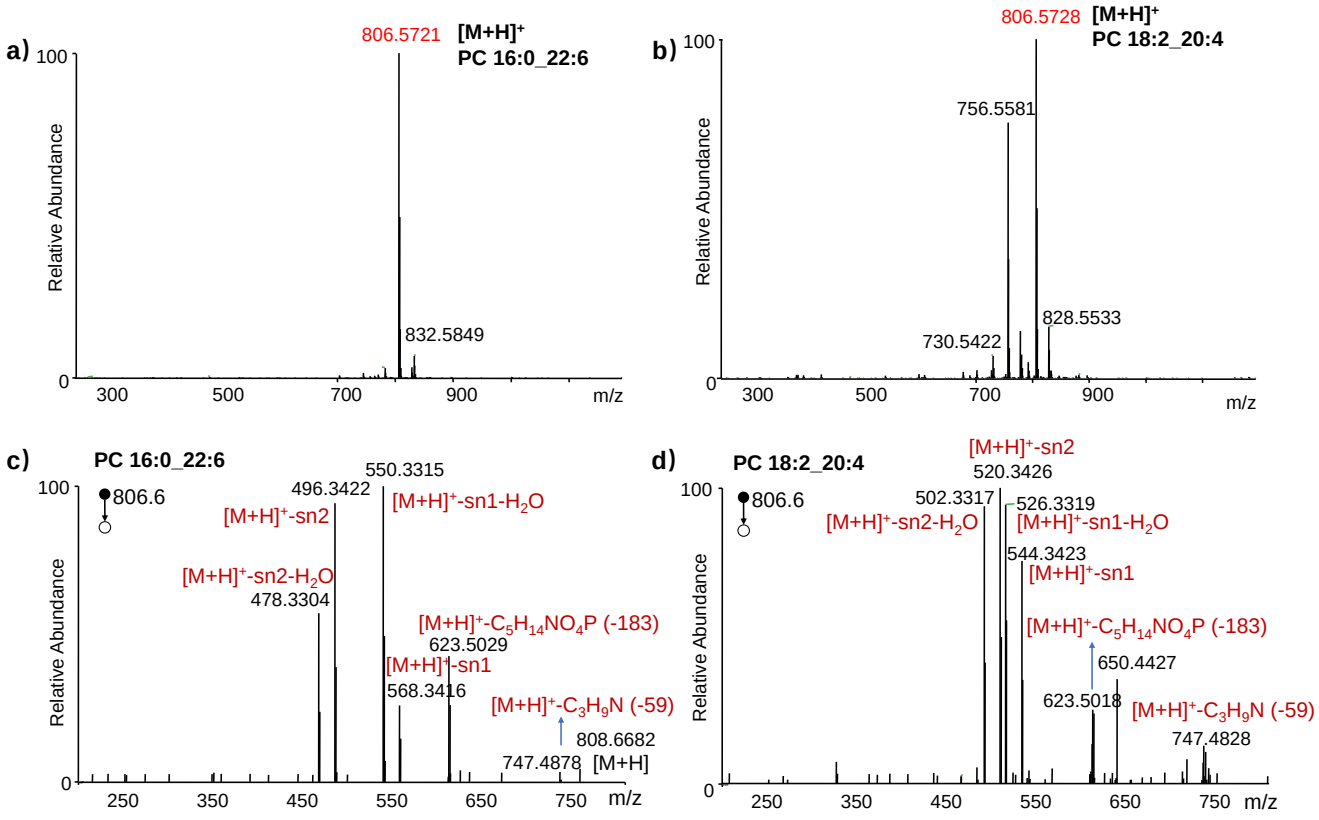

Fig. S12. Full mass and MS/MS spectra of PC 38:6 in the serum extract in positive ion mode. a, b) full mass spectrum of PC 38:6 at a) 9.33 min and b) 8.66 min; c, d) MS/MS spectrum of PC 38:6 at c) 9.33 min and d) 8.66 min. The “sn1” and “sn2” were used to discriminate the acyl fatty chains and don’t represent the actual sn-steric structure.

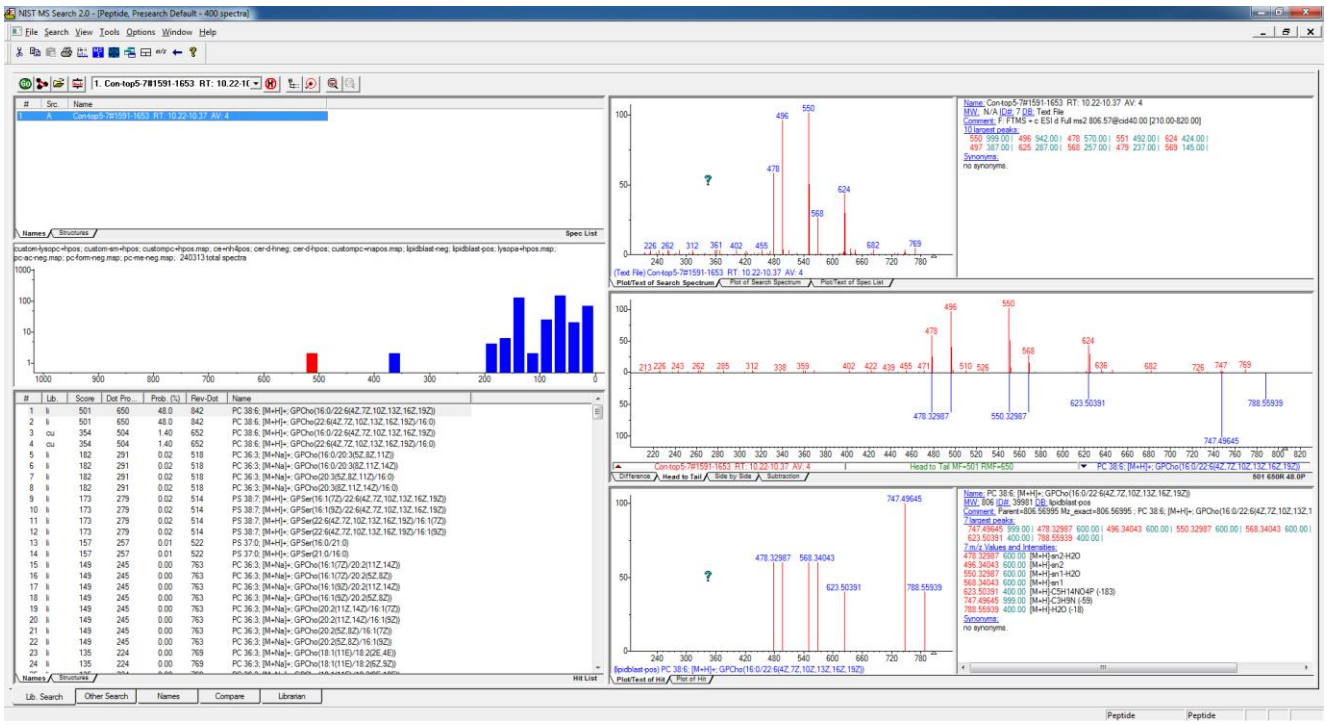

Fig. S13. Matching of the MS/MS spectrum of PC 38:6 in the serum extract at 9.33 min in the Lipid Blast database.

Fig. S14. Matching of the MS/MS spectrum of PC 38:6 in the serum extract at 8.66 min in the Lipid Blast database.

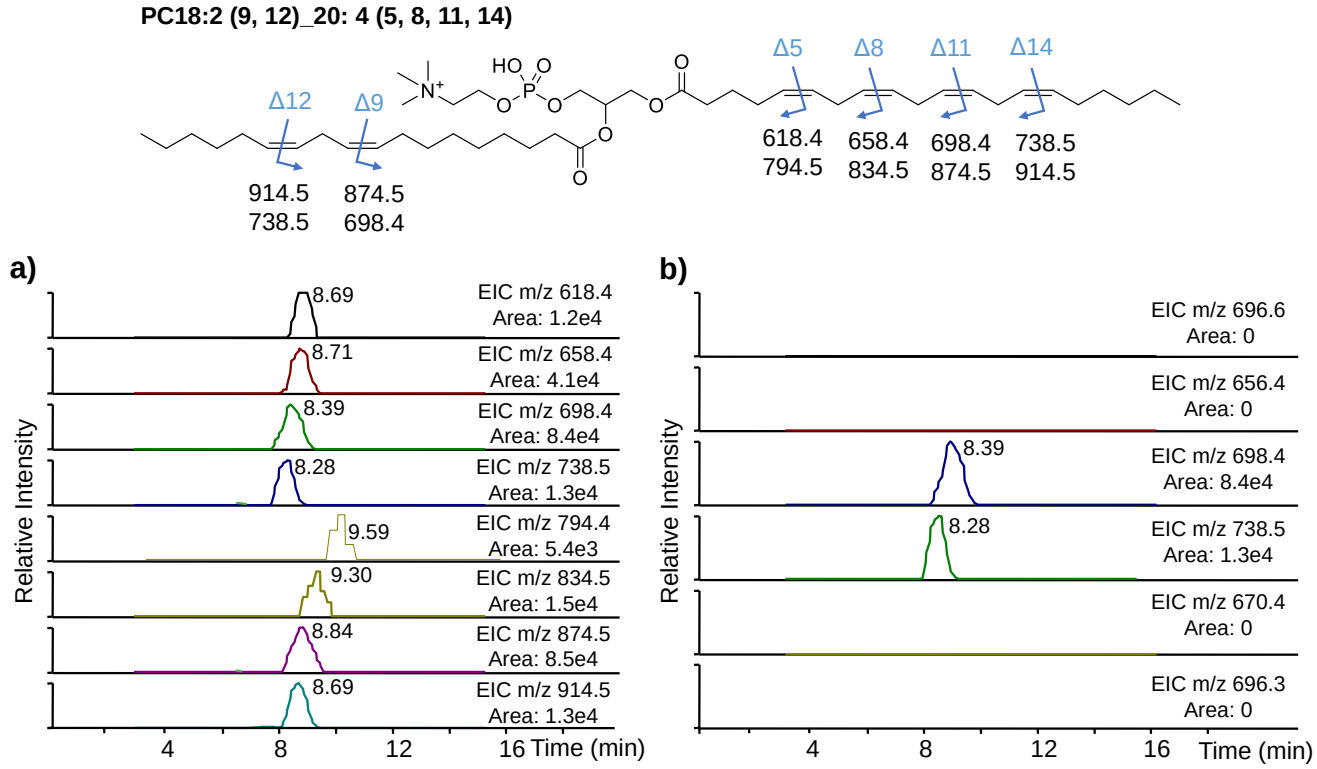

Fig. S15. EICs of the diagnostic ions for a) acyl chain 20:4 (5, 8, 11, 14) and b) acyl chain 18:2 in PC 18:2_20:4. EICs at *m/z* 696.6/656.4 correspond to the simulated diagnostic ions derived from the double bonds at Δ6 and Δ9 in the fatty acyl chain 18:2, EICs at *m/z* 698.4/738.5 correspond to that of the double bonds at Δ9 and Δ12, and EICs at *m/z* 670.4/696.3 correspond to that of the double bonds at Δ9 and Δ11. The chemical structure on the top show the positions of C=C bonds in PC 18:2_20:4 and the *m/z* values of the possible diagnostic fragment ions of its VACA reaction products via CID.

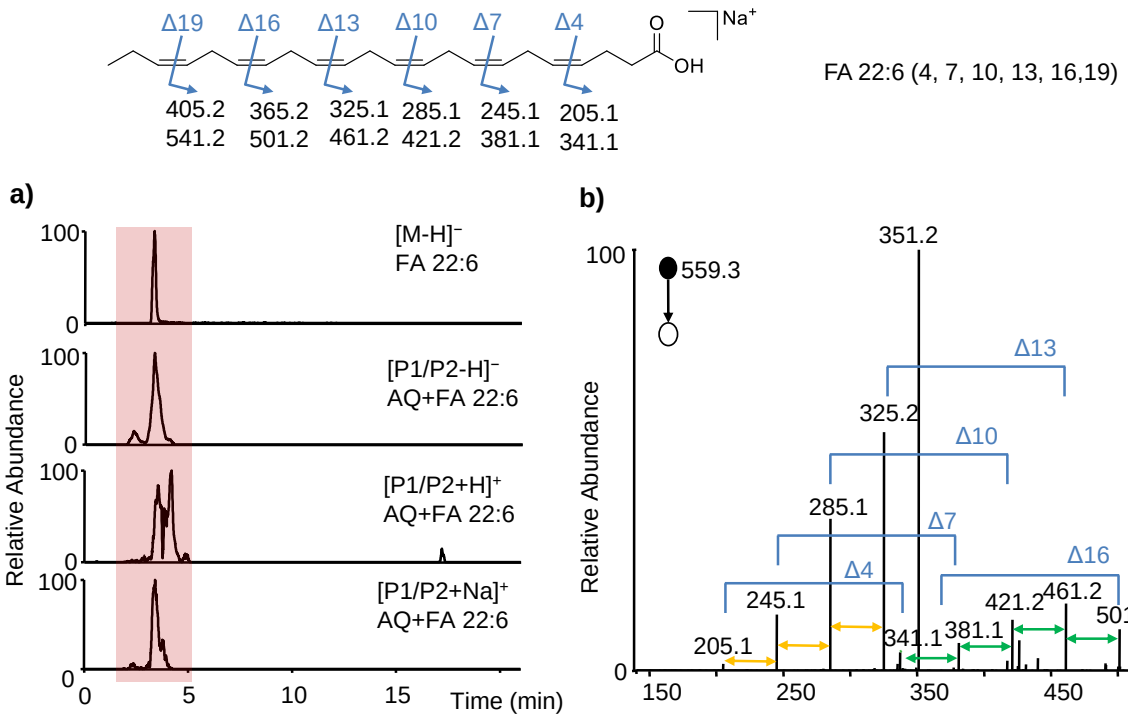

Fig. S16. Identification of the FA 22:6 in the serum extract. a) From top to the bottom: EICs of FA 22:6 at *m/z* 327.2 $[M-H]^-$, the VACA products of FA 22:6 in the negative (*m/z* 535.3, $[P1/P2-H]^-$) and positive (*m/z* 537.3 $[P1/P2+H]^+$ and 559.3 $[P1/P2+Na]^+$) ion modes. b) MS/MS spectrum of VACA products $[P1/P2+Na]^+$ at *m/z* 559.3. The chemical structure on the top shows the positions of C=C bonds and the possible *m/z* values of the diagnostic fragment ions. The diagnostic ion pair for C=C at Δ19 were not detected, and only five positions of C=C were inferred based on this MS/MS spectrum. Given the typical rule for the position of nonconjugated C=C bonds in fatty acids, we speculated that another position of C=C bond was located between C19 and C20. Hence, this FA was identified as FA 22:6 (4, 7, 10, 13, 16, 19).

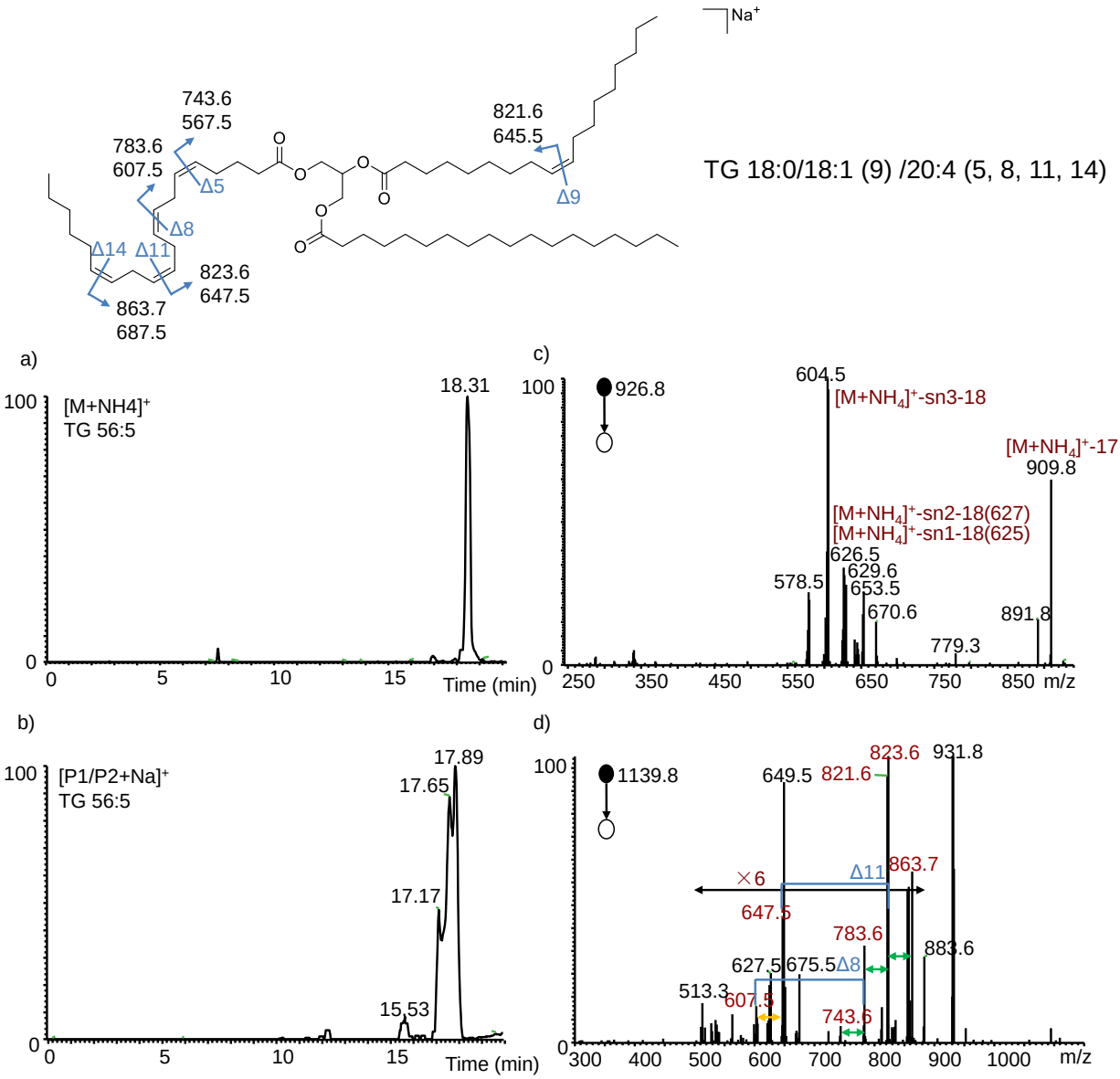

Fig. S17. Identification of the TG 56:5 in the serum extract. a) EICs of TG 56:5 at *m/z* 926.8 $[M+NH4]^+$. b) the VACA products of TG 56:5 in the positive (*m/z* 1139.8 $[P1/P2+Na]^+$ ion mode. c) MS/MS spectrum of TG 56:5 at *m/z* 926.8 $[M+NH4]^+$ at 18.31 min. d) average MS/MS spectra of VACA products $[P1/P2+Na]^+$ at *m/z* 1139.8 from 17.17~17.89 min. The chemical structure on the top shows the positions of C=C bonds and the possible *m/z* values of the diagnostic fragment ions for TG 18:0_18:1 (9)_20:4 (5, 8, 11, 14). Diagnostic ion pairs for C=C at Δ8 and Δ11 were detected for fatty acyl chain 20:4, while other C=C bond positions were detected with single diagnostic ions P1a. There also a diagnostic ion P1a at *m/z* 821.6 for another fatty acyl chain. Based on the outcome of LipidBlast (see Fig. S14), the structure of TG 56:5 with the highest score was TG 18:0_18:1_20:4. Therefore, the detailed structure this TG compound should be 18:0_18:1 (9)_20:4 (5, 8, 11,14).

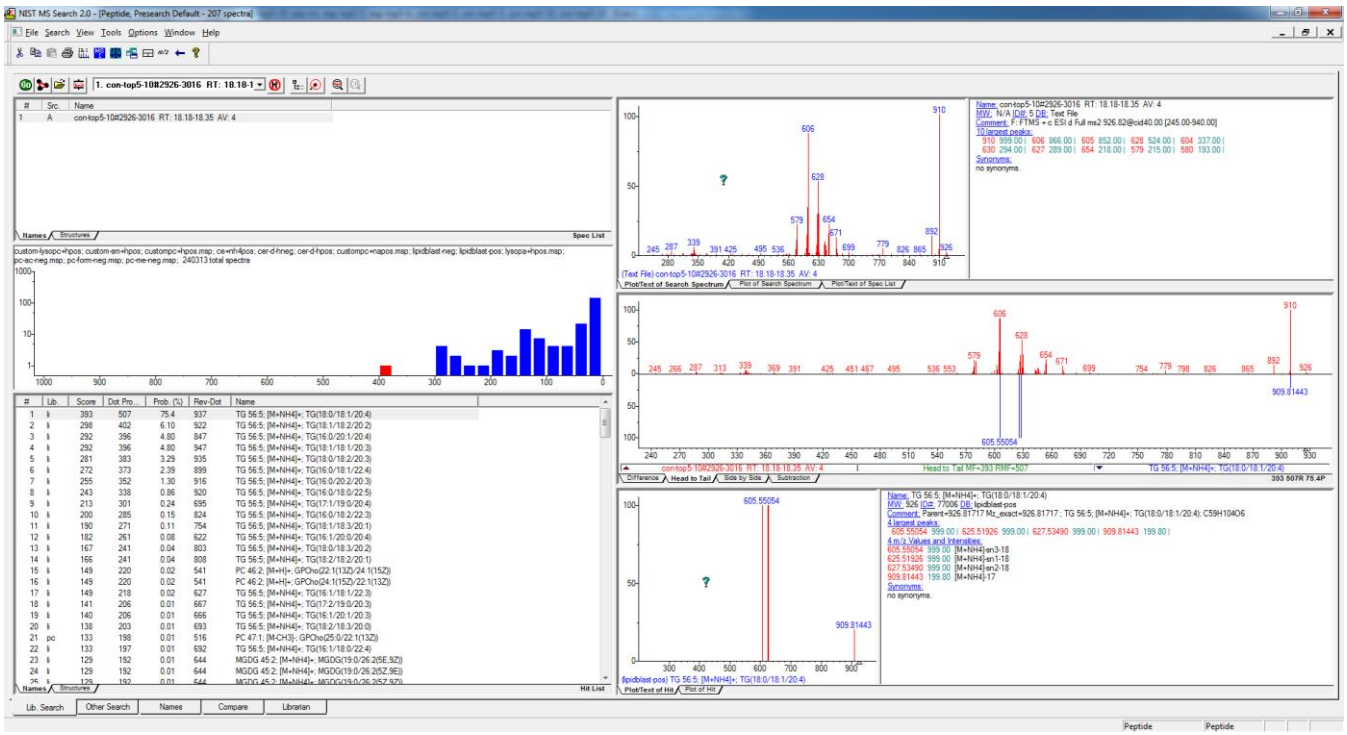

Fig. S18. Matching of the MS/MS spectrum of TG 56:5 in the serum extract at 18.31 min in the Lipid Blast database.

Supplementary Tables

Table S1. Statistics of the lipid numbers identified in human serum.

Lipids	FA	PC	PE	TG	SM	Cer	Total
Unidentified unsaturated lipids	0	9	16	41	25	0	96
Identified unsaturated lipids	12	45	5	21	2	1	86
Saturated lipids	3	15	3	10	4	1	36
Total	15	69	24	72	31	2	213

Table S2. Detailed structures of the lipids with the identified C=C bond positions.

Class	Structures with C=C positions
Fatty acids (FA) 12 (12)	FA 16:1 (9/11) FA 18:1 (9/11) FA 18:2 (9,12) FA 18:3 (9,12,15) FA 20:1 (11/13) FA 20:2 (11, 14) FA 20:3 (8, 11, 14) FA 20:4 (5, 8, 11, 14) FA 22:1 (13) FA 22:4 (7, 10, 13, 16) FA 22:5 (7, 10, 13, 16, 19) FA 22:6 (4, 7, 10, 13, 16, 19)
Lysophosphatidylcholines (LPC) 15 (17)	LPC 16:1 (9) LPC 18:1 (9 vs. 11) LPC 20:1 (11) LPC 18:2 (9, 12) LPC 20:2 (8, 11) LPC 18:3 (6, 9, 12) LPC 20:3 (8, 11, 14) LPC 20:4 (6, 9, 11, 14) LPC 22:4 (7, 10, 13, 16) LPC 20:5 (4, 7, 10, 13, 16) LPC 22:5 (4, 7, 10, 13, 16) LPC 22:6 (4, 7, 10, 13, 16, 19)
Phosphocholines (PC) 30 (36)	PC 16:0_18:1 (9 vs. 11) PC 18:0_18:1 (9) PC P-16:0_24:1 (15 vs.18) PC 14:0_18:2 (9, 12) PC 15:0_18:2 (9, 12) PC 16:0_18:2 (9, 12) PC P-16:0_18:2 (9, 12) PC 17:0_18:2 (9, 12) PC 18:0_18:2 (9, 12) PC 18:0_20:2 (8, 11) / PC 20:0_18:2 (9, 12) PC 18:2_18:2 (9, 12) PC P-16:0_20:2 (8, 11) PC P-18:0_22:2 (13, 16) / PC 18:2 (9, 12)_22:0 PC 18:0_18:3 (6, 9, 12) PC 17:0_20:3 (8, 11, 14) PC 18:0_20:3 (8, 11, 14) PC 15:0_20:4 (5, 8, 11, 14) PC 17:0_20:4 (5, 8, 11, 14)

	PC 17:0_22:4 (7, 10, 13, 16) PC 18:0_18:4 (3, 6, 9, 12) PC 18:1_20:4 (5, 8, 11, 14) PC 18:2_20:4 (8, 11, 14, 17) PC 18:0_22:4 (10, 13, 16, 19) PC P-20:0_24:4 (5, 8, 11, 14) PC 18:0_22:5 (4, 7, 10, 13, 16) PC P-20:0_22:5 (4, 7, 10, 13, 16) PC 16:0_22:6 (4, 7, 10, 13, 16, 19) PC 18:0_22:6 (4, 7, 10, 13, 16, 19)
Lysophosphatidylethanolamine (LPE) 1 (4)	LPE 18:1 (9) (standard)
Phosphoethanolamines (PE) 4 (16)	PE 16:0_18:2 (10,13) PE 18:2_20:2 (11, 14) PE 18:1 (9)_18:1 (9) (standard) PE P-18:2_20:2 (11, 14)
Cer 1(1)	Cer d18:1/16:0 (standard)
Sphingomyelins (SM) 2 (27)	SM d15:1_26:1 (17) SM d17:1_24:1 (15)
Triradylglycerolipids (TG) 21 (62)	TG 12:0_18:1 (15)_16:1 (13) TG 14:1_16:1 (10)_18:1 (12) TG 14:0_16:1 (10)_18:1 (11) TG 16:0_16:1 (10)_17:0 TG 16:0_16:1 (10)_18:1 (12) TG 16:0_16:0_18:1 (11) TG 16:0_17:1 (8)_18:2 (6, 9) TG 16:0_17:1 (8)_18:1 (9) TG 16:0_18:2 (9, 12)_18:2 (9, 12) TG 16:0_18:1 (9)_18:2 (9, 12) TG 16:0_18:1 (9)_18:1 (9) /16:0_18:1 (11)_18:1 (11) TG 17:0_18:1 (9)_18:2 (9, 12) TG 17:0_18:1 (9)_18:1 (9) TG 18:2 (9, 12)_18:2 (9, 12)_18:2 (9, 12) TG 18:1 (9)_18:1 (9)_18:2 (9, 12) TG 18:1 (9)_18:1 (9)_18:1 (9) TG 18:1 (9)_18:2 (9, 12)_20:4(5, 8, 11, 14) TG 18:1 (9)_18:2 (9, 12)_20:3 (8, 11, 14) TG 18:0_18:1 (17)_20:4(5, 8, 11, 14)

Note: "P-" represent the species of (1Z)-alkenyl ether (neutral Plasmalogen); the values after each subclass names are the number of identified unsaturated lipid species with specific C=C location, while the values in parenthesis are the number of all identified unsaturated lipids without analyisis of C=C location isomers.

Table S3. PC and LPC identified from human serum extract.

No.	Identification	RT (min)	Formula	Observed m/z	Calculated m/z	Error (ppm)	Adduct	Match details	Formula of neutral loss molecules for C=C analysis
1	LPC 14:0	1.28	$C_{22}H_{46}NO_7P$	468.3109	468.3090	4.1	[M+H]+	184.07387 300.00 $C_5H_{15}NO_4P$ m/z=184 240.10020 10.00 [M+H]-sn1-H_2O 258.11076 10.00 [M+H]-sn1 450.29844 999.00 [M+H]-H_2O (-18)	-
2	LPC 15:0	1.69	$C_{23}H_{48}NO_7P$	482.3260	482.3246	2.9	[M+H]+	184.07387 300.00 C5H15NO4P m/z=184 240.10021 10.00 [M+H]-sn1-H2O 258.11077 10.00 [M+H]-sn1 464.31409 999.00 [M+H]-H2O (-18)	-
3	LPC 16:1 (9)	1.44	$C_{24}H_{48}NO_7P$	494.3262	494.3246	3.2	[M+H]+	184.07387 300.00 C5H15NO4P m/z=184 240.10021 10.00 [M+H]-sn1-H2O 258.11077 10.00 [M+H]-sn1 476.31409 999.00 [M+H]-H2O (-18)	C_7H_{14}
4	LPC 16:0	2.16	$C_{24}H_{50}NO_7P$	496.3402	496.3403	-0.2	[M+H]+	184.07387 300.00 C5H15NO4P m/z=184 240.10023 10.00 [M+H]-sn1-H2O 258.11079 10.00 [M+H]-sn1 478.32975 999.00 [M+H]-H2O (-18)	-
5	LPC 17:1	1.88	$C_{25}H_{50}NO_7P$	508.3416	508.3403	2.6	[M+H]+	184.07387 300.00 C5H15NO4P m/z=184 240.10023 10.00 [M+H]-sn1-H2O 258.11079 10.00 [M+H]-sn1 490.32975 999.00 [M+H]-H2O (-18)	/
6	LPC 17:0	2.84	$C_{25}H_{52}NO_7P$	510.3579	510.3560	3.7	[M+H]+	184.07387 300.00 C5H15NO4P m/z=184 240.10024 10.00 [M+H]-sn1-H2O 258.11080 10.00 [M+H]-sn1 492.34540 999.00 [M+H]-H2O (-18)	-
7	LPC 18:3 (6, 9, 12)	1.98	$C_{26}H_{48}NO_7P$	518.3264	518.3246	3.5	[M+H]+	184.07387 300.00 C5H15NO4P m/z=184 240.10021 10.00 [M+H]-sn1-H2O 258.11077 10.00 [M+H]-sn1 500.31409 999.00 [M+H]-H2O (-18)	C_6H_{12}, C_9H_{16}, $C_{12}H_{20}$
8	LPC 18:2 (9, 12)	1.59	$C_{26}H_{50}NO_7P$	520.3423	520.3403	3.8	[M+H]+	184.07387 300.00 C5H15NO4P m/z=184 240.10026 10.00 [M+H]-sn1-H2O 258.11082 10.00 [M+H]-sn1 502.32978 999.00 [M+H]-H2O (-18)	C_6H_{12}, C_9H_{16}
9	LPC 18:1 (9)_18:1 (11)	2.38	$C_{26}H_{52}NO_7P$	522.3572	522.3560	2.3	[M+H]+	184.07387 300.00 C5H15NO4P m/z=184 240.10024 10.00 [M+H]-sn1-H2O 258.11080 10.00 [M+H]-sn1 504.34540 999.00 [M+H]-H2O (-18)	C_9H_{18}, $C_{11}H_{22}$
10	LPC P-18:0	2.86	$C_{26}H_{54}NO_6P$	508.3790	508.3767	4.5	[M+H]+	184.07387 300.00 C5H15NO4P m/z=184 224.10533 10.00 [M+H]-sn1-H2O 242.11589 10.00 [M+H]-sn1 490.36613 999.00 [M+H]-H2O (-18)	-
11	LPC 18:0	3.65	$C_{26}H_{54}NO_7P$	524.3734	524.3716	3.4	[M+H]+	184.07387 300.00 C5H15NO4P m/z=184 240.10023 10.00 [M+H]-sn1-H2O 258.11079 10.00 [M+H]-sn1 506.36103 999.00 [M+H]-H2O (-18)	-
12	LPC 20:5 (5, 8,11,14,17)	1.16	$C_{28}H_{48}NO_7P$	542.3264	542.3246	3.3	[M+H]+	184.07387 300.00 C5H15NO4P m/z=184 240.10021 10.00 [M+H]-sn1-H2O 258.11077 10.00 [M+H]-sn1 524.31409 999.00 [M+H]-H2O (-18)	C_3H_6, C_6H_{10}, C_9H_{14}, $C_{12}H_{18}$
13	LPC 20:4 (5, 8,11,14)	1.57	$C_{28}H_{50}NO_7P$	544.3404	544.3403	0.2	[M+H]+	184.07387 300.00 C5H15NO4P m/z=184 240.10026 10.00 [M+H]-sn1-H2O 258.11082 10.00 [M+H]-sn1 526.32978 999.00 [M+H]-H2O (-18)	C_6H_{12}, C_9H_{16}, $C_{12}H_{20}$, $C_{15}H_{24}$

14	LPC 20:3 (8,11,14)	2.01	$C_{28}H_{52}NO_7P$	546.3575	546.3560	2.7	[M+H]+	184.07387 300.00 C5H15NO4P m/z=184 240.10024 10.00 [M+H]-sn1-H2O 258.11080 10.00 [M+H]-sn1 528.34540 999.00 [M+H]-H2O (-18)	C_6H_{12}, C_9H_{16}, $C_{12}H_{20}$
15	LPC 20:2 (8, 11)	2.80	$C_{28}H_{54}NO_7P$	548.3730	548.3716	2.6	[M+H]+	184.07387 300.00 C5H15NO4P m/z=184 240.10023 10.00 [M+H]-sn1-H2O 258.11079 10.00 [M+H]-sn1 530.36103 999.00 [M+H]-H2O (-18)	C_9H_{18}, $C_{12}H_{22}$
16	LPC 20:1 (11)	3.81	$C_{28}H_{56}NO_7P$	550.3880	550.3873	1.3	[M+H]+	184.07387 300.00 C5H15NO4P m/z=184 240.10028 10.00 [M+H]-sn1-H2O 258.11084 10.00 [M+H]-sn1 532.37672 999.00 [M+H]-H2O (-18)	C_9H_{18}
17	LPC 20:0	5.36	$C_{28}H_{58}NO_7P$	552.4038	552.4029	1.6	[M+H]+	184.07387 300.00 C5H15NO4P m/z=184 240.10026 10.00 [M+H]-sn1-H2O 258.11082 10.00 [M+H]-sn1 534.39234 999.00 [M+H]-H2O (-18)	-
18	LPC 22:6 (4, 7, 10, 13, 16, 19)	1.47	$C_{30}H_{50}NO_7P$	568.3408	568.3403	0.9	[M+H]+	184.07387 300.00 C5H15NO4P m/z=184 240.10026 10.00 [M+H]-sn1-H2O 258.11082 10.00 [M+H]-sn1 550.32978 999.00 [M+H]-H2O (-18)	C_3H_6, C_6H_{10}, C_9H_{14}, $C_{12}H_{18}$, $C_{15}H_{22}$, $C_{18}H_{26}$
19	LPC 22:5 (7, 10, 13, 16, 19)	1.74	$C_{30}H_{52}NO_7P$	570.3557	570.3560	-0.5	[M+H]+	184.07387 300.00 C5H15NO4P m/z=184 240.10024 10.00 [M+H]-sn1-H2O 258.11080 10.00 [M+H]-sn1 552.34540 999.00 [M+H]-H2O (-18)	C_3H_6, C_6H_{10}, C_9H_{14}, $C_{12}H_{18}$, $C_{15}H_{22}$
20	LPC 22:5 (4, 7, 10, 13, 16)	2.07	$C_{30}H_{52}NO_7P$	570.3576	570.3560	2.8	[M+H]+	184.07387 300.00 C5H15NO4P m/z=184 240.10024 10.00 [M+H]-sn1-H2O 258.11080 10.00 [M+H]-sn1 552.34540 999.00 [M+H]-H2O (-18)	C_6H_{12}, C_9H_{16}, $C_{12}H_{20}$, $C_{15}H_{24}$
21	LPC 22:4 (7, 10, 13, 16)	2.50	$C_{30}H_{54}NO_7P$	572.3718	572.3716	0.4	[M+H]+	184.07387 300.00 C5H15NO4P m/z=184 240.10023 10.00 [M+H]-sn1-H2O 258.11079 10.00 [M+H]-sn1 554.36103 999.00 [M+H]-H2O (-18)	C_6H_{12}, C_9H_{16}, $C_{12}H_{20}$, $C_{15}H_{24}$
22	LPC 22:1	5.41	$C_{30}H_{60}NO_7P$	578.4198	578.4186	2.1	[M+H]+	184.07387 300.00 C5H15NO4P m/z=184 240.10031 10.00 [M+H]-sn1-H2O 258.11087 10.00 [M+H]-sn1 560.40803 999.00 [M+H]-H2O (-18)	/
23	LPC 22:0	6.59	$C_{30}H_{62}NO_7P$	580.4360	580.4342	3.1	[M+H]+	184.07387 300.00 C5H15NO4P m/z=184 240.10029 10.00 [M+H]-sn1-H2O 258.11085 10.00 [M+H]-sn1 562.42365 999.00 [M+H]-H2O (-18)	-
24	LPC 24:0	7.77	$C_{32}H_{66}NO_7P$	608.4677	608.4655	3.6	[M+H]+	184.07387 300.00 C5H15NO4P m/z=184 240.10032 10.00 [M+H]-sn1-H2O 258.11088 10.00 [M+H]-sn1 590.45496 999.00 [M+H]-H2O (-18)	-
25	LPC 26:1	8.2	$C_{34}H_{68}NO_7P$	634.4830	634.4812	2.9	[M+H]+	184.07387 300.00 C5H15NO4P m/z=184 240.10031 10.00 [M+H]-sn1-H2O 258.11087 10.00 [M+H]-sn1 616.47059 999.00 [M+H]-H2O (-18)	/
26	LPC 26:0	9.21	$C_{34}H_{70}NO_7P$	636.4978	636.4968	1.6	[M+H]+	184.07387 300.00 C5H15NO4P m/z=184 240.10035 10.00 [M+H]-sn1-H2O 258.11091 10.00 [M+H]-sn1 618.48627 999.00 [M+H]-H2O (-18)	-
27	PC P-16:0_14:0	10.31	$C_{38}H_{76}NO_7P$	690.5460	690.5438	3.2	[M+H]+	391.22511 100.00 [M+H]-sn1-C3H9N (-59) 450.29861 999.00 [M+H]-sn1 (alkenyl ether loss) 462.33497 10.00 [M+H]-sn2-H2O 480.34553 200.00 [M+H]-sn2 507.47773 10.00 [M+H]-C5H14NO4P (-183)	-
28	PC 15:0_16:0	10.40	$C_{39}H_{78}NO_8P$	720.5570	720.5543	3.8	[M+H]+	464.31425 600.00 [M+H]-sn2-H2O 478.32989 600.00 [M+H]-sn1-H2O 482.32481 600.00 [M+H]-sn2 496.34045 600.00 [M+H]-sn1	-

								537.48829 400.00 [M+H]-C5H14NO4P (-183) 661.48083 999.00 [M+H]-C3H9N (-59) 702.54377 400.00 [M+H]-H2O (-18)	
29	PC 14:0_18:2 (9, 12)	9.15	$C_{40}H_{76}NO_8P$	730.5418	730.5387	4.2	[M+H]+	450.29862 600.00 [M+H]-sn2-H2O 468.30918 600.00 [M+H]-sn2 502.32990 600.00 [M+H]-sn1-H2O 520.34046 600.00 [M+H]-sn1 547.47266 400.00 [M+H]-C5H14NO4P (-183) 671.46520 999.00 [M+H]-C3H9N (-59) 712.52814 400.00 [M+H]-H2O (-18)	C_6H_{12}, C_9H_{16}
30	PC P-16:0_16:0	11.83	$C_{40}H_{80}NO_7P$	718.5778	718.5751	3.8	[M+H]+	419.25642 100.00 [M+H]-sn1-C3H9N (-59) 462.33500 10.00 [M+H]-sn2-H2O 478.32992 999.00 [M+H]-sn1 (alkenyl ether loss) 480.34556 200.00 [M+H]-sn2 535.50904 10.00 [M+H]-C5H14NO4P (-183)	-
31	PC 16:0_16:0	11.11	$C_{40}H_{80}NO_8P$	734.5738	734.5694	6.0	[M+H]+	478.32987 600.00 [M+H]-sn1-H2O || [M+H]-sn2-H2O 496.34043 600.00 [M+H]-sn1 || [M+H]-sn2 551.50391 400.00 [M+H]-C5H14NO4P (-183) 675.49645 999.00 [M+H]-C3H9N (-59) 716.55939 400.00 [M+H]-H2O (-18)	-
32	PC 15:0_18:2 (9, 12)	10.30	$C_{41}H_{78}NO_8P$	744.5563	744.5538	3.4	[M+H]+	464.31425 600.00 [M+H]-sn2-H2O 482.32481 600.00 [M+H]-sn2 502.32989 600.00 [M+H]-sn1-H2O 520.34045 600.00 [M+H]-sn1 561.48829 400.00 [M+H]-C5H14NO4P (-183) 685.48083 999.00 [M+H]-C3H9N (-59) 726.54377 400.00 [M+H]-H2O (-18)	C_6H_{12}, C_9H_{16}
33	PC 16:0_18:2 (9, 12)	10.84	$C_{42}H_{80}NO_8P$	758.5721	758.5700	2.8	[M+H]+	478.32987 600.00 [M+H]-sn2-H2O 496.34043 600.00 [M+H]-sn2 502.32987 600.00 [M+H]-sn1-H2O 520.34043 600.00 [M+H]-sn1 575.50391 400.00 [M+H]-C5H14NO4P (-183) 699.49645 999.00 [M+H]-C3H9N (-59) 740.55939 400.00 [M+H]-H2O (-18)	C_6H_{12}, C_9H_{16}
34	PC P-16:0_18:2 (9, 12)	10.69	$C_{42}H_{80}NO_7P$	742.5781	742.5745	4.8	[M+H]+	263.23734 1.00 sn2-O 265.25298 1.00 sn1-O 460.28298 1.00 [M+H]-sn1-H2O 462.29862 1.00 [M+H]-sn2-H2O 478.29354 1.00 [M+H]-sn1 480.30918 1.00 [M+H]-sn2 601.51961 999.00 [M+H]-C2H8NO4P (-141) 724.52814 1.00 [M+H]-H2O (-18)	C_6H_{12}, C_9H_{16}
35	PC 16:0_18:1 (11) / PC 16:0_18:1 (9)	12.00	$C_{42}H_{82}NO_8P$	760.5876	760.5856	2.7	[M+H]+	478.32992 600.00 [M+H]-sn2-H2O 496.34048 600.00 [M+H]-sn2 504.34556 600.00 [M+H]-sn1-H2O 522.35612 600.00 [M+H]-sn1 577.51960 400.00 [M+H]-C5H14NO4P (-183) 701.51214 999.00 [M+H]-C3H9N (-59) 742.57508 400.00 [M+H]-H2O (-18)	C_9H_{18}, $C_{11}H_{22}$
36	PC 18:0_16:0	12.81	$C_{42}H_{84}NO_8P$	762.6037	762.6013	3.1	[M+H]+	478.32990 600.00 [M+H]-sn2-H2O 496.34046 600.00 [M+H]-sn2 506.36118 600.00 [M+H]-sn1-H2O 524.37174 600.00 [M+H]-sn1 579.53522 400.00 [M+H]-C5H14NO4P (-183) 703.52776 999.00 [M+H]-C3H9N (-59) 744.59070 400.00 [M+H]-H2O (-18)	-
37	PC 15:0_20:4 (5, 8, 11, 14)	9.72	$C_{43}H_{78}NO_8P$	768.5587	768.5543	5.7	[M+H]+	464.31425 600.00 [M+H]-sn2-H2O 482.32481 600.00 [M+H]-sn2 526.32989 600.00 [M+H]-sn1-H2O 544.34045 600.00 [M+H]-sn1	C_6H_{12}, C_9H_{16}, $C_{12}H_{20}$, $C_{15}H_{24}$

								585.48829 400.00 [M+H]-C5H14NO4P (-183) 709.48083 999.00 [M+H]-C3H9N (-59) 750.54377 400.00 [M+H]-H2O (-18)	
38	PC 17:0_18:2 (9, 12)	11.50	$C_{43}H_{82}NO_8P$	772.5871	772.5856	1.9	$[M+H]^+$	492.34556 600.00 [M+H]-sn2-H2O 502.32992 600.00 [M+H]-sn1-H2O 510.35612 600.00 [M+H]-sn2 520.34048 600.00 [M+H]-sn1 589.51960 400.00 [M+H]-C5H14NO4P (-183) 713.51214 999.00 [M+H]-C3H9N (-59) 754.57508 400.00 [M+H]-H2O (-18)	C_9H_{18}, $C_{11}H_{20}$
39	PC 18:3_18:3	8.50	$C_{44}H_{76}NO_8P$	800.5252	800.5207	5.7	$[M+Na]^+$	463.22271 40.00 [M+Na]-59-sn1 || [M+Na]-59-sn2 522.29621 20.00 [M+Na]-sn1-H2O || [M+Na]-sn2-H2O 540.30677 20.00 [M+Na]-sn1 || [M+Na]-sn2 617.45461 600.00 [M+Na]-C5H14NO4P (-183) 741.44715 999.00 [M+Na]-C3H9N (-59)	/
40	PC P-16:0_20:5	10.83	$C_{44}H_{78}NO_7P$	764.5615	764.5594	2.7	[M+H]+	462.33495 10.00 [M+H]-sn2-H2O 465.24073 100.00 [M+H]-sn1-C3H9N (-59) 480.34551 200.00 [M+H]-sn2 524.31423 999.00 [M+H]-sn1 (alkenyl ether loss) 581.49335 10.00 [M+H]-C5H14NO4P (-183)	/
41	PC 16:0_20:5	9.41	$C_{44}H_{78}NO_8P$	780.5564	780.5543	2.7	[M+H]+	478.32989 600.00 [M+H]-sn2-H2O 496.34045 600.00 [M+H]-sn2 524.31425 600.00 [M+H]-sn1-H2O 542.32481 600.00 [M+H]-sn1 597.48829 400.00 [M+H]-C5H14NO4P (-183) 721.48083 999.00 [M+H]-C3H9N (-59) 762.54377 400.00 [M+H]-H2O (-18)	/
42	PC 18:4 (3, 6, 9, 12)_18:0	9.92	$C_{44}H_{80}NO_8P$	782.5643	782.5699	-7.2	[M+H]+	502.32987 600.00 [M+H]-sn1-H2O || [M+H]-sn2-H2O 520.34043 600.00 [M+H]-sn1 || [M+H]-sn2 599.50391 400.00 [M+H]-C5H14NO4P (-183) 723.49645 999.00 [M+H]-C3H9N (-59) 764.55939 400.00 [M+H]-H2O (-18)	C_6H_{12}, C_9H_{16}, $C_{12}H_{20}$
43	PC 18:2 (9, 12)_18:2 (9, 12)	10.47	$C_{44}H_{80}NO_8P$	782.5732	782.5699	4.2	[M+H]+	478.32987 600.00 [M+H]-sn2-H2O 496.34043 600.00 [M+H]-sn2 526.32987 600.00 [M+H]-sn1-H2O 544.34043 600.00 [M+H]-sn1 599.50391 400.00 [M+H]-C5H14NO4P (-183) 723.49645 999.00 [M+H]-C3H9N (-59) 764.55939 400.00 [M+H]-H2O (-18)	C_9H_{16}, C_6H_{12}
44	PC 18:0_18:3 (6, 9, 12)	10.26	$C_{44}H_{82}NO_8P$	784.5861	784.5856	0.6	[M+H]+	502.32992 600.00 [M+H]-sn1-H2O 504.34556 600.00 [M+H]-sn2-H2O 520.34048 600.00 [M+H]-sn1 522.35612 600.00 [M+H]-sn2 601.51960 400.00 [M+H]-C5H14NO4P (-183) 725.51214 999.00 [M+H]-C3H9N (-59) 766.57508 400.00 [M+H]-H2O (-18)	C_6H_{12}, C_9H_{16}, $C_{12}H_{20}$
45	PC P-16:0_20:2 (11, 14)	11.46	$C_{44}H_{84}NO_7P$	770.6042	770.6063	-2.8	[M+H]+	462.33497 10.00 [M+H]-sn2-H2O 471.28767 100.00 [M+H]-sn1-C3H9N (-59) 480.34553 200.00 [M+H]-sn2 530.36117 999.00 [M+H]-sn1 (alkenyl ether loss) 587.54029 10.00 [M+H]-C5H14NO4P (-183)	C_6H_{12}, C_9H_{16}
46	PC 18:0_18:2 (9, 12)	12.04	$C_{44}H_{84}NO_8P$	786.6044	786.6013	4.0	[M+H]+	502.32990 600.00 [M+H]-sn1-H2O 506.36118 600.00 [M+H]-sn2-H2O 520.34046 600.00 [M+H]-sn1 524.37174 600.00 [M+H]-sn2 603.53522 400.00 [M+H]-C5H14NO4P (-183) 727.52776 999.00 [M+H]-C3H9N (-59) 768.59070 400.00 [M+H]-H2O (-18)	C_6H_{12}, C_9H_{16}

47	PC 18:0_18:1 (11)	13.15	$C_{44}H_{86}NO_8P$	788.6197	788.6170	3.5	[M+H]+	504.34559 600.00 [M+H]-sn1-H2O 506.36123 600.00 [M+H]-sn2-H2O 522.35615 600.00 [M+H]-sn1 524.37179 600.00 [M+H]-sn2 605.55091 400.00 [M+H]-C5H14NO4P (-183) 729.54345 999.00 [M+H]-C3H9N (-59) 770.60639 400.00 [M+H]-H2O (-18)	C_9H_{18}
48	PC 17:0_20:4 (5, 8, 11, 14)	11.3	$C_{45}H_{82}NO_8P$	796.5819	796.5856	-4.7	[M+H]+	492.34556 600.00 [M+H]-sn2-H2O 510.35612 600.00 [M+H]-sn2 526.32992 600.00 [M+H]-sn1-H2O 544.34048 600.00 [M+H]-sn1 613.51960 400.00 [M+H]-C5H14NO4P (-183) 737.51214 999.00 [M+H]-C3H9N (-59) 778.57508 400.00 [M+H]-H2O (-18)	C_6H_{12}, C_9H_{16}, $C_{12}H_{20}$, $C_{15}H_{24}$
49	PC 17:0_20:3 (8, 11, 14)	11.7	$C_{45}H_{84}NO_8P$	798.6031	798.6007	3.0	[M+H]+	492.34554 600.00 [M+H]-sn2-H2O 510.35610 600.00 [M+H]-sn2 528.34554 600.00 [M+H]-sn1-H2O 546.35610 600.00 [M+H]-sn1 615.53522 400.00 [M+H]-C5H14NO4P (-183) 739.52776 999.00 [M+H]-C3H9N (-59) 780.59070 400.00 [M+H]-H2O (-18)	C_6H_{12}, C_9H_{16}, $C_{12}H_{20}$
50	PC 16:0_22:6 (4, 7, 10, 13, 16, 19)	9.33	$C_{46}H_{80}NO_8P$	806.5721	806.5699	2.7	[M+H]+	478.32987 600.00 [M+H]-sn2-H2O 496.34043 600.00 [M+H]-sn2 550.32987 600.00 [M+H]-sn1-H2O 568.34043 600.00 [M+H]-sn1 623.50391 400.00 [M+H]-C5H14NO4P (-183) 747.49645 999.00 [M+H]-C3H9N (-59) 788.55939 400.00 [M+H]-H2O (-18)	C_3H_6, C_6H_{10}, C_9H_{14}, $C_{12}H_{18}$, $C_{15}H_{22}$, $C_{18}H_{26}$
51	PC 18:2 (9, 12)_20:4 (5, 8, 11, 14)	8.66	$C_{46}H_{80}NO_8P$	806.5728	806.5699	3.6	[M+H]+	478.32987 600.00 [M+H]-sn2-H2O 496.34043 600.00 [M+H]-sn2 550.32987 600.00 [M+H]-sn1-H2O 568.34043 600.00 [M+H]-sn1 623.50391 400.00 [M+H]-C5H14NO4P (-183) 747.49645 999.00 [M+H]-C3H9N (-59) 788.55939 400.00 [M+H]-H2O (-18)	C_6H_{12}, C_9H_{16}, , $C_{12}H_{20}$, $C_{15}H_{24}$,
52	PC 18:1 (9)_20:4 (5, 8, 11, 14)	10.60	$C_{46}H_{82}NO_8P$	808.5843	808.5851	-1.0	[M+H]+	504.34556 600.00 [M+H]-sn2-H2O 522.35612 600.00 [M+H]-sn2 526.32992 600.00 [M+H]-sn1-H2O 544.34048 600.00 [M+H]-sn1 625.51960 400.00 [M+H]-C5H14NO4P (-183) 749.51214 999.00 [M+H]-C3H9N (-59) 790.57508 400.00 [M+H]-H2O (-18)	C_9H_{18}, C_6H_{12}, C_9H_{16}, $C_{12}H_{20}$, $C_{15}H_{24}$
53	PC 18:0_20:4 (5, 8, 11, 14)	11.60	$C_{46}H_{84}NO_8P$	810.6036	810.6013	2.8	[M+H]+	506.36118 600.00 [M+H]-sn2-H2O 524.37174 600.00 [M+H]-sn2 526.32990 600.00 [M+H]-sn1-H2O 544.34046 600.00 [M+H]-sn1 627.53522 400.00 [M+H]-C5H14NO4P (-183) 751.52776 999.00 [M+H]-C3H9N (-59) 792.59070 400.00 [M+H]-H2O (-18)	C_6H_{12}, C_9H_{16}, $C_{12}H_{20}$, $C_{15}H_{24}$
54	PC 18:0_20:3 (8, 11, 14)	12.60	$C_{46}H_{86}NO_8P$	812.6182	812.6169	1.7	[M+H]+	506.36123 600.00 [M+H]-sn2-H2O 524.37179 600.00 [M+H]-sn2 528.34559 600.00 [M+H]-sn1-H2O 546.35615 600.00 [M+H]-sn1 629.55091 400.00 [M+H]-C5H14NO4P (-183) 753.54345 999.00 [M+H]-C3H9N (-59) 794.60639 400.00 [M+H]-H2O (-18)	C_6H_{12}, C_9H_{16}, $C_{12}H_{20}$
55	PC 18:2 (9, 12)_20:0	13.31	$C_{46}H_{88}NO_8P$	814.6330	814.6326	0.5	[M+H]+	502.32994 600.00 [M+H]-sn2-H2O 520.34050 600.00 [M+H]-sn2 534.39250 600.00 [M+H]-sn1-H2O 552.40306 600.00 [M+H]-sn1 631.56654 400.00 [M+H]-C5H14NO4P (-183)	C_6H_{12}, C_9H_{16}

								755.55908 999.00 [M+H]-C3H9N (-59) 796.62202 400.00 [M+H]-H2O (-18)	
56	PC 22:4 (10, 13, 16, 19)_17:0	11.98	$C_{47}H_{86}NO_8P$	846.6003	846.5983	2.4	[M+Na]+	483.28532 40.00 [M+Na]-59-sn2 489.23840 40.00 [M+Na]-59-sn1 542.35882 20.00 [M+Na]-sn2-H2O 548.31190 20.00 [M+Na]-sn1-H2O 560.36938 20.00 [M+Na]-sn2 566.32246 20.00 [M+Na]-sn1 663.53286 600.00 [M+Na]-C5H14NO4P (-183) 787.52540 999.00 [M+Na]-C3H9N (-59)	C_3H_6, C_6H_{10}, C_9H_{14}, $C_{12}H_{18}$
57	PC 18:1_22:6	10.10	$C_{48}H_{82}NO_8P$	832.5868	832.5856	1.4	[M+H]+	504.34556 600.00 [M+H]-sn2-H2O 522.35612 600.00 [M+H]-sn2 550.32992 600.00 [M+H]-sn1-H2O 568.34048 600.00 [M+H]-sn1 649.51960 400.00 [M+H]-C5H14NO4P (-183) 773.51214 999.00 [M+H]-C3H9N (-59) 814.57508 400.00 [M+H]-H2O (-18)	/
58	PC 18:0_22:6 (4, 7, 10, 13, 16, 19)	11.60	$C_{48}H_{84}NO_8P$	834.6008	834.6013	-0.6	[M+H]+	506.36118 600.00 [M+H]-sn2-H2O 524.37174 600.00 [M+H]-sn2 550.32990 600.00 [M+H]-sn1-H2O 568.34046 600.00 [M+H]-sn1 651.53522 400.00 [M+H]-C5H14NO4P (-183) 775.52776 999.00 [M+H]-C3H9N (-59) 816.59070 400.00 [M+H]-H2O (-18)	C_3H_6, C_6H_{10}, C_9H_{14}, $C_{12}H_{18}$, $C_{15}H_{22}$, $C_{18}H_{26}$
59	PC 18:0_22:5 (4, 7, 10, 13, 16)	12.30	$C_{48}H_{86}NO_8P$	836.6166	836.6170	-0.4	[M+H]+	506.36123 600.00 [M+H]-sn2-H2O 524.37179 600.00 [M+H]-sn2 552.34559 600.00 [M+H]-sn1-H2O 570.35615 600.00 [M+H]-sn1 653.55091 400.00 [M+H]-C5H14NO4P (-183) 777.54345 999.00 [M+H]-C3H9N (-59) 818.60639 400.00 [M+H]-H2O (-18)	C_3H_6, C_6H_{10}, C_9H_{14}, $C_{12}H_{18}$, $C_{15}H_{22}$, $C_{18}H_{26}$
60	PC 18:0_22:4 (7, 10, 13, 16)	12.90	$C_{48}H_{88}NO_8P$	838.6345	838.6326	2.3	[M+H]+	506.36122 600.00 [M+H]-sn2-H2O 524.37178 600.00 [M+H]-sn2 554.36122 600.00 [M+H]-sn1-H2O 572.37178 600.00 [M+H]-sn1 655.56654 400.00 [M+H]-C5H14NO4P (-183) 779.55908 999.00 [M+H]-C3H9N (-59) 820.62202 400.00 [M+H]-H2O (-18)	C_6H_{12}, C_9H_{16}, $C_{12}H_{20}$, $C_{15}H_{24}$
61	PC P-18:0_22:2 (13, 16)	13.86	$C_{48}H_{92}NO_7P$	848.6534	848.6504	3.6	[M+Na]+	307.30027 10.00 [M+Na]-183-Na-sn2 643.60291 40.00 [M+Na]-183-Na+H 665.58486 40.00 [M+Na]-C5H14NO4P (-183) 789.57740 999.00 [M+Na]-C3H9N (-59)	C_6H_{12}, C_9H_{16}
62	PC P-16:0_24:1 (18/15)	15.40	$C_{48}H_{94}NO_7P$	850.6725	850.6660	7.6	[M+Na]+	279.26904 10.00 [M+Na]-183-Na-sn2 645.61860 40.00 [M+Na]-183-Na+H 667.60055 40.00 [M+Na]-C5H14NO4P (-183) 791.59309 999.00 [M+Na]-C3H9N (-59)	C_9H_{18}, C_6H_{12}
63	PC P-20:0_22:5 (4, 7, 10, 13, 16)	12.20	$C_{50}H_{90}NO_7P$	870.6366	870.6347	2.2	[M+Na]+	335.33157 10.00 [M+Na]-183-Na-sn2 665.58729 40.00 [M+Na]-183-Na+H 687.56924 40.00 [M+Na]-C5H14NO4P (-183) 811.56178 999.00 [M+Na]-C3H9N (-59)	C_6H_{12}, C_9H_{16}, $C_{12}H_{20}$, $C_{15}H_{24}$
64	PC P-20:0_22:4 (7, 10, 13, 16)	13.55	$C_{50}H_{92}NO_7P$	872.6518	872.6509	1.0	[M+Na]+	307.30027 10.00 [M+Na]-183-Na-sn2 667.60291 40.00 [M+Na]-183-Na+H 689.58486 40.00 [M+Na]-C5H14NO4P (-183) 813.57740 999.00 [M+Na]-C3H9N (-59)	C_6H_{12}, C_9H_{16}, $C_{12}H_{20}$, $C_{15}H_{24}$
65	PC P-20:0_22:4	13.72	$C_{50}H_{92}NO_7P$	872.6555	872.6509	5.3	[M+Na]+	307.30027 10.00 [M+Na]-183-Na-sn2 667.60291 40.00 [M+Na]-183-Na+H 689.58486 40.00 [M+Na]-C5H14NO4P (-183) 813.57740 999.00 [M+Na]-C3H9N (-59)	/
66	PC P-18:0_26:1	16.33	$C_{51}H_{98}NO_8P$	906.7365	906.7291	8.2	[M+Na]+	511.31663 40.00 [M+Na]-59-sn2 521.30099 40.00 [M+Na]-59-sn1 570.39013 20.00 [M+Na]-sn2-H2O	/

								580.37449 20.00 [M+Na]-sn1-H2O 588.40069 20.00 [M+Na]-sn2 598.38505 20.00 [M+Na]-sn1 723.62673 600.00 [M+Na]-C5H14NO4P (-183) 847.61927 999.00 [M+Na]-C3H9N (-59)	
67	PC P-20:0_24:4 (5, 8, 11, 14)	15.16	$C_{52}H_{96}NO_7P$	900.6755	900.6822	-7.4	[M+Na]+	335.33158 10.00 [M+Na]-183-Na-sn2 695.63422 40.00 [M+Na]-183-Na+H 717.61617 40.00 [M+Na]-C5H14NO4P (-183) 841.60871 999.00 [M+Na]-C3H9N (-59)	C_6H_{12}, C_9H_{16}, $C_{12}H_{20}$, $C_{15}H_{24}$

Note: In the first column from right, “-” denotes the saturated lipids and “/” denotes the unsaturated lipids but the C=C bonds positions were not identified. The chemical formulas were simulated based on the exact masses of diagnostic ions P1b (only containing the C and H atoms). The match details in the second column from right include: *m/z* values of product ions, their intensities, and possible explanations. The (1Z)-alkenyl ether (neutral Plasmalogen) species is represented by the "P-" prefix in the second column from left.

Table S4. PE and LPE identified from human serum extract.

No.	Identification	RT (min)	Formula	Observed m/z	Calculated m/z	Error (ppm)	Adduct	Match details	Formula of neutral loss molecules for C=C analysis
1	LPE 16:0	2.55	$C_{21}H_{44}NO_7P$	454.2936	454.2934	0.4	[M+H]+	198.05329 10.00 [M+H]-sn1-H2O 216.06385 10.00 [M+H]-sn1 313.27428 999.00 [M+H]-C3H8NO6P (-141) 393.24061 200.00 [M+H]- (C2NH5+H20 (-61) 436.28281 999.00 [M+H]-H2O (-18)	-
2	LPE 18:2)	1.74	$C_{23}H_{44}NO_7P$	478.2946	478.2934	2.5	[M+H]+	198.05329 10.00 [M+H]-sn1-H2O 216.06385 10.00 [M+H]-sn1 337.27428 999.00 [M+H]-C3H8NO6P (-141) 417.24061 200.00 [M+H]- (C2NH5+H20 (-61) 460.28281 999.00 [M+H]-H2O (-18)	/
3	LPE 18:1 (9)	2.40	$C_{23}H_{46}NO_7P$	480.3103	480.3090	2.7	[M+H]+	198.05328 10.00 [M+H]-sn1-H2O 216.06384 10.00 [M+H]-sn1 339.28990 999.00 [M+H]-C3H8NO6P (-141) 419.25624 200.00 [M+H]- (C2NH5+H20 (-61) 462.29844 999.00 [M+H]-H2O (-18)	/
4	LPE 18:0	3.98	$C_{23}H_{48}NO_7P$	482.3259	482.3246	2.7	[M+H]+	198.05329 10.00 [M+H]-sn1-H2O 216.06385 10.00 [M+H]-sn1 341.30556 999.00 [M+H]-C3H8NO6P (-141) 421.27189 200.00 [M+H]- (C2NH5+H20 (-61) 464.31409 999.00 [M+H]-H2O (-18)	-
5	LPE (20:4)	1.67	$C_{25}H_{44}NO_7P$	502.2950	502.2910	8.0	[M+H]+	198.05329 10.00 [M+H]-sn1-H2O 216.06385 10.00 [M+H]-sn1 361.27428 999.00 [M+H]-C3H8NO6P (-141) 441.24061 200.00 [M+H]- (C2NH5+H20 (-61) 484.28281 999.00 [M+H]-H2O (-18)	/
6	PE (3:0_18:4)	1.80	$C_{26}H_{44}NO_8P$	530.2895	530.2883	2.2	[M+H]+	57.03402 1.00 sn1-O 254.07948 1.00 [M+H]-sn2-H2O 259.20606 1.00 sn2-O 272.09004 1.00 [M+H]-sn2 389.26918 999.00 [M+H]-C2H8NO4P (-141) 456.25152 1.00 [M+H]-sn1-H2O 474.26208 1.00 [M+H]-sn1 512.27772 1.00 [M+H]-H2O (-18)	/
7	LPE (22:6)	1.54	$C_{27}H_{44}NO_7P$	526.2941	526.2933	1.5	[M+H]+	198.05326 10.00 [M+H]-sn1-H2O 216.06382 10.00 [M+H]-sn1 385.27425 999.00 [M+H]-C3H8NO6P (-141) 465.24058 200.00 [M+H]- (C2NH5+H20 (-61) 508.28278 999.00 [M+H]-H2O (-18)	/
8	PE P-16:0_18:2	11.90	$C_{39}H_{74}NO_7P$	700.5300	700.5276	3.4	[M+H]+	266.28461 150.00 sn1 ether +C2H8NO3P-H3PO4 337.27439 200.00 [M+H]-C2H8NO4P-sn2 364.26151 999.00 sn1 ether + C2H8NO3P (+124) 559.50899 30.00 [M+H]-C2H8NO4P (-141) 682.51752 100.00 [M+H]-H2O (-18)	/
9	PE 16:0_18:2 (10, 13)	11.10	$C_{39}H_{74}NO_8P$	716.5250	716.5225	3.5	[M+H]+	239.23734 1.00 sn1-O 263.23734 1.00 sn2-O 436.28294 1.00 [M+H]-sn2-H2O 454.29350 1.00 [M+H]-sn2 460.28294 1.00 [M+H]-sn1-H2O 478.29350 1.00 [M+H]-sn1 575.50392 999.00 [M+H]-C2H8NO4P (-141) 698.51246 1.00 [M+H]-H2O (-18)	C_5H_{10}, C_8H_{14}
10	PE 16:0_18:1	12.30	$C_{39}H_{76}NO_8P$	740.5235	740.5201	4.6	[M+Na]+	415.22273 3.00 [M+Na]-43-SN2-H 441.23837 3.00 [M+Na]-43-SN1-H 599.50156 400.00 [M+Na]-C2H8NO4P (-141) 697.47845 999.00 [M+Na]-C2H5N (-43)	/

11	PE P-16:0_20:4	11.60	$C_{41}H_{74}NO_7P$	746.5105	746.5100	0.6	[M+Na]+	386.24346 100.00 sn1 ether +C2H8NO3P+Na (+124+23) 583.50899 40.00 [M+Na]-C2H8NO4P-Na+H 605.49094 50.00 [M+Na]-C2H8NO4P (-141) 623.50150 40.00 [M+Na]-C2H8NO4P+H20 (-141+18) 703.46783 999.00 [M+Na]-C2H5N (-43) 728.49947 20.00 [M+Na]-H20 (-18)	/
12	PE 18:1_18:2	11.12	$C_{41}H_{76}NO_8P$	742.5425	742.5387	5.1	[M+H]+	263.23734 1.00 sn2-O 265.25298 1.00 sn1-O 460.28298 1.00 [M+H]-sn1-H2O 462.29862 1.00 [M+H]-sn2-H2O 478.29354 1.00 [M+H]-sn1 480.30918 1.00 [M+H]-sn2 601.51961 999.00 [M+H]-C2H8NO4P (-141) 724.52814 1.00 [M+H]-H2O (-18)	/
13	PE P-18:0_18:2	13.10	$C_{41}H_{78}NO_7P$	728.5620	728.5589	4.3	[M+H]+	294.31589 150.00 sn1 ether +C2H8NO3P-H3PO4 337.27442 200.00 [M+H]-C2H8NO4P-sn2 392.29279 999.00 sn1 ether + C2H8NO3P (+124) 587.54030 30.00 [M+H]-C2H8NO4P (-141) 710.54883 100.00 [M+H]-H2O (-18)	/
14	PE 18:1_18:1	12.40	$C_{41}H_{78}NO_8P$	744.5571	744.5538	4.5	[M+H]+	265.25298 1.00 sn1-O || sn2-O 462.29861 1.00 [M+H]-sn1-H2O || [M+H]-sn2-H2O 480.30917 1.00 [M+H]-sn1 || [M+H]-sn2 603.53523 999.00 [M+H]-C2H8NO4P (-141) 726.54377 1.00 [M+H]-H2O (-18)	/
15	PE P-18:0_18:0	14.08	$C_{41}H_{82}NO_7P$	732.5857	732.5907	-6.8	[M+H]+	294.31589 150.00 sn1 ether +C2H8NO3P-H3PO4 341.30574 200.00 [M+H]-C2H8NO4P-sn2 392.29279 999.00 sn1 ether + C2H8NO3P (+124) 591.57162 30.00 [M+H]-C2H8NO4P (-141) 714.58015 100.00 [M+H]-H2O (-18)	-
16	PE P-16:0_22:6	10.49	$C_{43}H_{74}NO_7P$	748.5310	748.5281	3.9	[M+H]+	266.28461 150.00 sn1 ether +C2H8NO3P-H3PO4 364.26151 999.00 sn1 ether + C2H8NO3P (+124) 385.27439 200.00 [M+H]-C2H8NO4P-sn2 607.50899 30.00 [M+H]-C2H8NO4P (-141) 730.51752 100.00 [M+H]-H2O (-18)	/
17	PE P-16:0_22:5	11.40	$C_{43}H_{76}NO_7P$	750.5461	750.5438	3.0	[M+H]+	266.28461 150.00 sn1 ether +C2H8NO3P-H3PO4 364.26151 999.00 sn1 ether + C2H8NO3P (+124) 387.29008 200.00 [M+H]-C2H8NO4P-sn2 609.52468 30.00 [M+H]-C2H8NO4P (-141) 732.53321 100.00 [M+H]-H2O (-18)	/
18	PE 18:0_20:5	12.70	$C_{43}H_{76}NO_8P$	766.5391	766.5357	4.3	[M+H]+	267.26862 1.00 sn1-O 285.22170 1.00 sn2-O 464.31426 1.00 [M+H]-sn2-H2O 482.26734 1.00 [M+H]-sn1-H2O 482.32482 1.00 [M+H]-sn2 500.27790 1.00 [M+H]-sn1 625.51961 999.00 [M+H]-C2H8NO4P (-141) 748.52814 1.00 [M+H]-H2O (-18)	/
19	PE P-18:2 (9, 12)_20:2 (11, 14)	12.80	$C_{43}H_{78}NO_7P$	752.5631	752.5594	4.9	[M+H]+	294.31589 150.00 sn1 ether +C2H8NO3P-H3PO4 361.27442 200.00 [M+H]-C2H8NO4P-sn2 392.29279 999.00 sn1 ether + C2H8NO3P (+124) 611.54030 30.00 [M+H]-C2H8NO4P (-141) 734.54883 100.00 [M+H]-H2O (-18)	C_6H_{12}, C_9H_{16}
20	PE 18:2 (9, 12)_20:2 (11, 14)	12.17	$C_{43}H_{78}NO_8P$	768.5594	768.5543	6.6	[M+H]+	267.26862 1.00 sn1-O 287.23734 1.00 sn2-O 464.31425 1.00 [M+H]-sn2-H2O 482.32481 1.00 [M+H]-sn2 484.28297 1.00 [M+H]-sn1-H2O 502.29353 1.00 [M+H]-sn1 627.53523 999.00 [M+H]-C2H8NO4P (-141) 750.54377 1.00 [M+H]-H2O (-18)	C_6H_{12}, C_9H_{16}

21	PE P-18:0_20:3	12.48	$C_{43}H_{80}NO_7P$	754.5677	754.5751	-9.8	[M+H]+	294.31589 150.00 sn1 ether +C2H8NO3P-H3PO4 363.29011 200.00 [M+H]-C2H8NO4P-sn2 392.29279 999.00 sn1 ether + C2H8NO3P (+124) 613.55599 30.00 [M+H]-C2H8NO4P (-141) 736.56452 100.00 [M+H]-H2O (-18)	/
22	PE P-18:0_22:6	12.00	$C_{45}H_{78}NO_7P$	776.5609	776.5594	1.9	[M+H]+	294.31589 150.00 sn1 ether +C2H8NO3P-H3PO4 385.27442 200.00 [M+H]-C2H8NO4P-sn2 392.29279 999.00 sn1 ether + C2H8NO3P (+124) 635.54030 30.00 [M+H]-C2H8NO4P (-141) 758.54883 100.00 [M+H]-H2O (-18)	/
23	PE P-18:0_22:5	12.49	$C_{45}H_{80}NO_7P$	778.5767	778.5751	2.1	[M+H]+	294.31589 150.00 sn1 ether +C2H8NO3P-H3PO4 387.29011 200.00 [M+H]-C2H8NO4P-sn2 392.29279 999.00 sn1 ether + C2H8NO3P (+124) 637.55599 30.00 [M+H]-C2H8NO4P (-141) 760.56452 100.00 [M+H]-H2O (-18)	/
24	PE P-18:0_22:4	14.02	$C_{45}H_{82}NO_7P$	780.5941	780.5907	4.4	[M+H]+	322.34717 150.00 sn1 ether +C2H8NO3P-H3PO4 361.27446 200.00 [M+H]-C2H8NO4P-sn2 420.32407 999.00 sn1 ether + C2H8NO3P (+124) 639.57162 30.00 [M+H]-C2H8NO4P (-141) 762.58015 100.00 [M+H]-H2O (-18)	/

Note: In the first column from right, “-” denotes the saturated lipids and “/” denotes the unsaturated lipids but the C=C bonds positions were not identified. The chemical formulas were simulated based on the exact masses of diagnostic ions P1b (only containing the C and H atoms). The match details in the second column from right include: *m/z* values of product ions, their intensities, and possible explanations. The (1Z)-alkenyl ether (neutral Plasmalogen) species is represented by the "P-" prefix in the second column from left.

Table S5. Sphingolipids identified from human serum extract.

No.	Identification	RT (min)	Formula	Observed m/z	Calculated m/z	Error (ppm)	Adduct	Match details	Formula of neutral loss molecules for C=C analysis
1	SM d14:1 (4)/18:1 (9)	7.12	$C_{37}H_{74}N_2O_6P$	673.5318	673.5284	5.0	[M]+	490.46240 20.00 [M+]-C5H14NO4P (-183) 596.44438 50.00 [M+] (-18 -59) 614.45494 10.00 [M+]-C3H9N (-59) 655.51788 999.00 [M+]-H2O (-18)	/
2	SM d14:0/18:1	8.10	$C_{37}H_{76}N_2O_6P$	675.5469	675.5441	4.1	[M]+	492.47809 20.00 [M+]-C5H14NO4P (-183) 598.46007 50.00 [M+] (-18 -59) 616.47063 10.00 [M+]-C3H9N (-59) 657.53357 999.00 [M+]-H2O (-18)	/
3	SM d14:0/18:0	9.50	$C_{37}H_{78}N_2O_6P$	677.5619	677.5598	3.1	[M]+	494.49371 20.00 [M+]-C5H14NO4P (-183) 600.47569 50.00 [M+] (-18 -59) 618.48625 10.00 [M+]-C3H9N (-59) 659.54919 999.00 [M+]-H2O (-18)	-
4	SM d15:0/18:1)	9.60	$C_{38}H_{78}N_2O_6P$	689.5620	689.5597	3.3	[M]+	506.49371 20.00 [M+]-C5H14NO4P (-183) 612.47569 50.00 [M+] (-18 -59) 630.48625 10.00 [M+]-C3H9N (-59) 671.54919 999.00 [M+]-H2O (-18)	/
5	SM d16:1 (4)/18:1 (9)	8.60	$C_{39}H_{78}N_2O_6P$	701.5625	701.5597	4.0	[M]+	518.49371 20.00 [M+]-C5H14NO4P (-183) 624.47569 50.00 [M+] (-18 -59) 642.48625 10.00 [M+]-C3H9N (-59) 683.54919 999.00 [M+]-H2O (-18)	/
6	SM d14:1/20:0	10.60	$C_{39}H_{80}N_2O_6P$	703.5782	703.5754	4.0	[M]+	520.50934 20.00 [M+]-C5H14NO4P (-183) 626.49132 50.00 [M+] (-18 -59) 644.50188 10.00 [M+]-C3H9N (-59) 685.56482 999.00 [M+]-H2O (-18)	/
7	SM d14:0/20:0	10.30	$C_{39}H_{82}N_2O_6P$	705.5926	705.5911	2.2	[M]+	522.52502 20.00 [M+]-C5H14NO4P (-183) 628.50700 50.00 [M+] (-18 -59) 646.51756 10.00 [M+]-C3H9N (-59) 687.58050 999.00 [M+]-H2O (-18)	-
8	SM d17:1 (4)/18:1 (9)	9.90	$C_{40}H_{80}N_2O_6P$	715.5781	715.5754	3.8	[M]+	532.50934 20.00 [M+]-C5H14NO4P (-183) 638.49132 50.00 [M+] (-18 -59) 656.50188 10.00 [M+]-C3H9N (-59) 697.56482 999.00 [M+]-H2O (-18)	/
9	SM d18:1 (4)/18:1 (9)	9.95	$C_{41}H_{82}N_2O_6P$	729.5949	729.5911	5.2	[M]+	546.52502 20.00 [M+]-C5H14NO4P (-183) 652.50700 50.00 [M+] (-18 -59) 670.51756 10.00 [M+]-C3H9N (-59) 711.58050 999.00 [M+]-H2O (-18)	/
10	SM d14:1 (4)/22:0	12.10	$C_{41}H_{84}N_2O_6P$	731.6097	731.6067	4.1	[M]+	548.54065 20.00 [M+]-C5H14NO4P (-183) 654.52263 50.00 [M+] (-18 -59) 672.53319 10.00 [M+]-C3H9N (-59) 713.59613 999.00 [M+]-H2O (-18)	/
11	SM d14:0/22:0	11.90	$C_{41}H_{86}N_2O_6P$	733.6249	733.6218	4.2	[M]+	550.55634 20.00 [M+]-C5H14NO4P (-183) 656.53832 50.00 [M+] (-18 -59) 674.54888 10.00 [M+]-C3H9N (-59) 715.61182 999.00 [M+]-H2O (-18)	-
12	SM d14:1/24:1	12.00	$C_{43}H_{86}N_2O_6P$	757.6252	757.6224	3.7	[M]+	574.55634 20.00 [M+]-C5H14NO4P (-183) 680.53832 50.00 [M+] (-18 -59) 698.54888 10.00 [M+]-C3H9N (-59) 739.61182 999.00 [M+]-H2O (-18)	/
13	SM d14:0/24:1 (15)	13.40	$C_{43}H_{88}N_2O_6P$	759.6401	759.6380	2.8	[M]+	576.57196 20.00 [M+]-C5H14NO4P (-183) 682.55394 50.00 [M+] (-18 -59) 700.56450 10.00 [M+]-C3H9N (-59) 741.62744 999.00 [M+]-H2O (-18)	/
14	SM d14:1/26:1	13.03	$C_{45}H_{90}N_2O_6P$	785.6559	785.6536	2.9	[M]+	602.58759 20.00 [M+]-C5H14NO4P (-183) 708.56957 50.00 [M+] (-18 -59)	/

								726.58013 10.00 [M+]-C3H9N (-59) 767.64307 999.00 [M+]-H2O (-18)	
15	SM d16:1/24:1	13.32	$C_{45}H_{90}N_2O_6P$	785.6559	785.6536	2.9	[M]+	602.58759 20.00 [M+]-C5H14NO4P (-183) 708.56957 50.00 [M+] (-18 -59) 726.58013 10.00 [M+]-C3H9N (-59) 767.64307 999.00 [M+]-H2O (-18)	/
16	SM d14:0/26:1 (12)	14.68	$C_{45}H_{92}N_2O_6P$	787.6738	787.6693	5.7	[M]+	604.60327 20.00 [M+]-C5H14NO4P (-183) 710.58525 50.00 [M+] (-18 -59) 728.59581 10.00 [M+]-C3H9N (-59) 769.65875 999.00 [M+]-H2O (-18)	/
17	SM d15:0/24:1	14.20	$C_{44}H_{90}N_2O_6P$	795.6365	795.6356	1.2	[M+Na]+	612.56954 20.00 [M+Na]-C5H14NO4P (-183) 736.56208 999.00 [M+Na]-C3H9N (-59)	/
18	SM d15:1/26:1 (17)	14.05	$C_{46}H_{92}N_2O_6P$	799.6701	799.6693	1.0	[M]+	616.60327 20.00 [M+]-C5H14NO4P (-183) 722.58525 50.00 [M+] (-18 -59) 740.59581 10.00 [M+]-C3H9N (-59) 781.65875 999.00 [M+]-H2O (-18)	C_9H_{18}
19	SM d17:1/24:1 (15)	13.60	$C_{46}H_{92}N_2O_6P$	799.6709	799.6693	2.0	[M]+	616.60327 20.00 [M+]-C5H14NO4P (-183) 722.58525 50.00 [M+] (-18 -59) 740.59581 10.00 [M+]-C3H9N (-59) 781.65875 999.00 [M+]-H2O (-18)	C_9H_{18}
20	SM d15:0/26:1	15.40	$C_{46}H_{94}N_2O_6P$	801.6895	801.6849	5.7	[M]+	618.61890 20.00 [M+]-C5H14NO4P (-183) 724.60088 50.00 [M+] (-18 -59) 742.61144 10.00 [M+]-C3H9N (-59) 783.67438 999.00 [M+]-H2O (-18)	/
21	SM d14:1/26:1	13.50	$C_{47}H_{88}N_2O_6P$	807.6357	807.6356	0.2	[M+Na]+	624.56954 20.00 [M+Na]-C5H14NO4P (-183) 748.56208 999.00 [M+Na]-C3H9N (-59)	/
22	SM d14:0/26:0	12.80	$C_{45}H_{94}N_2O_6P$	811.6695	811.6669	3.3	[M+Na]+	628.60085 20.00 [M+Na]-C5H14NO4P (-183) 752.59339 999.00 [M+Na]-C3H9N (-59)	-
23	SM d18:1/24:1	14.62	$C_{47}H_{94}N_2O_6P$	813.6871	813.6849	2.7	[M]+	630.61890 20.00 [M+]-C5H14NO4P (-183) 736.60088 50.00 [M+] (-18 -59) 754.61144 10.00 [M+]-C3H9N (-59) 795.67438 999.00 [M+]-H2O (-18)	/
24	SM d18:1/24:1	14.78	$C_{47}H_{94}N_2O_6P$	813.6871	813.6849	2.7	[M]+	630.61890 20.00 [M+]-C5H14NO4P (-183) 736.60088 50.00 [M+] (-18 -59) 754.61144 10.00 [M+]-C3H9N (-59) 795.67438 999.00 [M+]-H2O (-18)	/
25	SM d18:1/24:1	16.02	$C_{47}H_{96}N_2O_6P$	815.7043	815.7006	4.5	[M]+	632.63458 20.00 [M+]-C5H14NO4P (-183) 738.61656 50.00 [M+] (-18 -59) 756.62712 10.00 [M+]-C3H9N (-59) 797.69006 999.00 [M+]-H2O (-18)	/
26	SM d16:0/26:1	15.11	$C_{47}H_{96}N_2O_6P$	815.7043	815.7006	4.5	[M]+	632.63458 20.00 [M+]-C5H14NO4P (-183) 738.61656 50.00 [M+] (-18 -59) 756.62712 10.00 [M+]-C3H9N (-59) 797.69006 999.00 [M+]-H2O (-18)	/
27	SM d19:1/24:1	15.45	$C_{48}H_{96}N_2O_6P$	827.7020	827.7006	1.7	[M]+	644.63458 20.00 [M+]-C5H14NO4P (-183) 750.61656 50.00 [M+] (-18 -59) 768.62712 10.00 [M+]-C3H9N (-59) 809.69006 999.00 [M+]-H2O (-18)	/
28	SM d17:1/26:1	15.23	$C_{48}H_{96}N_2O_6P$	827.7025	827.7006	2.3	[M]+	644.63458 20.00 [M+]-C5H14NO4P (-183) 750.61656 50.00 [M+] (-18 -59) 768.62712 10.00 [M+]-C3H9N (-59) 809.69006 999.00 [M+]-H2O (-18)	/
29	SM d17:1/26:1	14.96	$C_{48}H_{96}N_2O_6P$	827.7025	827.7006	2.3	[M]+	644.63458 20.00 [M+]-C5H14NO4P (-183) 750.61656 50.00 [M+] (-18 -59) 768.62712 10.00 [M+]-C3H9N (-59) 809.69006 999.00 [M+]-H2O (-18)	/
30	SM d18:1/26:1	15.84	$C_{49}H_{98}N_2O_6P$	841.7203	841.7163	4.8	[M]+	658.65021 20.00 [M+]-C5H14NO4P (-183) 764.63219 50.00 [M+] (-18 -59) 782.64275 10.00 [M+]-C3H9N (-59) 823.70569 999.00 [M+]-H2O (-18)	/

31	SM d18:1/26:0	16.81	$C_{49}H_{100}N_2O_6P$	843.7361	843.7319	5.0	[M]+	660.66583 20.00 [M+]-C5H14NO4P (-183) 766.64781 50.00 [M+] (-18 -59) 784.65837 10.00 [M+]-C3H9N (-59) 825.72131 999.00 [M+]-H2O (-18)	/

Note: In the first column from right, "-" denotes the saturated lipids and "/" denotes the unsaturated lipids but the C=C bonds positions were not identified. The chemical formulas were simulated based on the exact masses of diagnostic ions P1b (only containing the C and H atoms). The match details in the second column from right include: *m/z* values of product ions, their intensities, and possible explanations.

Table S6. TG and DG identified from human serum extract.

No.	Identification	RT (min)	Formula	Observed m/z	Calculated m/z	Error (ppm)	Adduct	Match details	Formula of neutral loss molecules for C=C analysis
1	TG 12:0_12:0_18:1	17.19	$C_{45}H_{84}O_6$	738.6624	738.6608	2.2	[M+NH4]+	439.37850 999.00 [M+NH4]-sn3-18 521.45670 999.00 [M+NH4]-sn1-18 || [M+NH4]-sn2-18 721.65803 199.80 [M+NH4]-17	/
2	TG 12:0_14:0_16:0	17.68	$C_{45}H_{86}O_6$	740.6769	740.6764	0.7	[M+NH4]+	467.40978 999.00 [M+NH4]-sn3-18 495.44106 999.00 [M+NH4]-sn2-18 523.47234 999.00 [M+NH4]-sn1-18 723.67367 199.80 [M+NH4]-17	/
3	TG 12:0_14:1_18:1	17.21	$C_{47}H_{86}O_6$	764.6797	764.6764	4.3	[M+NH4]+	465.39414 999.00 [M+NH4]-sn3-18 521.45670 999.00 [M+NH4]-sn2-18 547.47234 999.00 [M+NH4]-sn1-18 747.67367 199.80 [M+NH4]-17	/
4	TG 14:0_16:1_14:0	17.69	$C_{47}H_{88}O_6$	766.6952	766.6921	4.0	[M+NH4]+	493.42542 999.00 [M+NH4]-sn3-18 495.44106 999.00 [M+NH4]-sn2-18 549.48798 999.00 [M+NH4]-sn1-18 749.68931 199.80 [M+NH4]-17	/
5	TG 14:1_16:1_16:1	17.27	$C_{49}H_{88}O_6$	790.6920	790.6920	0.0	[M+NH4]+	519.44106 999.00 [M+NH4]-sn2-18 || [M+NH4]-sn3-18 547.47234 999.00 [M+NH4]-sn1-18 773.68931 199.80 [M+NH4]-17	/
6	TG 12:0_18:1 (15)_16:1 (13)	17.70	$C_{49}H_{90}O_6$	792.7109	792.7077	4.0	[M+NH4]+	493.42542 999.00 [M+NH4]-sn2-18 521.45670 999.00 [M+NH4]-sn3-18 575.50362 999.00 [M+NH4]-sn1-18 775.70495 199.80 [M+NH4]-17	C_3H_6
7	TG 14:0_16:0_16:1	18.00	$C_{49}H_{92}O_6$	794.7256	794.7233	2.9	[M+NH4]+	521.45670 999.00 [M+NH4]-sn2-18 523.47234 999.00 [M+NH4]-sn3-18 549.48798 999.00 [M+NH4]-sn1-18 777.72059 199.80 [M+NH4]-17	/
8	TG 14:0_16:0_16:0	18.23	$C_{49}H_{94}O_6$	796.7409	796.7390	2.4	[M+NH4]+	523.47234 999.00 [M+NH4]-sn2-18 || [M+NH4]-sn3-18 551.50362 999.00 [M+NH4]-sn1-18 779.73623 199.80 [M+NH4]-17	-
9	TG 14:1 (11)_16:1 (10)_18:1 (12)	17.71	$C_{51}H_{92}O_6$	818.7267	818.7233	4.2	[M+NH4]+	519.44106 999.00 [M+NH4]-sn3-18 547.47234 999.00 [M+NH4]-sn2-18 575.50362 999.00 [M+NH4]-sn1-18 801.72059 199.80 [M+NH4]-17	C_6H_{12}
10	TG 14:0_16:1 (10)_18:1 (11)	18.10	$C_{51}H_{94}O_6$	820.7413	820.7390	2.8	[M+NH4]+	521.45670 999.00 [M+NH4]-sn3-18 549.48798 999.00 [M+NH4]-sn2-18 575.50362 999.00 [M+NH4]-sn1-18 803.73623 199.80 [M+NH4]-17	C_9H_{18}
11	TG 14:0_16:0_18:1 (11)	18.23	$C_{51}H_{96}O_6$	822.7571	822.7546	3.0	[M+NH4]+	523.47234 999.00 [M+NH4]-sn3-18 549.48798 999.00 [M+NH4]-sn2-18 577.51926 999.00 [M+NH4]-sn1-18 805.75187 199.80 [M+NH4]-17	C_9H_{18}
12	TG 14:0_16:0_18:0	18.39	$C_{51}H_{98}O_6$	824.7736	824.7702	4.1	[M+NH4]+	551.50362 999.00 [M+NH4]-sn1-18 || [M+NH4]-sn2-18 || [M+NH4]-sn3-18 807.76751 199.80 [M+NH4]-17	-
13	TG 16:1_16:1_17:1	17.89	$C_{52}H_{94}O_6$	832.7391	832.7390	0.1	[M+NH4]+	547.47234 999.00 [M+NH4]-sn3-18 561.48798 999.00 [M+NH4]-sn1-18 || [M+NH4]-sn2-18 815.73623 199.80 [M+NH4]-17	/
14	TG 16:0_16:1_17:1	18.15	$C_{52}H_{96}O_6$	834.7552	834.7546	0.7	[M+NH4]+	549.48798 999.00 [M+NH4]-sn3-18 561.48798 999.00 [M+NH4]-sn1-18 563.50362 999.00 [M+NH4]-sn2-18 817.75187 199.80 [M+NH4]-17	/
15	TG 16:0_16:1 (10)_17:0	18.31	$C_{52}H_{98}O_6$	836.7757	836.7702	6.6	[M+NH4]+	549.48798 999.00 [M+NH4]-sn3-18 563.50362 999.00 [M+NH4]-sn1-18 565.51926 999.00 [M+NH4]-sn2-18 819.76751 199.80 [M+NH4]-17	C_6H_{12}

16	TG 16:0_16:0_17:0	18.45	$C_{52}H_{100}O_6$	838.7905	838.7859	5.5	[M+NH4]+	551.50362 999.00 [M+NH4]-sn3-18 565.51926 999.00 [M+NH4]-sn1-18 || [M+NH4]-sn2-18 821.78315 199.80 [M+NH4]-17	-
17	TG 16:1_16:1_18:3	17.40	$C_{53}H_{92}O_6$	842.7288	842.7233	6.5	[M+NH4]+	547.47234 999.00 [M+NH4]-sn3-18 571.47234 999.00 [M+NH4]-sn1-18 || [M+NH4]-sn2-18 825.72059 199.80 [M+NH4]-17	/
18	TG 16:1_16:1_18:2	17.75	$C_{53}H_{94}O_6$	844.7440	844.7390	5.9	[M+NH4]+	549.48798 999.00 [M+NH4]-sn3-18 571.47234 999.00 [M+NH4]-sn1-18 573.48798 999.00 [M+NH4]-sn2-18 827.73623 199.80 [M+NH4]-17	/
19	TG 16:0_16:1_18:2	18.20	$C_{53}H_{96}O_6$	846.7584	846.7545	4.5	[M+NH4]+	549.48798 999.00 [M+NH4]-sn3-18 573.48798 999.00 [M+NH4]-sn1-18 575.50362 999.00 [M+NH4]-sn2-18 829.75187 199.80 [M+NH4]-17	/
20	TG 16:0_16:1 (9)_18:1 (12)	18.02	$C_{53}H_{98}O_6$	848.7660	848.7702	-4.9	[M+NH4]+	549.48798 999.00 [M+NH4]-sn3-18 575.50362 999.00 [M+NH4]-sn1-18 577.51926 999.00 [M+NH4]-sn2-18 831.76751 199.80 [M+NH4]-17	C_6H_{12}
21	TG 16:0_16:0_18:1 (11)	18.23	$C_{53}H_{100}O_6$	850.7809	850.7859	-5.9	[M+NH4]+	551.50362 999.00 [M+NH4]-sn3-18 577.51926 999.00 [M+NH4]-sn1-18 || [M+NH4]-sn2-18 833.78315 199.80 [M+NH4]-17	C_9H_{18}
22	TG 16:0_16:0_18:0	18.50	$C_{53}H_{102}O_6$	852.8049	852.8015	4.0	[M+NH4]+	551.50362 999.00 [M+NH4]-sn3-18 579.53490 999.00 [M+NH4]-sn1-18 || [M+NH4]-sn2-18 835.79879 199.80 [M+NH4]-17	-
23	TG 16:1_17:1_18:2	17.91	$C_{54}H_{96}O_6$	858.7584	858.7546	4.4	[M+NH4]+	561.48798 999.00 [M+NH4]-sn3-18 573.48798 999.00 [M+NH4]-sn2-18 587.50362 999.00 [M+NH4]-sn1-18 841.75187 199.80 [M+NH4]-17	/
24	TG 16:0_17:1 (8)_18:2 (6, 9)	18.14	$C_{54}H_{98}O_6$	860.7744	860.7702	4.9	[M+NH4]+	563.50362 999.00 [M+NH4]-sn3-18 575.50362 999.00 [M+NH4]-sn2-18 587.50362 999.00 [M+NH4]-sn1-18 843.76751 199.80 [M+NH4]-17	C_9H_{18}, $C_{12}H_{22}$
25	TG 16:0_17:1 (8)_18:1 (9)	18.30	$C_{54}H_{100}O_6$	862.7907	862.7859	5.6	[M+NH4]+	563.50362 999.00 [M+NH4]-sn3-18 577.51926 999.00 [M+NH4]-sn2-18 589.51926 999.00 [M+NH4]-sn1-18 845.78315 199.80 [M+NH4]-17	C_9H_{18}
26	TG 16:0_17:0_18:1	18.45	$C_{54}H_{102}O_6$	864.8043	864.8015	3.2	[M+NH4]+	565.51926 999.00 [M+NH4]-sn3-18 577.51926 999.00 [M+NH4]-sn2-18 591.53490 999.00 [M+NH4]-sn1-18 847.79879 199.80 [M+NH4]-17	/
27	TG 16:1_18:3_18:3	17.07	$C_{55}H_{92}O_6$	866.7269	866.7233	4.2	[M+NH4]+	571.47234 999.00 [M+NH4]-sn2-18 || [M+NH4]-sn3-18 595.47234 999.00 [M+NH4]-sn1-18 849.72059 199.80 [M+NH4]-17	/
28	TG 16:0_17:0_18:0	18.56	$C_{54}H_{104}O_6$	866.8196	866.8172	2.8	[M+NH4]+	565.51926 999.00 [M+NH4]-sn3-18 579.53490 999.00 [M+NH4]-sn2-18 593.55054 999.00 [M+NH4]-sn1-18 849.81443 199.80 [M+NH4]-17	-
29	TG 16:1_18:2_18:3	17.58	$C_{55}H_{94}O_6$	868.7429	868.7390	4.5	[M+NH4]+	547.47234 999.00 [M+NH4]-sn3-18 597.48798 999.00 [M+NH4]-sn1-18 || [M+NH4]-sn2-18 851.73623 199.80 [M+NH4]-17	/
30	TG 16:1_18:2_18:3	17.43	$C_{55}H_{94}O_6$	868.7412	868.7390	2.5	[M+NH4]+	571.47234 999.00 [M+NH4]-sn2-18 573.48798 999.00 [M+NH4]-sn3-18 597.48798 999.00 [M+NH4]-sn1-18 851.73623 199.80 [M+NH4]-17	/
31	TG 16:1_18:2_18:2	17.81	$C_{55}H_{96}O_6$	870.7575	870.7546	3.3	[M+NH4]+	573.48798 999.00 [M+NH4]-sn2-18 575.50362 999.00 [M+NH4]-sn3-18 597.48798 999.00 [M+NH4]-sn1-18 853.75187 199.80 [M+NH4]-17	/
32	TG 16:0_18:2 (9, 12)_18:2 (9, 12)	18.05	$C_{55}H_{98}O_6$	872.7724	872.7702	2.5	[M+NH4]+	575.50362 999.00 [M+NH4]-sn2-18 || [M+NH4]-sn3-18 599.50362 999.00 [M+NH4]-sn1-18 855.76751 199.80 [M+NH4]-17	C_9H_{16}, C_6H_{12}

33	TG 16:0_18:1 (9)_18:2 (9, 12)	18.30	$C_{55}H_{100}O_6$	874.7879	874.7859	2.3	[M+NH4]+	575.50362 999.00 [M+NH4]-sn2-18 577.51926 999.00 [M+NH4]-sn3-18 601.51926 999.00 [M+NH4]-sn1-18 857.78315 199.80 [M+NH4]-17	C_9H_{16}, C_6H_{12}
34	TG 16:0_18:1 (9)_18:1 (9) / TG 16:0_18:1 (11)_18:1 (11)	18.37	$C_{55}H_{102}O_6$	876.8051	876.8015	4.1	[M+NH4]+	577.51926 999.00 [M+NH4]-sn2-18 || [M+NH4]-sn3-18 603.53490 999.00 [M+NH4]-sn1-18 859.79879 199.80 [M+NH4]-17	C_9H_{18}, C_7H_{14}
35	TG 16:0_18:0_18:1	18.51	$C_{55}H_{104}O_6$	878.8196	878.8172	2.7	[M+NH4]+	577.51926 999.00 [M+NH4]-sn2-18 579.53490 999.00 [M+NH4]-sn3-18 605.55054 999.00 [M+NH4]-sn1-18 861.81443 199.80 [M+NH4]-17	/
36	TG 16:0_18:0_18:0	18.62	$C_{55}H_{106}O_6$	880.8368	880.8328	4.5	[M+NH4]+	579.53490 999.00 [M+NH4]-sn2-18 || [M+NH4]-sn3-18 607.56618 999.00 [M+NH4]-sn1-18 863.83007 199.80 [M+NH4]-17	-
37	TG 17:2_18:2_18:2	17.70	$C_{56}H_{96}O_6$	882.7507	882.7546	-4.4	[M+NH4]+	585.48798 999.00 [M+NH4]-sn2-18 || [M+NH4]-sn3-18 599.50362 999.00 [M+NH4]-sn1-18 865.75187 199.80 [M+NH4]-17	/
38	TG 17:1_18:2_18:2	18.00	$C_{56}H_{98}O_6$	884.7725	884.7703	2.5	[M+NH4]+	587.50362 999.00 [M+NH4]-sn2-18 || [M+NH4]-sn3-18 599.50362 999.00 [M+NH4]-sn1-18 867.76751 199.80 [M+NH4]-17	/
39	TG 17:1_18:1_18:2	18.15	$C_{56}H_{100}O_6$	886.7875	886.7859	1.8	[M+NH4]+	587.50362 999.00 [M+NH4]-sn2-18 589.51926 999.00 [M+NH4]-sn3-18 601.51926 999.00 [M+NH4]-sn1-18 869.78315 199.80 [M+NH4]-17	/
40	TG 17:0_18:1 (9)_18:2 (9, 12)	18.31	$C_{56}H_{102}O_6$	888.8025	888.8015	1.1	[M+NH4]+	589.51926 999.00 [M+NH4]-sn2-18 591.53490 999.00 [M+NH4]-sn3-18 601.51926 999.00 [M+NH4]-sn1-18 871.79879 199.80 [M+NH4]-17	C_9H_{18}, C_6H_{12}, C_9H_{16}
41	TG 17:0_18:1 (9)_18:1 (9)	18.44	$C_{56}H_{104}O_6$	890.8170	890.8172	-0.2	[M+NH4]+	591.53490 999.00 [M+NH4]-sn2-18 || [M+NH4]-sn3-18 603.53490 999.00 [M+NH4]-sn1-18 873.81443 199.80 [M+NH4]-17	C_9H_{18}
42	TG 18:2_18:3_18:3	17.07	$C_{57}H_{94}O_6$	892.7433	892.7390	4.8	[M+NH4]+	595.47234 999.00 [M+NH4]-sn1-18 597.48798 999.00 [M+NH4]-sn2-18 || [M+NH4]-sn3-18 875.73623 199.80 [M+NH4]-17	/
43	TG 17:0_18:0_18:1	18.20	$C_{56}H_{106}O_6$	892.8358	892.8328	3.3	[M+NH4]+	591.53490 999.00 [M+NH4]-sn2-18 593.55054 999.00 [M+NH4]-sn3-18 605.55054 999.00 [M+NH4]-sn1-18 875.83007 199.80 [M+NH4]-17	/
44	TG 18:2 (9, 12)_18:2 (9, 12)_18:3 (9, 12, 15)	17.46	$C_{57}H_{96}O_6$	894.7566	894.7546	2.2	[M+NH4]+	573.48798 999.00 [M+NH4]-sn3-18 597.48798 999.00 [M+NH4]-sn2-18 623.50362 999.00 [M+NH4]-sn1-18 877.75187 199.80 [M+NH4]-17	C_3H_6, C_6H_{10}, C_9H_{14}, C_6H_{12}, C_9H_{16}
45	TG 16:0_18:0_19:0	18.65	$C_{56}H_{108}O_6$	894.8528	894.8484	4.9	[M+NH4]+	579.53490 999.00 [M+NH4]-sn3-18 593.55054 999.00 [M+NH4]-sn2-18 621.58182 999.00 [M+NH4]-sn1-18 877.84571 199.80 [M+NH4]-17	-
46	TG 18:2 (9, 12)_18:2 (9, 12)_18:2 (9, 12)	17.80	$C_{57}H_{98}O_6$	896.7700	896.7702	-0.2	[M+NH4]+	599.50362 999.00 [M+NH4]-sn1-18 || [M+NH4]-sn2-18 || [M+NH4]-sn3-18 879.76751 199.80 [M+NH4]-17	C_6H_{12}, C_9H_{16}
47	TG 18:1_18:2_18:2	18.05	$C_{57}H_{100}O_6$	898.7842	898.7859	-1.9	[M+NH4]+	599.50362 999.00 [M+NH4]-sn1-18 601.51926 999.00 [M+NH4]-sn2-18 || [M+NH4]-sn3-18 881.78315 199.80 [M+NH4]-17	/
48	TG 18:1 (9)_18:1 (9)_18:2 (9, 12)	18.23	$C_{57}H_{102}O_6$	900.8008	900.8015	-0.8	[M+NH4]+	601.51926 999.00 [M+NH4]-sn1-18 || [M+NH4]-sn2-18 603.53490 999.00 [M+NH4]-sn3-18 883.79879 199.80 [M+NH4]-17	C_6H_{12}, C_9H_{16}, C_9H_{18}
49	TG 18:1 (9)_18:1 (9)_18:1 (9)	18.40	$C_{57}H_{104}O_6$	902.8174	902.8172	0.3	[M+NH4]+	603.53490 999.00 [M+NH4]-sn1-18 || [M+NH4]-sn2-18 || [M+NH4]-sn3-18 885.81443 199.80 [M+NH4]-17	C_9H_{18}
50	TG 18:0_18:1_18:1	18.50	$C_{57}H_{106}O_6$	904.8350	904.8328	2.4	[M+NH4]+	603.53490 999.00 [M+NH4]-sn1-18 605.55054 999.00 [M+NH4]-sn2-18 || [M+NH4]-sn3-18 887.83007 199.80 [M+NH4]-17	/

51	TG 18:0_18:0_18:1	18.62	$C_{57}H_{108}O_6$	906.8516	906.8484	3.5	[M+NH4]+	605.55054 999.00 [M+NH4]-sn1-18 || [M+NH4]-sn2-18 607.56618 999.00 [M+NH4]-sn3-18 889.84571 199.80 [M+NH4]-17	/
52	TG 18:0_18:0_18:0	18.71	$C_{57}H_{110}O_6$	908.8676	908.8641	3.9	[M+NH4]+	607.56618 999.00 [M+NH4]-sn1-18 || [M+NH4]-sn2-18 || [M+NH4]-sn3-18 891.86135 199.80 [M+NH4]-17	-
53	TG 16:0_17:0_22:0	18.74	$C_{58}H_{112}O_6$	912.8018	912.8015	0.3	[M+NH4]+	565.51926 999.00 [M+NH4]-sn3-18 635.59746 999.00 [M+NH4]-sn2-18 649.61310 999.00 [M+NH4]-sn1-18 905.87699 199.80 [M+NH4]-17	-
54	TG 18:2_18:3_20:5	16.97	$C_{59}H_{94}O_6$	916.7426	916.7390	3.9	[M+NH4]+	597.48798 999.00 [M+NH4]-sn3-18 619.47234 999.00 [M+NH4]-sn1-18 621.48798 999.00 [M+NH4]-sn2-18 899.73623 199.80 [M+NH4]-17	/
55	TG 18:2_18:3_20:4	17.33	$C_{59}H_{96}O_6$	918.7552	918.7546	0.7	[M+NH4]+	597.48798 999.00 [M+NH4]-sn3-18 621.48798 999.00 [M+NH4]-sn1-18 623.50362 999.00 [M+NH4]-sn2-18 901.75187 199.80 [M+NH4]-17	/
56	TG 16:0_18:2_22:6	17.84	$C_{59}H_{98}O_6$	920.7692	920.7702	-1.1	[M+NH4]+	575.50362 999.00 [M+NH4]-sn3-18 623.50362 999.00 [M+NH4]-sn2-18 647.50362 999.00 [M+NH4]-sn1-18 903.76751 199.80 [M+NH4]-17	/
57	TG 16:1_18:0_21:0	18.66	$C_{58}H_{112}O_6$	920.8662	920.8641	2.3	[M+NH4]+	565.51926 999.00 [M+NH4]-sn3-18 635.59746 999.00 [M+NH4]-sn2-18 649.61310 999.00 [M+NH4]-sn1-18 905.87699 199.80 [M+NH4]-17	/
58	TG 18:1 (9)_18:2 (9, 12)_20:4 (5, 8, 11, 14)	17.96	$C_{59}H_{100}O_6$	922.7851	922.7859	-0.9	[M+NH4]+	603.53490 999.00 [M+NH4]-sn3-18 623.50362 999.00 [M+NH4]-sn1-18 || [M+NH4]-sn2-18 905.78315 199.80 [M+NH4]-17	C_6H_{12}, C_9H_{16}, $C_{12}H_{20}$, $C_{15}H_{24}$, C_9H_{18}
59	TG 18:1 (9)_18:2 (9, 12)_20:3 (8, 11, 14)	18.17	$C_{59}H_{102}O_6$	924.7965	924.8015	-5.4	[M+NH4]+	603.53490 999.00 [M+NH4]-sn3-18 625.51926 999.00 [M+NH4]-sn1-18 || [M+NH4]-sn2-18 907.79879 199.80 [M+NH4]-17	$C_6H_{12}O$, $C_9H_{16}O$, $C_9H_{18}O$
60	TG 18:0_18:1 (12)_20:4 (5, 8, 11, 14)	18.31	$C_{59}H_{104}O_6$	926.8163	926.8172	-1.0	[M+NH4]+	605.55054 999.00 [M+NH4]-sn3-18 625.51926 999.00 [M+NH4]-sn1-18 627.53490 999.00 [M+NH4]-sn2-18 909.81443 199.80 [M+NH4]-17	C_6H_{12}, C_9H_{16}, $C_{12}H_{20}$, $C_{15}H_{24}$
61	TG 18:1_18:2_20:1	18.37	$C_{59}H_{106}O_6$	928.8315	928.8328	-1.4	[M+NH4]+	601.51926 999.00 [M+NH4]-sn3-18 629.55054 999.00 [M+NH4]-sn1-18 631.56618 999.00 [M+NH4]-sn2-18 911.83007 199.80 [M+NH4]-17	/
62	TG 18:1_18:1_20:1	18.50	$C_{59}H_{108}O_6$	930.8444	930.8484	-4.3	[M+NH4]+	603.53490 999.00 [M+NH4]-sn3-18 631.56618 999.00 [M+NH4]-sn1-18 || [M+NH4]-sn2-18 913.84571 199.80 [M+NH4]-17	/
63	TG 20:0_16:1_20:1	18.60	$C_{59}H_{110}O_6$	932.8651	932.8641	1.1	[M+NH4]+	603.53490 999.00 [M+NH4]-sn3-18 633.58182 999.00 [M+NH4]-sn1-18 || [M+NH4]-sn2-18 915.86135 199.80 [M+NH4]-17	/
64	TG 18:0_18:1_20:0	18.70	$C_{59}H_{112}O_6$	934.8815	934.8797	1.9	[M+NH4]+	605.55054 999.00 [M+NH4]-sn3-18 633.58182 999.00 [M+NH4]-sn1-18 635.59746 999.00 [M+NH4]-sn2-18 917.87699 199.80 [M+NH4]-17	/
65	TG 18:0_16:0_22:0	18.80	$C_{59}H_{114}O_6$	936.8981	936.8954	3.0	[M+NH4]+	579.53490 999.00 [M+NH4]-sn3-18 649.61310 999.00 [M+NH4]-sn1-18 || [M+NH4]-sn2-18 919.89263 199.80 [M+NH4]-17	-
66	TG 18:2_18:3_22:6	17.15	$C_{61}H_{96}O_6$	942.7576	942.7546	3.2	[M+NH4]+	597.48798 999.00 [M+NH4]-sn3-18 645.48798 999.00 [M+NH4]-sn1-18 647.50362 999.00 [M+NH4]-sn2-18 925.75187 199.80 [M+NH4]-17	/
67	TG 18:2_18:2_22:6	17.50	$C_{61}H_{98}O_6$	944.7717	944.7702	1.6	$[M+NH4]^+$	599.50362 999.00 [M+NH4]-sn3-18 647.50362 999.00 [M+NH4]-sn1-18 || [M+NH4]-sn2-18 927.76751 199.80 [M+NH4]-17	/

68	TG 18:2_18:2_22:5	17.84	$C_{61}H_{100}O_6$	946.7875	946.7859	1.7	[M+NH4]+	601.51926 999.00 [M+NH4]-sn3-18 647.50362 999.00 [M+NH4]-sn1-18 649.51926 999.00 [M+NH4]-sn2-18 929.78315 199.80 [M+NH4]-17	/
69	TG 18:1_18:1_22:6	18.07	$C_{61}H_{102}O_6$	948.8015	948.8015	0.0	[M+NH4]+	603.53490 999.00 [M+NH4]-sn3-18 649.51926 999.00 [M+NH4]-sn1-18 || [M+NH4]-sn2-18 931.79879 199.80 [M+NH4]-17	/
70	DG 18:2_18:2	11.30	$C_{39}H_{68}O_5$	634.5427	634.5407	3.2	[M+NH4]+	337.27410 999.00 [M+NH4]-sn1 || [M+NH4]-sn2 599.52743 500.00 [M+NH4]-NH4-H2O (-17-18) 617.53799 200.00 [M+NH4]-NH4 (-17)	/
71	DG 18:1_18:2	13.10	$C_{39}H_{70}O_5$	636.5573	636.5564	1.5	[M+NH4]+	337.27410 999.00 [M+NH4]-sn1 339.28974 999.00 [M+NH4]-sn2 601.54307 500.00 [M+NH4]-NH4-H2O (-17-18) 619.55363 200.00 [M+NH4]-NH4 (-17)	/
72	DG 18:1_18:1	13.84	$C_{39}H_{72}O_5$	638.5778	638.5720	9.1	[M+NH4]+	339.28974 999.00 [M+NH4]-sn1 || [M+NH4]-sn2 603.55871 500.00 [M+NH4]-NH4-H2O (-17-18) 621.56927 200.00 [M+NH4]-NH4 (-17)	/

Note: In the first column from right, “-” denotes the saturated lipids and “/” denotes the unsaturated lipids but the C=C bonds positions were not identified. The chemical formulas were simulated based on the exact masses of diagnostic ions P1b (only containing the C and H atoms). The match details in the second column from right include: *m/z* values of product ions, their intensities, and possible explanations.

Table S7. Ceramide identified from human serum extract.

No.	Identification	RT (min)	Formula	Observed m/z	Calculated m/z	Error (ppm)	Adduct	Match details	Formula of neutral loss molecules for C=C analysis
1	Cer d18:0/22:0	16.40	$C_{40}H_{81}NO_3$	624.6296	624.6296	0.0	$[M+H]^+$	266.24837 999.00 LCB sphingo-base 284.25893 100.00 LCB sphingo-base + H_2O	-
2	Cer d18:1/16:0	1.61	$C_{34}H_{67}NO_3$	538.5219	538.5194	4.6	$[M+H]^+$	-	/

Note: In the first column from right, "-" denotes the saturated lipids and "/" denotes the unsaturated lipids but the C=C bonds positions were not identified. The chemical formulas were simulated based on the exact masses of diagnostic ions P1b (only containing the C and H atoms). The match details in the second column from right include: *m/z* values of product ions, their intensities, and possible explanations.

Table S8. FA identified from human serum extract.

NO.	Identification	RT (min)	Formula	Observed m/z	Calculated m/z	Error (ppm)	Adduct	Formula of neutral loss molecules for C=C analysis
1	16: 0	4.89	$C_{16}H_{32}O_2$	255.2317	255.2318	-0.4	$[M-H]^-$	-
2	16: 1 (9/11)	3.51	$C_{16}H_{30}O_2$	253.2168	253.2162	2.4	$[M-H]^-$	C_7H_{14}, C_5H_{10}
3	18: 0	6.27	$C_{18}H_{36}O_2$	283.2629	283.2631	-0.7	$[M-H]^-$	-
4	18: 1 (9/11)	5.06	$C_{18}H_{34}O_2$	281.2471	281.2475	-1.4	$[M-H]^-$	$C_{11}H_{22}$, C_9H_{18}
5	18: 2 (9, 12)	3.92	$C_{18}H_{32}O_2$	279.2323	279.2319	1.4	$[M-H]^-$	C_6H_{12}, C_9H_{16}
6	18: 3 (9, 12, 15)	2.84	$C_{18}H_{30}O_2$	277.2166	277.2162	1.4	$[M-H]^-$	C_3H_6, C_6H_{10}, C_9H_{14}
7	20: 0	7.51	$C_{20}H_{40}O_2$	311.2947	311.2944	1.0	$[M-H]^-$	-
8	20: 1 (11/13)	6.31	$C_{20}H_{38}O_2$	309.2787	309.2788	-0.3	$[M-H]^-$	C_9H_{18}, C_7H_{14}
9	20: 2 (11, 14)	5.32	$C_{20}H_{36}O_2$	307.2636	307.2632	1.3	$[M-H]^-$	C_6H_{12}, C_9H_{16}
10	20: 3 (8, 11, 14)	4.39	$C_{20}H_{34}O_2$	305.2478	305.2475	1.0	$[M-H]^-$	C_6H_{12}, C_9H_{16}
11	20: 4 (5, 8, 11, 14)	3.67	$C_{20}H_{32}O_2$	303.2322	303.2319	1.0	$[M-H]^-$	C_6H_{12}, C_9H_{16}, $C_{12}H_{20}$, $C_{15}H_{24}$
12	22: 1 (13)	7.51	$C_{22}H_{42}O_2$	337.3103	337.3103	0.0	$[M-H]^-$	C_9H_{18}
13	22: 4 (7, 10, 13, 16)	4.84	$C_{22}H_{36}O_2$	331.2629	331.2632	-0.9	$[M-H]^-$	C_6H_{12}, C_9H_{16}, $C_{12}H_{20}$, $C_{15}H_{24}$
14	22: 5 (7, 10, 13, 16, 19)	4.32	$C_{22}H_{34}O_2$	329.2474	329.2475	-0.3	$[M-H]^-$	C_3H_6, C_6H_{10}, C_9H_{14}, $C_{12}H_{18}$, $C_{15}H_{22}$
15	22: 6 (4, 7, 10, 13, 16, 19)	3.36	$C_{22}H_{32}O_2$	327.2324	327.2319	1.5	$[M-H]^-$	C_3H_6, C_6H_{10}, C_9H_{14}, $C_{12}H_{18}$, $C_{15}H_{22}$

Note: In the first column from right, "-" denotes the saturated lipids. The chemical formulas were simulated based on the exact masses of diagnostic ions P1b (only containing the C and H atoms). The match details in the second column from right include: *m/z* values of product ions, their intensities, and possible explanations.