SUPPLEMENTAL INFORMATION

Journal of Lipid Research: Methods paper

Widely-targeted quantitative lipidomics methodology by supercritical fluid chromatography coupled with fast-scanning triple quadrupole mass spectrometry

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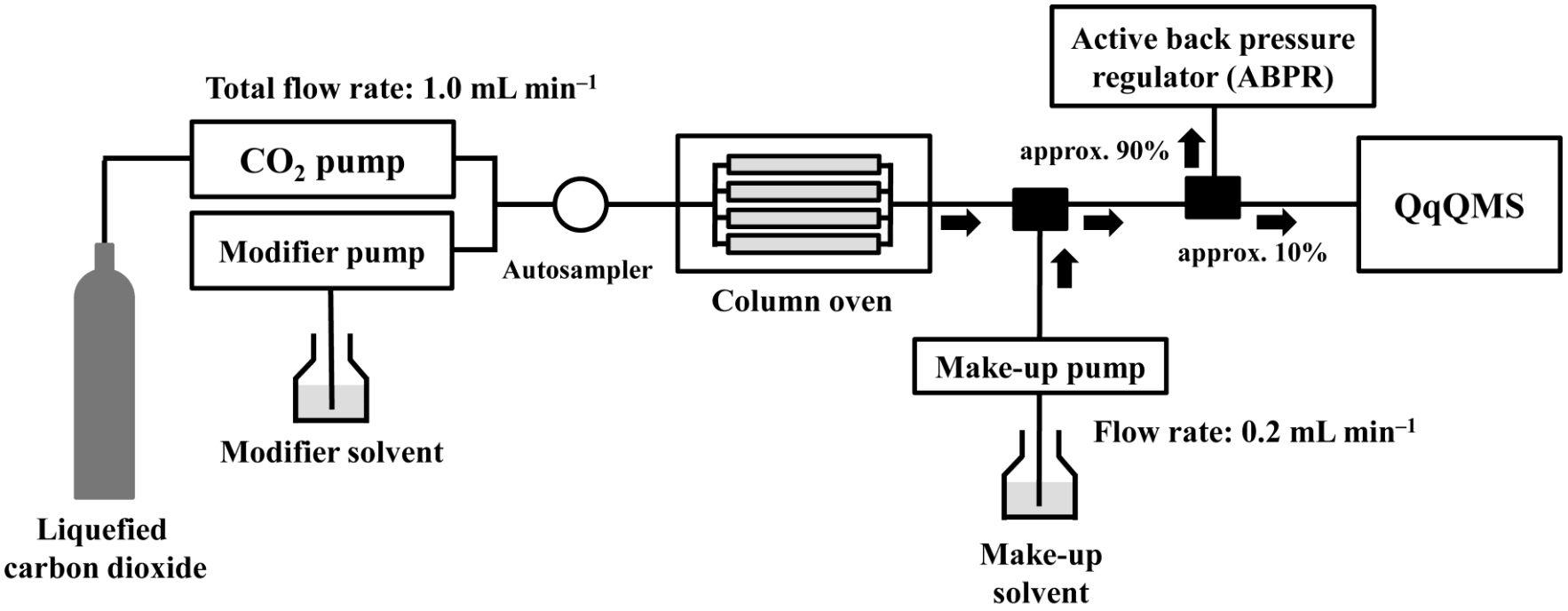
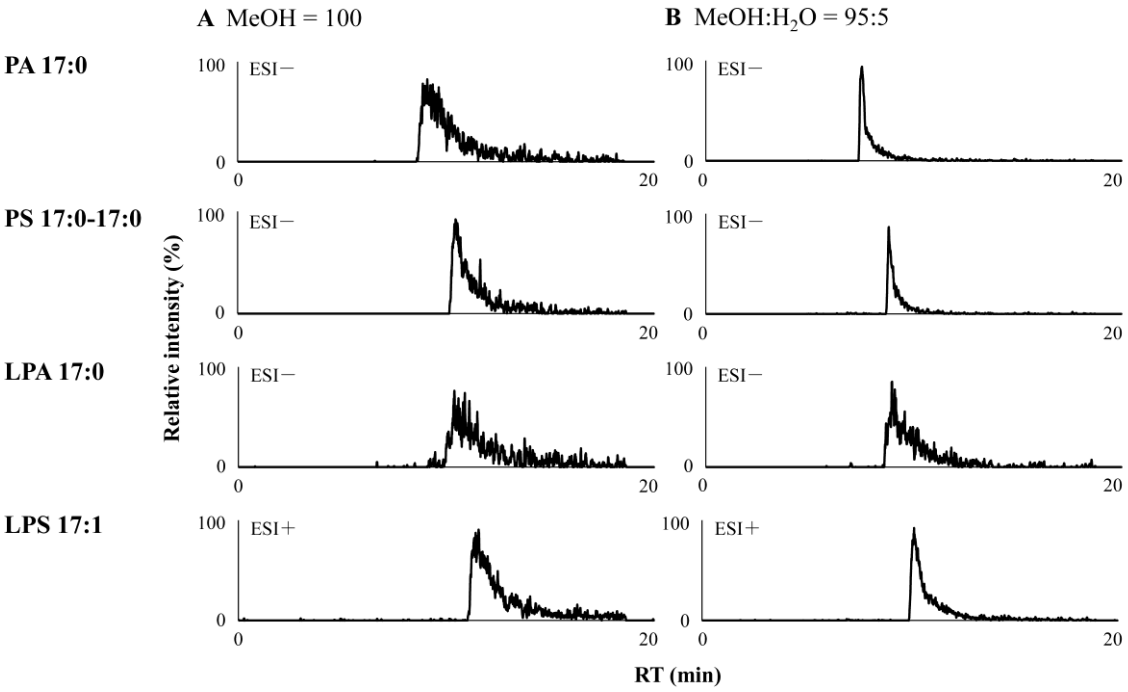
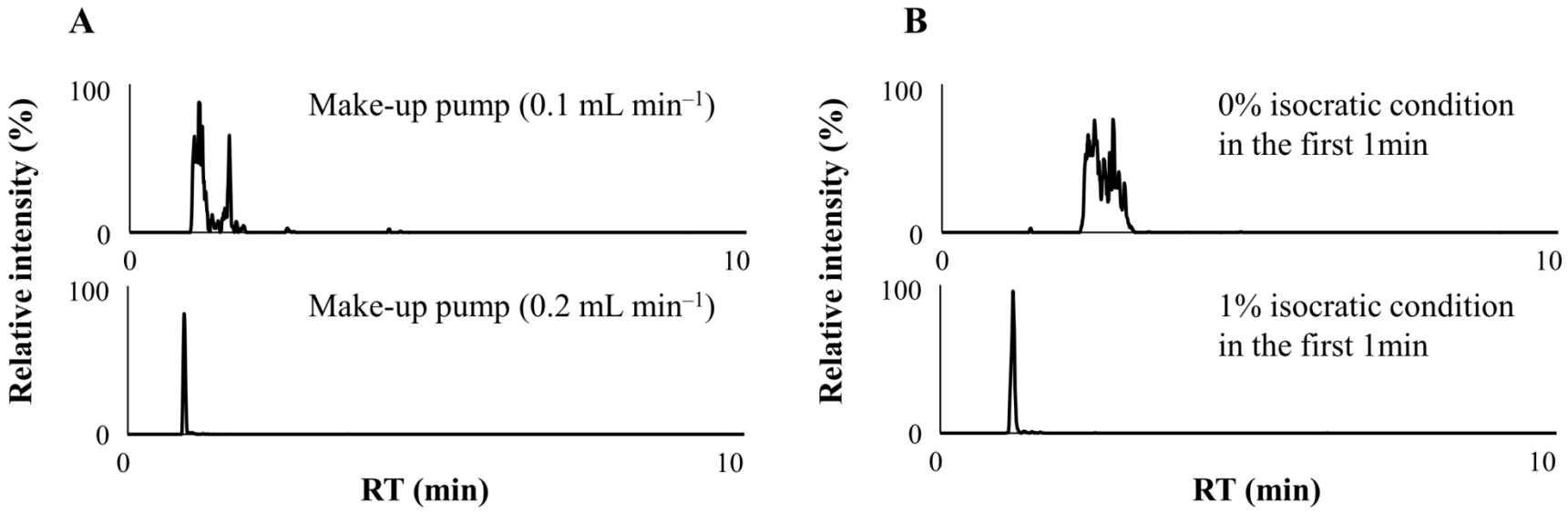


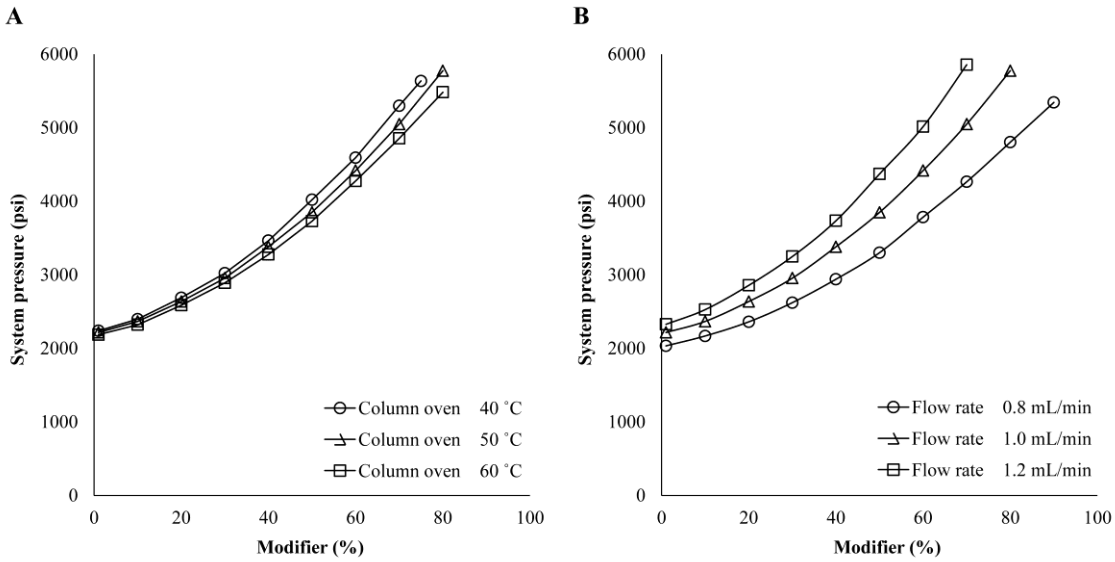
Supplemental Fig. S1: A schematic diagram of SFC/QqQMS system used in this study.



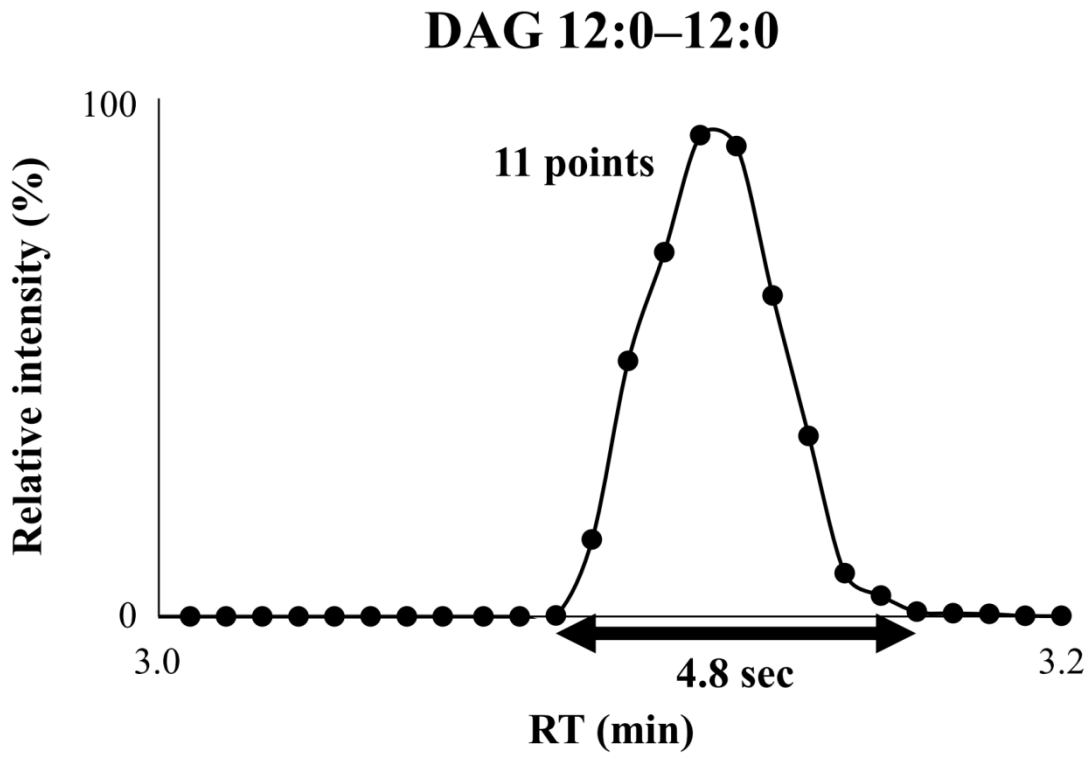
Supplemental Fig. S2: Improvement of peak shape of 4 polar lipids by addition of 5% water to the modifier solvent. (A) 100% methanol with 0.1% (w/v) ammonium acetate. (B) Methanol/water (95/5, v/v) with 0.1% (w/v) ammonium acetate.



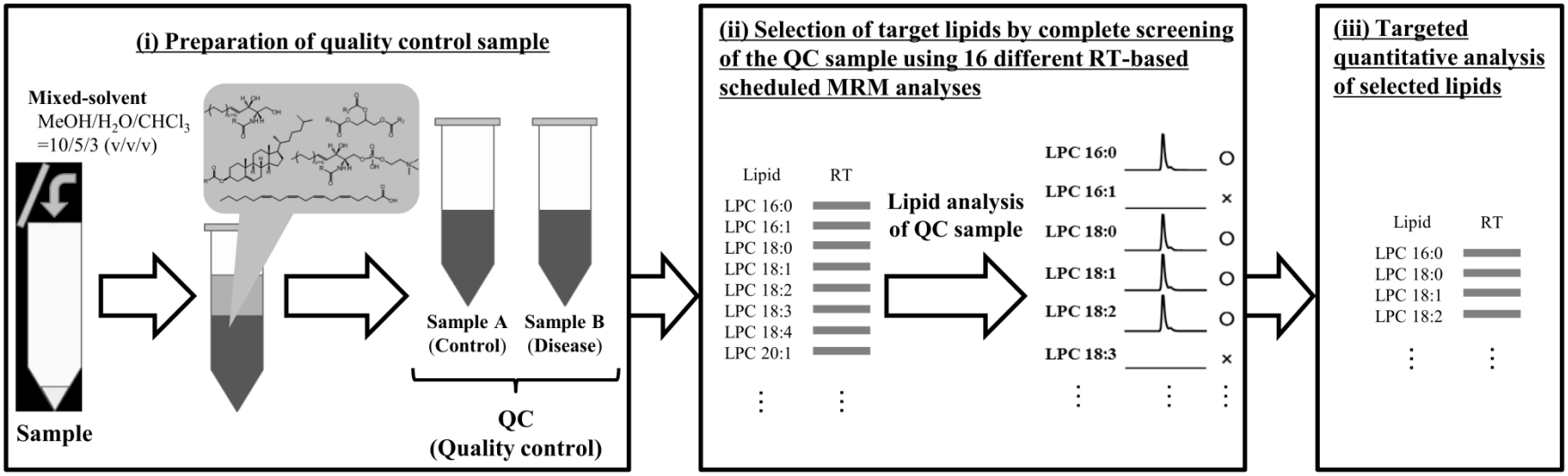
Supplemental Fig. S3: Improvement of peak shape of nonpolar lipid (CE 17:0) by optimization of flow rate of make-up pump (A) and modifier condition (B) in SFC/QqQMS with the BEH column.



Supplemental Fig. S4: Effect of column oven temperature and flow rate on system pressure under various mobile phase conditions. (A) Column oven temperature, 40 ˚C, 50 ˚C, and 60 ˚C; ABPR, 1500 psi; and flow rate 1.0 mL min^{-1}. (B) Column oven temperature, 50 ˚C; ABPR, 1500 psi; and flow rate 0.8 mL min^{-1}, 1.0 mL min^{-1}, and 1.2 mL min^{-1}.



Supplemental Fig. S5: Evaluation of number of data points per peak. The MRM parameters per one time-period were as follows: limit on number of MRM transitions, 150; dwell time, 1 ms; MS inter-scan and inter-channel delay, 2 ms; and polarity switch inter-scan, 15 ms.



Supplemental Fig. S6: Flowchart of the widely-targeted quantitative lipidomics methodology.

Supplemental Table S1: Features of representative lipidomics methodologies.

	DI/MS/MS	RP-LC/MS/MS	NP-LC/MS/MS	HILIC/MS/MS	SFC/MS/MS (in this study)
Throughput	+++	++	++	+	++
Sensitivity	+	+++	++	+++	+++
Identification of isomers	+	+++	++	++	+++
The number of lipids detected	+	+++	++	++	+++
Quantitative performance	+++	+	+++	+++	+++

Each characteristic was evaluated in three stages (+, ++, and +++).

Supplemental Table S2: Fatty acid composition used for the setting of theoretically calculated a comprehensive lipid MRM library.

Abbreviation	Main fatty acid	Abbreviation	Main fatty acid
12:0	Lauric acid	20:2	Eicosadienoic acid (*n*-6)
14:0	Myristic acid	20:3	Dihomo-γ-linoleic acid (*n*-6)
14:1	Myristoleic acid (*n*-5)	20:4	Arachidonic acid (*n*-6)
16:0	Palmitic acid	20:5	Eicosapentaenoic acid (*n*-3)
16:1	Palmitoleic acid (*n*-7)	22:6	Behenic acid
18:0	Stearic acid	22:1	Erucic acid (*n*-9)
18:1	Oleic acid (*n*-9)	22:2	Docosadienoic acid (*n*-6)
18:2	Linoleic acid (*n*-6)	22:3	Docosatorienoic acid (*n*-3)
18:3	α-Linoleic acid (*n*-3)	22:4	Docosatetraenoic acid (*n*-6)
18:4	Stearidonic acid (*n*-3)	22:5	Docosapentaenoic acid (*n*-3)
20:0	Arachidic acid	22:6	Docosahexaenoic acid (*n*-3)
20:1	Eicosenoic acid (*n*-9)		

Double bond positions (*n*).

Supplemental Table S3: MRM transition settings of 22 classes of lipids investigated.

Lipid class	Ion mode	The number of MRM transition	MS^1 (*m/z*)	MS^2 (*m/z*)	Cone voltage (V)	Collision energy (V)
LPC	ESI+	23	$[M + H]^+$	184.1	10	30
LPE	ESI+	23	$[M + H]^+$	$[M + H]^+ - 141.0$	30	20
LPG	ESI+	23	$[M + H]^+$	$[M + H]^+ - 172.0$	40	20
LPA	ESI−	23	$[M - H]^-$	153.8	10	20
LPI	ESI−	23	$[M - H]^-$	241	10	40
LPS	ESI+	23	$[M + H]^+$	$[M + H]^+ - 185.0$	30	20
PC	ESI−	529	$[M + CH_3COO]^-$	[Acyl FA (*sn*-1) − H]$^-$ and [Acyl FA (*sn*-2) − H]$^-$	15	40
Alkyl-acyl PC (e) and/or Alkenyl-acyl PC (p)	ESI+	319	$[M + H]^+$	[LPC FAe and/or FAp (*sn*-1) + H]$^+$ and [LPC − OH]$^+$	20	30
PE	ESI−	529	$[M - H]^-$	[Acyl FA (*sn*-1) − H]$^-$ and [Acyl FA (*sn*-2) − H]$^-$	50	25
Alkenyl-acyl PE (p)	ESI+	345	$[M + H]^+$	$[M - FA - (CH_2{=}COHCH_2OH)]^+$	20	30
PG	ESI−	529	$[M - H]^-$	[Acyl FA (*sn*-1) − H]$^-$ and [Acyl FA (*sn*-2) − H]$^-$	30	40
PA	ESI−	529	$[M - H]^-$	[Acyl FA (*sn*-1) − H]$^-$ and [Acyl FA (*sn*-2) − H]$^-$	20	40
PI	ESI−	529	$[M - H]^-$	[Acyl FA (*sn*-1) − H]$^-$ and [Acyl FA (*sn*-2) − H]$^-$	50	50
PS	ESI−	529	$[M - H]^-$	[Acyl FA (*sn*-1) − H]$^-$ and [Acyl FA (sn-2) − H]$^-$	30	50
SM	ESI+	23	$[M + H]^+$	184.1	50	30
Cer	ESI+	23	$[M + H]^+$	$[So\ dFA + H - H_2O]^+$	20	30
CE	ESI+	23	$[M + NH_4]^+$	369.4	20	10
MAG	ESI+	23	$[M + H]^+$	$[M + H - H_2O]^+$	10	10
DAG	ESI+	529	$[M + NH_4]^+$	$[M + NH_4 - NH_3 - Acyl\ FAFA\ (sn\text{-}1)]^+$ and $[M + NH_4 - NH_3 - Acyl\ FAFA\ (sn\text{-}2)]^+$	50	20

TAG	ESI+	167	$[M + NH_4]^+$	$[M + NH_4]^+$	10	10
FFA	ESI−	23	$[M – H]^-$	$[M – H]^-$	10	10

Ether-linked isobaric species of plasmanyl (e) and plasmenyl (p) analogs of glycerophospholipids.

Acyl positions of glycerolipids (*sn*-1 and *sn*-2).

Supplemental Table S4: Comparison of SFC separation behavior of lipid classes with six kinds of SFC columns.

Lipid class	RT (min) (Mean ± SD) (n = 5)					
	BEH	2-EP	2-PIC	DEA	DIOL	1-AA
CE 17:0	0.92 ± 0.02	2.47 ± 0.09	2.82 ± 0.01	1.19 ± 0.01	1.32 ± 0.01	4.18 ± 0.01
TAG 17:0-17:0-17:0	1.00 ± 0.01	2.79 ± 0.01	2.98 ± 0.00	1.22 ± 0.05	1.78 ± 0.03	4.11 ± 0.01
FFA 17:0	2.98 ± 0.01	3.22 ± 0.01	3.53 ± 0.02	4.05 ± 0.01	3.01 ± 0.01	3.66 ± 0.02
DAG 12:0-12:0	3.13 ± 0.02	3.29 ± 0.02	3.41 ± 0.02	3.08 ± 0.01	3.13 ± 0.01	4.14 ± 0.00
MAG 17:0	4.17 ± 0.02	4.06 ± 0.03	4.30 ± 0.01	4.06 ± 0.02	4.03 ± 0.00	4.50 ± 0.01
Cer d18:1-17:0	4.50 ± 0.01	4.44 ± 0.00	4.54 ± 0.01	4.48 ± 0.01	4.40 ± 0.01	4.77 ± 0.01
PG 17:0-17:0	6.77 ± 0.01	5.72 ± 0.01	6.81 ± 0.00	8.86 ± 0.01	6.39 ± 0.00	6.75 ± 0.01
PE 17:0-17:0	6.94 ± 0.01	5.53 ± 0.01	5.95 ± 0.00	6.11 ± 0.01	5.75 ± 0.01	6.51 ± 0.00
PA 17:0-17:0	7.12 ± 0.03	9.23 ± 0.52	8.55 ± 0.25	12.37 ± 0.02	6.07 ± 0.01	7.66 ± 0.19
LPG 17:1	7.94 ± 0.01	6.39 ± 0.01	8.24 ± 0.01	11.04 ± 0.02	7.22 ± 0.01	7.46 ± 0.00
LPE 17:1	8.30 ± 0.01	6.16 ± 0.01	6.92 ± 0.00	7.49 ± 0.01	7.13 ± 0.00	7.25 ± 0.00
PI 17:0-14:1	8.30 ± 0.01	6.51 ± 0.01	9.05 ± 0.01	12.21 ± 0.01	8.01 ± 0.01	8.35 ± 0.01
PS 17:0-17:0	8.80 ± 0.02	6.79 ± 0.07	8.35 ± 0.02	12.27 ± 0.02	7.43 ± 0.01	8.51 ± 0.08
LPA 17:0	8.97 ± 0.17	n.d.	10.85 ± 0.29	17.40 ± 0.06	7.32 ± 0.02	9.55 ± 0.53
LPI 17:1	9.33 ± 0.01	7.14 ± 0.04	10.41 ± 0.00	14.27 ± 0.02	9.27 ± 0.00	9.01 ± 0.02
LPS 17:1	10.19 ± 0.05	8.11 ± 0.36	10.10 ± 0.02	15.51 ± 0.02	9.02 ± 0.01	9.54 ± 0.11
PC 17:0-17:0	10.21 ± 0.02	6.73 ± 0.02	5.48 ± 0.01	5.36 ± 0.01	5.50 ± 0.01	6.34 ± 0.00
SM d18:1-17:0	11.38 ± 0.03	7.50 ± 0.02	5.90 ± 0.01	5.78 ± 0.01	6.11 ± 0.01	6.80 ± 0.00
LPC 17:0	11.86 ± 0.03	7.68 ± 0.02	6.19 ± 0.01	6.08 ± 0.01	6.49 ± 0.01	6.97 ± 0.00

Supplemental Table S5: In-house lipid MRM library.

Method 1: DAG and PA (1)								
No	Name	Precursor	CV (V)	Product	CE (V)	RT setting (min)	IonMode	Ion
1	DAG 12:0-12:0	474.4	50	257.2	20	3.25	ES+	1
2	DAG 12:0-14:0	502.4	50	257.2	20	3.25	ES+	1
3	DAG 12:0-14:0	502.4	50	285.3	20	3.25	ES+	2
4	DAG 12:0-14:1	500.4	50	257.2	20	3.25	ES+	1
5	DAG 12:0-14:1	500.4	50	283.3	20	3.25	ES+	2
6	DAG 12:0-16:0	530.5	50	257.2	20	3.25	ES+	1
7	DAG 12:0-16:0	530.5	50	313.3	20	3.25	ES+	2
8	DAG 12:0-16:1	528.5	50	257.2	20	3.25	ES+	1
9	DAG 12:0-16:1	528.5	50	311.3	20	3.25	ES+	2
10	DAG 12:0-18:0	558.5	50	257.2	20	3.25	ES+	1
11	DAG 12:0-18:0	558.5	50	341.3	20	3.25	ES+	2
12	DAG 12:0-18:1	556.5	50	257.2	20	3.25	ES+	1
13	DAG 12:0-18:1	556.5	50	339.3	20	3.25	ES+	2
14	DAG 12:0-18:2	554.5	50	257.2	20	3.25	ES+	1
15	DAG 12:0-18:2	554.5	50	337.3	20	3.25	ES+	2
16	DAG 12:0-18:3	552.5	50	257.2	20	3.25	ES+	1
17	DAG 12:0-18:3	552.5	50	335.3	20	3.25	ES+	2
18	DAG 12:0-18:4	550.4	50	257.2	20	3.25	ES+	1
19	DAG 12:0-18:4	550.4	50	333.3	20	3.25	ES+	2
20	DAG 12:0-20:0	586.5	50	257.2	20	3.25	ES+	1
21	DAG 12:0-20:0	586.5	50	369.4	20	3.25	ES+	2
22	DAG 12:0-20:1	584.5	50	257.2	20	3.25	ES+	1
23	DAG 12:0-20:1	584.5	50	367.3	20	3.25	ES+	2
24	DAG 12:0-20:2	582.5	50	257.2	20	3.25	ES+	1
25	DAG 12:0-20:2	582.5	50	365.3	20	3.25	ES+	2
26	DAG 12:0-20:3	580.5	50	257.2	20	3.25	ES+	1
27	DAG 12:0-20:3	580.5	50	363.3	20	3.25	ES+	2
28	DAG 12:0-20:4	578.5	50	257.2	20	3.25	ES+	1
29	DAG 12:0-20:4	578.5	50	361.3	20	3.25	ES+	2
30	DAG 12:0-20:5	576.5	50	257.2	20	3.25	ES+	1
31	DAG 12:0-20:5	576.5	50	359.3	20	3.25	ES+	2
32	DAG 12:0-22:0	614.6	50	257.2	20	3.25	ES+	1

33	DAG 12:0-22:0	614.6	50	397.4	20	3.25	ES+	2
34	DAG 12:0-22:1	612.6	50	257.2	20	3.25	ES+	1
35	DAG 12:0-22:1	612.6	50	395.4	20	3.25	ES+	2
36	DAG 12:0-22:2	610.5	50	257.2	20	3.25	ES+	1
37	DAG 12:0-22:2	610.5	50	393.4	20	3.25	ES+	2
38	DAG 12:0-22:3	608.5	50	257.2	20	3.25	ES+	1
39	DAG 12:0-22:3	608.5	50	391.3	20	3.25	ES+	2
40	DAG 12:0-22:4	606.5	50	257.2	20	3.25	ES+	1
41	DAG 12:0-22:4	606.5	50	389.3	20	3.25	ES+	2
42	DAG 12:0-22:5	604.5	50	257.2	20	3.25	ES+	1
43	DAG 12:0-22:5	604.5	50	387.3	20	3.25	ES+	2
44	DAG 12:0-22:6	602.5	50	257.2	20	3.25	ES+	1
45	DAG 12:0-22:6	602.5	50	385.3	20	3.25	ES+	2
46	DAG 14:0-14:0	530.5	50	285.3	20	3.25	ES+	1
47	DAG 14:0-14:1	528.5	50	283.3	20	3.25	ES+	1
48	DAG 14:0-14:1	528.5	50	285.3	20	3.25	ES+	2
49	DAG 14:0-16:0	558.5	50	285.3	20	3.25	ES+	1
50	DAG 14:0-16:0	558.5	50	313.3	20	3.25	ES+	2
51	DAG 14:0-16:1	556.5	50	285.3	20	3.25	ES+	1
52	DAG 14:0-16:1	556.5	50	311.3	20	3.25	ES+	2
53	DAG 14:0-18:0	586.5	50	285.3	20	3.25	ES+	1
54	DAG 14:0-18:0	586.5	50	341.3	20	3.25	ES+	2
55	DAG 14:0-18:1	584.5	50	285.3	20	3.25	ES+	1
56	DAG 14:0-18:1	584.5	50	339.3	20	3.25	ES+	2
57	DAG 14:0-18:2	582.5	50	285.3	20	3.25	ES+	1
58	DAG 14:0-18:2	582.5	50	337.3	20	3.25	ES+	2
59	DAG 14:0-18:3	580.5	50	285.3	20	3.25	ES+	1
60	DAG 14:0-18:3	580.5	50	335.3	20	3.25	ES+	2
61	DAG 14:0-18:4	578.5	50	285.3	20	3.25	ES+	1
62	DAG 14:0-18:4	578.5	50	333.3	20	3.25	ES+	2
63	DAG 14:0-20:0	614.6	50	285.3	20	3.25	ES+	1
64	DAG 14:0-20:0	614.6	50	369.4	20	3.25	ES+	2
65	DAG 14:0-20:1	612.6	50	285.3	20	3.25	ES+	1
66	DAG 14:0-20:1	612.6	50	367.3	20	3.25	ES+	2
67	DAG 14:0-20:2	610.5	50	285.3	20	3.25	ES+	1

68	DAG 14:0-20:2	610.5	50	365.3	20	3.25	ES+	2
69	DAG 14:0-20:3	608.5	50	285.3	20	3.25	ES+	1
70	DAG 14:0-20:3	608.5	50	363.3	20	3.25	ES+	2
71	DAG 14:0-20:4	606.5	50	285.3	20	3.25	ES+	1
72	DAG 14:0-20:4	606.5	50	361.3	20	3.25	ES+	2
73	DAG 14:0-20:5	604.5	50	285.3	20	3.25	ES+	1
74	DAG 14:0-20:5	604.5	50	359.3	20	3.25	ES+	2
75	DAG 14:0-22:0	642.6	50	285.3	20	3.25	ES+	1
76	DAG 14:0-22:0	642.6	50	397.4	20	3.25	ES+	2
77	DAG 14:0-22:1	640.6	50	285.3	20	3.25	ES+	1
78	DAG 14:0-22:1	640.6	50	395.4	20	3.25	ES+	2
79	DAG 14:0-22:2	638.6	50	285.3	20	3.25	ES+	1
80	DAG 14:0-22:2	638.6	50	393.4	20	3.25	ES+	2
81	DAG 14:0-22:3	636.6	50	285.3	20	3.25	ES+	1
82	DAG 14:0-22:3	636.6	50	391.3	20	3.25	ES+	2
83	DAG 14:0-22:4	634.5	50	285.3	20	3.25	ES+	1
84	DAG 14:0-22:4	634.5	50	389.3	20	3.25	ES+	2
85	DAG 14:0-22:5	632.5	50	285.3	20	3.25	ES+	1
86	DAG 14:0-22:5	632.5	50	387.3	20	3.25	ES+	2
87	DAG 14:0-22:6	630.5	50	285.3	20	3.25	ES+	1
88	DAG 14:0-22:6	630.5	50	385.3	20	3.25	ES+	2
89	DAG 14:1-14:1	526.4	50	283.3	20	3.25	ES+	1
90	DAG 14:1-16:0	556.5	50	283.3	20	3.25	ES+	1
91	DAG 14:1-16:0	556.5	50	313.3	20	3.25	ES+	2
92	DAG 14:1-16:1	554.5	50	283.3	20	3.25	ES+	1
93	DAG 14:1-16:1	554.5	50	311.3	20	3.25	ES+	2
94	DAG 14:1-18:0	584.5	50	283.3	20	3.25	ES+	1
95	DAG 14:1-18:0	584.5	50	341.3	20	3.25	ES+	2
96	DAG 14:1-18:1	582.5	50	283.3	20	3.25	ES+	1
97	DAG 14:1-18:1	582.5	50	339.3	20	3.25	ES+	2
98	DAG 14:1-18:2	580.5	50	283.3	20	3.25	ES+	1
99	DAG 14:1-18:2	580.5	50	337.3	20	3.25	ES+	2
100	DAG 14:1-18:3	578.5	50	283.3	20	3.25	ES+	1
101	DAG 14:1-18:3	578.5	50	335.3	20	3.25	ES+	2
102	DAG 14:1-18:4	576.5	50	283.3	20	3.25	ES+	1

103	DAG 14:1-18:4	576.5	50	333.3	20	3.25	ES+	2
104	DAG 14:1-20:0	612.6	50	283.3	20	3.25	ES+	1
105	DAG 14:1-20:0	612.6	50	369.4	20	3.25	ES+	2
106	DAG 14:1-20:1	610.5	50	283.3	20	3.25	ES+	1
107	DAG 14:1-20:1	610.5	50	367.3	20	3.25	ES+	2
108	DAG 14:1-20:2	608.5	50	283.3	20	3.25	ES+	1
109	DAG 14:1-20:2	608.5	50	365.3	20	3.25	ES+	2
110	DAG 14:1-20:3	606.5	50	283.3	20	3.25	ES+	1
111	DAG 14:1-20:3	606.5	50	363.3	20	3.25	ES+	2
112	DAG 14:1-20:4	604.5	50	283.3	20	3.25	ES+	1
113	DAG 14:1-20:4	604.5	50	361.3	20	3.25	ES+	2
114	DAG 14:1-20:5	602.5	50	283.3	20	3.25	ES+	1
115	DAG 14:1-20:5	602.5	50	359.3	20	3.25	ES+	2
116	DAG 14:1-22:0	640.6	50	283.3	20	3.25	ES+	1
117	DAG 14:1-22:0	640.6	50	397.4	20	3.25	ES+	2
118	DAG 14:1-22:1	638.6	50	283.3	20	3.25	ES+	1
119	DAG 14:1-22:1	638.6	50	395.4	20	3.25	ES+	2
120	DAG 14:1-22:2	636.6	50	283.3	20	3.25	ES+	1
121	DAG 14:1-22:2	636.6	50	393.4	20	3.25	ES+	2
122	DAG 14:1-22:3	634.5	50	283.3	20	3.25	ES+	1
123	DAG 14:1-22:3	634.5	50	391.3	20	3.25	ES+	2
124	DAG 14:1-22:4	632.5	50	283.3	20	3.25	ES+	1
125	DAG 14:1-22:4	632.5	50	389.3	20	3.25	ES+	2
126	DAG 14:1-22:5	630.5	50	283.3	20	3.25	ES+	1
127	DAG 14:1-22:5	630.5	50	387.3	20	3.25	ES+	2
128	DAG 14:1-22:6	628.5	50	283.3	20	3.25	ES+	1
129	DAG 14:1-22:6	628.5	50	385.3	20	3.25	ES+	2
130	DAG 16:0-16:0	586.5	50	313.3	20	3.25	ES+	1
131	DAG 16:0-16:1	584.5	50	311.3	20	3.25	ES+	1
132	DAG 16:0-16:1	584.5	50	313.3	20	3.25	ES+	2
133	DAG 16:0-18:0	614.6	50	313.3	20	3.25	ES+	1
134	DAG 16:0-18:0	614.6	50	341.3	20	3.25	ES+	2
135	DAG 16:0-18:1	612.6	50	313.3	20	3.25	ES+	1
136	DAG 16:0-18:1	612.6	50	339.3	20	3.25	ES+	2
137	DAG 16:0-18:2	610.5	50	313.3	20	3.25	ES+	1

138	DAG 16:0-18:2	610.5	50	337.3	20	3.25	ES+	2
139	DAG 16:0-18:3	608.5	50	313.3	20	3.25	ES+	1
140	DAG 16:0-18:3	608.5	50	335.3	20	3.25	ES+	2
141	DAG 16:0-18:4	606.5	50	313.3	20	3.25	ES+	1
142	DAG 16:0-18:4	606.5	50	333.3	20	3.25	ES+	2
143	PA 12:0-12:0	535.3	20	199.3	40	12.43	ES-	1
144	PA 12:0-14:0	563.4	20	199.3	40	12.43	ES-	1
145	PA 12:0-14:0	563.4	20	227.3	40	12.43	ES-	2
146	PA 12:0-14:1	561.4	20	199.3	40	12.43	ES-	1
147	PA 12:0-14:1	561.4	20	225.3	40	12.43	ES-	2
148	PA 12:0-16:0	591.4	20	199.3	40	12.43	ES-	1
149	PA 12:0-16:0	591.4	20	255.3	40	12.43	ES-	2
150	PA 12:0-16:1	589.4	20	199.3	40	12.43	ES-	1
151	PA 12:0-16:1	589.4	20	253.3	40	12.43	ES-	2
152	PA 12:0-18:0	619.4	20	199.3	40	12.43	ES-	1
153	PA 12:0-18:0	619.4	20	283.3	40	12.43	ES-	2
154	PA 12:0-18:1	617.4	20	199.3	40	12.43	ES-	1
155	PA 12:0-18:1	617.4	20	281.3	40	12.43	ES-	2
156	PA 12:0-18:2	615.4	20	199.3	40	12.43	ES-	1
157	PA 12:0-18:2	615.4	20	279.3	40	12.43	ES-	2
158	PA 12:0-18:3	613.4	20	199.3	40	12.43	ES-	1
159	PA 12:0-18:3	613.4	20	277.3	40	12.43	ES-	2
160	PA 12:0-18:4	611.4	20	199.3	40	12.43	ES-	1
161	PA 12:0-18:4	611.4	20	275.3	40	12.43	ES-	2
162	PA 12:0-20:0	647.5	20	199.3	40	12.43	ES-	1
163	PA 12:0-20:0	647.5	20	311.2	40	12.43	ES-	2
164	PA 12:0-20:1	645.5	20	199.3	40	12.43	ES-	1
165	PA 12:0-20:1	645.5	20	309.2	40	12.43	ES-	2
166	PA 12:0-20:2	643.4	20	199.3	40	12.43	ES-	1
167	PA 12:0-20:2	643.4	20	307.2	40	12.43	ES-	2
168	PA 12:0-20:3	641.4	20	199.3	40	12.43	ES-	1
169	PA 12:0-20:3	641.4	20	305.2	40	12.43	ES-	2
170	PA 12:0-20:4	639.4	20	199.3	40	12.43	ES-	1
171	PA 12:0-20:4	639.4	20	303.2	40	12.43	ES-	2
172	PA 12:0-20:5	637.4	20	199.3	40	12.43	ES-	1

173	PA 12:0-20:5	637.4	20	301.2	40	12.43	ES-	2
174	PA 12:0-22:0	675.5	20	199.3	40	12.43	ES-	1
175	PA 12:0-22:0	675.5	20	339.2	40	12.43	ES-	2
176	PA 12:0-22:1	673.5	20	199.3	40	12.43	ES-	1
177	PA 12:0-22:1	673.5	20	337.2	40	12.43	ES-	2
178	PA 12:0-22:2	671.5	20	199.3	40	12.43	ES-	1
179	PA 12:0-22:2	671.5	20	335.2	40	12.43	ES-	2
180	PA 12:0-22:3	669.5	20	199.3	40	12.43	ES-	1
181	PA 12:0-22:3	669.5	20	333.2	40	12.43	ES-	2
182	PA 12:0-22:4	667.4	20	199.3	40	12.43	ES-	1
183	PA 12:0-22:4	667.4	20	331.2	40	12.43	ES-	2
184	PA 12:0-22:5	665.4	20	199.3	40	12.43	ES-	1
185	PA 12:0-22:5	665.4	20	329.2	40	12.43	ES-	2
186	PA 12:0-22:6	663.4	20	199.3	40	12.43	ES-	1
187	PA 12:0-22:6	663.4	20	327.2	40	12.43	ES-	2
188	PA 14:0-14:0	591.4	20	227.3	40	12.43	ES-	1
189	PA 14:0-14:1	589.4	20	225.3	40	12.43	ES-	1
190	PA 14:0-14:1	589.4	20	227.3	40	12.43	ES-	2
191	PA 14:0-16:0	619.4	20	227.3	40	12.43	ES-	1
192	PA 14:0-16:0	619.4	20	255.3	40	12.43	ES-	2
193	PA 14:0-16:1	617.4	20	227.3	40	12.43	ES-	1
194	PA 14:0-16:1	617.4	20	253.3	40	12.43	ES-	2
195	PA 14:0-18:0	647.5	20	227.3	40	12.43	ES-	1
196	PA 14:0-18:0	647.5	20	283.3	40	12.43	ES-	2
197	PA 14:0-18:1	645.5	20	227.3	40	12.43	ES-	1
198	PA 14:0-18:1	645.5	20	281.3	40	12.43	ES-	2
199	PA 14:0-18:2	643.4	20	227.3	40	12.43	ES-	1
200	PA 14:0-18:2	643.4	20	279.3	40	12.43	ES-	2
201	PA 14:0-18:3	641.4	20	227.3	40	12.43	ES-	1
202	PA 14:0-18:3	641.4	20	277.3	40	12.43	ES-	2
203	PA 14:0-18:4	639.4	20	227.3	40	12.43	ES-	1
204	PA 14:0-18:4	639.4	20	275.3	40	12.43	ES-	2
205	PA 14:0-20:0	675.5	20	227.3	40	12.43	ES-	1
206	PA 14:0-20:0	675.5	20	311.2	40	12.43	ES-	2
207	PA 14:0-20:1	673.5	20	227.3	40	12.43	ES-	1

208	PA 14:0-20:1	673.5	20	309.2	40	12.43	ES-	2
209	PA 14:0-20:2	671.5	20	227.3	40	12.43	ES-	1
210	PA 14:0-20:2	671.5	20	307.2	40	12.43	ES-	2
211	PA 14:0-20:3	669.5	20	227.3	40	12.43	ES-	1
212	PA 14:0-20:3	669.5	20	305.2	40	12.43	ES-	2
213	PA 14:0-20:4	667.4	20	227.3	40	12.43	ES-	1
214	PA 14:0-20:4	667.4	20	303.2	40	12.43	ES-	2
215	PA 14:0-20:5	665.4	20	227.3	40	12.43	ES-	1
216	PA 14:0-20:5	665.4	20	301.2	40	12.43	ES-	2
217	PA 14:0-22:0	703.5	20	227.3	40	12.43	ES-	1
218	PA 14:0-22:0	703.5	20	339.2	40	12.43	ES-	2
219	PA 14:0-22:1	701.5	20	227.3	40	12.43	ES-	1
220	PA 14:0-22:1	701.5	20	337.2	40	12.43	ES-	2
221	PA 14:0-22:2	699.5	20	227.3	40	12.43	ES-	1
222	PA 14:0-22:2	699.5	20	335.2	40	12.43	ES-	2
223	PA 14:0-22:3	697.5	20	227.3	40	12.43	ES-	1
224	PA 14:0-22:3	697.5	20	333.2	40	12.43	ES-	2
225	PA 14:0-22:4	695.5	20	227.3	40	12.43	ES-	1
226	PA 14:0-22:4	695.5	20	331.2	40	12.43	ES-	2
227	PA 14:0-22:5	693.5	20	227.3	40	12.43	ES-	1
228	PA 14:0-22:5	693.5	20	329.2	40	12.43	ES-	2
229	PA 14:0-22:6	691.4	20	227.3	40	12.43	ES-	1
230	PA 14:0-22:6	691.4	20	327.2	40	12.43	ES-	2
231	PA 14:1-14:1	587.4	20	225.3	40	12.43	ES-	1
232	PA 14:1-16:0	617.4	20	225.3	40	12.43	ES-	1
233	PA 14:1-16:0	617.4	20	255.3	40	12.43	ES-	2
234	PA 14:1-16:1	615.4	20	225.3	40	12.43	ES-	1
235	PA 14:1-16:1	615.4	20	253.3	40	12.43	ES-	2
236	PA 14:1-18:0	645.5	20	225.3	40	12.43	ES-	1
237	PA 14:1-18:0	645.5	20	283.3	40	12.43	ES-	2
238	PA 14:1-18:1	643.4	20	225.3	40	12.43	ES-	1
239	PA 14:1-18:1	643.4	20	281.3	40	12.43	ES-	2
240	PA 14:1-18:2	641.4	20	225.3	40	12.43	ES-	1
241	PA 14:1-18:2	641.4	20	279.3	40	12.43	ES-	2
242	PA 14:1-18:3	639.4	20	225.3	40	12.43	ES-	1

243	PA 14:1-18:3	639.4	20	277.3	40	12.43	ES-	2
244	PA 14:1-18:4	637.4	20	225.3	40	12.43	ES-	1
245	PA 14:1-18:4	637.4	20	275.3	40	12.43	ES-	2
246	PA 14:1-20:0	673.5	20	225.3	40	12.43	ES-	1
247	PA 14:1-20:0	673.5	20	311.2	40	12.43	ES-	2
248	PA 14:1-20:1	671.5	20	225.3	40	12.43	ES-	1
249	PA 14:1-20:1	671.5	20	309.2	40	12.43	ES-	2
250	PA 14:1-20:2	669.5	20	225.3	40	12.43	ES-	1
251	PA 14:1-20:2	669.5	20	307.2	40	12.43	ES-	2
252	PA 14:1-20:3	667.4	20	225.3	40	12.43	ES-	1
253	PA 14:1-20:3	667.4	20	305.2	40	12.43	ES-	2
254	PA 14:1-20:4	665.4	20	225.3	40	12.43	ES-	1
255	PA 14:1-20:4	665.4	20	303.2	40	12.43	ES-	2
256	PA 14:1-20:5	663.4	20	225.3	40	12.43	ES-	1
257	PA 14:1-20:5	663.4	20	301.2	40	12.43	ES-	2
258	PA 14:1-22:0	701.5	20	225.3	40	12.43	ES-	1
259	PA 14:1-22:0	701.5	20	339.2	40	12.43	ES-	2
260	PA 14:1-22:1	699.5	20	225.3	40	12.43	ES-	1
261	PA 14:1-22:1	699.5	20	337.2	40	12.43	ES-	2
262	PA 14:1-22:2	697.5	20	225.3	40	12.43	ES-	1
263	PA 14:1-22:2	697.5	20	335.2	40	12.43	ES-	2
264	PA 14:1-22:3	695.5	20	225.3	40	12.43	ES-	1
265	PA 14:1-22:3	695.5	20	333.2	40	12.43	ES-	2
266	PA 14:1-22:4	693.5	20	225.3	40	12.43	ES-	1
267	PA 14:1-22:4	693.5	20	331.2	40	12.43	ES-	2
268	PA 14:1-22:5	691.4	20	225.3	40	12.43	ES-	1
269	PA 14:1-22:5	691.4	20	329.2	40	12.43	ES-	2
270	PA 14:1-22:6	689.4	20	225.3	40	12.43	ES-	1
271	PA 14:1-22:6	689.4	20	327.2	40	12.43	ES-	2
272	PA 16:0-16:0	647.5	20	255.3	40	12.43	ES-	1
273	PA 16:0-16:1	645.5	20	253.3	40	12.43	ES-	1
274	PA 16:0-16:1	645.5	20	255.3	40	12.43	ES-	2
275	PA 16:0-18:0	675.5	20	255.3	40	12.43	ES-	1
276	PA 16:0-18:0	675.5	20	283.3	40	12.43	ES-	2
277	PA 16:0-18:1	673.5	20	255.3	40	12.43	ES-	1

278	PA 16:0-18:1	673.5	20	281.3	40	12.43	ES-	2
279	PA 16:0-18:2	671.5	20	255.3	40	12.43	ES-	1
280	PA 16:0-18:2	671.5	20	279.3	40	12.43	ES-	2
281	PA 16:0-18:3	669.5	20	255.3	40	12.43	ES-	1
282	PA 16:0-18:3	669.5	20	277.3	40	12.43	ES-	2
283	PA 16:0-18:4	667.4	20	255.3	40	12.43	ES-	1
284	PA 16:0-18:4	667.4	20	275.3	40	12.43	ES-	2

Method 2: DAG and PA (2)

No	Name	Precursor	CV (V)	Product	CE (V)	RT setting (min)	IonMode	Ion
1	DAG 16:0-20:0	642.6	50	313.3	20	3.25	ES+	1
2	DAG 16:0-20:0	642.6	50	369.4	20	3.25	ES+	2
3	DAG 16:0-20:1	640.6	50	313.3	20	3.25	ES+	1
4	DAG 16:0-20:1	640.6	50	367.3	20	3.25	ES+	2
5	DAG 16:0-20:2	638.6	50	313.3	20	3.25	ES+	1
6	DAG 16:0-20:2	638.6	50	365.3	20	3.25	ES+	2
7	DAG 16:0-20:3	636.6	50	313.3	20	3.25	ES+	1
8	DAG 16:0-20:3	636.6	50	363.3	20	3.25	ES+	2
9	DAG 16:0-20:4	634.5	50	313.3	20	3.25	ES+	1
10	DAG 16:0-20:4	634.5	50	361.3	20	3.25	ES+	2
11	DAG 16:0-20:5	632.5	50	313.3	20	3.25	ES+	1
12	DAG 16:0-20:5	632.5	50	359.3	20	3.25	ES+	2
13	DAG 16:0-22:0	670.6	50	313.3	20	3.25	ES+	1
14	DAG 16:0-22:0	670.6	50	397.4	20	3.25	ES+	2
15	DAG 16:0-22:1	668.6	50	313.3	20	3.25	ES+	1
16	DAG 16:0-22:1	668.6	50	395.4	20	3.25	ES+	2
17	DAG 16:0-22:2	666.6	50	313.3	20	3.25	ES+	1
18	DAG 16:0-22:2	666.6	50	393.4	20	3.25	ES+	2
19	DAG 16:0-22:3	664.6	50	313.3	20	3.25	ES+	1
20	DAG 16:0-22:3	664.6	50	391.3	20	3.25	ES+	2
21	DAG 16:0-22:4	662.6	50	313.3	20	3.25	ES+	1
22	DAG 16:0-22:4	662.6	50	389.3	20	3.25	ES+	2
23	DAG 16:0-22:5	660.6	50	313.3	20	3.25	ES+	1
24	DAG 16:0-22:5	660.6	50	387.3	20	3.25	ES+	2
25	DAG 16:0-22:6	658.5	50	313.3	20	3.25	ES+	1
26	DAG 16:0-22:6	658.5	50	385.3	20	3.25	ES+	2

27	DAG 16:1-16:1	582.5	50	311.3	20	3.25	ES+	1
28	DAG 16:1-18:0	612.6	50	311.3	20	3.25	ES+	1
29	DAG 16:1-18:0	612.6	50	341.3	20	3.25	ES+	2
30	DAG 16:1-18:1	610.5	50	311.3	20	3.25	ES+	1
31	DAG 16:1-18:1	610.5	50	339.3	20	3.25	ES+	2
32	DAG 16:1-18:2	608.5	50	311.3	20	3.25	ES+	1
33	DAG 16:1-18:2	608.5	50	337.3	20	3.25	ES+	2
34	DAG 16:1-18:3	606.5	50	311.3	20	3.25	ES+	1
35	DAG 16:1-18:3	606.5	50	335.3	20	3.25	ES+	2
36	DAG 16:1-18:4	604.5	50	311.3	20	3.25	ES+	1
37	DAG 16:1-18:4	604.5	50	333.3	20	3.25	ES+	2
38	DAG 16:1-20:0	640.6	50	311.3	20	3.25	ES+	1
39	DAG 16:1-20:0	640.6	50	369.4	20	3.25	ES+	2
40	DAG 16:1-20:1	638.6	50	311.3	20	3.25	ES+	1
41	DAG 16:1-20:1	638.6	50	367.3	20	3.25	ES+	2
42	DAG 16:1-20:2	636.6	50	311.3	20	3.25	ES+	1
43	DAG 16:1-20:2	636.6	50	365.3	20	3.25	ES+	2
44	DAG 16:1-20:3	634.5	50	311.3	20	3.25	ES+	1
45	DAG 16:1-20:3	634.5	50	363.3	20	3.25	ES+	2
46	DAG 16:1-20:4	632.5	50	311.3	20	3.25	ES+	1
47	DAG 16:1-20:4	632.5	50	361.3	20	3.25	ES+	2
48	DAG 16:1-20:5	630.5	50	311.3	20	3.25	ES+	1
49	DAG 16:1-20:5	630.5	50	359.3	20	3.25	ES+	2
50	DAG 16:1-22:0	668.6	50	311.3	20	3.25	ES+	1
51	DAG 16:1-22:0	668.6	50	397.4	20	3.25	ES+	2
52	DAG 16:1-22:1	666.6	50	311.3	20	3.25	ES+	1
53	DAG 16:1-22:1	666.6	50	395.4	20	3.25	ES+	2
54	DAG 16:1-22:2	664.6	50	311.3	20	3.25	ES+	1
55	DAG 16:1-22:2	664.6	50	393.4	20	3.25	ES+	2
56	DAG 16:1-22:3	662.6	50	311.3	20	3.25	ES+	1
57	DAG 16:1-22:3	662.6	50	391.3	20	3.25	ES+	2
58	DAG 16:1-22:4	660.6	50	311.3	20	3.25	ES+	1
59	DAG 16:1-22:4	660.6	50	389.3	20	3.25	ES+	2
60	DAG 16:1-22:5	658.5	50	311.3	20	3.25	ES+	1
61	DAG 16:1-22:5	658.5	50	387.3	20	3.25	ES+	2

62	DAG 16:1-22:6	656.5	50	311.3	20	3.25	ES+	1
63	DAG 16:1-22:6	656.5	50	385.3	20	3.25	ES+	2
64	DAG 18:0-18:0	642.6	50	341.3	20	3.25	ES+	1
65	DAG 18:0-18:1	640.6	50	339.3	20	3.25	ES+	1
66	DAG 18:0-18:1	640.6	50	341.3	20	3.25	ES+	2
67	DAG 18:0-18:2	638.6	50	337.3	20	3.25	ES+	1
68	DAG 18:0-18:2	638.6	50	341.3	20	3.25	ES+	2
69	DAG 18:0-18:3	636.6	50	335.3	20	3.25	ES+	1
70	DAG 18:0-18:3	636.6	50	341.3	20	3.25	ES+	2
71	DAG 18:0-18:4	634.5	50	333.3	20	3.25	ES+	1
72	DAG 18:0-18:4	634.5	50	341.3	20	3.25	ES+	2
73	DAG 18:0-20:0	670.6	50	341.3	20	3.25	ES+	1
74	DAG 18:0-20:0	670.6	50	369.4	20	3.25	ES+	2
75	DAG 18:0-20:1	668.6	50	341.3	20	3.25	ES+	1
76	DAG 18:0-20:1	668.6	50	367.3	20	3.25	ES+	2
77	DAG 18:0-20:2	666.6	50	341.3	20	3.25	ES+	1
78	DAG 18:0-20:2	666.6	50	365.3	20	3.25	ES+	2
79	DAG 18:0-20:3	664.6	50	341.3	20	3.25	ES+	1
80	DAG 18:0-20:3	664.6	50	363.3	20	3.25	ES+	2
81	DAG 18:0-20:4	662.6	50	341.3	20	3.25	ES+	1
82	DAG 18:0-20:4	662.6	50	361.3	20	3.25	ES+	2
83	DAG 18:0-20:5	660.6	50	341.3	20	3.25	ES+	1
84	DAG 18:0-20:5	660.6	50	359.3	20	3.25	ES+	2
85	DAG 18:0-22:0	698.7	50	341.3	20	3.25	ES+	1
86	DAG 18:0-22:0	698.7	50	397.4	20	3.25	ES+	2
87	DAG 18:0-22:1	696.7	50	341.3	20	3.25	ES+	1
88	DAG 18:0-22:1	696.7	50	395.4	20	3.25	ES+	2
89	DAG 18:0-22:2	694.6	50	341.3	20	3.25	ES+	1
90	DAG 18:0-22:2	694.6	50	393.4	20	3.25	ES+	2
91	DAG 18:0-22:3	692.6	50	341.3	20	3.25	ES+	1
92	DAG 18:0-22:3	692.6	50	391.3	20	3.25	ES+	2
93	DAG 18:0-22:4	690.6	50	341.3	20	3.25	ES+	1
94	DAG 18:0-22:4	690.6	50	389.3	20	3.25	ES+	2
95	DAG 18:0-22:5	688.6	50	341.3	20	3.25	ES+	1
96	DAG 18:0-22:5	688.6	50	387.3	20	3.25	ES+	2

97	DAG 18:0-22:6	686.6	50	341.3	20	3.25	ES+	1
98	DAG 18:0-22:6	686.6	50	385.3	20	3.25	ES+	2
99	DAG 18:1-18:1	638.6	50	339.3	20	3.25	ES+	1
100	DAG 18:1-18:2	636.6	50	337.3	20	3.25	ES+	1
101	DAG 18:1-18:2	636.6	50	339.3	20	3.25	ES+	2
102	DAG 18:1-18:3	634.5	50	335.3	20	3.25	ES+	1
103	DAG 18:1-18:3	634.5	50	339.3	20	3.25	ES+	2
104	DAG 18:1-18:4	632.5	50	333.3	20	3.25	ES+	1
105	DAG 18:1-18:4	632.5	50	339.3	20	3.25	ES+	2
106	DAG 18:1-20:0	668.6	50	339.3	20	3.25	ES+	1
107	DAG 18:1-20:0	668.6	50	369.4	20	3.25	ES+	2
108	DAG 18:1-20:1	666.6	50	339.3	20	3.25	ES+	1
109	DAG 18:1-20:1	666.6	50	367.3	20	3.25	ES+	2
110	DAG 18:1-20:2	664.6	50	339.3	20	3.25	ES+	1
111	DAG 18:1-20:2	664.6	50	365.3	20	3.25	ES+	2
112	DAG 18:1-20:3	662.6	50	339.3	20	3.25	ES+	1
113	DAG 18:1-20:3	662.6	50	363.3	20	3.25	ES+	2
114	DAG 18:1-20:4	660.6	50	339.3	20	3.25	ES+	1
115	DAG 18:1-20:4	660.6	50	361.3	20	3.25	ES+	2
116	DAG 18:1-20:5	658.5	50	339.3	20	3.25	ES+	1
117	DAG 18:1-20:5	658.5	50	359.3	20	3.25	ES+	2
118	DAG 18:1-22:0	696.7	50	339.3	20	3.25	ES+	1
119	DAG 18:1-22:0	696.7	50	397.4	20	3.25	ES+	2
120	DAG 18:1-22:1	694.6	50	339.3	20	3.25	ES+	1
121	DAG 18:1-22:1	694.6	50	395.4	20	3.25	ES+	2
122	DAG 18:1-22:2	692.6	50	339.3	20	3.25	ES+	1
123	DAG 18:1-22:2	692.6	50	393.4	20	3.25	ES+	2
124	DAG 18:1-22:3	690.6	50	339.3	20	3.25	ES+	1
125	DAG 18:1-22:3	690.6	50	391.3	20	3.25	ES+	2
126	DAG 18:1-22:4	688.6	50	339.3	20	3.25	ES+	1
127	DAG 18:1-22:4	688.6	50	389.3	20	3.25	ES+	2
128	DAG 18:1-22:5	686.6	50	339.3	20	3.25	ES+	1
129	DAG 18:1-22:5	686.6	50	387.3	20	3.25	ES+	2
130	DAG 18:1-22:6	684.6	50	339.3	20	3.25	ES+	1
131	DAG 18:1-22:6	684.6	50	385.3	20	3.25	ES+	2

132	DAG 18:2-18:2	634.5	50	337.3	20	3.25	ES+	1
133	DAG 18:2-18:3	632.5	50	335.3	20	3.25	ES+	1
134	DAG 18:2-18:3	632.5	50	337.3	20	3.25	ES+	2
135	DAG 18:2-18:4	630.5	50	333.3	20	3.25	ES+	1
136	DAG 18:2-18:4	630.5	50	337.3	20	3.25	ES+	2
137	DAG 18:2-20:0	666.6	50	337.3	20	3.25	ES+	1
138	DAG 18:2-20:0	666.6	50	369.4	20	3.25	ES+	2
139	DAG 18:2-20:1	664.6	50	337.3	20	3.25	ES+	1
140	DAG 18:2-20:1	664.6	50	367.3	20	3.25	ES+	2
141	DAG 18:2-20:2	662.6	50	337.3	20	3.25	ES+	1
142	DAG 18:2-20:2	662.6	50	365.3	20	3.25	ES+	2
143	DAG 18:2-20:3	660.6	50	337.3	20	3.25	ES+	1
144	DAG 18:2-20:3	660.6	50	363.3	20	3.25	ES+	2
145	DAG 18:2-20:4	658.5	50	337.3	20	3.25	ES+	1
146	DAG 18:2-20:4	658.5	50	361.3	20	3.25	ES+	2
147	DAG 18:2-20:5	656.5	50	337.3	20	3.25	ES+	1
148	DAG 18:2-20:5	656.5	50	359.3	20	3.25	ES+	2
149	PA 16:0-20:0	703.5	20	255.3	40	12.43	ES-	1
150	PA 16:0-20:0	703.5	20	311.2	40	12.43	ES-	2
151	PA 16:0-20:1	701.5	20	255.3	40	12.43	ES-	1
152	PA 16:0-20:1	701.5	20	309.2	40	12.43	ES-	2
153	PA 16:0-20:2	699.5	20	255.3	40	12.43	ES-	1
154	PA 16:0-20:2	699.5	20	307.2	40	12.43	ES-	2
155	PA 16:0-20:3	697.5	20	255.3	40	12.43	ES-	1
156	PA 16:0-20:3	697.5	20	305.2	40	12.43	ES-	2
157	PA 16:0-20:4	695.5	20	255.3	40	12.43	ES-	1
158	PA 16:0-20:4	695.5	20	303.2	40	12.43	ES-	2
159	PA 16:0-20:5	693.5	20	255.3	40	12.43	ES-	1
160	PA 16:0-20:5	693.5	20	301.2	40	12.43	ES-	2
161	PA 16:0-22:0	731.6	20	255.3	40	12.43	ES-	1
162	PA 16:0-22:0	731.6	20	339.2	40	12.43	ES-	2
163	PA 16:0-22:1	729.5	20	255.3	40	12.43	ES-	1
164	PA 16:0-22:1	729.5	20	337.2	40	12.43	ES-	2
165	PA 16:0-22:2	727.5	20	255.3	40	12.43	ES-	1
166	PA 16:0-22:2	727.5	20	335.2	40	12.43	ES-	2

167	PA 16:0-22:3	725.5	20	255.3	40	12.43	ES-	1
168	PA 16:0-22:3	725.5	20	333.2	40	12.43	ES-	2
169	PA 16:0-22:4	723.5	20	255.3	40	12.43	ES-	1
170	PA 16:0-22:4	723.5	20	331.2	40	12.43	ES-	2
171	PA 16:0-22:5	721.5	20	255.3	40	12.43	ES-	1
172	PA 16:0-22:5	721.5	20	329.2	40	12.43	ES-	2
173	PA 16:0-22:6	719.5	20	255.3	40	12.43	ES-	1
174	PA 16:0-22:6	719.5	20	327.2	40	12.43	ES-	2
175	PA 16:1-16:1	643.4	20	253.3	40	12.43	ES-	1
176	PA 16:1-18:0	673.5	20	253.3	40	12.43	ES-	1
177	PA 16:1-18:0	673.5	20	283.3	40	12.43	ES-	2
178	PA 16:1-18:1	671.5	20	253.3	40	12.43	ES-	1
179	PA 16:1-18:1	671.5	20	281.3	40	12.43	ES-	2
180	PA 16:1-18:2	669.5	20	253.3	40	12.43	ES-	1
181	PA 16:1-18:2	669.5	20	279.3	40	12.43	ES-	2
182	PA 16:1-18:3	667.4	20	253.3	40	12.43	ES-	1
183	PA 16:1-18:3	667.4	20	277.3	40	12.43	ES-	2
184	PA 16:1-18:4	665.4	20	253.3	40	12.43	ES-	1
185	PA 16:1-18:4	665.4	20	275.3	40	12.43	ES-	2
186	PA 16:1-20:0	701.5	20	253.3	40	12.43	ES-	1
187	PA 16:1-20:0	701.5	20	311.2	40	12.43	ES-	2
188	PA 16:1-20:1	699.5	20	253.3	40	12.43	ES-	1
189	PA 16:1-20:1	699.5	20	309.2	40	12.43	ES-	2
190	PA 16:1-20:2	697.5	20	253.3	40	12.43	ES-	1
191	PA 16:1-20:2	697.5	20	307.2	40	12.43	ES-	2
192	PA 16:1-20:3	695.5	20	253.3	40	12.43	ES-	1
193	PA 16:1-20:3	695.5	20	305.2	40	12.43	ES-	2
194	PA 16:1-20:4	693.5	20	253.3	40	12.43	ES-	1
195	PA 16:1-20:4	693.5	20	303.2	40	12.43	ES-	2
196	PA 16:1-20:5	691.4	20	253.3	40	12.43	ES-	1
197	PA 16:1-20:5	691.4	20	301.2	40	12.43	ES-	2
198	PA 16:1-22:0	729.5	20	253.3	40	12.43	ES-	1
199	PA 16:1-22:0	729.5	20	339.2	40	12.43	ES-	2
200	PA 16:1-22:1	727.5	20	253.3	40	12.43	ES-	1
201	PA 16:1-22:1	727.5	20	337.2	40	12.43	ES-	2

202	PA 16:1-22:2	725.5	20	253.3	40	12.43	ES-	1
203	PA 16:1-22:2	725.5	20	335.2	40	12.43	ES-	2
204	PA 16:1-22:3	723.5	20	253.3	40	12.43	ES-	1
205	PA 16:1-22:3	723.5	20	333.2	40	12.43	ES-	2
206	PA 16:1-22:4	721.5	20	253.3	40	12.43	ES-	1
207	PA 16:1-22:4	721.5	20	331.2	40	12.43	ES-	2
208	PA 16:1-22:5	719.5	20	253.3	40	12.43	ES-	1
209	PA 16:1-22:5	719.5	20	329.2	40	12.43	ES-	2
210	PA 16:1-22:6	717.5	20	253.3	40	12.43	ES-	1
211	PA 16:1-22:6	717.5	20	327.2	40	12.43	ES-	2
212	PA 17:0-17:0	675.5	20	269.3	40	12.43	ES-	1
213	PA 18:0-18:0	703.5	20	283.3	40	12.43	ES-	1
214	PA 18:0-18:1	701.5	20	281.3	40	12.43	ES-	1
215	PA 18:0-18:1	701.5	20	283.3	40	12.43	ES-	2
216	PA 18:0-18:2	699.5	20	279.3	40	12.43	ES-	1
217	PA 18:0-18:2	699.5	20	283.3	40	12.43	ES-	2
218	PA 18:0-18:3	697.5	20	277.3	40	12.43	ES-	1
219	PA 18:0-18:3	697.5	20	283.3	40	12.43	ES-	2
220	PA 18:0-18:4	695.5	20	275.3	40	12.43	ES-	1
221	PA 18:0-18:4	695.5	20	283.3	40	12.43	ES-	2
222	PA 18:0-20:0	731.6	20	283.3	40	12.43	ES-	1
223	PA 18:0-20:0	731.6	20	311.2	40	12.43	ES-	2
224	PA 18:0-20:1	729.5	20	283.3	40	12.43	ES-	1
225	PA 18:0-20:1	729.5	20	309.2	40	12.43	ES-	2
226	PA 18:0-20:2	727.5	20	283.3	40	12.43	ES-	1
227	PA 18:0-20:2	727.5	20	307.2	40	12.43	ES-	2
228	PA 18:0-20:3	725.5	20	283.3	40	12.43	ES-	1
229	PA 18:0-20:3	725.5	20	305.2	40	12.43	ES-	2
230	PA 18:0-20:4	723.5	20	283.3	40	12.43	ES-	1
231	PA 18:0-20:4	723.5	20	303.2	40	12.43	ES-	2
232	PA 18:0-20:5	721.5	20	283.3	40	12.43	ES-	1
233	PA 18:0-20:5	721.5	20	301.2	40	12.43	ES-	2
234	PA 18:0-22:0	759.6	20	283.3	40	12.43	ES-	1
235	PA 18:0-22:0	759.6	20	339.2	40	12.43	ES-	2
236	PA 18:0-22:1	757.6	20	283.3	40	12.43	ES-	1

237	PA 18:0-22:1	757.6	20	337.2	40	12.43	ES-	2
238	PA 18:0-22:2	755.6	20	283.3	40	12.43	ES-	1
239	PA 18:0-22:2	755.6	20	335.2	40	12.43	ES-	2
240	PA 18:0-22:3	753.5	20	283.3	40	12.43	ES-	1
241	PA 18:0-22:3	753.5	20	333.2	40	12.43	ES-	2
242	PA 18:0-22:4	751.5	20	283.3	40	12.43	ES-	1
243	PA 18:0-22:4	751.5	20	331.2	40	12.43	ES-	2
244	PA 18:0-22:5	749.5	20	283.3	40	12.43	ES-	1
245	PA 18:0-22:5	749.5	20	329.2	40	12.43	ES-	2
246	PA 18:0-22:6	747.5	20	283.3	40	12.43	ES-	1
247	PA 18:0-22:6	747.5	20	327.2	40	12.43	ES-	2
248	PA 18:1-18:1	699.5	20	281.3	40	12.43	ES-	1
249	PA 18:1-18:2	697.5	20	279.3	40	12.43	ES-	1
250	PA 18:1-18:2	697.5	20	281.3	40	12.43	ES-	2
251	PA 18:1-18:3	695.5	20	277.3	40	12.43	ES-	1
252	PA 18:1-18:3	695.5	20	281.3	40	12.43	ES-	2
253	PA 18:1-18:4	693.5	20	275.3	40	12.43	ES-	1
254	PA 18:1-18:4	693.5	20	281.3	40	12.43	ES-	2
255	PA 18:1-20:0	729.5	20	281.3	40	12.43	ES-	1
256	PA 18:1-20:0	729.5	20	311.2	40	12.43	ES-	2
257	PA 18:1-20:1	727.5	20	281.3	40	12.43	ES-	1
258	PA 18:1-20:1	727.5	20	309.2	40	12.43	ES-	2
259	PA 18:1-20:2	725.5	20	281.3	40	12.43	ES-	1
260	PA 18:1-20:2	725.5	20	307.2	40	12.43	ES-	2
261	PA 18:1-20:3	723.5	20	281.3	40	12.43	ES-	1
262	PA 18:1-20:3	723.5	20	305.2	40	12.43	ES-	2
263	PA 18:1-20:4	721.5	20	281.3	40	12.43	ES-	1
264	PA 18:1-20:4	721.5	20	303.2	40	12.43	ES-	2
265	PA 18:1-20:5	719.5	20	281.3	40	12.43	ES-	1
266	PA 18:1-20:5	719.5	20	301.2	40	12.43	ES-	2
267	PA 18:1-22:0	757.6	20	281.3	40	12.43	ES-	1
268	PA 18:1-22:0	757.6	20	339.2	40	12.43	ES-	2
269	PA 18:1-22:1	755.6	20	281.3	40	12.43	ES-	1
270	PA 18:1-22:1	755.6	20	337.2	40	12.43	ES-	2
271	PA 18:1-22:2	753.5	20	281.3	40	12.43	ES-	1

272	PA 18:1-22:2	753.5	20	335.2	40	12.43	ES-	2
273	PA 18:1-22:3	751.5	20	281.3	40	12.43	ES-	1
274	PA 18:1-22:3	751.5	20	333.2	40	12.43	ES-	2
275	PA 18:1-22:4	749.5	20	281.3	40	12.43	ES-	1
276	PA 18:1-22:4	749.5	20	331.2	40	12.43	ES-	2
277	PA 18:1-22:5	747.5	20	281.3	40	12.43	ES-	1
278	PA 18:1-22:5	747.5	20	329.2	40	12.43	ES-	2
279	PA 18:1-22:6	745.5	20	281.3	40	12.43	ES-	1
280	PA 18:1-22:6	745.5	20	327.2	40	12.43	ES-	2
281	PA 18:2-18:2	695.5	20	279.3	40	12.43	ES-	1
282	PA 18:2-18:3	693.5	20	277.3	40	12.43	ES-	1
283	PA 18:2-18:3	693.5	20	279.3	40	12.43	ES-	2
284	PA 18:2-18:4	691.4	20	275.3	40	12.43	ES-	1
285	PA 18:2-18:4	691.4	20	279.3	40	12.43	ES-	2
286	PA 18:2-20:0	727.5	20	279.3	40	12.43	ES-	1
287	PA 18:2-20:0	727.5	20	311.2	40	12.43	ES-	2
288	PA 18:2-20:1	725.5	20	279.3	40	12.43	ES-	1
289	PA 18:2-20:1	725.5	20	309.2	40	12.43	ES-	2
290	PA 18:2-20:2	723.5	20	279.3	40	12.43	ES-	1
291	PA 18:2-20:2	723.5	20	307.2	40	12.43	ES-	2
292	PA 18:2-20:3	721.5	20	279.3	40	12.43	ES-	1
293	PA 18:2-20:3	721.5	20	305.2	40	12.43	ES-	2
294	PA 18:2-20:4	719.5	20	279.3	40	12.43	ES-	1
295	PA 18:2-20:4	719.5	20	303.2	40	12.43	ES-	2
296	PA 18:2-20:5	717.5	20	279.3	40	12.43	ES-	1
297	PA 18:2-20:5	717.5	20	301.2	40	12.43	ES-	2

Method 3: DAG and PA (3)

No	Name	Precursor	CV (V)	Product	CE (V)	RT setting (min)	IonMode	Ion
1	DAG 18:2-22:0	694.6	50	337.3	20	3.25	ES+	1
2	DAG 18:2-22:0	694.6	50	397.4	20	3.25	ES+	2
3	DAG 18:2-22:1	692.6	50	337.3	20	3.25	ES+	1
4	DAG 18:2-22:1	692.6	50	395.4	20	3.25	ES+	2
5	DAG 18:2-22:2	690.6	50	337.3	20	3.25	ES+	1
6	DAG 18:2-22:2	690.6	50	393.4	20	3.25	ES+	2
7	DAG 18:2-22:3	688.6	50	337.3	20	3.25	ES+	1

8	DAG 18:2-22:3	688.6	50	391.3	20	3.25	ES+	2
9	DAG 18:2-22:4	686.6	50	337.3	20	3.25	ES+	1
10	DAG 18:2-22:4	686.6	50	389.3	20	3.25	ES+	2
11	DAG 18:2-22:5	684.6	50	337.3	20	3.25	ES+	1
12	DAG 18:2-22:5	684.6	50	387.3	20	3.25	ES+	2
13	DAG 18:2-22:6	682.5	50	337.3	20	3.25	ES+	1
14	DAG 18:2-22:6	682.5	50	385.3	20	3.25	ES+	2
15	DAG 18:3-18:3	630.5	50	335.3	20	3.25	ES+	1
16	DAG 18:3-18:4	628.5	50	333.3	20	3.25	ES+	1
17	DAG 18:3-18:4	628.5	50	335.3	20	3.25	ES+	2
18	DAG 18:3-20:0	664.6	50	335.3	20	3.25	ES+	1
19	DAG 18:3-20:0	664.6	50	369.4	20	3.25	ES+	2
20	DAG 18:3-20:1	662.6	50	335.3	20	3.25	ES+	1
21	DAG 18:3-20:1	662.6	50	367.3	20	3.25	ES+	2
22	DAG 18:3-20:2	660.6	50	335.3	20	3.25	ES+	1
23	DAG 18:3-20:2	660.6	50	365.3	20	3.25	ES+	2
24	DAG 18:3-20:3	658.5	50	335.3	20	3.25	ES+	1
25	DAG 18:3-20:3	658.5	50	363.3	20	3.25	ES+	2
26	DAG 18:3-20:4	656.5	50	335.3	20	3.25	ES+	1
27	DAG 18:3-20:4	656.5	50	361.3	20	3.25	ES+	2
28	DAG 18:3-20:5	654.5	50	335.3	20	3.25	ES+	1
29	DAG 18:3-20:5	654.5	50	359.3	20	3.25	ES+	2
30	DAG 18:3-22:0	692.6	50	335.3	20	3.25	ES+	1
31	DAG 18:3-22:0	692.6	50	397.4	20	3.25	ES+	2
32	DAG 18:3-22:1	690.6	50	335.3	20	3.25	ES+	1
33	DAG 18:3-22:1	690.6	50	395.4	20	3.25	ES+	2
34	DAG 18:3-22:2	688.6	50	335.3	20	3.25	ES+	1
35	DAG 18:3-22:2	688.6	50	393.4	20	3.25	ES+	2
36	DAG 18:3-22:3	686.6	50	335.3	20	3.25	ES+	1
37	DAG 18:3-22:3	686.6	50	391.3	20	3.25	ES+	2
38	DAG 18:3-22:4	684.6	50	335.3	20	3.25	ES+	1
39	DAG 18:3-22:4	684.6	50	389.3	20	3.25	ES+	2
40	DAG 18:3-22:5	682.5	50	335.3	20	3.25	ES+	1
41	DAG 18:3-22:5	682.5	50	387.3	20	3.25	ES+	2
42	DAG 18:3-22:6	680.5	50	335.3	20	3.25	ES+	1

43	DAG 18:3-22:6	680.5	50	385.3	20	3.25	ES+	2
44	DAG 18:4-18:4	626.5	50	333.3	20	3.25	ES+	1
45	DAG 18:4-20:0	662.6	50	333.3	20	3.25	ES+	1
46	DAG 18:4-20:0	662.6	50	369.4	20	3.25	ES+	2
47	DAG 18:4-20:1	660.6	50	333.3	20	3.25	ES+	1
48	DAG 18:4-20:1	660.6	50	367.3	20	3.25	ES+	2
49	DAG 18:4-20:2	658.5	50	333.3	20	3.25	ES+	1
50	DAG 18:4-20:2	658.5	50	365.3	20	3.25	ES+	2
51	DAG 18:4-20:3	656.5	50	333.3	20	3.25	ES+	1
52	DAG 18:4-20:3	656.5	50	363.3	20	3.25	ES+	2
53	DAG 18:4-20:4	654.5	50	333.3	20	3.25	ES+	1
54	DAG 18:4-20:4	654.5	50	361.3	20	3.25	ES+	2
55	DAG 18:4-20:5	652.5	50	333.3	20	3.25	ES+	1
56	DAG 18:4-20:5	652.5	50	359.3	20	3.25	ES+	2
57	DAG 18:4-22:0	690.6	50	333.3	20	3.25	ES+	1
58	DAG 18:4-22:0	690.6	50	397.4	20	3.25	ES+	2
59	DAG 18:4-22:1	688.6	50	333.3	20	3.25	ES+	1
60	DAG 18:4-22:1	688.6	50	395.4	20	3.25	ES+	2
61	DAG 18:4-22:2	686.6	50	333.3	20	3.25	ES+	1
62	DAG 18:4-22:2	686.6	50	393.4	20	3.25	ES+	2
63	DAG 18:4-22:3	684.6	50	333.3	20	3.25	ES+	1
64	DAG 18:4-22:3	684.6	50	391.3	20	3.25	ES+	2
65	DAG 18:4-22:4	682.5	50	333.3	20	3.25	ES+	1
66	DAG 18:4-22:4	682.5	50	389.3	20	3.25	ES+	2
67	DAG 18:4-22:5	680.5	50	333.3	20	3.25	ES+	1
68	DAG 18:4-22:5	680.5	50	387.3	20	3.25	ES+	2
69	DAG 18:4-22:6	678.5	50	333.3	20	3.25	ES+	1
70	DAG 18:4-22:6	678.5	50	385.3	20	3.25	ES+	2
71	DAG 20:0-20:0	698.7	50	369.4	20	3.25	ES+	1
72	DAG 20:0-20:1	696.7	50	367.3	20	3.25	ES+	1
73	DAG 20:0-20:1	696.7	50	369.4	20	3.25	ES+	2
74	DAG 20:0-20:2	694.6	50	365.3	20	3.25	ES+	1
75	DAG 20:0-20:2	694.6	50	369.4	20	3.25	ES+	2
76	DAG 20:0-20:3	692.6	50	363.3	20	3.25	ES+	1
77	DAG 20:0-20:3	692.6	50	369.4	20	3.25	ES+	2

78	DAG 20:0-20:4	690.6	50	361.3	20	3.25	ES+	1
79	DAG 20:0-20:4	690.6	50	369.4	20	3.25	ES+	2
80	DAG 20:0-20:5	688.6	50	359.3	20	3.25	ES+	1
81	DAG 20:0-20:5	688.6	50	369.4	20	3.25	ES+	2
82	DAG 20:0-22:0	726.7	50	369.4	20	3.25	ES+	1
83	DAG 20:0-22:0	726.7	50	397.4	20	3.25	ES+	2
84	DAG 20:0-22:1	724.7	50	369.4	20	3.25	ES+	1
85	DAG 20:0-22:1	724.7	50	395.4	20	3.25	ES+	2
86	DAG 20:0-22:2	722.7	50	369.4	20	3.25	ES+	1
87	DAG 20:0-22:2	722.7	50	393.4	20	3.25	ES+	2
88	DAG 20:0-22:3	720.7	50	369.4	20	3.25	ES+	1
89	DAG 20:0-22:3	720.7	50	391.3	20	3.25	ES+	2
90	DAG 20:0-22:4	718.6	50	369.4	20	3.25	ES+	1
91	DAG 20:0-22:4	718.6	50	389.3	20	3.25	ES+	2
92	DAG 20:0-22:5	716.6	50	369.4	20	3.25	ES+	1
93	DAG 20:0-22:5	716.6	50	387.3	20	3.25	ES+	2
94	DAG 20:0-22:6	714.6	50	369.4	20	3.25	ES+	1
95	DAG 20:0-22:6	714.6	50	385.3	20	3.25	ES+	2
96	DAG 20:1-20:1	694.6	50	367.3	20	3.25	ES+	1
97	DAG 20:1-20:2	692.6	50	365.3	20	3.25	ES+	1
98	DAG 20:1-20:2	692.6	50	367.3	20	3.25	ES+	2
99	DAG 20:1-20:3	690.6	50	363.3	20	3.25	ES+	1
100	DAG 20:1-20:3	690.6	50	367.3	20	3.25	ES+	2
101	DAG 20:1-20:4	688.6	50	361.3	20	3.25	ES+	1
102	DAG 20:1-20:4	688.6	50	367.3	20	3.25	ES+	2
103	DAG 20:1-20:5	686.6	50	359.3	20	3.25	ES+	1
104	DAG 20:1-20:5	686.6	50	367.3	20	3.25	ES+	2
105	DAG 20:1-22:0	724.7	50	367.3	20	3.25	ES+	1
106	DAG 20:1-22:0	724.7	50	397.4	20	3.25	ES+	2
107	DAG 20:1-22:1	722.7	50	367.3	20	3.25	ES+	1
108	DAG 20:1-22:1	722.7	50	395.4	20	3.25	ES+	2
109	DAG 20:1-22:2	720.7	50	367.3	20	3.25	ES+	1
110	DAG 20:1-22:2	720.7	50	393.4	20	3.25	ES+	2
111	DAG 20:1-22:3	718.6	50	367.3	20	3.25	ES+	1
112	DAG 20:1-22:3	718.6	50	391.3	20	3.25	ES+	2

113	DAG 20:1-22:4	716.6	50	367.3	20	3.25	ES+	1
114	DAG 20:1-22:4	716.6	50	389.3	20	3.25	ES+	2
115	DAG 20:1-22:5	714.6	50	367.3	20	3.25	ES+	1
116	DAG 20:1-22:5	714.6	50	387.3	20	3.25	ES+	2
117	DAG 20:1-22:6	712.6	50	367.3	20	3.25	ES+	1
118	DAG 20:1-22:6	712.6	50	385.3	20	3.25	ES+	2
119	DAG 20:2-20:2	690.6	50	365.3	20	3.25	ES+	1
120	DAG 20:2-20:3	688.6	50	363.3	20	3.25	ES+	1
121	DAG 20:2-20:3	688.6	50	365.3	20	3.25	ES+	2
122	DAG 20:2-20:4	686.6	50	361.3	20	3.25	ES+	1
123	DAG 20:2-20:4	686.6	50	365.3	20	3.25	ES+	2
124	DAG 20:2-20:5	684.6	50	359.3	20	3.25	ES+	1
125	DAG 20:2-20:5	684.6	50	365.3	20	3.25	ES+	2
126	DAG 20:2-22:0	722.7	50	365.3	20	3.25	ES+	1
127	DAG 20:2-22:0	722.7	50	397.4	20	3.25	ES+	2
128	DAG 20:2-22:1	720.7	50	365.3	20	3.25	ES+	1
129	DAG 20:2-22:1	720.7	50	395.4	20	3.25	ES+	2
130	DAG 20:2-22:2	718.6	50	365.3	20	3.25	ES+	1
131	DAG 20:2-22:2	718.6	50	393.4	20	3.25	ES+	2
132	DAG 20:2-22:3	716.6	50	365.3	20	3.25	ES+	1
133	DAG 20:2-22:3	716.6	50	391.3	20	3.25	ES+	2
134	DAG 20:2-22:4	714.6	50	365.3	20	3.25	ES+	1
135	DAG 20:2-22:4	714.6	50	389.3	20	3.25	ES+	2
136	DAG 20:2-22:5	712.6	50	365.3	20	3.25	ES+	1
137	DAG 20:2-22:5	712.6	50	387.3	20	3.25	ES+	2
138	DAG 20:2-22:6	710.6	50	365.3	20	3.25	ES+	1
139	DAG 20:2-22:6	710.6	50	385.3	20	3.25	ES+	2
140	DAG 20:3-20:3	686.6	50	363.3	20	3.25	ES+	1
141	DAG 20:3-20:4	684.6	50	361.3	20	3.25	ES+	1
142	DAG 20:3-20:4	684.6	50	363.3	20	3.25	ES+	2
143	DAG 20:3-20:5	682.5	50	359.3	20	3.25	ES+	1
144	DAG 20:3-20:5	682.5	50	363.3	20	3.25	ES+	2
145	PA 18:2-22:0	755.6	20	279.3	40	12.43	ES-	1
146	PA 18:2-22:0	755.6	20	339.2	40	12.43	ES-	2
147	PA 18:2-22:1	753.5	20	279.3	40	12.43	ES-	1

148	PA 18:2-22:1	753.5	20	337.2	40	12.43	ES-	2
149	PA 18:2-22:2	751.5	20	279.3	40	12.43	ES-	1
150	PA 18:2-22:2	751.5	20	335.2	40	12.43	ES-	2
151	PA 18:2-22:3	749.5	20	279.3	40	12.43	ES-	1
152	PA 18:2-22:3	749.5	20	333.2	40	12.43	ES-	2
153	PA 18:2-22:4	747.5	20	279.3	40	12.43	ES-	1
154	PA 18:2-22:4	747.5	20	331.2	40	12.43	ES-	2
155	PA 18:2-22:5	745.5	20	279.3	40	12.43	ES-	1
156	PA 18:2-22:5	745.5	20	329.2	40	12.43	ES-	2
157	PA 18:2-22:6	743.5	20	279.3	40	12.43	ES-	1
158	PA 18:2-22:6	743.5	20	327.2	40	12.43	ES-	2
159	PA 18:3-18:3	691.4	20	277.3	40	12.43	ES-	1
160	PA 18:3-18:4	689.4	20	275.3	40	12.43	ES-	1
161	PA 18:3-18:4	689.4	20	277.3	40	12.43	ES-	2
162	PA 18:3-20:0	725.5	20	277.3	40	12.43	ES-	1
163	PA 18:3-20:0	725.5	20	311.2	40	12.43	ES-	2
164	PA 18:3-20:1	723.5	20	277.3	40	12.43	ES-	1
165	PA 18:3-20:1	723.5	20	309.2	40	12.43	ES-	2
166	PA 18:3-20:2	721.5	20	277.3	40	12.43	ES-	1
167	PA 18:3-20:2	721.5	20	307.2	40	12.43	ES-	2
168	PA 18:3-20:3	719.5	20	277.3	40	12.43	ES-	1
169	PA 18:3-20:3	719.5	20	305.2	40	12.43	ES-	2
170	PA 18:3-20:4	717.5	20	277.3	40	12.43	ES-	1
171	PA 18:3-20:4	717.5	20	303.2	40	12.43	ES-	2
172	PA 18:3-20:5	715.4	20	277.3	40	12.43	ES-	1
173	PA 18:3-20:5	715.4	20	301.2	40	12.43	ES-	2
174	PA 18:3-22:0	753.5	20	277.3	40	12.43	ES-	1
175	PA 18:3-22:0	753.5	20	339.2	40	12.43	ES-	2
176	PA 18:3-22:1	751.5	20	277.3	40	12.43	ES-	1
177	PA 18:3-22:1	751.5	20	337.2	40	12.43	ES-	2
178	PA 18:3-22:2	749.5	20	277.3	40	12.43	ES-	1
179	PA 18:3-22:2	749.5	20	335.2	40	12.43	ES-	2
180	PA 18:3-22:3	747.5	20	277.3	40	12.43	ES-	1
181	PA 18:3-22:3	747.5	20	333.2	40	12.43	ES-	2
182	PA 18:3-22:4	745.5	20	277.3	40	12.43	ES-	1

183	PA 18:3-22:4	745.5	20	331.2	40	12.43	ES-	2
184	PA 18:3-22:5	743.5	20	277.3	40	12.43	ES-	1
185	PA 18:3-22:5	743.5	20	329.2	40	12.43	ES-	2
186	PA 18:3-22:6	741.5	20	277.3	40	12.43	ES-	1
187	PA 18:3-22:6	741.5	20	327.2	40	12.43	ES-	2
188	PA 18:4-18:4	687.4	20	275.3	40	12.43	ES-	1
189	PA 18:4-20:0	723.5	20	275.3	40	12.43	ES-	1
190	PA 18:4-20:0	723.5	20	311.2	40	12.43	ES-	2
191	PA 18:4-20:1	721.5	20	275.3	40	12.43	ES-	1
192	PA 18:4-20:1	721.5	20	309.2	40	12.43	ES-	2
193	PA 18:4-20:2	719.5	20	275.3	40	12.43	ES-	1
194	PA 18:4-20:2	719.5	20	307.2	40	12.43	ES-	2
195	PA 18:4-20:3	717.5	20	275.3	40	12.43	ES-	1
196	PA 18:4-20:3	717.5	20	305.2	40	12.43	ES-	2
197	PA 18:4-20:4	715.4	20	275.3	40	12.43	ES-	1
198	PA 18:4-20:4	715.4	20	303.2	40	12.43	ES-	2
199	PA 18:4-20:5	713.4	20	275.3	40	12.43	ES-	1
200	PA 18:4-20:5	713.4	20	301.2	40	12.43	ES-	2
201	PA 18:4-22:0	751.5	20	275.3	40	12.43	ES-	1
202	PA 18:4-22:0	751.5	20	339.2	40	12.43	ES-	2
203	PA 18:4-22:1	749.5	20	275.3	40	12.43	ES-	1
204	PA 18:4-22:1	749.5	20	337.2	40	12.43	ES-	2
205	PA 18:4-22:2	747.5	20	275.3	40	12.43	ES-	1
206	PA 18:4-22:2	747.5	20	335.2	40	12.43	ES-	2
207	PA 18:4-22:3	745.5	20	275.3	40	12.43	ES-	1
208	PA 18:4-22:3	745.5	20	333.2	40	12.43	ES-	2
209	PA 18:4-22:4	743.5	20	275.3	40	12.43	ES-	1
210	PA 18:4-22:4	743.5	20	331.2	40	12.43	ES-	2
211	PA 18:4-22:5	741.5	20	275.3	40	12.43	ES-	1
212	PA 18:4-22:5	741.5	20	329.2	40	12.43	ES-	2
213	PA 18:4-22:6	739.4	20	275.3	40	12.43	ES-	1
214	PA 18:4-22:6	739.4	20	327.2	40	12.43	ES-	2
215	PA 20:0-20:0	759.6	20	311.2	40	12.43	ES-	1
216	PA 20:0-20:1	757.6	20	309.2	40	12.43	ES-	1
217	PA 20:0-20:1	757.6	20	311.2	40	12.43	ES-	2

218	PA 20:0-20:2	755.6	20	307.2	40	12.43	ES-	1
219	PA 20:0-20:2	755.6	20	311.2	40	12.43	ES-	2
220	PA 20:0-20:3	753.5	20	305.2	40	12.43	ES-	1
221	PA 20:0-20:3	753.5	20	311.2	40	12.43	ES-	2
222	PA 20:0-20:4	751.5	20	303.2	40	12.43	ES-	1
223	PA 20:0-20:4	751.5	20	311.2	40	12.43	ES-	2
224	PA 20:0-20:5	749.5	20	301.2	40	12.43	ES-	1
225	PA 20:0-20:5	749.5	20	311.2	40	12.43	ES-	2
226	PA 20:0-22:0	787.6	20	311.2	40	12.43	ES-	1
227	PA 20:0-22:0	787.6	20	339.2	40	12.43	ES-	2
228	PA 20:0-22:1	785.6	20	311.2	40	12.43	ES-	1
229	PA 20:0-22:1	785.6	20	337.2	40	12.43	ES-	2
230	PA 20:0-22:2	783.6	20	311.2	40	12.43	ES-	1
231	PA 20:0-22:2	783.6	20	335.2	40	12.43	ES-	2
232	PA 20:0-22:3	781.6	20	311.2	40	12.43	ES-	1
233	PA 20:0-22:3	781.6	20	333.2	40	12.43	ES-	2
234	PA 20:0-22:4	779.6	20	311.2	40	12.43	ES-	1
235	PA 20:0-22:4	779.6	20	331.2	40	12.43	ES-	2
236	PA 20:0-22:5	777.5	20	311.2	40	12.43	ES-	1
237	PA 20:0-22:5	777.5	20	329.2	40	12.43	ES-	2
238	PA 20:0-22:6	775.5	20	311.2	40	12.43	ES-	1
239	PA 20:0-22:6	775.5	20	327.2	40	12.43	ES-	2
240	PA 20:1-20:1	755.6	20	309.2	40	12.43	ES-	1
241	PA 20:1-20:2	753.5	20	307.2	40	12.43	ES-	1
242	PA 20:1-20:2	753.5	20	309.2	40	12.43	ES-	2
243	PA 20:1-20:3	751.5	20	305.2	40	12.43	ES-	1
244	PA 20:1-20:3	751.5	20	309.2	40	12.43	ES-	2
245	PA 20:1-20:4	749.5	20	303.2	40	12.43	ES-	1
246	PA 20:1-20:4	749.5	20	309.2	40	12.43	ES-	2
247	PA 20:1-20:5	747.5	20	301.2	40	12.43	ES-	1
248	PA 20:1-20:5	747.5	20	309.2	40	12.43	ES-	2
249	PA 20:1-22:0	785.6	20	309.2	40	12.43	ES-	1
250	PA 20:1-22:0	785.6	20	339.2	40	12.43	ES-	2
251	PA 20:1-22:1	783.6	20	309.2	40	12.43	ES-	1
252	PA 20:1-22:1	783.6	20	337.2	40	12.43	ES-	2

253	PA 20:1-22:2	781.6	20	309.2	40	12.43	ES-	1
254	PA 20:1-22:2	781.6	20	335.2	40	12.43	ES-	2
255	PA 20:1-22:3	779.6	20	309.2	40	12.43	ES-	1
256	PA 20:1-22:3	779.6	20	333.2	40	12.43	ES-	2
257	PA 20:1-22:4	777.5	20	309.2	40	12.43	ES-	1
258	PA 20:1-22:4	777.5	20	331.2	40	12.43	ES-	2
259	PA 20:1-22:5	775.5	20	309.2	40	12.43	ES-	1
260	PA 20:1-22:5	775.5	20	329.2	40	12.43	ES-	2
261	PA 20:1-22:6	773.5	20	309.2	40	12.43	ES-	1
262	PA 20:1-22:6	773.5	20	327.2	40	12.43	ES-	2
263	PA 20:2-20:2	751.5	20	307.2	40	12.43	ES-	1
264	PA 20:2-20:3	749.5	20	305.2	40	12.43	ES-	1
265	PA 20:2-20:3	749.5	20	307.2	40	12.43	ES-	2
266	PA 20:2-20:4	747.5	20	303.2	40	12.43	ES-	1
267	PA 20:2-20:4	747.5	20	307.2	40	12.43	ES-	2
268	PA 20:2-20:5	745.5	20	301.2	40	12.43	ES-	1
269	PA 20:2-20:5	745.5	20	307.2	40	12.43	ES-	2
270	PA 20:2-22:0	783.6	20	307.2	40	12.43	ES-	1
271	PA 20:2-22:0	783.6	20	339.2	40	12.43	ES-	2
272	PA 20:2-22:1	781.6	20	307.2	40	12.43	ES-	1
273	PA 20:2-22:1	781.6	20	337.2	40	12.43	ES-	2
274	PA 20:2-22:2	779.6	20	307.2	40	12.43	ES-	1
275	PA 20:2-22:2	779.6	20	335.2	40	12.43	ES-	2
276	PA 20:2-22:3	777.5	20	307.2	40	12.43	ES-	1
277	PA 20:2-22:3	777.5	20	333.2	40	12.43	ES-	2
278	PA 20:2-22:4	775.5	20	307.2	40	12.43	ES-	1
279	PA 20:2-22:4	775.5	20	331.2	40	12.43	ES-	2
280	PA 20:2-22:5	773.5	20	307.2	40	12.43	ES-	1
281	PA 20:2-22:5	773.5	20	329.2	40	12.43	ES-	2
282	PA 20:2-22:6	771.5	20	307.2	40	12.43	ES-	1
283	PA 20:2-22:6	771.5	20	327.2	40	12.43	ES-	2
284	PA 20:3-20:3	747.5	20	305.2	40	12.43	ES-	1
285	PA 20:3-20:4	745.5	20	303.2	40	12.43	ES-	1
286	PA 20:3-20:4	745.5	20	305.2	40	12.43	ES-	2
287	PA 20:3-20:5	743.5	20	301.2	40	12.43	ES-	1

288	PA 20:3-20:5	743.5	20	305.2	40	12.43	ES-	2

Method 4: DAG and PA (4)

No	Name	Precursor	CV (V)	Product	CE (V)	RT setting (min)	IonMode	Ion
1	DAG 20:3-22:0	720.7	50	363.3	20	3.25	ES+	1
2	DAG 20:3-22:0	720.7	50	397.4	20	3.25	ES+	2
3	DAG 20:3-22:1	718.6	50	363.3	20	3.25	ES+	1
4	DAG 20:3-22:1	718.6	50	395.4	20	3.25	ES+	2
5	DAG 20:3-22:2	716.6	50	363.3	20	3.25	ES+	1
6	DAG 20:3-22:2	716.6	50	393.4	20	3.25	ES+	2
7	DAG 20:3-22:3	714.6	50	363.3	20	3.25	ES+	1
8	DAG 20:3-22:3	714.6	50	391.3	20	3.25	ES+	2
9	DAG 20:3-22:4	712.6	50	363.3	20	3.25	ES+	1
10	DAG 20:3-22:4	712.6	50	389.3	20	3.25	ES+	2
11	DAG 20:3-22:5	710.6	50	363.3	20	3.25	ES+	1
12	DAG 20:3-22:5	710.6	50	387.3	20	3.25	ES+	2
13	DAG 20:3-22:6	708.6	50	363.3	20	3.25	ES+	1
14	DAG 20:3-22:6	708.6	50	385.3	20	3.25	ES+	2
15	DAG 20:4-20:4	682.5	50	361.3	20	3.25	ES+	1
16	DAG 20:4-20:5	680.5	50	359.3	20	3.25	ES+	1
17	DAG 20:4-20:5	680.5	50	361.3	20	3.25	ES+	2
18	DAG 20:4-22:0	718.6	50	361.3	20	3.25	ES+	1
19	DAG 20:4-22:0	718.6	50	397.4	20	3.25	ES+	2
20	DAG 20:4-22:1	716.6	50	361.3	20	3.25	ES+	1
21	DAG 20:4-22:1	716.6	50	395.3	20	3.25	ES+	2
22	DAG 20:4-22:2	714.6	50	361.3	20	3.25	ES+	1
23	DAG 20:4-22:2	714.6	50	393.3	20	3.25	ES+	2
24	DAG 20:4-22:3	712.6	50	361.3	20	3.25	ES+	1
25	DAG 20:4-22:3	712.6	50	391.3	20	3.25	ES+	2
26	DAG 20:4-22:4	710.6	50	361.3	20	3.25	ES+	1
27	DAG 20:4-22:4	710.6	50	389.3	20	3.25	ES+	2
28	DAG 20:4-22:5	708.6	50	361.3	20	3.25	ES+	1
29	DAG 20:4-22:5	708.6	50	387.3	20	3.25	ES+	2
30	DAG 20:4-22:6	706.5	50	361.3	20	3.25	ES+	1
31	DAG 20:4-22:6	706.5	50	385.3	20	3.25	ES+	2
32	DAG 20:5-20:5	678.5	50	359.3	20	3.25	ES+	1

33	DAG 20:5-22:0	716.6	50	359.3	20	3.25	ES+	1
34	DAG 20:5-22:0	716.6	50	397.4	20	3.25	ES+	2
35	DAG 20:5-22:1	714.6	50	359.3	20	3.25	ES+	1
36	DAG 20:5-22:1	714.6	50	395.3	20	3.25	ES+	2
37	DAG 20:5-22:2	712.6	50	359.3	20	3.25	ES+	1
38	DAG 20:5-22:2	712.6	50	393.3	20	3.25	ES+	2
39	DAG 20:5-22:3	710.6	50	359.3	20	3.25	ES+	1
40	DAG 20:5-22:3	710.6	50	391.3	20	3.25	ES+	2
41	DAG 20:5-22:4	708.6	50	359.3	20	3.25	ES+	1
42	DAG 20:5-22:4	708.6	50	389.3	20	3.25	ES+	2
43	DAG 20:5-22:5	706.5	50	359.3	20	3.25	ES+	1
44	DAG 20:5-22:5	706.5	50	387.3	20	3.25	ES+	2
45	DAG 20:5-22:6	704.5	50	359.3	20	3.25	ES+	1
46	DAG 20:5-22:6	704.5	50	385.3	20	3.25	ES+	2
47	DAG 22:0-22:0	754.7	50	397.4	20	3.25	ES+	1
48	DAG 22:0-22:1	752.7	50	395.4	20	3.25	ES+	1
49	DAG 22:0-22:1	752.7	50	397.4	20	3.25	ES+	2
50	DAG 22:0-22:2	750.7	50	393.4	20	3.25	ES+	1
51	DAG 22:0-22:2	750.7	50	397.4	20	3.25	ES+	2
52	DAG 22:0-22:3	748.7	50	391.3	20	3.25	ES+	1
53	DAG 22:0-22:3	748.7	50	397.4	20	3.25	ES+	2
54	DAG 22:0-22:4	746.7	50	389.3	20	3.25	ES+	1
55	DAG 22:0-22:4	746.7	50	397.4	20	3.25	ES+	2
56	DAG 22:0-22:5	744.7	50	387.3	20	3.25	ES+	1
57	DAG 22:0-22:5	744.7	50	397.4	20	3.25	ES+	2
58	DAG 22:0-22:6	742.6	50	385.3	20	3.25	ES+	1
59	DAG 22:0-22:6	742.6	50	397.4	20	3.25	ES+	2
60	DAG 22:1-22:1	750.7	50	395.4	20	3.25	ES+	1
61	DAG 22:1-22:2	748.7	50	393.4	20	3.25	ES+	1
62	DAG 22:1-22:2	748.7	50	395.4	20	3.25	ES+	2
63	DAG 22:1-22:3	746.7	50	391.3	20	3.25	ES+	1
64	DAG 22:1-22:3	746.7	50	395.4	20	3.25	ES+	2
65	DAG 22:1-22:4	744.7	50	389.3	20	3.25	ES+	1
66	DAG 22:1-22:4	744.7	50	395.4	20	3.25	ES+	2
67	DAG 22:1-22:5	742.6	50	387.3	20	3.25	ES+	1

68	DAG 22:1-22:5	742.6	50	395.4	20	3.25	ES+	2
69	DAG 22:1-22:6	740.6	50	385.3	20	3.25	ES+	1
70	DAG 22:1-22:6	740.6	50	395.4	20	3.25	ES+	2
71	DAG 22:2-22:2	746.7	50	393.4	20	3.25	ES+	1
72	DAG 22:2-22:3	744.7	50	391.3	20	3.25	ES+	1
73	DAG 22:2-22:3	744.7	50	393.4	20	3.25	ES+	2
74	DAG 22:2-22:4	742.6	50	389.3	20	3.25	ES+	1
75	DAG 22:2-22:4	742.6	50	393.4	20	3.25	ES+	2
76	DAG 22:2-22:5	740.6	50	387.3	20	3.25	ES+	1
77	DAG 22:2-22:5	740.6	50	393.4	20	3.25	ES+	2
78	DAG 22:2-22:6	738.6	50	385.3	20	3.25	ES+	1
79	DAG 22:2-22:6	738.6	50	393.4	20	3.25	ES+	2
80	DAG 22:3-22:3	742.6	50	391.3	20	3.25	ES+	1
81	DAG 22:3-22:4	740.6	50	389.3	20	3.25	ES+	1
82	DAG 22:3-22:4	740.6	50	391.3	20	3.25	ES+	2
83	DAG 22:3-22:5	738.6	50	387.3	20	3.25	ES+	1
84	DAG 22:3-22:5	738.6	50	391.3	20	3.25	ES+	2
85	DAG 22:3-22:6	736.6	50	385.3	20	3.25	ES+	1
86	DAG 22:3-22:6	736.6	50	391.3	20	3.25	ES+	2
87	DAG 22:4-22:4	738.6	50	389.3	20	3.25	ES+	1
88	DAG 22:4-22:5	736.6	50	387.3	20	3.25	ES+	1
89	DAG 22:4-22:5	736.6	50	389.3	20	3.25	ES+	2
90	DAG 22:4-22:6	734.6	50	385.3	20	3.25	ES+	1
91	DAG 22:4-22:6	734.6	50	389.3	20	3.25	ES+	2
92	DAG 22:5-22:5	734.6	50	387.3	20	3.25	ES+	1
93	DAG 22:5-22:6	732.6	50	385.3	20	3.25	ES+	1
94	DAG 22:5-22:6	732.6	50	387.3	20	3.25	ES+	2
95	DAG 22:6-22:6	730.5	50	385.3	20	3.25	ES+	1
96	PA 20:3-22:0	781.6	20	305.2	40	12.43	ES-	1
97	PA 20:3-22:0	781.6	20	339.2	40	12.43	ES-	2
98	PA 20:3-22:1	779.6	20	305.2	40	12.43	ES-	1
99	PA 20:3-22:1	779.6	20	337.2	40	12.43	ES-	2
100	PA 20:3-22:2	777.5	20	305.2	40	12.43	ES-	1
101	PA 20:3-22:2	777.5	20	335.2	40	12.43	ES-	2
102	PA 20:3-22:3	775.5	20	305.2	40	12.43	ES-	1

103	PA 20:3-22:3	775.5	20	333.2	40	12.43	ES-	2
104	PA 20:3-22:4	773.5	20	305.2	40	12.43	ES-	1
105	PA 20:3-22:4	773.5	20	331.2	40	12.43	ES-	2
106	PA 20:3-22:5	771.5	20	305.2	40	12.43	ES-	1
107	PA 20:3-22:5	771.5	20	329.2	40	12.43	ES-	2
108	PA 20:3-22:6	769.5	20	305.2	40	12.43	ES-	1
109	PA 20:3-22:6	769.5	20	327.2	40	12.43	ES-	2
110	PA 20:4-20:4	743.5	20	303.2	40	12.43	ES-	1
111	PA 20:4-20:5	741.5	20	301.2	40	12.43	ES-	1
112	PA 20:4-20:5	741.5	20	303.2	40	12.43	ES-	2
113	PA 20:4-22:0	779.6	20	303.2	40	12.43	ES-	1
114	PA 20:4-22:0	779.6	20	339.2	40	12.43	ES-	2
115	PA 20:4-22:1	777.5	20	303.2	40	12.43	ES-	1
116	PA 20:4-22:1	777.5	20	337.2	40	12.43	ES-	2
117	PA 20:4-22:2	775.5	20	303.2	40	12.43	ES-	1
118	PA 20:4-22:2	775.5	20	335.2	40	12.43	ES-	2
119	PA 20:4-22:3	773.5	20	303.2	40	12.43	ES-	1
120	PA 20:4-22:3	773.5	20	333.2	40	12.43	ES-	2
121	PA 20:4-22:4	771.5	20	303.2	40	12.43	ES-	1
122	PA 20:4-22:4	771.5	20	331.2	40	12.43	ES-	2
123	PA 20:4-22:5	769.5	20	303.2	40	12.43	ES-	1
124	PA 20:4-22:5	769.5	20	329.2	40	12.43	ES-	2
125	PA 20:4-22:6	767.5	20	303.2	40	12.43	ES-	1
126	PA 20:4-22:6	767.5	20	327.2	40	12.43	ES-	2
127	PA 20:5-20:5	739.4	20	301.2	40	12.43	ES-	1
128	PA 20:5-22:0	777.5	20	301.2	40	12.43	ES-	1
129	PA 20:5-22:0	777.5	20	339.2	40	12.43	ES-	2
130	PA 20:5-22:1	775.5	20	301.2	40	12.43	ES-	1
131	PA 20:5-22:1	775.5	20	337.2	40	12.43	ES-	2
132	PA 20:5-22:2	773.5	20	301.2	40	12.43	ES-	1
133	PA 20:5-22:2	773.5	20	335.2	40	12.43	ES-	2
134	PA 20:5-22:3	771.5	20	301.2	40	12.43	ES-	1
135	PA 20:5-22:3	771.5	20	333.2	40	12.43	ES-	2
136	PA 20:5-22:4	769.5	20	301.2	40	12.43	ES-	1
137	PA 20:5-22:4	769.5	20	331.2	40	12.43	ES-	2

138	PA 20:5-22:5	767.5	20	301.2	40	12.43	ES-	1
139	PA 20:5-22:5	767.5	20	329.2	40	12.43	ES-	2
140	PA 20:5-22:6	765.5	20	301.2	40	12.43	ES-	1
141	PA 20:5-22:6	765.5	20	327.2	40	12.43	ES-	2
142	PA 22:0-22:0	815.7	20	339.2	40	12.43	ES-	1
143	PA 22:0-22:1	813.6	20	337.2	40	12.43	ES-	1
144	PA 22:0-22:1	813.6	20	339.2	40	12.43	ES-	2
145	PA 22:0-22:2	811.6	20	335.2	40	12.43	ES-	1
146	PA 22:0-22:2	811.6	20	339.2	40	12.43	ES-	2
147	PA 22:0-22:3	809.6	20	333.2	40	12.43	ES-	1
148	PA 22:0-22:3	809.6	20	339.2	40	12.43	ES-	2
149	PA 22:0-22:4	807.6	20	331.2	40	12.43	ES-	1
150	PA 22:0-22:4	807.6	20	339.2	40	12.43	ES-	2
151	PA 22:0-22:5	805.6	20	329.2	40	12.43	ES-	1
152	PA 22:0-22:5	805.6	20	339.2	40	12.43	ES-	2
153	PA 22:0-22:6	803.6	20	327.2	40	12.43	ES-	1
154	PA 22:0-22:6	803.6	20	339.2	40	12.43	ES-	2
155	PA 22:1-22:1	811.6	20	337.2	40	12.43	ES-	1
156	PA 22:1-22:2	809.6	20	335.2	40	12.43	ES-	1
157	PA 22:1-22:2	809.6	20	337.2	40	12.43	ES-	2
158	PA 22:1-22:3	807.6	20	333.2	40	12.43	ES-	1
159	PA 22:1-22:3	807.6	20	337.2	40	12.43	ES-	2
160	PA 22:1-22:4	805.6	20	331.2	40	12.43	ES-	1
161	PA 22:1-22:4	805.6	20	337.2	40	12.43	ES-	2
162	PA 22:1-22:5	803.6	20	329.2	40	12.43	ES-	1
163	PA 22:1-22:5	803.6	20	337.2	40	12.43	ES-	2
164	PA 22:1-22:6	801.5	20	327.2	40	12.43	ES-	1
165	PA 22:1-22:6	801.5	20	337.2	40	12.43	ES-	2
166	PA 22:2-22:2	807.6	20	335.2	40	12.43	ES-	1
167	PA 22:2-22:3	805.6	20	333.2	40	12.43	ES-	1
168	PA 22:2-22:3	805.6	20	335.2	40	12.43	ES-	2
169	PA 22:2-22:4	803.6	20	331.2	40	12.43	ES-	1
170	PA 22:2-22:4	803.6	20	335.2	40	12.43	ES-	2
171	PA 22:2-22:5	801.5	20	329.2	40	12.43	ES-	1
172	PA 22:2-22:5	801.5	20	335.2	40	12.43	ES-	2

173	PA 22:2-22:6	799.5	20	327.2	40	12.43	ES-	1
174	PA 22:2-22:6	799.5	20	335.2	40	12.43	ES-	2
175	PA 22:3-22:3	803.6	20	333.2	40	12.43	ES-	1
176	PA 22:3-22:4	801.5	20	331.2	40	12.43	ES-	1
177	PA 22:3-22:4	801.5	20	333.2	40	12.43	ES-	2
178	PA 22:3-22:5	799.5	20	329.2	40	12.43	ES-	1
179	PA 22:3-22:5	799.5	20	333.2	40	12.43	ES-	2
180	PA 22:3-22:6	797.5	20	327.2	40	12.43	ES-	1
181	PA 22:3-22:6	797.5	20	333.2	40	12.43	ES-	2
182	PA 22:4-22:4	799.5	20	331.2	40	12.43	ES-	1
183	PA 22:4-22:5	797.5	20	329.2	40	12.43	ES-	1
184	PA 22:4-22:5	797.5	20	331.2	40	12.43	ES-	2
185	PA 22:4-22:6	795.5	20	327.2	40	12.43	ES-	1
186	PA 22:4-22:6	795.5	20	331.2	40	12.43	ES-	2
187	PA 22:5-22:5	795.5	20	329.2	40	12.43	ES-	1
188	PA 22:5-22:6	793.5	20	327.2	40	12.43	ES-	1
189	PA 22:5-22:6	793.5	20	329.2	40	12.43	ES-	2
190	PA 22:6-22:6	791.5	20	327.2	40	12.43	ES-	1

Method 5: PCe and PI (1)

No	Name	Precursor	CV (V)	Product	CE (V)	RT setting (min)	IonMode	Ion
1	PC 16:0e-12:0	664.5	20	422.3	30	5.40	ES+	1
2	PC 16:0e-12:0	664.5	20	482.4	30	5.40	ES+	2
3	PC 16:0e-14:0	692.6	20	450.3	30	5.40	ES+	1
4	PC 16:0e-14:0	692.6	20	482.4	30	5.40	ES+	2
5	PC 16:0e-14:1	690.5	20	448.3	30	5.40	ES+	1
6	PC 16:0e-14:1	690.5	20	482.4	30	5.40	ES+	2
7	PC 16:0e-16:0	720.6	20	478.3	30	5.40	ES+	1
8	PC 16:0e-16:0	720.6	20	482.4	30	5.40	ES+	2
9	PC 16:0e-16:1	718.6	20	476.3	30	5.40	ES+	1
10	PC 16:0e-16:1	718.6	20	482.4	30	5.40	ES+	2
11	PC 16:0e-18:0	748.6	20	482.4	30	5.40	ES+	1
12	PC 16:0e-18:0	748.6	20	506.3	30	5.40	ES+	2
13	PC 16:0e-18:1	746.6	20	482.4	30	5.40	ES+	1
14	PC 16:0e-18:1	746.6	20	504.3	30	5.40	ES+	2
15	PC 16:0e-18:2	744.6	20	482.4	30	5.40	ES+	1

16	PC 16:0e-18:2	744.6	20	502.3	30	5.40	ES+	2
17	PC 16:0e-18:3	742.6	20	482.4	30	5.40	ES+	1
18	PC 16:0e-18:3	742.6	20	500.3	30	5.40	ES+	2
19	PC 16:0e-18:4	740.6	20	482.4	30	5.40	ES+	1
20	PC 16:0e-18:4	740.6	20	498.3	30	5.40	ES+	2
21	PC 16:0e-20:0	776.7	20	482.4	30	5.40	ES+	1
22	PC 16:0e-20:0	776.7	20	534.3	30	5.40	ES+	2
23	PC 16:0e-20:1	774.6	20	482.4	30	5.40	ES+	1
24	PC 16:0e-20:1	774.6	20	532.3	30	5.40	ES+	2
25	PC 16:0e-20:2	772.6	20	482.4	30	5.40	ES+	1
26	PC 16:0e-20:2	772.6	20	530.3	30	5.40	ES+	2
27	PC 16:0e-20:3	770.6	20	482.4	30	5.40	ES+	1
28	PC 16:0e-20:3	770.6	20	528.3	30	5.40	ES+	2
29	PC 16:0e-20:4	768.6	20	482.4	30	5.40	ES+	1
30	PC 16:0e-20:4	768.6	20	526.3	30	5.40	ES+	2
31	PC 16:0e-20:5	766.6	20	482.4	30	5.40	ES+	1
32	PC 16:0e-20:5	766.6	20	524.3	30	5.40	ES+	2
33	PC 16:0e-22:0	804.7	20	482.4	30	5.40	ES+	1
34	PC 16:0e-22:0	804.7	20	562.3	30	5.40	ES+	2
35	PC 16:0e-22:1	802.7	20	482.4	30	5.40	ES+	1
36	PC 16:0e-22:1	802.7	20	560.3	30	5.40	ES+	2
37	PC 16:0e-22:2	800.7	20	482.4	30	5.40	ES+	1
38	PC 16:0e-22:2	800.7	20	558.3	30	5.40	ES+	2
39	PC 16:0e-22:3	798.6	20	482.4	30	5.40	ES+	1
40	PC 16:0e-22:3	798.6	20	556.3	30	5.40	ES+	2
41	PC 16:0e-22:4	796.6	20	482.4	30	5.40	ES+	1
42	PC 16:0e-22:4	796.6	20	554.3	30	5.40	ES+	2
43	PC 16:0e-22:5	794.6	20	482.4	30	5.40	ES+	1
44	PC 16:0e-22:5	794.6	20	552.3	30	5.40	ES+	2
45	PC 16:0e-22:6	792.6	20	482.4	30	5.40	ES+	1
46	PC 16:0e-22:6	792.6	20	550.3	30	5.40	ES+	2
47	PC 16:1e-12:0	662.5	20	422.3	30	5.40	ES+	1
48	PC 16:1e-12:0	662.5	20	480.4	30	5.40	ES+	2
49	PC 16:1e-14:0	690.5	20	450.3	30	5.40	ES+	1
50	PC 16:1e-14:0	690.5	20	480.4	30	5.40	ES+	2

51	PC 16:1e-14:1	688.5	20	448.3	30	5.40	ES+	1
52	PC 16:1e-14:1	688.5	20	480.4	30	5.40	ES+	2
53	PC 16:1e-16:0	718.6	20	478.3	30	5.40	ES+	1
54	PC 16:1e-16:0	718.6	20	480.4	30	5.40	ES+	2
55	PC 16:1e-16:1	716.6	20	476.3	30	5.40	ES+	1
56	PC 16:1e-16:1	716.6	20	480.4	30	5.40	ES+	2
57	PC 16:1e-18:0	746.6	20	480.4	30	5.40	ES+	1
58	PC 16:1e-18:0	746.6	20	506.3	30	5.40	ES+	2
59	PC 16:1e-18:1	744.6	20	480.4	30	5.40	ES+	1
60	PC 16:1e-18:1	744.6	20	504.3	30	5.40	ES+	2
61	PC 16:1e-18:2	742.6	20	480.4	30	5.40	ES+	1
62	PC 16:1e-18:2	742.6	20	502.3	30	5.40	ES+	2
63	PC 16:1e-18:3	740.6	20	480.4	30	5.40	ES+	1
64	PC 16:1e-18:3	740.6	20	500.3	30	5.40	ES+	2
65	PC 16:1e-18:4	738.5	20	480.4	30	5.40	ES+	1
66	PC 16:1e-18:4	738.5	20	498.3	30	5.40	ES+	2
67	PC 16:1e-20:0	774.6	20	480.4	30	5.40	ES+	1
68	PC 16:1e-20:0	774.6	20	534.3	30	5.40	ES+	2
69	PC 16:1e-20:1	772.6	20	480.4	30	5.40	ES+	1
70	PC 16:1e-20:1	772.6	20	532.3	30	5.40	ES+	2
71	PC 16:1e-20:2	770.6	20	480.4	30	5.40	ES+	1
72	PC 16:1e-20:2	770.6	20	530.3	30	5.40	ES+	2
73	PC 16:1e-20:3	768.6	20	480.4	30	5.40	ES+	1
74	PC 16:1e-20:3	768.6	20	528.3	30	5.40	ES+	2
75	PC 16:1e-20:4	766.6	20	480.4	30	5.40	ES+	1
76	PC 16:1e-20:4	766.6	20	526.3	30	5.40	ES+	2
77	PC 16:1e-20:5	764.6	20	480.4	30	5.40	ES+	1
78	PC 16:1e-20:5	764.6	20	524.3	30	5.40	ES+	2
79	PC 16:1e-22:0	802.7	20	480.4	30	5.40	ES+	1
80	PC 16:1e-22:0	802.7	20	562.3	30	5.40	ES+	2
81	PC 16:1e-22:1	800.7	20	480.4	30	5.40	ES+	1
82	PC 16:1e-22:1	800.7	20	560.3	30	5.40	ES+	2
83	PC 16:1e-22:2	798.6	20	480.4	30	5.40	ES+	1
84	PC 16:1e-22:2	798.6	20	558.3	30	5.40	ES+	2
85	PC 16:1e-22:3	796.6	20	480.4	30	5.40	ES+	1

86	PC 16:1e-22:3	796.6	20	556.3	30	5.40	ES+	2
87	PC 16:1e-22:4	794.6	20	480.4	30	5.40	ES+	1
88	PC 16:1e-22:4	794.6	20	554.3	30	5.40	ES+	2
89	PC 16:1e-22:5	792.6	20	480.4	30	5.40	ES+	1
90	PC 16:1e-22:5	792.6	20	552.3	30	5.40	ES+	2
91	PC 16:1e-22:6	790.6	20	480.4	30	5.40	ES+	1
92	PC 16:1e-22:6	790.6	20	550.3	30	5.40	ES+	2
93	PI 12:0-12:0	697.4	50	199.3	50	12.06	ES-	1
94	PI 12:0-14:0	725.4	50	199.3	50	12.06	ES-	1
95	PI 12:0-14:0	725.4	50	227.3	50	12.06	ES-	2
96	PI 12:0-14:1	723.4	50	199.3	50	12.06	ES-	1
97	PI 12:0-14:1	723.4	50	225.3	50	12.06	ES-	2
98	PI 12:0-16:0	753.5	50	199.3	50	12.06	ES-	1
99	PI 12:0-16:0	753.5	50	255.3	50	12.06	ES-	2
100	PI 12:0-16:1	751.4	50	199.3	50	12.06	ES-	1
101	PI 12:0-16:1	751.4	50	253.3	50	12.06	ES-	2
102	PI 12:0-18:0	781.5	50	199.3	50	12.06	ES-	1
103	PI 12:0-18:0	781.5	50	283.3	50	12.06	ES-	2
104	PI 12:0-18:1	779.5	50	199.3	50	12.06	ES-	1
105	PI 12:0-18:1	779.5	50	281.3	50	12.06	ES-	2
106	PI 12:0-18:2	777.5	50	199.3	50	12.06	ES-	1
107	PI 12:0-18:2	777.5	50	279.3	50	12.06	ES-	2
108	PI 12:0-18:3	775.4	50	199.3	50	12.06	ES-	1
109	PI 12:0-18:3	775.4	50	277.3	50	12.06	ES-	2
110	PI 12:0-18:4	773.4	50	199.3	50	12.06	ES-	1
111	PI 12:0-18:4	773.4	50	275.3	50	12.06	ES-	2
112	PI 12:0-20:0	809.5	50	199.3	50	12.06	ES-	1
113	PI 12:0-20:0	809.5	50	311.2	50	12.06	ES-	2
114	PI 12:0-20:1	807.5	50	199.3	50	12.06	ES-	1
115	PI 12:0-20:1	807.5	50	309.2	50	12.06	ES-	2
116	PI 12:0-20:2	805.5	50	199.3	50	12.06	ES-	1
117	PI 12:0-20:2	805.5	50	307.2	50	12.06	ES-	2
118	PI 12:0-20:3	803.5	50	199.3	50	12.06	ES-	1
119	PI 12:0-20:3	803.5	50	305.2	50	12.06	ES-	2
120	PI 12:0-20:4	801.5	50	199.3	50	12.06	ES-	1

121	PI 12:0-20:4	801.5	50	303.2	50	12.06	ES-	2
122	PI 12:0-20:5	799.4	50	199.3	50	12.06	ES-	1
123	PI 12:0-20:5	799.4	50	301.2	50	12.06	ES-	2
124	PI 12:0-22:0	837.5	50	199.3	50	12.06	ES-	1
125	PI 12:0-22:0	837.5	50	339.2	50	12.06	ES-	2
126	PI 12:0-22:1	835.5	50	199.3	50	12.06	ES-	1
127	PI 12:0-22:1	835.5	50	337.2	50	12.06	ES-	2
128	PI 12:0-22:2	833.5	50	199.3	50	12.06	ES-	1
129	PI 12:0-22:2	833.5	50	335.2	50	12.06	ES-	2
130	PI 12:0-22:3	831.5	50	199.3	50	12.06	ES-	1
131	PI 12:0-22:3	831.5	50	333.2	50	12.06	ES-	2
132	PI 12:0-22:4	829.5	50	199.3	50	12.06	ES-	1
133	PI 12:0-22:4	829.5	50	331.2	50	12.06	ES-	2
134	PI 12:0-22:5	827.5	50	199.3	50	12.06	ES-	1
135	PI 12:0-22:5	827.5	50	329.2	50	12.06	ES-	2
136	PI 12:0-22:6	825.5	50	199.3	50	12.06	ES-	1
137	PI 12:0-22:6	825.5	50	327.2	50	12.06	ES-	2
138	PI 14:0-14:0	753.5	50	227.3	50	12.06	ES-	1
139	PI 14:0-14:1	751.4	50	225.3	50	12.06	ES-	1
140	PI 14:0-14:1	751.4	50	227.3	50	12.06	ES-	2
141	PI 14:0-16:0	781.5	50	227.3	50	12.06	ES-	1
142	PI 14:0-16:0	781.5	50	255.3	50	12.06	ES-	2
143	PI 14:0-16:1	779.5	50	227.3	50	12.06	ES-	1
144	PI 14:0-16:1	779.5	50	253.3	50	12.06	ES-	2
145	PI 14:0-18:0	809.5	50	227.3	50	12.06	ES-	1
146	PI 14:0-18:0	809.5	50	283.3	50	12.06	ES-	2
147	PI 14:0-18:1	807.5	50	227.3	50	12.06	ES-	1
148	PI 14:0-18:1	807.5	50	281.3	50	12.06	ES-	2
149	PI 14:0-18:2	805.5	50	227.3	50	12.06	ES-	1
150	PI 14:0-18:2	805.5	50	279.3	50	12.06	ES-	2
151	PI 14:0-18:3	803.5	50	227.3	50	12.06	ES-	1
152	PI 14:0-18:3	803.5	50	277.3	50	12.06	ES-	2
153	PI 14:0-18:4	801.5	50	227.3	50	12.06	ES-	1
154	PI 14:0-18:4	801.5	50	275.3	50	12.06	ES-	2
155	PI 14:0-20:0	837.5	50	227.3	50	12.06	ES-	1

156	PI 14:0-20:0	837.5	50	311.2	50	12.06	ES-	2
157	PI 14:0-20:1	835.5	50	227.3	50	12.06	ES-	1
158	PI 14:0-20:1	835.5	50	309.2	50	12.06	ES-	2
159	PI 14:0-20:2	833.5	50	227.3	50	12.06	ES-	1
160	PI 14:0-20:2	833.5	50	307.2	50	12.06	ES-	2
161	PI 14:0-20:3	831.5	50	227.3	50	12.06	ES-	1
162	PI 14:0-20:3	831.5	50	305.2	50	12.06	ES-	2
163	PI 14:0-20:4	829.5	50	227.3	50	12.06	ES-	1
164	PI 14:0-20:4	829.5	50	303.2	50	12.06	ES-	2
165	PI 14:0-20:5	827.5	50	227.3	50	12.06	ES-	1
166	PI 14:0-20:5	827.5	50	301.2	50	12.06	ES-	2
167	PI 14:0-22:0	865.6	50	227.3	50	12.06	ES-	1
168	PI 14:0-22:0	865.6	50	339.2	50	12.06	ES-	2
169	PI 14:0-22:1	863.6	50	227.3	50	12.06	ES-	1
170	PI 14:0-22:1	863.6	50	337.2	50	12.06	ES-	2
171	PI 14:0-22:2	861.5	50	227.3	50	12.06	ES-	1
172	PI 14:0-22:2	861.5	50	335.2	50	12.06	ES-	2
173	PI 14:0-22:3	859.5	50	227.3	50	12.06	ES-	1
174	PI 14:0-22:3	859.5	50	333.2	50	12.06	ES-	2
175	PI 14:0-22:4	857.5	50	227.3	50	12.06	ES-	1
176	PI 14:0-22:4	857.5	50	331.2	50	12.06	ES-	2
177	PI 14:0-22:5	855.5	50	227.3	50	12.06	ES-	1
178	PI 14:0-22:5	855.5	50	329.2	50	12.06	ES-	2
179	PI 14:0-22:6	853.5	50	227.3	50	12.06	ES-	1
180	PI 14:0-22:6	853.5	50	327.2	50	12.06	ES-	2
181	PI 14:1-14:1	749.4	50	225.3	50	12.06	ES-	1
182	PI 14:1-16:0	779.5	50	225.3	50	12.06	ES-	1
183	PI 14:1-16:0	779.5	50	255.3	50	12.06	ES-	2
184	PI 14:1-16:1	777.5	50	225.3	50	12.06	ES-	1
185	PI 14:1-16:1	777.5	50	253.3	50	12.06	ES-	2
186	PI 14:1-18:0	807.5	50	225.3	50	12.06	ES-	1
187	PI 14:1-18:0	807.5	50	283.3	50	12.06	ES-	2
188	PI 14:1-18:1	805.5	50	225.3	50	12.06	ES-	1
189	PI 14:1-18:1	805.5	50	281.3	50	12.06	ES-	2
190	PI 14:1-18:2	803.5	50	225.3	50	12.06	ES-	1

191	PI 14:1-18:2	803.5	50	279.3	50	12.06	ES-	2
192	PI 14:1-18:3	801.5	50	225.3	50	12.06	ES-	1
193	PI 14:1-18:3	801.5	50	277.3	50	12.06	ES-	2
194	PI 14:1-18:4	799.4	50	225.3	50	12.06	ES-	1
195	PI 14:1-18:4	799.4	50	275.3	50	12.06	ES-	2
196	PI 14:1-20:0	835.5	50	225.3	50	12.06	ES-	1
197	PI 14:1-20:0	835.5	50	311.2	50	12.06	ES-	2
198	PI 14:1-20:1	833.5	50	225.3	50	12.06	ES-	1
199	PI 14:1-20:1	833.5	50	309.2	50	12.06	ES-	2
200	PI 14:1-20:2	831.5	50	225.3	50	12.06	ES-	1
201	PI 14:1-20:2	831.5	50	307.2	50	12.06	ES-	2
202	PI 14:1-20:3	829.5	50	225.3	50	12.06	ES-	1
203	PI 14:1-20:3	829.5	50	305.2	50	12.06	ES-	2
204	PI 14:1-20:4	827.5	50	225.3	50	12.06	ES-	1
205	PI 14:1-20:4	827.5	50	303.2	50	12.06	ES-	2
206	PI 14:1-20:5	825.5	50	225.3	50	12.06	ES-	1
207	PI 14:1-20:5	825.5	50	301.2	50	12.06	ES-	2
208	PI 14:1-22:0	863.6	50	225.3	50	12.06	ES-	1
209	PI 14:1-22:0	863.6	50	339.2	50	12.06	ES-	2
210	PI 14:1-22:1	861.5	50	225.3	50	12.06	ES-	1
211	PI 14:1-22:1	861.5	50	337.2	50	12.06	ES-	2
212	PI 14:1-22:2	859.5	50	225.3	50	12.06	ES-	1
213	PI 14:1-22:2	859.5	50	335.2	50	12.06	ES-	2
214	PI 14:1-22:3	857.5	50	225.3	50	12.06	ES-	1
215	PI 14:1-22:3	857.5	50	333.2	50	12.06	ES-	2
216	PI 14:1-22:4	855.5	50	225.3	50	12.06	ES-	1
217	PI 14:1-22:4	855.5	50	331.2	50	12.06	ES-	2
218	PI 14:1-22:5	853.5	50	225.3	50	12.06	ES-	1
219	PI 14:1-22:5	853.5	50	329.2	50	12.06	ES-	2
220	PI 14:1-22:6	851.5	50	225.3	50	12.06	ES-	1
221	PI 14:1-22:6	851.5	50	327.2	50	12.06	ES-	2
222	PI 16:0-16:0	809.5	50	255.3	50	12.06	ES-	1
223	PI 16:0-16:1	807.5	50	253.3	50	12.06	ES-	1
224	PI 16:0-16:1	807.5	50	255.3	50	12.06	ES-	2
225	PI 16:0-18:0	837.5	50	255.3	50	12.06	ES-	1

226	PI 16:0-18:0	837.5	50	283.3	50	12.06	ES-	2
227	PI 16:0-18:1	835.5	50	255.3	50	12.06	ES-	1
228	PI 16:0-18:1	835.5	50	281.3	50	12.06	ES-	2
229	PI 16:0-18:2	833.5	50	255.3	50	12.06	ES-	1
230	PI 16:0-18:2	833.5	50	279.3	50	12.06	ES-	2
231	PI 16:0-18:3	831.5	50	255.3	50	12.06	ES-	1
232	PI 16:0-18:3	831.5	50	277.3	50	12.06	ES-	2
233	PI 16:0-18:4	829.5	50	255.3	50	12.06	ES-	1
234	PI 16:0-18:4	829.5	50	275.3	50	12.06	ES-	2

Method 6: PCe and PI (2)

No	Name	Precursor	CV (V)	Product	CE (V)	RT setting (min)	IonMode	Ion
1	PC 18:0e-12:0	692.6	20	422.3	30	5.40	ES+	1
2	PC 18:0e-12:0	692.6	20	510.4	30	5.40	ES+	2
3	PC 18:0e-14:0	720.6	20	450.3	30	5.40	ES+	1
4	PC 18:0e-14:0	720.6	20	510.4	30	5.40	ES+	2
5	PC 18:0e-14:1	718.6	20	448.3	30	5.40	ES+	1
6	PC 18:0e-14:1	718.6	20	510.4	30	5.40	ES+	2
7	PC 18:0e-16:0	748.6	20	478.3	30	5.40	ES+	1
8	PC 18:0e-16:0	748.6	20	510.4	30	5.40	ES+	2
9	PC 18:0e-16:1	746.6	20	476.3	30	5.40	ES+	1
10	PC 18:0e-16:1	746.6	20	510.4	30	5.40	ES+	2
11	PC 18:0e-18:0	776.7	20	506.3	30	5.40	ES+	1
12	PC 18:0e-18:0	776.7	20	510.4	30	5.40	ES+	2
13	PC 18:0e-18:1	774.6	20	504.3	30	5.40	ES+	1
14	PC 18:0e-18:1	774.6	20	510.4	30	5.40	ES+	2
15	PC 18:0e-18:2	772.6	20	502.3	30	5.40	ES+	1
16	PC 18:0e-18:2	772.6	20	510.4	30	5.40	ES+	2
17	PC 18:0e-18:3	770.6	20	500.3	30	5.40	ES+	1
18	PC 18:0e-18:3	770.6	20	510.4	30	5.40	ES+	2
19	PC 18:0e-18:4	768.6	20	498.3	30	5.40	ES+	1
20	PC 18:0e-18:4	768.6	20	510.4	30	5.40	ES+	2
21	PC 18:0e-20:0	804.7	20	510.4	30	5.40	ES+	1
22	PC 18:0e-20:0	804.7	20	534.3	30	5.40	ES+	2
23	PC 18:0e-20:1	802.7	20	510.4	30	5.40	ES+	1
24	PC 18:0e-20:1	802.7	20	532.3	30	5.40	ES+	2

25	PC 18:0e-20:2	800.7	20	510.4	30	5.40	ES+	1
26	PC 18:0e-20:2	800.7	20	530.3	30	5.40	ES+	2
27	PC 18:0e-20:3	798.6	20	510.4	30	5.40	ES+	1
28	PC 18:0e-20:3	798.6	20	528.3	30	5.40	ES+	2
29	PC 18:0e-20:4	796.6	20	510.4	30	5.40	ES+	1
30	PC 18:0e-20:4	796.6	20	526.3	30	5.40	ES+	2
31	PC 18:0e-20:5	794.6	20	510.4	30	5.40	ES+	1
32	PC 18:0e-20:5	794.6	20	524.3	30	5.40	ES+	2
33	PC 18:0e-22:0	832.7	20	510.4	30	5.40	ES+	1
34	PC 18:0e-22:0	832.7	20	562.3	30	5.40	ES+	2
35	PC 18:0e-22:1	830.7	20	510.4	30	5.40	ES+	1
36	PC 18:0e-22:1	830.7	20	560.3	30	5.40	ES+	2
37	PC 18:0e-22:2	828.7	20	510.4	30	5.40	ES+	1
38	PC 18:0e-22:2	828.7	20	558.3	30	5.40	ES+	2
39	PC 18:0e-22:3	826.7	20	510.4	30	5.40	ES+	1
40	PC 18:0e-22:3	826.7	20	556.3	30	5.40	ES+	2
41	PC 18:0e-22:4	824.7	20	510.4	30	5.40	ES+	1
42	PC 18:0e-22:4	824.7	20	554.3	30	5.40	ES+	2
43	PC 18:0e-22:5	822.6	20	510.4	30	5.40	ES+	1
44	PC 18:0e-22:5	822.6	20	552.3	30	5.40	ES+	2
45	PC 18:0e-22:6	820.6	20	510.4	30	5.40	ES+	1
46	PC 18:0e-22:6	820.6	20	550.3	30	5.40	ES+	2
47	PC 18:1e-12:0	690.5	20	422.3	30	5.40	ES+	1
48	PC 18:1e-12:0	690.5	20	508.4	30	5.40	ES+	2
49	PC 18:1e-14:0	718.6	20	450.3	30	5.40	ES+	1
50	PC 18:1e-14:0	718.6	20	508.4	30	5.40	ES+	2
51	PC 18:1e-14:1	716.6	20	448.3	30	5.40	ES+	1
52	PC 18:1e-14:1	716.6	20	508.4	30	5.40	ES+	2
53	PC 18:1e-16:0	746.6	20	478.3	30	5.40	ES+	1
54	PC 18:1e-16:0	746.6	20	508.4	30	5.40	ES+	2
55	PC 18:1e-16:1	744.6	20	476.3	30	5.40	ES+	1
56	PC 18:1e-16:1	744.6	20	508.4	30	5.40	ES+	2
57	PC 18:1e-18:0	774.6	20	506.3	30	5.40	ES+	1
58	PC 18:1e-18:0	774.6	20	508.4	30	5.40	ES+	2
59	PC 18:1e-18:1	772.6	20	504.3	30	5.40	ES+	1

60	PC 18:1e-18:1	772.6	20	508.4	30	5.40	ES+	2
61	PC 18:1e-18:2	770.6	20	502.3	30	5.40	ES+	1
62	PC 18:1e-18:2	770.6	20	508.4	30	5.40	ES+	2
63	PC 18:1e-18:3	768.6	20	500.3	30	5.40	ES+	1
64	PC 18:1e-18:3	768.6	20	508.4	30	5.40	ES+	2
65	PC 18:1e-18:4	766.6	20	498.3	30	5.40	ES+	1
66	PC 18:1e-18:4	766.6	20	508.4	30	5.40	ES+	2
67	PC 18:1e-20:0	802.7	20	508.4	30	5.40	ES+	1
68	PC 18:1e-20:0	802.7	20	534.3	30	5.40	ES+	2
69	PC 18:1e-20:1	800.7	20	508.4	30	5.40	ES+	1
70	PC 18:1e-20:1	800.7	20	532.3	30	5.40	ES+	2
71	PC 18:1e-20:2	798.6	20	508.4	30	5.40	ES+	1
72	PC 18:1e-20:2	798.6	20	530.3	30	5.40	ES+	2
73	PC 18:1e-20:3	796.6	20	508.4	30	5.40	ES+	1
74	PC 18:1e-20:3	796.6	20	528.3	30	5.40	ES+	2
75	PC 18:1e-20:4	794.6	20	508.4	30	5.40	ES+	1
76	PC 18:1e-20:4	794.6	20	526.3	30	5.40	ES+	2
77	PC 18:1e-20:5	792.6	20	508.4	30	5.40	ES+	1
78	PC 18:1e-20:5	792.6	20	524.3	30	5.40	ES+	2
79	PC 18:1e-22:0	830.7	20	508.4	30	5.40	ES+	1
80	PC 18:1e-22:0	830.7	20	562.3	30	5.40	ES+	2
81	PC 18:1e-22:1	828.7	20	508.4	30	5.40	ES+	1
82	PC 18:1e-22:1	828.7	20	560.3	30	5.40	ES+	2
83	PC 18:1e-22:2	826.7	20	508.4	30	5.40	ES+	1
84	PC 18:1e-22:2	826.7	20	558.3	30	5.40	ES+	2
85	PC 18:1e-22:3	824.7	20	508.4	30	5.40	ES+	1
86	PC 18:1e-22:3	824.7	20	556.3	30	5.40	ES+	2
87	PC 18:1e-22:4	822.6	20	508.4	30	5.40	ES+	1
88	PC 18:1e-22:4	822.6	20	554.3	30	5.40	ES+	2
89	PC 18:1e-22:5	820.6	20	508.4	30	5.40	ES+	1
90	PC 18:1e-22:5	820.6	20	552.3	30	5.40	ES+	2
91	PC 18:1e-22:6	818.6	20	508.4	30	5.40	ES+	1
92	PC 18:1e-22:6	818.6	20	550.3	30	5.40	ES+	2
93	PI 16:0-20:0	865.6	50	255.3	50	12.06	ES-	1
94	PI 16:0-20:0	865.6	50	311.2	50	12.06	ES-	2

95	PI 16:0-20:1	863.6	50	255.3	50	12.06	ES-	1
96	PI 16:0-20:1	863.6	50	309.2	50	12.06	ES-	2
97	PI 16:0-20:2	861.5	50	255.3	50	12.06	ES-	1
98	PI 16:0-20:2	861.5	50	307.2	50	12.06	ES-	2
99	PI 16:0-20:3	859.5	50	255.3	50	12.06	ES-	1
100	PI 16:0-20:3	859.5	50	305.2	50	12.06	ES-	2
101	PI 16:0-20:4	857.5	50	255.3	50	12.06	ES-	1
102	PI 16:0-20:4	857.5	50	303.2	50	12.06	ES-	2
103	PI 16:0-20:5	855.5	50	255.3	50	12.06	ES-	1
104	PI 16:0-20:5	855.5	50	301.2	50	12.06	ES-	2
105	PI 16:0-22:0	893.6	50	255.3	50	12.06	ES-	1
106	PI 16:0-22:0	893.6	50	339.2	50	12.06	ES-	2
107	PI 16:0-22:1	891.6	50	255.3	50	12.06	ES-	1
108	PI 16:0-22:1	891.6	50	337.2	50	12.06	ES-	2
109	PI 16:0-22:2	889.6	50	255.3	50	12.06	ES-	1
110	PI 16:0-22:2	889.6	50	335.2	50	12.06	ES-	2
111	PI 16:0-22:3	887.6	50	255.3	50	12.06	ES-	1
112	PI 16:0-22:3	887.6	50	333.2	50	12.06	ES-	2
113	PI 16:0-22:4	885.5	50	255.3	50	12.06	ES-	1
114	PI 16:0-22:4	885.5	50	331.2	50	12.06	ES-	2
115	PI 16:0-22:5	883.5	50	255.3	50	12.06	ES-	1
116	PI 16:0-22:5	883.5	50	329.2	50	12.06	ES-	2
117	PI 16:0-22:6	881.5	50	255.3	50	12.06	ES-	1
118	PI 16:0-22:6	881.5	50	327.2	50	12.06	ES-	2
119	PI 16:1-16:1	805.5	50	253.3	50	12.06	ES-	1
120	PI 16:1-18:0	835.5	50	253.3	50	12.06	ES-	1
121	PI 16:1-18:0	835.5	50	283.3	50	12.06	ES-	2
122	PI 16:1-18:1	833.5	50	253.3	50	12.06	ES-	1
123	PI 16:1-18:1	833.5	50	281.3	50	12.06	ES-	2
124	PI 16:1-18:2	831.5	50	253.3	50	12.06	ES-	1
125	PI 16:1-18:2	831.5	50	279.3	50	12.06	ES-	2
126	PI 16:1-18:3	829.5	50	253.3	50	12.06	ES-	1
127	PI 16:1-18:3	829.5	50	277.3	50	12.06	ES-	2
128	PI 16:1-18:4	827.5	50	253.3	50	12.06	ES-	1
129	PI 16:1-18:4	827.5	50	275.3	50	12.06	ES-	2

130	PI 16:1-20:0	863.6	50	253.3	50	12.06	ES-	1
131	PI 16:1-20:0	863.6	50	311.2	50	12.06	ES-	2
132	PI 16:1-20:1	861.5	50	253.3	50	12.06	ES-	1
133	PI 16:1-20:1	861.5	50	309.2	50	12.06	ES-	2
134	PI 16:1-20:2	859.5	50	253.3	50	12.06	ES-	1
135	PI 16:1-20:2	859.5	50	307.2	50	12.06	ES-	2
136	PI 16:1-20:3	857.5	50	253.3	50	12.06	ES-	1
137	PI 16:1-20:3	857.5	50	305.2	50	12.06	ES-	2
138	PI 16:1-20:4	855.5	50	253.3	50	12.06	ES-	1
139	PI 16:1-20:4	855.5	50	303.2	50	12.06	ES-	2
140	PI 16:1-20:5	853.5	50	253.3	50	12.06	ES-	1
141	PI 16:1-20:5	853.5	50	301.2	50	12.06	ES-	2
142	PI 16:1-22:0	891.6	50	253.3	50	12.06	ES-	1
143	PI 16:1-22:0	891.6	50	339.2	50	12.06	ES-	2
144	PI 16:1-22:1	889.6	50	253.3	50	12.06	ES-	1
145	PI 16:1-22:1	889.6	50	337.2	50	12.06	ES-	2
146	PI 16:1-22:2	887.6	50	253.3	50	12.06	ES-	1
147	PI 16:1-22:2	887.6	50	335.2	50	12.06	ES-	2
148	PI 16:1-22:3	885.5	50	253.3	50	12.06	ES-	1
149	PI 16:1-22:3	885.5	50	333.2	50	12.06	ES-	2
150	PI 16:1-22:4	883.5	50	253.3	50	12.06	ES-	1
151	PI 16:1-22:4	883.5	50	331.2	50	12.06	ES-	2
152	PI 16:1-22:5	881.5	50	253.3	50	12.06	ES-	1
153	PI 16:1-22:5	881.5	50	329.2	50	12.06	ES-	2
154	PI 16:1-22:6	879.5	50	253.3	50	12.06	ES-	1
155	PI 16:1-22:6	879.5	50	327.2	50	12.06	ES-	2
156	PI 17:0-14:1	793.5	50	225.3	50	12.06	ES-	1
157	PI 17:0-14:1	793.5	50	269.3	50	12.06	ES-	2
158	PI 18:0-18:0	865.6	50	283.3	50	12.06	ES-	1
159	PI 18:0-18:1	863.6	50	281.3	50	12.06	ES-	1
160	PI 18:0-18:1	863.6	50	283.3	50	12.06	ES-	2
161	PI 18:0-18:2	861.5	50	279.3	50	12.06	ES-	1
162	PI 18:0-18:2	861.5	50	283.3	50	12.06	ES-	2
163	PI 18:0-18:3	859.5	50	277.3	50	12.06	ES-	1
164	PI 18:0-18:3	859.5	50	283.3	50	12.06	ES-	2

165	PI 18:0-18:4	857.5	50	275.3	50	12.06	ES-	1
166	PI 18:0-18:4	857.5	50	283.3	50	12.06	ES-	2
167	PI 18:0-20:0	893.6	50	283.3	50	12.06	ES-	1
168	PI 18:0-20:0	893.6	50	311.2	50	12.06	ES-	2
169	PI 18:0-20:1	891.6	50	283.3	50	12.06	ES-	1
170	PI 18:0-20:1	891.6	50	309.2	50	12.06	ES-	2
171	PI 18:0-20:2	889.6	50	283.3	50	12.06	ES-	1
172	PI 18:0-20:2	889.6	50	307.2	50	12.06	ES-	2
173	PI 18:0-20:3	887.6	50	283.3	50	12.06	ES-	1
174	PI 18:0-20:3	887.6	50	305.2	50	12.06	ES-	2
175	PI 18:0-20:4	885.5	50	283.3	50	12.06	ES-	1
176	PI 18:0-20:4	885.5	50	303.2	50	12.06	ES-	2
177	PI 18:0-20:5	883.5	50	283.3	50	12.06	ES-	1
178	PI 18:0-20:5	883.5	50	301.2	50	12.06	ES-	2
179	PI 18:0-22:0	921.6	50	283.3	50	12.06	ES-	1
180	PI 18:0-22:0	921.6	50	339.2	50	12.06	ES-	2
181	PI 18:0-22:1	919.6	50	283.3	50	12.06	ES-	1
182	PI 18:0-22:1	919.6	50	337.2	50	12.06	ES-	2
183	PI 18:0-22:2	917.6	50	283.3	50	12.06	ES-	1
184	PI 18:0-22:2	917.6	50	335.2	50	12.06	ES-	2
185	PI 18:0-22:3	915.6	50	283.3	50	12.06	ES-	1
186	PI 18:0-22:3	915.6	50	333.2	50	12.06	ES-	2
187	PI 18:0-22:4	913.6	50	283.3	50	12.06	ES-	1
188	PI 18:0-22:4	913.6	50	331.2	50	12.06	ES-	2
189	PI 18:0-22:5	911.6	50	283.3	50	12.06	ES-	1
190	PI 18:0-22:5	911.6	50	329.2	50	12.06	ES-	2
191	PI 18:0-22:6	909.5	50	283.3	50	12.06	ES-	1
192	PI 18:0-22:6	909.5	50	327.2	50	12.06	ES-	2
193	PI 18:1-18:1	861.5	50	281.3	50	12.06	ES-	1
194	PI 18:1-18:2	859.5	50	279.3	50	12.06	ES-	1
195	PI 18:1-18:2	859.5	50	281.3	50	12.06	ES-	2
196	PI 18:1-18:3	857.5	50	277.3	50	12.06	ES-	1
197	PI 18:1-18:3	857.5	50	281.3	50	12.06	ES-	2
198	PI 18:1-18:4	855.5	50	275.3	50	12.06	ES-	1
199	PI 18:1-18:4	855.5	50	281.3	50	12.06	ES-	2

200	PI 18:1-20:0	891.6	50	281.3	50	12.06	ES-	1
201	PI 18:1-20:0	891.6	50	311.2	50	12.06	ES-	2
202	PI 18:1-20:1	889.6	50	281.3	50	12.06	ES-	1
203	PI 18:1-20:1	889.6	50	309.2	50	12.06	ES-	2
204	PI 18:1-20:2	887.6	50	281.3	50	12.06	ES-	1
205	PI 18:1-20:2	887.6	50	307.2	50	12.06	ES-	2
206	PI 18:1-20:3	885.5	50	281.3	50	12.06	ES-	1
207	PI 18:1-20:3	885.5	50	305.2	50	12.06	ES-	2
208	PI 18:1-20:4	883.5	50	281.3	50	12.06	ES-	1
209	PI 18:1-20:4	883.5	50	303.2	50	12.06	ES-	2
210	PI 18:1-20:5	881.5	50	281.3	50	12.06	ES-	1
211	PI 18:1-20:5	881.5	50	301.2	50	12.06	ES-	2
212	PI 18:1-22:0	919.6	50	281.3	50	12.06	ES-	1
213	PI 18:1-22:0	919.6	50	339.2	50	12.06	ES-	2
214	PI 18:1-22:1	917.6	50	281.3	50	12.06	ES-	1
215	PI 18:1-22:1	917.6	50	337.2	50	12.06	ES-	2
216	PI 18:1-22:2	915.6	50	281.3	50	12.06	ES-	1
217	PI 18:1-22:2	915.6	50	335.2	50	12.06	ES-	2
218	PI 18:1-22:3	913.6	50	281.3	50	12.06	ES-	1
219	PI 18:1-22:3	913.6	50	333.2	50	12.06	ES-	2
220	PI 18:1-22:4	911.6	50	281.3	50	12.06	ES-	1
221	PI 18:1-22:4	911.6	50	331.2	50	12.06	ES-	2
222	PI 18:1-22:5	909.5	50	281.3	50	12.06	ES-	1
223	PI 18:1-22:5	909.5	50	329.2	50	12.06	ES-	2
224	PI 18:1-22:6	907.5	50	281.3	50	12.06	ES-	1
225	PI 18:1-22:6	907.5	50	327.2	50	12.06	ES-	2
226	PI 18:2-18:2	857.5	50	279.3	50	12.06	ES-	1
227	PI 18:2-18:3	855.5	50	277.3	50	12.06	ES-	1
228	PI 18:2-18:3	855.5	50	279.3	50	12.06	ES-	2
229	PI 18:2-18:4	853.5	50	275.3	50	12.06	ES-	1
230	PI 18:2-18:4	853.5	50	279.3	50	12.06	ES-	2
231	PI 18:2-20:0	889.6	50	279.3	50	12.06	ES-	1
232	PI 18:2-20:0	889.6	50	311.2	50	12.06	ES-	2
233	PI 18:2-20:1	887.6	50	279.3	50	12.06	ES-	1
234	PI 18:2-20:1	887.6	50	309.2	50	12.06	ES-	2

235	PI 18:2-20:2	885.5	50	279.3	50	12.06	ES-	1
236	PI 18:2-20:2	885.5	50	307.2	50	12.06	ES-	2
237	PI 18:2-20:3	883.5	50	279.3	50	12.06	ES-	1
238	PI 18:2-20:3	883.5	50	305.2	50	12.06	ES-	2
239	PI 18:2-20:4	881.5	50	279.3	50	12.06	ES-	1
240	PI 18:2-20:4	881.5	50	303.2	50	12.06	ES-	2
241	PI 18:2-20:5	879.5	50	279.3	50	12.06	ES-	1
242	PI 18:2-20:5	879.5	50	301.2	50	12.06	ES-	2

Method 7: PCe and PI (3)

No	Name	Precursor	CV (V)	Product	CE (V)	RT setting (min)	IonMode	Ion
1	PC 18:2e-12:0	688.5	20	422.3	30	5.40	ES+	1
2	PC 18:2e-12:0	688.5	20	506.4	30	5.40	ES+	2
3	PC 18:2e-14:0	716.6	20	450.3	30	5.40	ES+	1
4	PC 18:2e-14:0	716.6	20	506.4	30	5.40	ES+	2
5	PC 18:2e-14:1	714.5	20	448.3	30	5.40	ES+	1
6	PC 18:2e-14:1	714.5	20	506.4	30	5.40	ES+	2
7	PC 18:2e-16:0	744.6	20	478.3	30	5.40	ES+	1
8	PC 18:2e-16:0	744.6	20	506.4	30	5.40	ES+	2
9	PC 18:2e-16:1	742.6	20	476.3	30	5.40	ES+	1
10	PC 18:2e-16:1	742.6	20	506.4	30	5.40	ES+	2
11	PC 18:2e-18:0	772.6	20	506.3	30	5.40	ES+	1
12	PC 18:2e-18:1	770.6	20	504.3	30	5.40	ES+	1
13	PC 18:2e-18:1	770.6	20	506.4	30	5.40	ES+	2
14	PC 18:2e-18:2	768.6	20	502.3	30	5.40	ES+	1
15	PC 18:2e-18:2	768.6	20	506.4	30	5.40	ES+	2
16	PC 18:2e-18:3	766.6	20	500.3	30	5.40	ES+	1
17	PC 18:2e-18:3	766.6	20	506.4	30	5.40	ES+	2
18	PC 18:2e-18:4	764.6	20	498.3	30	5.40	ES+	1
19	PC 18:2e-18:4	764.6	20	506.4	30	5.40	ES+	2
20	PC 18:2e-20:0	800.7	20	506.4	30	5.40	ES+	1
21	PC 18:2e-20:0	800.7	20	534.3	30	5.40	ES+	2
22	PC 18:2e-20:1	798.6	20	506.4	30	5.40	ES+	1
23	PC 18:2e-20:1	798.6	20	532.3	30	5.40	ES+	2
24	PC 18:2e-20:2	796.6	20	506.4	30	5.40	ES+	1
25	PC 18:2e-20:2	796.6	20	530.3	30	5.40	ES+	2

26	PC 18:2e-20:3	794.6	20	506.4	30	5.40	ES+	1
27	PC 18:2e-20:3	794.6	20	528.3	30	5.40	ES+	2
28	PC 18:2e-20:4	792.6	20	506.4	30	5.40	ES+	1
29	PC 18:2e-20:4	792.6	20	526.3	30	5.40	ES+	2
30	PC 18:2e-20:5	790.6	20	506.4	30	5.40	ES+	1
31	PC 18:2e-20:5	790.6	20	524.3	30	5.40	ES+	2
32	PC 18:2e-22:0	828.7	20	506.4	30	5.40	ES+	1
33	PC 18:2e-22:0	828.7	20	562.3	30	5.40	ES+	2
34	PC 18:2e-22:1	826.7	20	506.4	30	5.40	ES+	1
35	PC 18:2e-22:1	826.7	20	560.3	30	5.40	ES+	2
36	PC 18:2e-22:2	824.7	20	506.4	30	5.40	ES+	1
37	PC 18:2e-22:2	824.7	20	558.3	30	5.40	ES+	2
38	PC 18:2e-22:3	822.6	20	506.4	30	5.40	ES+	1
39	PC 18:2e-22:3	822.6	20	556.3	30	5.40	ES+	2
40	PC 18:2e-22:4	820.6	20	506.4	30	5.40	ES+	1
41	PC 18:2e-22:4	820.6	20	554.3	30	5.40	ES+	2
42	PC 18:2e-22:5	818.6	20	506.4	30	5.40	ES+	1
43	PC 18:2e-22:5	818.6	20	552.3	30	5.40	ES+	2
44	PC 18:2e-22:6	816.6	20	506.4	30	5.40	ES+	1
45	PC 18:2e-22:6	816.6	20	550.3	30	5.40	ES+	2
46	PI 18:2-22:0	917.6	50	279.3	50	12.06	ES-	1
47	PI 18:2-22:0	917.6	50	339.2	50	12.06	ES-	2
48	PI 18:2-22:1	915.6	50	279.3	50	12.06	ES-	1
49	PI 18:2-22:1	915.6	50	337.2	50	12.06	ES-	2
50	PI 18:2-22:2	913.6	50	279.3	50	12.06	ES-	1
51	PI 18:2-22:2	913.6	50	335.2	50	12.06	ES-	2
52	PI 18:2-22:3	911.6	50	279.3	50	12.06	ES-	1
53	PI 18:2-22:3	911.6	50	333.2	50	12.06	ES-	2
54	PI 18:2-22:4	909.5	50	279.3	50	12.06	ES-	1
55	PI 18:2-22:4	909.5	50	331.2	50	12.06	ES-	2
56	PI 18:2-22:5	907.5	50	279.3	50	12.06	ES-	1
57	PI 18:2-22:5	907.5	50	329.2	50	12.06	ES-	2
58	PI 18:2-22:6	905.5	50	279.3	50	12.06	ES-	1
59	PI 18:2-22:6	905.5	50	327.2	50	12.06	ES-	2
60	PI 18:3-18:3	853.5	50	277.3	50	12.06	ES-	1

61	PI 18:3-18:4	851.5	50	275.3	50	12.06	ES-	1
62	PI 18:3-18:4	851.5	50	277.3	50	12.06	ES-	2
63	PI 18:3-20:0	887.6	50	277.3	50	12.06	ES-	1
64	PI 18:3-20:0	887.6	50	311.2	50	12.06	ES-	2
65	PI 18:3-20:1	885.5	50	277.3	50	12.06	ES-	1
66	PI 18:3-20:1	885.5	50	309.2	50	12.06	ES-	2
67	PI 18:3-20:2	883.5	50	277.3	50	12.06	ES-	1
68	PI 18:3-20:2	883.5	50	307.2	50	12.06	ES-	2
69	PI 18:3-20:3	881.5	50	277.3	50	12.06	ES-	1
70	PI 18:3-20:3	881.5	50	305.2	50	12.06	ES-	2
71	PI 18:3-20:4	879.5	50	277.3	50	12.06	ES-	1
72	PI 18:3-20:4	879.5	50	303.2	50	12.06	ES-	2
73	PI 18:3-20:5	877.5	50	277.3	50	12.06	ES-	1
74	PI 18:3-20:5	877.5	50	301.2	50	12.06	ES-	2
75	PI 18:3-22:0	915.6	50	277.3	50	12.06	ES-	1
76	PI 18:3-22:0	915.6	50	339.2	50	12.06	ES-	2
77	PI 18:3-22:1	913.6	50	277.3	50	12.06	ES-	1
78	PI 18:3-22:1	913.6	50	337.2	50	12.06	ES-	2
79	PI 18:3-22:2	911.6	50	277.3	50	12.06	ES-	1
80	PI 18:3-22:2	911.6	50	335.2	50	12.06	ES-	2
81	PI 18:3-22:3	909.5	50	277.3	50	12.06	ES-	1
82	PI 18:3-22:3	909.5	50	333.2	50	12.06	ES-	2
83	PI 18:3-22:4	907.5	50	277.3	50	12.06	ES-	1
84	PI 18:3-22:4	907.5	50	331.2	50	12.06	ES-	2
85	PI 18:3-22:5	905.5	50	277.3	50	12.06	ES-	1
86	PI 18:3-22:5	905.5	50	329.2	50	12.06	ES-	2
87	PI 18:3-22:6	903.5	50	277.3	50	12.06	ES-	1
88	PI 18:3-22:6	903.5	50	327.2	50	12.06	ES-	2
89	PI 18:4-18:4	849.5	50	275.3	50	12.06	ES-	1
90	PI 18:4-20:0	885.5	50	275.3	50	12.06	ES-	1
91	PI 18:4-20:0	885.5	50	311.2	50	12.06	ES-	2
92	PI 18:4-20:1	883.5	50	275.3	50	12.06	ES-	1
93	PI 18:4-20:1	883.5	50	309.2	50	12.06	ES-	2
94	PI 18:4-20:2	881.5	50	275.3	50	12.06	ES-	1
95	PI 18:4-20:2	881.5	50	307.2	50	12.06	ES-	2

96	PI 18:4-20:3	879.5	50	275.3	50	12.06	ES-	1
97	PI 18:4-20:3	879.5	50	305.2	50	12.06	ES-	2
98	PI 18:4-20:4	877.5	50	275.3	50	12.06	ES-	1
99	PI 18:4-20:4	877.5	50	303.2	50	12.06	ES-	2
100	PI 18:4-20:5	875.5	50	275.3	50	12.06	ES-	1
101	PI 18:4-20:5	875.5	50	301.2	50	12.06	ES-	2
102	PI 18:4-22:0	913.6	50	275.3	50	12.06	ES-	1
103	PI 18:4-22:0	913.6	50	339.2	50	12.06	ES-	2
104	PI 18:4-22:1	911.6	50	275.3	50	12.06	ES-	1
105	PI 18:4-22:1	911.6	50	337.2	50	12.06	ES-	2
106	PI 18:4-22:2	909.5	50	275.3	50	12.06	ES-	1
107	PI 18:4-22:2	909.5	50	335.2	50	12.06	ES-	2
108	PI 18:4-22:3	907.5	50	275.3	50	12.06	ES-	1
109	PI 18:4-22:3	907.5	50	333.2	50	12.06	ES-	2
110	PI 18:4-22:4	905.5	50	275.3	50	12.06	ES-	1
111	PI 18:4-22:4	905.5	50	331.2	50	12.06	ES-	2
112	PI 18:4-22:5	903.5	50	275.3	50	12.06	ES-	1
113	PI 18:4-22:5	903.5	50	329.2	50	12.06	ES-	2
114	PI 18:4-22:6	901.5	50	275.3	50	12.06	ES-	1
115	PI 18:4-22:6	901.5	50	327.2	50	12.06	ES-	2
116	PI 20:0-20:0	921.6	50	311.2	50	12.06	ES-	1
117	PI 20:0-20:1	919.6	50	309.2	50	12.06	ES-	1
118	PI 20:0-20:1	919.6	50	311.2	50	12.06	ES-	2
119	PI 20:0-20:2	917.6	50	307.2	50	12.06	ES-	1
120	PI 20:0-20:2	917.6	50	311.2	50	12.06	ES-	2
121	PI 20:0-20:3	915.6	50	305.2	50	12.06	ES-	1
122	PI 20:0-20:3	915.6	50	311.2	50	12.06	ES-	2
123	PI 20:0-20:4	913.6	50	303.2	50	12.06	ES-	1
124	PI 20:0-20:4	913.6	50	311.2	50	12.06	ES-	2
125	PI 20:0-20:5	911.6	50	301.2	50	12.06	ES-	1
126	PI 20:0-20:5	911.6	50	311.2	50	12.06	ES-	2
127	PI 20:0-22:0	949.7	50	311.2	50	12.06	ES-	1
128	PI 20:0-22:0	949.7	50	339.2	50	12.06	ES-	2
129	PI 20:0-22:1	947.7	50	311.2	50	12.06	ES-	1
130	PI 20:0-22:1	947.7	50	337.2	50	12.06	ES-	2

131	PI 20:0-22:2	945.6	50	311.2	50	12.06	ES-	1
132	PI 20:0-22:2	945.6	50	335.2	50	12.06	ES-	2
133	PI 20:0-22:3	943.6	50	311.2	50	12.06	ES-	1
134	PI 20:0-22:3	943.6	50	333.2	50	12.06	ES-	2
135	PI 20:0-22:4	941.6	50	311.2	50	12.06	ES-	1
136	PI 20:0-22:4	941.6	50	331.2	50	12.06	ES-	2
137	PI 20:0-22:5	939.6	50	311.2	50	12.06	ES-	1
138	PI 20:0-22:5	939.6	50	329.2	50	12.06	ES-	2
139	PI 20:0-22:6	937.6	50	311.2	50	12.06	ES-	1
140	PI 20:0-22:6	937.6	50	327.2	50	12.06	ES-	2
141	PI 20:1-20:1	917.6	50	309.2	50	12.06	ES-	1
142	PI 20:1-20:2	915.6	50	307.2	50	12.06	ES-	1
143	PI 20:1-20:2	915.6	50	309.2	50	12.06	ES-	2
144	PI 20:1-20:3	913.6	50	305.2	50	12.06	ES-	1
145	PI 20:1-20:3	913.6	50	309.2	50	12.06	ES-	2
146	PI 20:1-20:4	911.6	50	303.2	50	12.06	ES-	1
147	PI 20:1-20:4	911.6	50	309.2	50	12.06	ES-	2
148	PI 20:1-20:5	909.5	50	301.2	50	12.06	ES-	1
149	PI 20:1-20:5	909.5	50	309.2	50	12.06	ES-	2
150	PI 20:1-22:0	947.7	50	309.2	50	12.06	ES-	1
151	PI 20:1-22:0	947.7	50	339.2	50	12.06	ES-	2
152	PI 20:1-22:1	945.6	50	309.2	50	12.06	ES-	1
153	PI 20:1-22:1	945.6	50	337.2	50	12.06	ES-	2
154	PI 20:1-22:2	943.6	50	309.2	50	12.06	ES-	1
155	PI 20:1-22:2	943.6	50	335.2	50	12.06	ES-	2
156	PI 20:1-22:3	941.6	50	309.2	50	12.06	ES-	1
157	PI 20:1-22:3	941.6	50	333.2	50	12.06	ES-	2
158	PI 20:1-22:4	939.6	50	309.2	50	12.06	ES-	1
159	PI 20:1-22:4	939.6	50	331.2	50	12.06	ES-	2
160	PI 20:1-22:5	937.6	50	309.2	50	12.06	ES-	1
161	PI 20:1-22:5	937.6	50	329.2	50	12.06	ES-	2
162	PI 20:1-22:6	935.6	50	309.2	50	12.06	ES-	1
163	PI 20:1-22:6	935.6	50	327.2	50	12.06	ES-	2
164	PI 20:2-20:2	913.6	50	307.2	50	12.06	ES-	1
165	PI 20:2-20:3	911.6	50	305.2	50	12.06	ES-	1

166	PI 20:2-20:3	911.6	50	307.2	50	12.06	ES-	2
167	PI 20:2-20:4	909.5	50	303.2	50	12.06	ES-	1
168	PI 20:2-20:4	909.5	50	307.2	50	12.06	ES-	2
169	PI 20:2-20:5	907.5	50	301.2	50	12.06	ES-	1
170	PI 20:2-20:5	907.5	50	307.2	50	12.06	ES-	2
171	PI 20:2-22:0	945.6	50	307.2	50	12.06	ES-	1
172	PI 20:2-22:0	945.6	50	339.2	50	12.06	ES-	2
173	PI 20:2-22:1	943.6	50	307.2	50	12.06	ES-	1
174	PI 20:2-22:1	943.6	50	337.2	50	12.06	ES-	2
175	PI 20:2-22:2	941.6	50	307.2	50	12.06	ES-	1
176	PI 20:2-22:2	941.6	50	335.2	50	12.06	ES-	2
177	PI 20:2-22:3	939.6	50	307.2	50	12.06	ES-	1
178	PI 20:2-22:3	939.6	50	333.2	50	12.06	ES-	2
179	PI 20:2-22:4	937.6	50	307.2	50	12.06	ES-	1
180	PI 20:2-22:4	937.6	50	331.2	50	12.06	ES-	2
181	PI 20:2-22:5	935.6	50	307.2	50	12.06	ES-	1
182	PI 20:2-22:5	935.6	50	329.2	50	12.06	ES-	2
183	PI 20:2-22:6	933.5	50	307.2	50	12.06	ES-	1
184	PI 20:2-22:6	933.5	50	327.2	50	12.06	ES-	2
185	PI 20:3-20:3	909.5	50	305.2	50	12.06	ES-	1
186	PI 20:3-20:4	907.5	50	303.2	50	12.06	ES-	1
187	PI 20:3-20:4	907.5	50	305.2	50	12.06	ES-	2
188	PI 20:3-20:5	905.5	50	301.2	50	12.06	ES-	1
189	PI 20:3-20:5	905.5	50	305.2	50	12.06	ES-	2

Method 8: LPLs, SM, Cer, and FFA

No	Name	Precursor	CV (V)	Product	CE (V)	RT setting (min)	IonMode	Ion
1	LPC 12:0	440.3	10	184.1	30	6.12	ES+	1
2	LPC 14:0	468.3	10	184.1	30	6.12	ES+	1
3	LPC 14:1	466.3	10	184.1	30	6.12	ES+	1
4	LPC 16:0	496.3	10	184.1	30	6.12	ES+	1
5	LPC 16:1	494.3	10	184.1	30	6.12	ES+	1
6	LPC 17:0	510.4	10	184.1	30	6.12	ES+	1
7	LPC 18:0	524.4	10	184.1	30	6.12	ES+	1
8	LPC 18:1	522.4	10	184.1	30	6.12	ES+	1
9	LPC 18:2	520.3	10	184.1	30	6.12	ES+	1

10	LPC 18:3	518.3	10	184.1	30	6.12	ES+	1
11	LPC 18:4	516.3	10	184.1	30	6.12	ES+	1
12	LPC 20:0	552.4	10	184.1	30	6.12	ES+	1
13	LPC 20:1	550.4	10	184.1	30	6.12	ES+	1
14	LPC 20:2	548.4	10	184.1	30	6.12	ES+	1
15	LPC 20:3	546.4	10	184.1	30	6.12	ES+	1
16	LPC 20:4	544.3	10	184.1	30	6.12	ES+	1
17	LPC 20:5	542.3	10	184.1	30	6.12	ES+	1
18	LPC 22:0	580.4	10	184.1	30	6.12	ES+	1
19	LPC 22:1	578.4	10	184.1	30	6.12	ES+	1
20	LPC 22:2	576.4	10	184.1	30	6.12	ES+	1
21	LPC 22:3	574.4	10	184.1	30	6.12	ES+	1
22	LPC 22:4	572.4	10	184.1	30	6.12	ES+	1
23	LPC 22:5	570.4	10	184.1	30	6.12	ES+	1
24	LPC 22:6	568.3	10	184.1	30	6.12	ES+	1
25	LPE 12:0	398.2	30	257.1	20	7.45	ES+	1
26	LPE 14:0	426.3	30	285.2	20	7.45	ES+	1
27	LPE 14:1	424.2	30	283.1	20	7.45	ES+	1
28	LPE 16:0	454.3	30	313.2	20	7.45	ES+	1
29	LPE 16:1	452.3	30	311.2	20	7.45	ES+	1
30	LPE 17:1	466.3	30	325.2	20	7.45	ES+	1
31	LPE 18:0	482.3	30	341.2	20	7.45	ES+	1
32	LPE 18:1	480.3	30	339.2	20	7.45	ES+	1
33	LPE 18:2	478.3	30	337.2	20	7.45	ES+	1
34	LPE 18:3	476.3	30	335.2	20	7.45	ES+	1
35	LPE 18:4	474.3	30	333.2	20	7.45	ES+	1
36	LPE 20:0	510.4	30	369.3	20	7.45	ES+	1
37	LPE 20:1	508.3	30	367.2	20	7.45	ES+	1
38	LPE 20:2	506.3	30	365.2	20	7.45	ES+	1
39	LPE 20:3	504.3	30	363.2	20	7.45	ES+	1
40	LPE 20:4	502.3	30	361.2	20	7.45	ES+	1
41	LPE 20:5	500.3	30	359.2	20	7.45	ES+	1
42	LPE 22:0	538.4	30	397.3	20	7.45	ES+	1
43	LPE 22:1	536.4	30	395.3	20	7.45	ES+	1
44	LPE 22:2	534.4	30	393.3	20	7.45	ES+	1

45	LPE 22:3	532.3	30	391.2	20	7.45	ES+	1
46	LPE 22:4	530.3	30	389.2	20	7.45	ES+	1
47	LPE 22:5	528.3	30	387.2	20	7.45	ES+	1
48	LPE 22:6	526.3	30	385.2	20	7.45	ES+	1
49	LPG 12:0	429.2	40	257.2	20	10.87	ES+	1
50	LPG 14:0	457.3	40	285.2	20	10.87	ES+	1
51	LPG 14:1	455.2	40	283.2	20	10.87	ES+	1
52	LPG 16:0	485.3	40	313.3	20	10.87	ES+	1
53	LPG 16:1	483.3	40	311.3	20	10.87	ES+	1
54	LPG 17:1	497.3	40	325.2	20	10.87	ES+	1
55	LPG 18:0	513.3	40	341.3	20	10.87	ES+	1
56	LPG 18:1	511.3	40	339.3	20	10.87	ES+	1
57	LPG 18:2	509.3	40	337.3	20	10.87	ES+	1
58	LPG 18:3	507.3	40	335.3	20	10.87	ES+	1
59	LPG 18:4	505.3	40	333.2	20	10.87	ES+	1
60	LPG 20:0	541.3	40	369.3	20	10.87	ES+	1
61	LPG 20:1	539.3	40	367.3	20	10.87	ES+	1
62	LPG 20:2	537.3	40	365.3	20	10.87	ES+	1
63	LPG 20:3	535.3	40	363.3	20	10.87	ES+	1
64	LPG 20:4	533.3	40	361.3	20	10.87	ES+	1
65	LPG 20:5	531.3	40	359.3	20	10.87	ES+	1
66	LPG 22:0	569.4	40	397.4	20	10.87	ES+	1
67	LPG 22:1	567.4	40	395.3	20	10.87	ES+	1
68	LPG 22:2	565.3	40	393.3	20	10.87	ES+	1
69	LPG 22:3	563.3	40	391.3	20	10.87	ES+	1
70	LPG 22:4	561.3	40	389.3	20	10.87	ES+	1
71	LPG 22:5	559.3	40	387.3	20	10.87	ES+	1
72	LPG 22:6	557.3	40	385.3	20	10.87	ES+	1
73	LPS 12:0	442.2	30	257.1	20	15.36	ES+	1
74	LPS 14:0	470.3	30	285.1	20	15.36	ES+	1
75	LPS 14:1	468.2	30	283.1	20	15.36	ES+	1
76	LPS 16:0	498.3	30	313.2	20	15.36	ES+	1
77	LPS 16:1	496.3	30	311.2	20	15.36	ES+	1
78	LPS 17:1	510.3	30	325.2	20	15.36	ES+	1
79	LPS 18:0	526.3	30	341.2	20	15.36	ES+	1

80	LPS 18:1	524.3	30	339.2	20	15.36	ES+	1
81	LPS 18:2	522.3	30	337.2	20	15.36	ES+	1
82	LPS 18:3	520.3	30	335.2	20	15.36	ES+	1
83	LPS 18:4	518.3	30	333.1	20	15.36	ES+	1
84	LPS 20:0	554.3	30	369.2	20	15.36	ES+	1
85	LPS 20:1	552.3	30	367.2	20	15.36	ES+	1
86	LPS 20:2	550.3	30	365.2	20	15.36	ES+	1
87	LPS 20:3	548.3	30	363.2	20	15.36	ES+	1
88	LPS 20:4	546.3	30	361.2	20	15.36	ES+	1
89	LPS 20:5	544.3	30	359.2	20	15.36	ES+	1
90	LPS 22:0	582.4	30	397.3	20	15.36	ES+	1
91	LPS 22:1	580.4	30	395.2	20	15.36	ES+	1
92	LPS 22:2	578.3	30	393.2	20	15.36	ES+	1
93	LPS 22:3	576.3	30	391.2	20	15.36	ES+	1
94	LPS 22:4	574.3	30	389.2	20	15.36	ES+	1
95	LPS 22:5	572.3	30	387.2	20	15.36	ES+	1
96	LPS 22:6	570.3	30	385.2	20	15.36	ES+	1
97	SM d18:1-12:0	647.5	50	184.1	30	5.83	ES+	1
98	SM d18:1-14:0	675.5	50	184.1	30	5.83	ES+	1
99	SM d18:1-14:1	673.5	50	184.1	30	5.83	ES+	1
100	SM d18:1-16:0	703.6	50	184.1	30	5.83	ES+	1
101	SM d18:1-16:1	701.6	50	184.1	30	5.83	ES+	1
102	SM d18:1-17:0	717.6	50	184.1	30	5.83	ES+	1
103	SM d18:1-18:0	731.6	50	184.1	30	5.83	ES+	1
104	SM d18:1-18:1	729.6	50	184.1	30	5.83	ES+	1
105	SM d18:1-18:2	727.6	50	184.1	30	5.83	ES+	1
106	SM d18:1-18:3	725.6	50	184.1	30	5.83	ES+	1
107	SM d18:1-18:4	723.5	50	184.1	30	5.83	ES+	1
108	SM d18:1-20:0	759.6	50	184.1	30	5.83	ES+	1
109	SM d18:1-20:1	757.6	50	184.1	30	5.83	ES+	1
110	SM d18:1-20:2	755.6	50	184.1	30	5.83	ES+	1
111	SM d18:1-20:3	753.6	50	184.1	30	5.83	ES+	1
112	SM d18:1-20:4	751.6	50	184.1	30	5.83	ES+	1
113	SM d18:1-20:5	749.6	50	184.1	30	5.83	ES+	1
114	SM d18:1-22:0	787.7	50	184.1	30	5.83	ES+	1

115	SM d18:1-22:1	785.7	50	184.1	30	5.83	ES+	1
116	SM d18:1-22:2	783.6	50	184.1	30	5.83	ES+	1
117	SM d18:1-22:3	781.6	50	184.1	30	5.83	ES+	1
118	SM d18:1-22:4	779.6	50	184.1	30	5.83	ES+	1
119	SM d18:1-22:5	777.6	50	184.1	30	5.83	ES+	1
120	SM d18:1-22:6	775.6	50	184.1	30	5.83	ES+	1
121	Cer d18:1-12:0	482.5	20	264.3	30	4.48	ES+	1
122	Cer d18:1-14:0	510.5	20	264.3	30	4.48	ES+	1
123	Cer d18:1-14:1	508.5	20	264.3	30	4.48	ES+	1
124	Cer d18:1-16:0	538.5	20	264.3	30	4.48	ES+	1
125	Cer d18:1-16:1	536.5	20	264.3	30	4.48	ES+	1
126	Cer d18:1-17:0	552.5	20	264.3	30	4.48	ES+	1
127	Cer d18:1-18:0	566.6	20	264.3	30	4.48	ES+	1
128	Cer d18:1-18:1	564.5	20	264.3	30	4.48	ES+	1
129	Cer d18:1-18:2	562.5	20	264.3	30	4.48	ES+	1
130	Cer d18:1-18:3	560.5	20	264.3	30	4.48	ES+	1
131	Cer d18:1-18:4	558.5	20	264.3	30	4.48	ES+	1
132	Cer d18:1-20:0	594.6	20	264.3	30	4.48	ES+	1
133	Cer d18:1-20:1	592.6	20	264.3	30	4.48	ES+	1
134	Cer d18:1-20:2	590.6	20	264.3	30	4.48	ES+	1
135	Cer d18:1-20:3	588.5	20	264.3	30	4.48	ES+	1
136	Cer d18:1-20:4	586.5	20	264.3	30	4.48	ES+	1
137	Cer d18:1-20:5	584.5	20	264.3	30	4.48	ES+	1
138	Cer d18:1-22:0	622.6	20	264.3	30	4.48	ES+	1
139	Cer d18:1-22:1	620.6	20	264.3	30	4.48	ES+	1
140	Cer d18:1-22:2	618.6	20	264.3	30	4.48	ES+	1
141	Cer d18:1-22:3	616.6	20	264.3	30	4.48	ES+	1
142	Cer d18:1-22:4	614.6	20	264.3	30	4.48	ES+	1
143	Cer d18:1-22:5	612.5	20	264.3	30	4.48	ES+	1
144	Cer d18:1-22:6	610.5	20	264.3	30	4.48	ES+	1
145	CE 12:0	586.6	20	369.3	10	1.12	ES+	1
146	CE 14:0	614.6	20	369.3	10	1.12	ES+	1
147	CE 14:1	612.6	20	369.3	10	1.12	ES+	1
148	CE 16:0	642.6	20	369.3	10	1.12	ES+	1
149	CE 16:1	640.6	20	369.3	10	1.12	ES+	1

150	CE 17:0	656.6	20	369.3	10	1.12	ES+	1
151	CE 18:0	670.6	20	369.3	10	1.12	ES+	1
152	CE 18:1	668.6	20	369.3	10	1.12	ES+	1
153	CE 18:2	666.6	20	369.3	10	1.12	ES+	1
154	CE 18:3	664.6	20	369.3	10	1.12	ES+	1
155	CE 18:4	662.6	20	369.3	10	1.12	ES+	1
156	CE 20:0	698.7	20	369.3	10	1.12	ES+	1
157	CE 20:1	696.7	20	369.3	10	1.12	ES+	1
158	CE 20:2	694.6	20	369.3	10	1.12	ES+	1
159	CE 20:3	692.6	20	369.3	10	1.12	ES+	1
160	CE 20:4	690.6	20	369.3	10	1.12	ES+	1
161	CE 20:5	688.6	20	369.3	10	1.12	ES+	1
162	CE 22:0	726.7	20	369.3	10	1.12	ES+	1
163	CE 22:1	724.7	20	369.3	10	1.12	ES+	1
164	CE 22:2	722.7	20	369.3	10	1.12	ES+	1
165	CE 22:3	720.7	20	369.3	10	1.12	ES+	1
166	CE 22:4	718.6	20	369.3	10	1.12	ES+	1
167	CE 22:5	716.6	20	369.3	10	1.12	ES+	1
168	CE 22:6	714.6	20	369.3	10	1.12	ES+	1
169	MAG 12:0	275.2	10	257.2	10	3.97	ES+	1
170	MAG 14:0	303.3	10	285.3	10	3.97	ES+	1
171	MAG 14:1	301.3	10	283.3	10	3.97	ES+	1
172	MAG 16:0	331.3	10	313.3	10	3.97	ES+	1
173	MAG 16:1	329.3	10	311.3	10	3.97	ES+	1
174	MAG 17:0	345.3	10	327.3	10	3.97	ES+	1
175	MAG 18:0	359.3	10	341.3	10	3.97	ES+	1
176	MAG 18:1	357.3	10	339.3	10	3.97	ES+	1
177	MAG 18:2	355.3	10	337.3	10	3.97	ES+	1
178	MAG 18:3	353.3	10	335.3	10	3.97	ES+	1
179	MAG 18:4	351.3	10	333.3	10	3.97	ES+	1
180	MAG 20:0	387.4	10	369.4	10	3.97	ES+	1
181	MAG 20:1	385.4	10	367.4	10	3.97	ES+	1
182	MAG 20:2	383.3	10	365.3	10	3.97	ES+	1
183	MAG 20:3	381.3	10	363.3	10	3.97	ES+	1
184	MAG 20:4	379.3	10	361.3	10	3.97	ES+	1

185	MAG 20:5	377.3	10	359.3	10	3.97	ES+	1
186	MAG 22:0	415.4	10	397.4	10	3.97	ES+	1
187	MAG 22:1	413.4	10	395.4	10	3.97	ES+	1
188	MAG 22:2	411.4	10	393.4	10	3.97	ES+	1
189	MAG 22:3	409.4	10	391.4	10	3.97	ES+	1
190	MAG 22:4	407.3	10	389.3	10	3.97	ES+	1
191	MAG 22:5	405.3	10	387.3	10	3.97	ES+	1
192	MAG 22:6	403.3	10	385.3	10	3.97	ES+	1
193	LPI 12:0	515.2	10	240.9	40	14.02	ES-	1
194	LPI 14:0	543.3	10	240.9	40	14.02	ES-	1
195	LPI 14:1	541.2	10	240.9	40	14.02	ES-	1
196	LPI 16:0	571.3	10	240.9	40	14.02	ES-	1
197	LPI 16:1	569.3	10	240.9	40	14.02	ES-	1
198	LPI 17:1	583.3	10	240.9	40	14.02	ES-	1
199	LPI 18:0	599.3	10	240.9	40	14.02	ES-	1
200	LPI 18:1	597.3	10	240.9	40	14.02	ES-	1
201	LPI 18:2	595.3	10	240.9	40	14.02	ES-	1
202	LPI 18:3	593.3	10	240.9	40	14.02	ES-	1
203	LPI 18:4	591.3	10	240.9	40	14.02	ES-	1
204	LPI 20:0	627.4	10	240.9	40	14.02	ES-	1
205	LPI 20:1	625.3	10	240.9	40	14.02	ES-	1
206	LPI 20:2	623.3	10	240.9	40	14.02	ES-	1
207	LPI 20:3	621.3	10	240.9	40	14.02	ES-	1
208	LPI 20:4	619.3	10	240.9	40	14.02	ES-	1
209	LPI 20:5	617.3	10	240.9	40	14.02	ES-	1
210	LPI 22:0	655.4	10	240.9	40	14.02	ES-	1
211	LPI 22:1	653.4	10	240.9	40	14.02	ES-	1
212	LPI 22:2	651.4	10	240.9	40	14.02	ES-	1
213	LPI 22:3	649.3	10	240.9	40	14.02	ES-	1
214	LPI 22:4	647.3	10	240.9	40	14.02	ES-	1
215	LPI 22:5	645.3	10	240.9	40	14.02	ES-	1
216	LPI 22:6	643.3	10	240.9	40	14.02	ES-	1
217	LPA 12:0	353.2	10	152.8	20	17.43	ES-	1
218	LPA 14:0	381.2	10	152.8	20	17.43	ES-	1
219	LPA 14:1	379.2	10	152.8	20	17.43	ES-	1

220	LPA 16:0	409.2	10	152.8	20	17.43	ES-	1
221	LPA 16:1	407.2	10	152.8	20	17.43	ES-	1
222	LPA 17:0	423.3	10	152.8	20	17.43	ES-	1
223	LPA 18:0	437.3	10	152.8	20	17.43	ES-	1
224	LPA 18:1	435.3	10	152.8	20	17.43	ES-	1
225	LPA 18:2	433.2	10	152.8	20	17.43	ES-	1
226	LPA 18:3	431.2	10	152.8	20	17.43	ES-	1
227	LPA 18:4	429.2	10	152.8	20	17.43	ES-	1
228	LPA 20:0	465.3	10	152.8	20	17.43	ES-	1
229	LPA 20:1	463.3	10	152.8	20	17.43	ES-	1
230	LPA 20:2	461.3	10	152.8	20	17.43	ES-	1
231	LPA 20:3	459.3	10	152.8	20	17.43	ES-	1
232	LPA 20:4	457.2	10	152.8	20	17.43	ES-	1
233	LPA 20:5	455.2	10	152.8	20	17.43	ES-	1
234	LPA 22:0	493.3	10	152.8	20	17.43	ES-	1
235	LPA 22:1	491.3	10	152.8	20	17.43	ES-	1
236	LPA 22:2	489.3	10	152.8	20	17.43	ES-	1
237	LPA 22:3	487.3	10	152.8	20	17.43	ES-	1
238	LPA 22:4	485.3	10	152.8	20	17.43	ES-	1
239	LPA 22:5	483.3	10	152.8	20	17.43	ES-	1
240	LPA 22:6	481.2	10	152.8	20	17.43	ES-	1
241	FFA 12:0	199.2	10	199.2	10	4.02	ES-	1
242	FFA 14:0	227.2	10	227.2	10	4.02	ES-	1
243	FFA 14:1	225.2	10	225.2	10	4.02	ES-	1
244	FFA 16:0	255.2	10	255.2	10	4.02	ES-	1
245	FFA 16:1	253.2	10	253.2	10	4.02	ES-	1
246	FFA 17:0	269.2	10	269.2	10	4.02	ES-	1
247	FFA 18:0	283.3	10	283.3	10	4.02	ES-	1
248	FFA 18:1	281.2	10	281.2	10	4.02	ES-	1
249	FFA 18:2	279.2	10	279.2	10	4.02	ES-	1
250	FFA 18:3	277.2	10	277.2	10	4.02	ES-	1
251	FFA 18:4	275.2	10	275.2	10	4.02	ES-	1
252	FFA 20:0	311.3	10	311.3	10	4.02	ES-	1
253	FFA 20:1	309.3	10	309.3	10	4.02	ES-	1
254	FFA 20:2	307.3	10	307.3	10	4.02	ES-	1

255	FFA 20:3	305.2	10	305.2	10	4.02	ES-	1
256	FFA 20:4	303.2	10	303.2	10	4.02	ES-	1
257	FFA 20:5	301.2	10	301.2	10	4.02	ES-	1
258	FFA 22:0	339.3	10	339.3	10	4.02	ES-	1
259	FFA 22:1	337.3	10	337.3	10	4.02	ES-	1
260	FFA 22:2	335.3	10	335.3	10	4.02	ES-	1
261	FFA 22:3	333.3	10	333.3	10	4.02	ES-	1
262	FFA 22:4	331.3	10	331.3	10	4.02	ES-	1
263	FFA 22:5	329.2	10	329.2	10	4.02	ES-	1
264	FFA 22:6	327.2	10	327.2	10	4.02	ES-	1

Method 9: PC, PE, PG, and PS (1)

No	Name	Precursor	CV (V)	Product	CE (V)	RT setting (min)	IonMode	Ion
1	PC 12:0-12:0	680.5	15	199.3	40	5.46	ES-	1
2	PC 12:0-14:0	708.5	15	199.3	40	5.46	ES-	1
3	PC 12:0-14:0	708.5	15	227.3	40	5.46	ES-	2
4	PC 12:0-14:1	706.5	15	199.3	40	5.46	ES-	1
5	PC 12:0-14:1	706.5	15	225.3	40	5.46	ES-	2
6	PC 12:0-16:0	736.5	15	199.3	40	5.46	ES-	1
7	PC 12:0-16:0	736.5	15	255.3	40	5.46	ES-	2
8	PC 12:0-16:1	734.5	15	199.3	40	5.46	ES-	1
9	PC 12:0-16:1	734.5	15	253.3	40	5.46	ES-	2
10	PC 12:0-18:0	764.5	15	199.3	40	5.46	ES-	1
11	PC 12:0-18:0	764.5	15	283.3	40	5.46	ES-	2
12	PC 12:0-18:1	762.5	15	199.3	40	5.46	ES-	1
13	PC 12:0-18:1	762.5	15	281.3	40	5.46	ES-	2
14	PC 12:0-18:2	760.5	15	199.3	40	5.46	ES-	1
15	PC 12:0-18:2	760.5	15	279.3	40	5.46	ES-	2
16	PC 12:0-18:3	758.5	15	199.3	40	5.46	ES-	1
17	PC 12:0-18:3	758.5	15	277.3	40	5.46	ES-	2
18	PC 12:0-18:4	756.5	15	199.3	40	5.46	ES-	1
19	PC 12:0-18:4	756.5	15	275.3	40	5.46	ES-	2
20	PC 12:0-20:0	792.6	15	199.3	40	5.46	ES-	1
21	PC 12:0-20:0	792.6	15	311.2	40	5.46	ES-	2
22	PC 12:0-20:1	790.6	15	199.3	40	5.46	ES-	1
23	PC 12:0-20:1	790.6	15	309.2	40	5.46	ES-	2

24	PC 12:0-20:2	788.5	15	199.3	40	5.46	ES-	1
25	PC 12:0-20:2	788.5	15	307.2	40	5.46	ES-	2
26	PC 12:0-20:3	786.5	15	199.3	40	5.46	ES-	1
27	PC 12:0-20:3	786.5	15	305.2	40	5.46	ES-	2
28	PC 12:0-20:4	784.5	15	199.3	40	5.46	ES-	1
29	PC 12:0-20:4	784.5	15	303.2	40	5.46	ES-	2
30	PC 12:0-20:5	782.5	15	199.3	40	5.46	ES-	1
31	PC 12:0-20:5	782.5	15	301.2	40	5.46	ES-	2
32	PC 12:0-22:0	820.6	15	199.3	40	5.46	ES-	1
33	PC 12:0-22:0	820.6	15	339.2	40	5.46	ES-	2
34	PC 12:0-22:1	818.6	15	199.3	40	5.46	ES-	1
35	PC 12:0-22:1	818.6	15	337.2	40	5.46	ES-	2
36	PC 12:0-22:2	816.6	15	199.3	40	5.46	ES-	1
37	PC 12:0-22:2	816.6	15	335.2	40	5.46	ES-	2
38	PC 12:0-22:3	814.6	15	199.3	40	5.46	ES-	1
39	PC 12:0-22:3	814.6	15	333.2	40	5.46	ES-	2
40	PC 12:0-22:4	812.5	15	199.3	40	5.46	ES-	1
41	PC 12:0-22:4	812.5	15	331.2	40	5.46	ES-	2
42	PC 12:0-22:5	810.5	15	199.3	40	5.46	ES-	1
43	PC 12:0-22:5	810.5	15	329.2	40	5.46	ES-	2
44	PC 12:0-22:6	808.5	15	199.3	40	5.46	ES-	1
45	PC 12:0-22:6	808.5	15	327.2	40	5.46	ES-	2
46	PC 14:0-14:0	736.5	15	227.3	40	5.46	ES-	1
47	PC 14:0-14:1	734.5	15	225.3	40	5.46	ES-	1
48	PC 14:0-14:1	734.5	15	227.3	40	5.46	ES-	2
49	PC 14:0-16:0	764.5	15	227.3	40	5.46	ES-	1
50	PC 14:0-16:0	764.5	15	255.3	40	5.46	ES-	2
51	PC 14:0-16:1	762.5	15	227.3	40	5.46	ES-	1
52	PC 14:0-16:1	762.5	15	253.3	40	5.46	ES-	2
53	PC 14:0-18:0	792.6	15	227.3	40	5.46	ES-	1
54	PC 14:0-18:0	792.6	15	283.3	40	5.46	ES-	2
55	PC 14:0-18:1	790.6	15	227.3	40	5.46	ES-	1
56	PC 14:0-18:1	790.6	15	281.3	40	5.46	ES-	2
57	PC 14:0-18:2	788.5	15	227.3	40	5.46	ES-	1
58	PC 14:0-18:2	788.5	15	279.3	40	5.46	ES-	2

59	PC 14:0-18:3	786.5	15	227.3	40	5.46	ES-	1
60	PC 14:0-18:3	786.5	15	277.3	40	5.46	ES-	2
61	PC 14:0-18:4	784.5	15	227.3	40	5.46	ES-	1
62	PC 14:0-18:4	784.5	15	275.3	40	5.46	ES-	2
63	PC 14:0-20:0	820.6	15	227.3	40	5.46	ES-	1
64	PC 14:0-20:0	820.6	15	311.2	40	5.46	ES-	2
65	PC 14:0-20:1	818.6	15	227.3	40	5.46	ES-	1
66	PC 14:0-20:1	818.6	15	309.2	40	5.46	ES-	2
67	PC 14:0-20:2	816.6	15	227.3	40	5.46	ES-	1
68	PC 14:0-20:2	816.6	15	307.2	40	5.46	ES-	2
69	PC 14:0-20:3	814.6	15	227.3	40	5.46	ES-	1
70	PC 14:0-20:3	814.6	15	305.2	40	5.46	ES-	2
71	PC 14:0-20:4	812.5	15	227.3	40	5.46	ES-	1
72	PC 14:0-20:4	812.5	15	303.2	40	5.46	ES-	2
73	PC 14:0-20:5	810.5	15	227.3	40	5.46	ES-	1
74	PC 14:0-20:5	810.5	15	301.2	40	5.46	ES-	2
75	PC 14:0-22:0	848.6	15	227.3	40	5.46	ES-	1
76	PC 14:0-22:0	848.6	15	339.2	40	5.46	ES-	2
77	PC 14:0-22:1	846.6	15	227.3	40	5.46	ES-	1
78	PC 14:0-22:1	846.6	15	337.2	40	5.46	ES-	2
79	PC 14:0-22:2	844.6	15	227.3	40	5.46	ES-	1
80	PC 14:0-22:2	844.6	15	335.2	40	5.46	ES-	2
81	PC 14:0-22:3	842.6	15	227.3	40	5.46	ES-	1
82	PC 14:0-22:3	842.6	15	333.2	40	5.46	ES-	2
83	PC 14:0-22:4	840.6	15	227.3	40	5.46	ES-	1
84	PC 14:0-22:4	840.6	15	331.2	40	5.46	ES-	2
85	PC 14:0-22:5	838.6	15	227.3	40	5.46	ES-	1
86	PC 14:0-22:5	838.6	15	329.2	40	5.46	ES-	2
87	PC 14:0-22:6	836.5	15	227.3	40	5.46	ES-	1
88	PC 14:0-22:6	836.5	15	327.2	40	5.46	ES-	2
89	PC 14:1-14:1	732.5	15	225.3	40	5.46	ES-	1
90	PC 14:1-16:0	762.5	15	225.3	40	5.46	ES-	1
91	PC 14:1-16:0	762.5	15	255.3	40	5.46	ES-	2
92	PC 14:1-16:1	760.5	15	225.3	40	5.46	ES-	1
93	PC 14:1-16:1	760.5	15	253.3	40	5.46	ES-	2

94	PC 14:1-18:0	790.6	15	225.3	40	5.46	ES-	1
95	PC 14:1-18:0	790.6	15	283.3	40	5.46	ES-	2
96	PC 14:1-18:1	788.5	15	225.3	40	5.46	ES-	1
97	PC 14:1-18:1	788.5	15	281.3	40	5.46	ES-	2
98	PC 14:1-18:2	786.5	15	225.3	40	5.46	ES-	1
99	PC 14:1-18:2	786.5	15	279.3	40	5.46	ES-	2
100	PC 14:1-18:3	784.5	15	225.3	40	5.46	ES-	1
101	PC 14:1-18:3	784.5	15	277.3	40	5.46	ES-	2
102	PC 14:1-18:4	782.5	15	225.3	40	5.46	ES-	1
103	PC 14:1-18:4	782.5	15	275.3	40	5.46	ES-	2
104	PC 14:1-20:0	818.6	15	225.3	40	5.46	ES-	1
105	PC 14:1-20:0	818.6	15	311.2	40	5.46	ES-	2
106	PC 14:1-20:1	816.6	15	225.3	40	5.46	ES-	1
107	PC 14:1-20:1	816.6	15	309.2	40	5.46	ES-	2
108	PC 14:1-20:2	814.6	15	225.3	40	5.46	ES-	1
109	PC 14:1-20:2	814.6	15	307.2	40	5.46	ES-	2
110	PC 14:1-20:3	812.5	15	225.3	40	5.46	ES-	1
111	PC 14:1-20:3	812.5	15	305.2	40	5.46	ES-	2
112	PC 14:1-20:4	810.5	15	225.3	40	5.46	ES-	1
113	PC 14:1-20:4	810.5	15	303.2	40	5.46	ES-	2
114	PC 14:1-20:5	808.5	15	225.3	40	5.46	ES-	1
115	PC 14:1-20:5	808.5	15	301.2	40	5.46	ES-	2
116	PC 14:1-22:0	846.6	15	225.3	40	5.46	ES-	1
117	PC 14:1-22:0	846.6	15	339.2	40	5.46	ES-	2
118	PC 14:1-22:1	844.6	15	225.3	40	5.46	ES-	1
119	PC 14:1-22:1	844.6	15	337.2	40	5.46	ES-	2
120	PC 14:1-22:2	842.6	15	225.3	40	5.46	ES-	1
121	PC 14:1-22:2	842.6	15	335.2	40	5.46	ES-	2
122	PC 14:1-22:3	840.6	15	225.3	40	5.46	ES-	1
123	PC 14:1-22:3	840.6	15	333.2	40	5.46	ES-	2
124	PC 14:1-22:4	838.6	15	225.3	40	5.46	ES-	1
125	PC 14:1-22:4	838.6	15	331.2	40	5.46	ES-	2
126	PC 14:1-22:5	836.5	15	225.3	40	5.46	ES-	1
127	PC 14:1-22:5	836.5	15	329.2	40	5.46	ES-	2
128	PC 14:1-22:6	834.5	15	225.3	40	5.46	ES-	1

129	PC 14:1-22:6	834.5	15	327.2	40	5.46	ES-	2
130	PC 16:0-16:0	792.6	15	255.3	40	5.46	ES-	1
131	PC 16:0-16:1	790.6	15	253.3	40	5.46	ES-	1
132	PC 16:0-16:1	790.6	15	255.3	40	5.46	ES-	2
133	PC 16:0-18:0	820.6	15	255.3	40	5.46	ES-	1
134	PC 16:0-18:0	820.6	15	283.3	40	5.46	ES-	2
135	PC 16:0-18:1	818.6	15	255.3	40	5.46	ES-	1
136	PC 16:0-18:1	818.6	15	281.3	40	5.46	ES-	2
137	PC 16:0-18:2	816.6	15	255.3	40	5.46	ES-	1
138	PC 16:0-18:2	816.6	15	279.3	40	5.46	ES-	2
139	PC 16:0-18:3	814.6	15	255.3	40	5.46	ES-	1
140	PC 16:0-18:3	814.6	15	277.3	40	5.46	ES-	2
141	PC 16:0-18:4	812.5	15	255.3	40	5.46	ES-	1
142	PC 16:0-18:4	812.5	15	275.3	40	5.46	ES-	2
143	PE 12:0-12:0	578.4	50	199.3	25	6.32	ES-	1
144	PE 12:0-14:0	606.4	50	199.3	25	6.32	ES-	1
145	PE 12:0-14:0	606.4	50	227.3	25	6.32	ES-	2
146	PE 12:0-14:1	604.4	50	199.3	25	6.32	ES-	1
147	PE 12:0-14:1	604.4	50	225.3	25	6.32	ES-	2
148	PE 12:0-16:0	634.4	50	199.3	25	6.32	ES-	1
149	PE 12:0-16:0	634.4	50	255.3	25	6.32	ES-	2
150	PE 12:0-16:1	632.4	50	199.3	25	6.32	ES-	1
151	PE 12:0-16:1	632.4	50	253.3	25	6.32	ES-	2
152	PE 12:0-18:0	662.5	50	199.3	25	6.32	ES-	1
153	PE 12:0-18:0	662.5	50	283.3	25	6.32	ES-	2
154	PE 12:0-18:1	660.5	50	199.3	25	6.32	ES-	1
155	PE 12:0-18:1	660.5	50	281.3	25	6.32	ES-	2
156	PE 12:0-18:2	658.4	50	199.3	25	6.32	ES-	1
157	PE 12:0-18:2	658.4	50	279.3	25	6.32	ES-	2
158	PE 12:0-18:3	656.4	50	199.3	25	6.32	ES-	1
159	PE 12:0-18:3	656.4	50	277.3	25	6.32	ES-	2
160	PE 12:0-18:4	654.4	50	199.3	25	6.32	ES-	1
161	PE 12:0-18:4	654.4	50	275.3	25	6.32	ES-	2
162	PE 12:0-20:0	690.5	50	199.3	25	6.32	ES-	1
163	PE 12:0-20:0	690.5	50	311.2	25	6.32	ES-	2

164	PE 12:0-20:1	688.5	50	199.3	25	6.32	ES-	1
165	PE 12:0-20:1	688.5	50	309.2	25	6.32	ES-	2
166	PE 12:0-20:2	686.5	50	199.3	25	6.32	ES-	1
167	PE 12:0-20:2	686.5	50	307.2	25	6.32	ES-	2
168	PE 12:0-20:3	684.5	50	199.3	25	6.32	ES-	1
169	PE 12:0-20:3	684.5	50	305.2	25	6.32	ES-	2
170	PE 12:0-20:4	682.4	50	199.3	25	6.32	ES-	1
171	PE 12:0-20:4	682.4	50	303.2	25	6.32	ES-	2
172	PE 12:0-20:5	680.4	50	199.3	25	6.32	ES-	1
173	PE 12:0-20:5	680.4	50	301.2	25	6.32	ES-	2
174	PE 12:0-22:0	718.5	50	199.3	25	6.32	ES-	1
175	PE 12:0-22:0	718.5	50	339.2	25	6.32	ES-	2
176	PE 12:0-22:1	716.5	50	199.3	25	6.32	ES-	1
177	PE 12:0-22:1	716.5	50	337.2	25	6.32	ES-	2
178	PE 12:0-22:2	714.5	50	199.3	25	6.32	ES-	1
179	PE 12:0-22:2	714.5	50	335.2	25	6.32	ES-	2
180	PE 12:0-22:3	712.5	50	199.3	25	6.32	ES-	1
181	PE 12:0-22:3	712.5	50	333.2	25	6.32	ES-	2
182	PE 12:0-22:4	710.5	50	199.3	25	6.32	ES-	1
183	PE 12:0-22:4	710.5	50	331.2	25	6.32	ES-	2
184	PE 12:0-22:5	708.5	50	199.3	25	6.32	ES-	1
185	PE 12:0-22:5	708.5	50	329.2	25	6.32	ES-	2
186	PE 12:0-22:6	706.4	50	199.3	25	6.32	ES-	1
187	PE 12:0-22:6	706.4	50	327.2	25	6.32	ES-	2
188	PE 14:0-14:0	634.4	50	227.3	25	6.32	ES-	1
189	PE 14:0-14:1	632.4	50	225.3	25	6.32	ES-	1
190	PE 14:0-14:1	632.4	50	227.3	25	6.32	ES-	2
191	PE 14:0-16:0	662.5	50	227.3	25	6.32	ES-	1
192	PE 14:0-16:0	662.5	50	255.3	25	6.32	ES-	2
193	PE 14:0-16:1	660.5	50	227.3	25	6.32	ES-	1
194	PE 14:0-16:1	660.5	50	253.3	25	6.32	ES-	2
195	PE 14:0-18:0	690.5	50	227.3	25	6.32	ES-	1
196	PE 14:0-18:0	690.5	50	283.3	25	6.32	ES-	2
197	PE 14:0-18:1	688.5	50	227.3	25	6.32	ES-	1
198	PE 14:0-18:1	688.5	50	281.3	25	6.32	ES-	2

199	PE 14:0-18:2	686.5	50	227.3	25	6.32	ES-	1
200	PE 14:0-18:2	686.5	50	279.3	25	6.32	ES-	2
201	PE 14:0-18:3	684.5	50	227.3	25	6.32	ES-	1
202	PE 14:0-18:3	684.5	50	277.3	25	6.32	ES-	2
203	PE 14:0-18:4	682.4	50	227.3	25	6.32	ES-	1
204	PE 14:0-18:4	682.4	50	275.3	25	6.32	ES-	2
205	PE 14:0-20:0	718.5	50	227.3	25	6.32	ES-	1
206	PE 14:0-20:0	718.5	50	311.2	25	6.32	ES-	2
207	PE 14:0-20:1	716.5	50	227.3	25	6.32	ES-	1
208	PE 14:0-20:1	716.5	50	309.2	25	6.32	ES-	2
209	PE 14:0-20:2	714.5	50	227.3	25	6.32	ES-	1
210	PE 14:0-20:2	714.5	50	307.2	25	6.32	ES-	2
211	PE 14:0-20:3	712.5	50	227.3	25	6.32	ES-	1
212	PE 14:0-20:3	712.5	50	305.2	25	6.32	ES-	2
213	PE 14:0-20:4	710.5	50	227.3	25	6.32	ES-	1
214	PE 14:0-20:4	710.5	50	303.2	25	6.32	ES-	2
215	PE 14:0-20:5	708.5	50	227.3	25	6.32	ES-	1
216	PE 14:0-20:5	708.5	50	301.2	25	6.32	ES-	2
217	PE 14:0-22:0	746.6	50	227.3	25	6.32	ES-	1
218	PE 14:0-22:0	746.6	50	339.2	25	6.32	ES-	2
219	PE 14:0-22:1	744.6	50	227.3	25	6.32	ES-	1
220	PE 14:0-22:1	744.6	50	337.2	25	6.32	ES-	2
221	PE 14:0-22:2	742.5	50	227.3	25	6.32	ES-	1
222	PE 14:0-22:2	742.5	50	335.2	25	6.32	ES-	2
223	PE 14:0-22:3	740.5	50	227.3	25	6.32	ES-	1
224	PE 14:0-22:3	740.5	50	333.2	25	6.32	ES-	2
225	PE 14:0-22:4	738.5	50	227.3	25	6.32	ES-	1
226	PE 14:0-22:4	738.5	50	331.2	25	6.32	ES-	2
227	PE 14:0-22:5	736.5	50	227.3	25	6.32	ES-	1
228	PE 14:0-22:5	736.5	50	329.2	25	6.32	ES-	2
229	PE 14:0-22:6	734.5	50	227.3	25	6.32	ES-	1
230	PE 14:0-22:6	734.5	50	327.2	25	6.32	ES-	2
231	PE 14:1-14:1	630.4	50	225.3	25	6.32	ES-	1
232	PE 14:1-16:0	660.5	50	225.3	25	6.32	ES-	1
233	PE 14:1-16:0	660.5	50	255.3	25	6.32	ES-	2

234	PE 14:1-16:1	658.4	50	225.3	25	6.32	ES-	1
235	PE 14:1-16:1	658.4	50	253.3	25	6.32	ES-	2
236	PE 14:1-18:0	688.5	50	225.3	25	6.32	ES-	1
237	PE 14:1-18:0	688.5	50	283.3	25	6.32	ES-	2
238	PE 14:1-18:1	686.5	50	225.3	25	6.32	ES-	1
239	PE 14:1-18:1	686.5	50	281.3	25	6.32	ES-	2
240	PE 14:1-18:2	684.5	50	225.3	25	6.32	ES-	1
241	PE 14:1-18:2	684.5	50	279.3	25	6.32	ES-	2
242	PE 14:1-18:3	682.4	50	225.3	25	6.32	ES-	1
243	PE 14:1-18:3	682.4	50	277.3	25	6.32	ES-	2
244	PE 14:1-18:4	680.4	50	225.3	25	6.32	ES-	1
245	PE 14:1-18:4	680.4	50	275.3	25	6.32	ES-	2
246	PE 14:1-20:0	716.5	50	225.3	25	6.32	ES-	1
247	PE 14:1-20:0	716.5	50	311.2	25	6.32	ES-	2
248	PE 14:1-20:1	714.5	50	225.3	25	6.32	ES-	1
249	PE 14:1-20:1	714.5	50	309.2	25	6.32	ES-	2
250	PE 14:1-20:2	712.5	50	225.3	25	6.32	ES-	1
251	PE 14:1-20:2	712.5	50	307.2	25	6.32	ES-	2
252	PE 14:1-20:3	710.5	50	225.3	25	6.32	ES-	1
253	PE 14:1-20:3	710.5	50	305.2	25	6.32	ES-	2
254	PE 14:1-20:4	708.5	50	225.3	25	6.32	ES-	1
255	PE 14:1-20:4	708.5	50	303.2	25	6.32	ES-	2
256	PE 14:1-20:5	706.4	50	225.3	25	6.32	ES-	1
257	PE 14:1-20:5	706.4	50	301.2	25	6.32	ES-	2
258	PE 14:1-22:0	744.6	50	225.3	25	6.32	ES-	1
259	PE 14:1-22:0	744.6	50	339.2	25	6.32	ES-	2
260	PE 14:1-22:1	742.5	50	225.3	25	6.32	ES-	1
261	PE 14:1-22:1	742.5	50	337.2	25	6.32	ES-	2
262	PE 14:1-22:2	740.5	50	225.3	25	6.32	ES-	1
263	PE 14:1-22:2	740.5	50	335.2	25	6.32	ES-	2
264	PE 14:1-22:3	738.5	50	225.3	25	6.32	ES-	1
265	PE 14:1-22:3	738.5	50	333.2	25	6.32	ES-	2
266	PE 14:1-22:4	736.5	50	225.3	25	6.32	ES-	1
267	PE 14:1-22:4	736.5	50	331.2	25	6.32	ES-	2
268	PE 14:1-22:5	734.5	50	225.3	25	6.32	ES-	1

269	PE 14:1-22:5	734.5	50	329.2	25	6.32	ES-	2
270	PE 14:1-22:6	732.5	50	225.3	25	6.32	ES-	1
271	PE 14:1-22:6	732.5	50	327.2	25	6.32	ES-	2
272	PE 16:0-16:0	690.5	50	255.3	25	6.32	ES-	1
273	PE 16:0-16:1	688.5	50	253.3	25	6.32	ES-	1
274	PE 16:0-16:1	688.5	50	255.3	25	6.32	ES-	2
275	PE 16:0-18:0	718.5	50	255.3	25	6.32	ES-	1
276	PE 16:0-18:0	718.5	50	283.3	25	6.32	ES-	2
277	PE 16:0-18:1	716.5	50	255.3	25	6.32	ES-	1
278	PE 16:0-18:1	716.5	50	281.3	25	6.32	ES-	2
279	PE 16:0-18:2	714.5	50	255.3	25	6.32	ES-	1
280	PE 16:0-18:2	714.5	50	279.3	25	6.32	ES-	2
281	PE 16:0-18:3	712.5	50	255.3	25	6.32	ES-	1
282	PE 16:0-18:3	712.5	50	277.3	25	6.32	ES-	2
283	PE 16:0-18:4	710.5	50	255.3	25	6.32	ES-	1
284	PE 16:0-18:4	710.5	50	275.3	25	6.32	ES-	2
285	PG 12:0-12:0	609.4	30	199.3	40	8.99	ES-	1
286	PG 12:0-14:0	637.4	30	199.3	40	8.99	ES-	1
287	PG 12:0-14:0	637.4	30	227.3	40	8.99	ES-	2
288	PG 12:0-14:1	635.4	30	199.3	40	8.99	ES-	1
289	PG 12:0-14:1	635.4	30	225.3	40	8.99	ES-	2
290	PG 12:0-16:0	665.4	30	199.3	40	8.99	ES-	1
291	PG 12:0-16:0	665.4	30	255.3	40	8.99	ES-	2
292	PG 12:0-16:1	663.4	30	199.3	40	8.99	ES-	1
293	PG 12:0-16:1	663.4	30	253.3	40	8.99	ES-	2
294	PG 12:0-18:0	693.5	30	199.3	40	8.99	ES-	1
295	PG 12:0-18:0	693.5	30	283.3	40	8.99	ES-	2
296	PG 12:0-18:1	691.5	30	199.3	40	8.99	ES-	1
297	PG 12:0-18:1	691.5	30	281.3	40	8.99	ES-	2
298	PG 12:0-18:2	689.4	30	199.3	40	8.99	ES-	1
299	PG 12:0-18:2	689.4	30	279.3	40	8.99	ES-	2
300	PG 12:0-18:3	687.4	30	199.3	40	8.99	ES-	1
301	PG 12:0-18:3	687.4	30	277.3	40	8.99	ES-	2
302	PG 12:0-18:4	685.4	30	199.3	40	8.99	ES-	1
303	PG 12:0-18:4	685.4	30	275.3	40	8.99	ES-	2

304	PG 12:0-20:0	721.5	30	199.3	40	8.99	ES-	1
305	PG 12:0-20:0	721.5	30	311.2	40	8.99	ES-	2
306	PG 12:0-20:1	719.5	30	199.3	40	8.99	ES-	1
307	PG 12:0-20:1	719.5	30	309.2	40	8.99	ES-	2
308	PG 12:0-20:2	717.5	30	199.3	40	8.99	ES-	1
309	PG 12:0-20:2	717.5	30	307.2	40	8.99	ES-	2
310	PG 12:0-20:3	715.5	30	199.3	40	8.99	ES-	1
311	PG 12:0-20:3	715.5	30	305.2	40	8.99	ES-	2
312	PG 12:0-20:4	713.4	30	199.3	40	8.99	ES-	1
313	PG 12:0-20:4	713.4	30	303.2	40	8.99	ES-	2
314	PG 12:0-20:5	711.4	30	199.3	40	8.99	ES-	1
315	PG 12:0-20:5	711.4	30	301.2	40	8.99	ES-	2
316	PG 12:0-22:0	749.5	30	199.3	40	8.99	ES-	1
317	PG 12:0-22:0	749.5	30	339.2	40	8.99	ES-	2
318	PG 12:0-22:1	747.5	30	199.3	40	8.99	ES-	1
319	PG 12:0-22:1	747.5	30	337.2	40	8.99	ES-	2
320	PG 12:0-22:2	745.5	30	199.3	40	8.99	ES-	1
321	PG 12:0-22:2	745.5	30	335.2	40	8.99	ES-	2
322	PG 12:0-22:3	743.5	30	199.3	40	8.99	ES-	1
323	PG 12:0-22:3	743.5	30	333.2	40	8.99	ES-	2
324	PG 12:0-22:4	741.5	30	199.3	40	8.99	ES-	1
325	PG 12:0-22:4	741.5	30	331.2	40	8.99	ES-	2
326	PG 12:0-22:5	739.5	30	199.3	40	8.99	ES-	1
327	PG 12:0-22:5	739.5	30	329.2	40	8.99	ES-	2
328	PG 12:0-22:6	737.4	30	199.3	40	8.99	ES-	1
329	PG 12:0-22:6	737.4	30	327.2	40	8.99	ES-	2
330	PG 14:0-14:0	665.4	30	227.3	40	8.99	ES-	1
331	PG 14:0-14:1	663.4	30	225.3	40	8.99	ES-	1
332	PG 14:0-14:1	663.4	30	227.3	40	8.99	ES-	2
333	PG 14:0-16:0	693.5	30	227.3	40	8.99	ES-	1
334	PG 14:0-16:0	693.5	30	255.3	40	8.99	ES-	2
335	PG 14:0-16:1	691.5	30	227.3	40	8.99	ES-	1
336	PG 14:0-16:1	691.5	30	253.3	40	8.99	ES-	2
337	PG 14:0-18:0	721.5	30	227.3	40	8.99	ES-	1
338	PG 14:0-18:0	721.5	30	283.3	40	8.99	ES-	2

339	PG 14:0-18:1	719.5	30	227.3	40	8.99	ES-	1
340	PG 14:0-18:1	719.5	30	281.3	40	8.99	ES-	2
341	PG 14:0-18:2	717.5	30	227.3	40	8.99	ES-	1
342	PG 14:0-18:2	717.5	30	279.3	40	8.99	ES-	2
343	PG 14:0-18:3	715.5	30	227.3	40	8.99	ES-	1
344	PG 14:0-18:3	715.5	30	277.3	40	8.99	ES-	2
345	PG 14:0-18:4	713.4	30	227.3	40	8.99	ES-	1
346	PG 14:0-18:4	713.4	30	275.3	40	8.99	ES-	2
347	PG 14:0-20:0	749.5	30	227.3	40	8.99	ES-	1
348	PG 14:0-20:0	749.5	30	311.2	40	8.99	ES-	2
349	PG 14:0-20:1	747.5	30	227.3	40	8.99	ES-	1
350	PG 14:0-20:1	747.5	30	309.2	40	8.99	ES-	2
351	PG 14:0-20:2	745.5	30	227.3	40	8.99	ES-	1
352	PG 14:0-20:2	745.5	30	307.2	40	8.99	ES-	2
353	PG 14:0-20:3	743.5	30	227.3	40	8.99	ES-	1
354	PG 14:0-20:3	743.5	30	305.2	40	8.99	ES-	2
355	PG 14:0-20:4	741.5	30	227.3	40	8.99	ES-	1
356	PG 14:0-20:4	741.5	30	303.2	40	8.99	ES-	2
357	PG 14:0-20:5	739.5	30	227.3	40	8.99	ES-	1
358	PG 14:0-20:5	739.5	30	301.2	40	8.99	ES-	2
359	PG 14:0-22:0	777.6	30	227.3	40	8.99	ES-	1
360	PG 14:0-22:0	777.6	30	339.2	40	8.99	ES-	2
361	PG 14:0-22:1	775.5	30	227.3	40	8.99	ES-	1
362	PG 14:0-22:1	775.5	30	337.2	40	8.99	ES-	2
363	PG 14:0-22:2	773.5	30	227.3	40	8.99	ES-	1
364	PG 14:0-22:2	773.5	30	335.2	40	8.99	ES-	2
365	PG 14:0-22:3	771.5	30	227.3	40	8.99	ES-	1
366	PG 14:0-22:3	771.5	30	333.2	40	8.99	ES-	2
367	PG 14:0-22:4	769.5	30	227.3	40	8.99	ES-	1
368	PG 14:0-22:4	769.5	30	331.2	40	8.99	ES-	2
369	PG 14:0-22:5	767.5	30	227.3	40	8.99	ES-	1
370	PG 14:0-22:5	767.5	30	329.2	40	8.99	ES-	2
371	PG 14:0-22:6	765.5	30	227.3	40	8.99	ES-	1
372	PG 14:0-22:6	765.5	30	327.2	40	8.99	ES-	2
373	PG 14:1-14:1	661.4	30	225.3	40	8.99	ES-	1

374	PG 14:1-16:0	691.5	30	225.3	40	8.99	ES-	1
375	PG 14:1-16:0	691.5	30	255.3	40	8.99	ES-	2
376	PG 14:1-16:1	689.4	30	225.3	40	8.99	ES-	1
377	PG 14:1-16:1	689.4	30	253.3	40	8.99	ES-	2
378	PG 14:1-18:0	719.5	30	225.3	40	8.99	ES-	1
379	PG 14:1-18:0	719.5	30	283.3	40	8.99	ES-	2
380	PG 14:1-18:1	717.5	30	225.3	40	8.99	ES-	1
381	PG 14:1-18:1	717.5	30	281.3	40	8.99	ES-	2
382	PG 14:1-18:2	715.5	30	225.3	40	8.99	ES-	1
383	PG 14:1-18:2	715.5	30	279.3	40	8.99	ES-	2
384	PG 14:1-18:3	713.4	30	225.3	40	8.99	ES-	1
385	PG 14:1-18:3	713.4	30	277.3	40	8.99	ES-	2
386	PG 14:1-18:4	711.4	30	225.3	40	8.99	ES-	1
387	PG 14:1-18:4	711.4	30	275.3	40	8.99	ES-	2
388	PG 14:1-20:0	747.5	30	225.3	40	8.99	ES-	1
389	PG 14:1-20:0	747.5	30	311.2	40	8.99	ES-	2
390	PG 14:1-20:1	745.5	30	225.3	40	8.99	ES-	1
391	PG 14:1-20:1	745.5	30	309.2	40	8.99	ES-	2
392	PG 14:1-20:2	743.5	30	225.3	40	8.99	ES-	1
393	PG 14:1-20:2	743.5	30	307.2	40	8.99	ES-	2
394	PG 14:1-20:3	741.5	30	225.3	40	8.99	ES-	1
395	PG 14:1-20:3	741.5	30	305.2	40	8.99	ES-	2
396	PG 14:1-20:4	739.5	30	225.3	40	8.99	ES-	1
397	PG 14:1-20:4	739.5	30	303.2	40	8.99	ES-	2
398	PG 14:1-20:5	737.4	30	225.3	40	8.99	ES-	1
399	PG 14:1-20:5	737.4	30	301.2	40	8.99	ES-	2
400	PG 14:1-22:0	775.5	30	225.3	40	8.99	ES-	1
401	PG 14:1-22:0	775.5	30	339.2	40	8.99	ES-	2
402	PG 14:1-22:1	773.5	30	225.3	40	8.99	ES-	1
403	PG 14:1-22:1	773.5	30	337.2	40	8.99	ES-	2
404	PG 14:1-22:2	771.5	30	225.3	40	8.99	ES-	1
405	PG 14:1-22:2	771.5	30	335.2	40	8.99	ES-	2
406	PG 14:1-22:3	769.5	30	225.3	40	8.99	ES-	1
407	PG 14:1-22:3	769.5	30	333.2	40	8.99	ES-	2
408	PG 14:1-22:4	767.5	30	225.3	40	8.99	ES-	1

409	PG 14:1-22:4	767.5	30	331.2	40	8.99	ES-	2
410	PG 14:1-22:5	765.5	30	225.3	40	8.99	ES-	1
411	PG 14:1-22:5	765.5	30	329.2	40	8.99	ES-	2
412	PG 14:1-22:6	763.5	30	225.3	40	8.99	ES-	1
413	PG 14:1-22:6	763.5	30	327.2	40	8.99	ES-	2
414	PG 16:0-16:0	721.5	30	255.3	40	8.99	ES-	1
415	PG 16:0-16:1	719.5	30	253.3	40	8.99	ES-	1
416	PG 16:0-16:1	719.5	30	255.3	40	8.99	ES-	2
417	PG 16:0-18:0	749.5	30	255.3	40	8.99	ES-	1
418	PG 16:0-18:0	749.5	30	283.3	40	8.99	ES-	2
419	PG 16:0-18:1	747.5	30	255.3	40	8.99	ES-	1
420	PG 16:0-18:1	747.5	30	281.3	40	8.99	ES-	2
421	PG 16:0-18:2	745.5	30	255.3	40	8.99	ES-	1
422	PG 16:0-18:2	745.5	30	279.3	40	8.99	ES-	2
423	PG 16:0-18:3	743.5	30	255.3	40	8.99	ES-	1
424	PG 16:0-18:3	743.5	30	277.3	40	8.99	ES-	2
425	PG 16:0-18:4	741.5	30	255.3	40	8.99	ES-	1
426	PG 16:0-18:4	741.5	30	275.3	40	8.99	ES-	2
427	PS 12:0-12:0	622.4	30	199.3	50	12.23	ES-	1
428	PS 12:0-14:0	650.4	30	199.3	50	12.23	ES-	1
429	PS 12:0-14:0	650.4	30	227.3	50	12.23	ES-	2
430	PS 12:0-14:1	648.4	30	199.3	50	12.23	ES-	1
431	PS 12:0-14:1	648.4	30	225.3	50	12.23	ES-	2
432	PS 12:0-16:0	678.4	30	199.3	50	12.23	ES-	1
433	PS 12:0-16:0	678.4	30	255.3	50	12.23	ES-	2
434	PS 12:0-16:1	676.4	30	199.3	50	12.23	ES-	1
435	PS 12:0-16:1	676.4	30	253.3	50	12.23	ES-	2
436	PS 12:0-18:0	706.5	30	199.3	50	12.23	ES-	1
437	PS 12:0-18:0	706.5	30	283.3	50	12.23	ES-	2
438	PS 12:0-18:1	704.5	30	199.3	50	12.23	ES-	1
439	PS 12:0-18:1	704.5	30	281.3	50	12.23	ES-	2
440	PS 12:0-18:2	702.4	30	199.3	50	12.23	ES-	1
441	PS 12:0-18:2	702.4	30	279.3	50	12.23	ES-	2
442	PS 12:0-18:3	700.4	30	199.3	50	12.23	ES-	1
443	PS 12:0-18:3	700.4	30	277.3	50	12.23	ES-	2

444	PS 12:0-18:4	698.4	30	199.3	50	12.23	ES-	1
445	PS 12:0-18:4	698.4	30	275.3	50	12.23	ES-	2
446	PS 12:0-20:0	734.5	30	199.3	50	12.23	ES-	1
447	PS 12:0-20:0	734.5	30	311.2	50	12.23	ES-	2
448	PS 12:0-20:1	732.5	30	199.3	50	12.23	ES-	1
449	PS 12:0-20:1	732.5	30	309.2	50	12.23	ES-	2
450	PS 12:0-20:2	730.5	30	199.3	50	12.23	ES-	1
451	PS 12:0-20:2	730.5	30	307.2	50	12.23	ES-	2
452	PS 12:0-20:3	728.5	30	199.3	50	12.23	ES-	1
453	PS 12:0-20:3	728.5	30	305.2	50	12.23	ES-	2
454	PS 12:0-20:4	726.4	30	199.3	50	12.23	ES-	1
455	PS 12:0-20:4	726.4	30	303.2	50	12.23	ES-	2
456	PS 12:0-20:5	724.4	30	199.3	50	12.23	ES-	1
457	PS 12:0-20:5	724.4	30	301.2	50	12.23	ES-	2
458	PS 12:0-22:0	762.5	30	199.3	50	12.23	ES-	1
459	PS 12:0-22:0	762.5	30	339.2	50	12.23	ES-	2
460	PS 12:0-22:1	760.5	30	199.3	50	12.23	ES-	1
461	PS 12:0-22:1	760.5	30	337.2	50	12.23	ES-	2
462	PS 12:0-22:2	758.5	30	199.3	50	12.23	ES-	1
463	PS 12:0-22:2	758.5	30	335.2	50	12.23	ES-	2
464	PS 12:0-22:3	756.5	30	199.3	50	12.23	ES-	1
465	PS 12:0-22:3	756.5	30	333.2	50	12.23	ES-	2
466	PS 12:0-22:4	754.5	30	199.3	50	12.23	ES-	1
467	PS 12:0-22:4	754.5	30	331.2	50	12.23	ES-	2
468	PS 12:0-22:5	752.5	30	199.3	50	12.23	ES-	1
469	PS 12:0-22:5	752.5	30	329.2	50	12.23	ES-	2
470	PS 12:0-22:6	750.4	30	199.3	50	12.23	ES-	1
471	PS 12:0-22:6	750.4	30	327.2	50	12.23	ES-	2
472	PS 14:0-14:0	678.4	30	227.3	50	12.23	ES-	1
473	PS 14:0-14:1	676.4	30	225.3	50	12.23	ES-	1
474	PS 14:0-14:1	676.4	30	227.3	50	12.23	ES-	2
475	PS 14:0-16:0	706.5	30	227.3	50	12.23	ES-	1
476	PS 14:0-16:0	706.5	30	255.3	50	12.23	ES-	2
477	PS 14:0-16:1	704.5	30	227.3	50	12.23	ES-	1
478	PS 14:0-16:1	704.5	30	253.3	50	12.23	ES-	2

479	PS 14:0-18:0	734.5	30	227.3	50	12.23	ES-	1
480	PS 14:0-18:0	734.5	30	283.3	50	12.23	ES-	2
481	PS 14:0-18:1	732.5	30	227.3	50	12.23	ES-	1
482	PS 14:0-18:1	732.5	30	281.3	50	12.23	ES-	2
483	PS 14:0-18:2	730.5	30	227.3	50	12.23	ES-	1
484	PS 14:0-18:2	730.5	30	279.3	50	12.23	ES-	2
485	PS 14:0-18:3	728.5	30	227.3	50	12.23	ES-	1
486	PS 14:0-18:3	728.5	30	277.3	50	12.23	ES-	2
487	PS 14:0-18:4	726.4	30	227.3	50	12.23	ES-	1
488	PS 14:0-18:4	726.4	30	275.3	50	12.23	ES-	2
489	PS 14:0-20:0	762.5	30	227.3	50	12.23	ES-	1
490	PS 14:0-20:0	762.5	30	311.2	50	12.23	ES-	2
491	PS 14:0-20:1	760.5	30	227.3	50	12.23	ES-	1
492	PS 14:0-20:1	760.5	30	309.2	50	12.23	ES-	2
493	PS 14:0-20:2	758.5	30	227.3	50	12.23	ES-	1
494	PS 14:0-20:2	758.5	30	307.2	50	12.23	ES-	2
495	PS 14:0-20:3	756.5	30	227.3	50	12.23	ES-	1
496	PS 14:0-20:3	756.5	30	305.2	50	12.23	ES-	2
497	PS 14:0-20:4	754.5	30	227.3	50	12.23	ES-	1
498	PS 14:0-20:4	754.5	30	303.2	50	12.23	ES-	2
499	PS 14:0-20:5	752.5	30	227.3	50	12.23	ES-	1
500	PS 14:0-20:5	752.5	30	301.2	50	12.23	ES-	2
501	PS 14:0-22:0	790.6	30	227.3	50	12.23	ES-	1
502	PS 14:0-22:0	790.6	30	339.2	50	12.23	ES-	2
503	PS 14:0-22:1	788.5	30	227.3	50	12.23	ES-	1
504	PS 14:0-22:1	788.5	30	337.2	50	12.23	ES-	2
505	PS 14:0-22:2	786.5	30	227.3	50	12.23	ES-	1
506	PS 14:0-22:2	786.5	30	335.2	50	12.23	ES-	2
507	PS 14:0-22:3	784.5	30	227.3	50	12.23	ES-	1
508	PS 14:0-22:3	784.5	30	333.2	50	12.23	ES-	2
509	PS 14:0-22:4	782.5	30	227.3	50	12.23	ES-	1
510	PS 14:0-22:4	782.5	30	331.2	50	12.23	ES-	2
511	PS 14:0-22:5	780.5	30	227.3	50	12.23	ES-	1
512	PS 14:0-22:5	780.5	30	329.2	50	12.23	ES-	2
513	PS 14:0-22:6	778.5	30	227.3	50	12.23	ES-	1

514	PS 14:0-22:6	778.5	30	327.2	50	12.23	ES-	2
515	PS 14:1-14:1	674.4	30	225.3	50	12.23	ES-	1
516	PS 14:1-16:0	704.5	30	225.3	50	12.23	ES-	1
517	PS 14:1-16:0	704.5	30	255.3	50	12.23	ES-	2
518	PS 14:1-16:1	702.4	30	225.3	50	12.23	ES-	1
519	PS 14:1-16:1	702.4	30	253.3	50	12.23	ES-	2
520	PS 14:1-18:0	732.5	30	225.3	50	12.23	ES-	1
521	PS 14:1-18:0	732.5	30	283.3	50	12.23	ES-	2
522	PS 14:1-18:1	730.5	30	225.3	50	12.23	ES-	1
523	PS 14:1-18:1	730.5	30	281.3	50	12.23	ES-	2
524	PS 14:1-18:2	728.5	30	225.3	50	12.23	ES-	1
525	PS 14:1-18:2	728.5	30	279.3	50	12.23	ES-	2
526	PS 14:1-18:3	726.4	30	225.3	50	12.23	ES-	1
527	PS 14:1-18:3	726.4	30	277.3	50	12.23	ES-	2
528	PS 14:1-18:4	724.4	30	225.3	50	12.23	ES-	1
529	PS 14:1-18:4	724.4	30	275.3	50	12.23	ES-	2
530	PS 14:1-20:0	760.5	30	225.3	50	12.23	ES-	1
531	PS 14:1-20:0	760.5	30	311.2	50	12.23	ES-	2
532	PS 14:1-20:1	758.5	30	225.3	50	12.23	ES-	1
533	PS 14:1-20:1	758.5	30	309.2	50	12.23	ES-	2
534	PS 14:1-20:2	756.5	30	225.3	50	12.23	ES-	1
535	PS 14:1-20:2	756.5	30	307.2	50	12.23	ES-	2
536	PS 14:1-20:3	754.5	30	225.3	50	12.23	ES-	1
537	PS 14:1-20:3	754.5	30	305.2	50	12.23	ES-	2
538	PS 14:1-20:4	752.5	30	225.3	50	12.23	ES-	1
539	PS 14:1-20:4	752.5	30	303.2	50	12.23	ES-	2
540	PS 14:1-20:5	750.4	30	225.3	50	12.23	ES-	1
541	PS 14:1-20:5	750.4	30	301.2	50	12.23	ES-	2
542	PS 14:1-22:0	788.5	30	225.3	50	12.23	ES-	1
543	PS 14:1-22:0	788.5	30	339.2	50	12.23	ES-	2
544	PS 14:1-22:1	786.5	30	225.3	50	12.23	ES-	1
545	PS 14:1-22:1	786.5	30	337.2	50	12.23	ES-	2
546	PS 14:1-22:2	784.5	30	225.3	50	12.23	ES-	1
547	PS 14:1-22:2	784.5	30	335.2	50	12.23	ES-	2
548	PS 14:1-22:3	782.5	30	225.3	50	12.23	ES-	1

549	PS 14:1-22:3	782.5	30	333.2	50	12.23	ES-	2
550	PS 14:1-22:4	780.5	30	225.3	50	12.23	ES-	1
551	PS 14:1-22:4	780.5	30	331.2	50	12.23	ES-	2
552	PS 14:1-22:5	778.5	30	225.3	50	12.23	ES-	1
553	PS 14:1-22:5	778.5	30	329.2	50	12.23	ES-	2
554	PS 14:1-22:6	776.5	30	225.3	50	12.23	ES-	1
555	PS 14:1-22:6	776.5	30	327.2	50	12.23	ES-	2
556	PS 16:0-16:0	734.5	30	255.3	50	12.23	ES-	1
557	PS 16:0-16:1	732.5	30	253.3	50	12.23	ES-	1
558	PS 16:0-16:1	732.5	30	255.3	50	12.23	ES-	2
559	PS 16:0-18:0	762.5	30	255.3	50	12.23	ES-	1
560	PS 16:0-18:0	762.5	30	283.3	50	12.23	ES-	2
561	PS 16:0-18:1	760.5	30	255.3	50	12.23	ES-	1
562	PS 16:0-18:1	760.5	30	281.3	50	12.23	ES-	2
563	PS 16:0-18:2	758.5	30	255.3	50	12.23	ES-	1
564	PS 16:0-18:2	758.5	30	279.3	50	12.23	ES-	2
565	PS 16:0-18:3	756.5	30	255.3	50	12.23	ES-	1
566	PS 16:0-18:3	756.5	30	277.3	50	12.23	ES-	2
567	PS 16:0-18:4	754.5	30	255.3	50	12.23	ES-	1
568	PS 16:0-18:4	754.5	30	275.3	50	12.23	ES-	2

Method 10: PC, PE, PG, and PS (2)

No	Name	Precursor	CV (V)	Product	CE (V)	RT setting (min)	IonMode	Ion
1	PC 16:0-20:0	848.6	15	255.3	40	5.46	ES-	1
2	PC 16:0-20:0	848.6	15	311.2	40	5.46	ES-	2
3	PC 16:0-20:1	846.6	15	255.3	40	5.46	ES-	1
4	PC 16:0-20:1	846.6	15	309.2	40	5.46	ES-	2
5	PC 16:0-20:2	844.6	15	255.3	40	5.46	ES-	1
6	PC 16:0-20:2	844.6	15	307.2	40	5.46	ES-	2
7	PC 16:0-20:3	842.6	15	255.3	40	5.46	ES-	1
8	PC 16:0-20:3	842.6	15	305.2	40	5.46	ES-	2
9	PC 16:0-20:4	840.6	15	255.3	40	5.46	ES-	1
10	PC 16:0-20:4	840.6	15	303.2	40	5.46	ES-	2
11	PC 16:0-20:5	838.6	15	255.3	40	5.46	ES-	1
12	PC 16:0-20:5	838.6	15	301.2	40	5.46	ES-	2
13	PC 16:0-22:0	876.7	15	255.3	40	5.46	ES-	1

14	PC 16:0-22:0	876.7	15	339.2	40	5.46	ES-	2
15	PC 16:0-22:1	874.7	15	255.3	40	5.46	ES-	1
16	PC 16:0-22:1	874.7	15	337.2	40	5.46	ES-	2
17	PC 16:0-22:2	872.6	15	255.3	40	5.46	ES-	1
18	PC 16:0-22:2	872.6	15	335.2	40	5.46	ES-	2
19	PC 16:0-22:3	870.6	15	255.3	40	5.46	ES-	1
20	PC 16:0-22:3	870.6	15	333.2	40	5.46	ES-	2
21	PC 16:0-22:4	868.6	15	255.3	40	5.46	ES-	1
22	PC 16:0-22:4	868.6	15	331.2	40	5.46	ES-	2
23	PC 16:0-22:5	866.6	15	255.3	40	5.46	ES-	1
24	PC 16:0-22:5	866.6	15	329.2	40	5.46	ES-	2
25	PC 16:0-22:6	864.6	15	255.3	40	5.46	ES-	1
26	PC 16:0-22:6	864.6	15	327.2	40	5.46	ES-	2
27	PC 16:1-16:1	788.5	15	253.3	40	5.46	ES-	1
28	PC 16:1-18:0	818.6	15	253.3	40	5.46	ES-	1
29	PC 16:1-18:0	818.6	15	283.3	40	5.46	ES-	2
30	PC 16:1-18:1	816.6	15	253.3	40	5.46	ES-	1
31	PC 16:1-18:1	816.6	15	281.3	40	5.46	ES-	2
32	PC 16:1-18:2	814.6	15	253.3	40	5.46	ES-	1
33	PC 16:1-18:2	814.6	15	279.3	40	5.46	ES-	2
34	PC 16:1-18:3	812.5	15	253.3	40	5.46	ES-	1
35	PC 16:1-18:3	812.5	15	277.3	40	5.46	ES-	2
36	PC 16:1-18:4	810.5	15	253.3	40	5.46	ES-	1
37	PC 16:1-18:4	810.5	15	275.3	40	5.46	ES-	2
38	PC 16:1-20:0	846.6	15	253.3	40	5.46	ES-	1
39	PC 16:1-20:0	846.6	15	311.2	40	5.46	ES-	2
40	PC 16:1-20:1	844.6	15	253.3	40	5.46	ES-	1
41	PC 16:1-20:1	844.6	15	309.2	40	5.46	ES-	2
42	PC 16:1-20:2	842.6	15	253.3	40	5.46	ES-	1
43	PC 16:1-20:2	842.6	15	307.2	40	5.46	ES-	2
44	PC 16:1-20:3	840.6	15	253.3	40	5.46	ES-	1
45	PC 16:1-20:3	840.6	15	305.2	40	5.46	ES-	2
46	PC 16:1-20:4	838.6	15	253.3	40	5.46	ES-	1
47	PC 16:1-20:4	838.6	15	303.2	40	5.46	ES-	2
48	PC 16:1-20:5	836.5	15	253.3	40	5.46	ES-	1

49	PC 16:1-20:5	836.5	15	301.2	40	5.46	ES-	2
50	PC 16:1-22:0	874.7	15	253.3	40	5.46	ES-	1
51	PC 16:1-22:0	874.7	15	339.2	40	5.46	ES-	2
52	PC 16:1-22:1	872.6	15	253.3	40	5.46	ES-	1
53	PC 16:1-22:1	872.6	15	337.2	40	5.46	ES-	2
54	PC 16:1-22:2	870.6	15	253.3	40	5.46	ES-	1
55	PC 16:1-22:2	870.6	15	335.2	40	5.46	ES-	2
56	PC 16:1-22:3	868.6	15	253.3	40	5.46	ES-	1
57	PC 16:1-22:3	868.6	15	333.2	40	5.46	ES-	2
58	PC 16:1-22:4	866.6	15	253.3	40	5.46	ES-	1
59	PC 16:1-22:4	866.6	15	331.2	40	5.46	ES-	2
60	PC 16:1-22:5	864.6	15	253.3	40	5.46	ES-	1
61	PC 16:1-22:5	864.6	15	329.2	40	5.46	ES-	2
62	PC 16:1-22:6	862.6	15	253.3	40	5.46	ES-	1
63	PC 16:1-22:6	862.6	15	327.2	40	5.46	ES-	2
64	PC 17:0-17:0	820.6	15	269.3	40	5.46	ES-	1
65	PC 18:0-18:0	848.6	15	283.3	40	5.46	ES-	1
66	PC 18:0-18:1	846.6	15	281.3	40	5.46	ES-	1
67	PC 18:0-18:1	846.6	15	283.3	40	5.46	ES-	2
68	PC 18:0-18:2	844.6	15	279.3	40	5.46	ES-	1
69	PC 18:0-18:2	844.6	15	283.3	40	5.46	ES-	2
70	PC 18:0-18:3	842.6	15	277.3	40	5.46	ES-	1
71	PC 18:0-18:3	842.6	15	283.3	40	5.46	ES-	2
72	PC 18:0-18:4	840.6	15	275.3	40	5.46	ES-	1
73	PC 18:0-18:4	840.6	15	283.3	40	5.46	ES-	2
74	PC 18:0-20:0	876.7	15	283.3	40	5.46	ES-	1
75	PC 18:0-20:0	876.7	15	311.2	40	5.46	ES-	2
76	PC 18:0-20:1	874.7	15	283.3	40	5.46	ES-	1
77	PC 18:0-20:1	874.7	15	309.2	40	5.46	ES-	2
78	PC 18:0-20:2	872.6	15	283.3	40	5.46	ES-	1
79	PC 18:0-20:2	872.6	15	307.2	40	5.46	ES-	2
80	PC 18:0-20:3	870.6	15	283.3	40	5.46	ES-	1
81	PC 18:0-20:3	870.6	15	305.2	40	5.46	ES-	2
82	PC 18:0-20:4	868.6	15	283.3	40	5.46	ES-	1
83	PC 18:0-20:4	868.6	15	303.2	40	5.46	ES-	2

84	PC 18:0-20:5	866.6	15	283.3	40	5.46	ES-	1
85	PC 18:0-20:5	866.6	15	301.2	40	5.46	ES-	2
86	PC 18:0-22:0	904.7	15	283.3	40	5.46	ES-	1
87	PC 18:0-22:0	904.7	15	339.2	40	5.46	ES-	2
88	PC 18:0-22:1	902.7	15	283.3	40	5.46	ES-	1
89	PC 18:0-22:1	902.7	15	337.2	40	5.46	ES-	2
90	PC 18:0-22:2	900.7	15	283.3	40	5.46	ES-	1
91	PC 18:0-22:2	900.7	15	335.2	40	5.46	ES-	2
92	PC 18:0-22:3	898.7	15	283.3	40	5.46	ES-	1
93	PC 18:0-22:3	898.7	15	333.2	40	5.46	ES-	2
94	PC 18:0-22:4	896.6	15	283.3	40	5.46	ES-	1
95	PC 18:0-22:4	896.6	15	331.2	40	5.46	ES-	2
96	PC 18:0-22:5	894.6	15	283.3	40	5.46	ES-	1
97	PC 18:0-22:5	894.6	15	329.2	40	5.46	ES-	2
98	PC 18:0-22:6	892.6	15	283.3	40	5.46	ES-	1
99	PC 18:0-22:6	892.6	15	327.2	40	5.46	ES-	2
100	PC 18:1-18:1	844.6	15	281.3	40	5.46	ES-	1
101	PC 18:1-18:2	842.6	15	279.3	40	5.46	ES-	1
102	PC 18:1-18:2	842.6	15	281.3	40	5.46	ES-	2
103	PC 18:1-18:3	840.6	15	277.3	40	5.46	ES-	1
104	PC 18:1-18:3	840.6	15	281.3	40	5.46	ES-	2
105	PC 18:1-18:4	838.6	15	275.3	40	5.46	ES-	1
106	PC 18:1-18:4	838.6	15	281.3	40	5.46	ES-	2
107	PC 18:1-20:0	874.7	15	281.3	40	5.46	ES-	1
108	PC 18:1-20:0	874.7	15	311.2	40	5.46	ES-	2
109	PC 18:1-20:1	872.6	15	281.3	40	5.46	ES-	1
110	PC 18:1-20:1	872.6	15	309.2	40	5.46	ES-	2
111	PC 18:1-20:2	870.6	15	281.3	40	5.46	ES-	1
112	PC 18:1-20:2	870.6	15	307.2	40	5.46	ES-	2
113	PC 18:1-20:3	868.6	15	281.3	40	5.46	ES-	1
114	PC 18:1-20:3	868.6	15	305.2	40	5.46	ES-	2
115	PC 18:1-20:4	866.6	15	281.3	40	5.46	ES-	1
116	PC 18:1-20:4	866.6	15	303.2	40	5.46	ES-	2
117	PC 18:1-20:5	864.6	15	281.3	40	5.46	ES-	1
118	PC 18:1-20:5	864.6	15	301.2	40	5.46	ES-	2

119	PC 18:1-22:0	902.7	15	281.3	40	5.46	ES-	1
120	PC 18:1-22:0	902.7	15	339.2	40	5.46	ES-	2
121	PC 18:1-22:1	900.7	15	281.3	40	5.46	ES-	1
122	PC 18:1-22:1	900.7	15	337.2	40	5.46	ES-	2
123	PC 18:1-22:2	898.7	15	281.3	40	5.46	ES-	1
124	PC 18:1-22:2	898.7	15	335.2	40	5.46	ES-	2
125	PC 18:1-22:3	896.6	15	281.3	40	5.46	ES-	1
126	PC 18:1-22:3	896.6	15	333.2	40	5.46	ES-	2
127	PC 18:1-22:4	894.6	15	281.3	40	5.46	ES-	1
128	PC 18:1-22:4	894.6	15	331.2	40	5.46	ES-	2
129	PC 18:1-22:5	892.6	15	281.3	40	5.46	ES-	1
130	PC 18:1-22:5	892.6	15	329.2	40	5.46	ES-	2
131	PC 18:1-22:6	890.6	15	281.3	40	5.46	ES-	1
132	PC 18:1-22:6	890.6	15	327.2	40	5.46	ES-	2
133	PC 18:2-18:2	840.6	15	279.3	40	5.46	ES-	1
134	PC 18:2-18:3	838.6	15	277.3	40	5.46	ES-	1
135	PC 18:2-18:3	838.6	15	279.3	40	5.46	ES-	2
136	PC 18:2-18:4	836.5	15	275.3	40	5.46	ES-	1
137	PC 18:2-18:4	836.5	15	279.3	40	5.46	ES-	2
138	PC 18:2-20:0	872.6	15	279.3	40	5.46	ES-	1
139	PC 18:2-20:0	872.6	15	311.2	40	5.46	ES-	2
140	PC 18:2-20:1	870.6	15	279.3	40	5.46	ES-	1
141	PC 18:2-20:1	870.6	15	309.2	40	5.46	ES-	2
142	PC 18:2-20:2	868.6	15	279.3	40	5.46	ES-	1
143	PC 18:2-20:2	868.6	15	307.2	40	5.46	ES-	2
144	PC 18:2-20:3	866.6	15	279.3	40	5.46	ES-	1
145	PC 18:2-20:3	866.6	15	305.2	40	5.46	ES-	2
146	PC 18:2-20:4	864.6	15	279.3	40	5.46	ES-	1
147	PC 18:2-20:4	864.6	15	303.2	40	5.46	ES-	2
148	PC 18:2-20:5	862.6	15	279.3	40	5.46	ES-	1
149	PC 18:2-20:5	862.6	15	301.2	40	5.46	ES-	2
150	PE 16:0-20:0	746.6	50	255.3	25	6.32	ES-	1
151	PE 16:0-20:0	746.6	50	311.2	25	6.32	ES-	2
152	PE 16:0-20:1	744.6	50	255.3	25	6.32	ES-	1
153	PE 16:0-20:1	744.6	50	309.2	25	6.32	ES-	2

154	PE 16:0-20:2	742.5	50	255.3	25	6.32	ES-	1
155	PE 16:0-20:2	742.5	50	307.2	25	6.32	ES-	2
156	PE 16:0-20:3	740.5	50	255.3	25	6.32	ES-	1
157	PE 16:0-20:3	740.5	50	305.2	25	6.32	ES-	2
158	PE 16:0-20:4	738.5	50	255.3	25	6.32	ES-	1
159	PE 16:0-20:4	738.5	50	303.2	25	6.32	ES-	2
160	PE 16:0-20:5	736.5	50	255.3	25	6.32	ES-	1
161	PE 16:0-20:5	736.5	50	301.2	25	6.32	ES-	2
162	PE 16:0-22:0	774.6	50	255.3	25	6.32	ES-	1
163	PE 16:0-22:0	774.6	50	339.2	25	6.32	ES-	2
164	PE 16:0-22:1	772.6	50	255.3	25	6.32	ES-	1
165	PE 16:0-22:1	772.6	50	337.2	25	6.32	ES-	2
166	PE 16:0-22:2	770.6	50	255.3	25	6.32	ES-	1
167	PE 16:0-22:2	770.6	50	335.2	25	6.32	ES-	2
168	PE 16:0-22:3	768.6	50	255.3	25	6.32	ES-	1
169	PE 16:0-22:3	768.6	50	333.2	25	6.32	ES-	2
170	PE 16:0-22:4	766.5	50	255.3	25	6.32	ES-	1
171	PE 16:0-22:4	766.5	50	331.2	25	6.32	ES-	2
172	PE 16:0-22:5	764.5	50	255.3	25	6.32	ES-	1
173	PE 16:0-22:5	764.5	50	329.2	25	6.32	ES-	2
174	PE 16:0-22:6	762.5	50	255.3	25	6.32	ES-	1
175	PE 16:0-22:6	762.5	50	327.2	25	6.32	ES-	2
176	PE 16:1-16:1	686.5	50	253.3	25	6.32	ES-	1
177	PE 16:1-18:0	716.5	50	253.3	25	6.32	ES-	1
178	PE 16:1-18:0	716.5	50	283.3	25	6.32	ES-	2
179	PE 16:1-18:1	714.5	50	253.3	25	6.32	ES-	1
180	PE 16:1-18:1	714.5	50	281.3	25	6.32	ES-	2
181	PE 16:1-18:2	712.5	50	253.3	25	6.32	ES-	1
182	PE 16:1-18:2	712.5	50	279.3	25	6.32	ES-	2
183	PE 16:1-18:3	710.5	50	253.3	25	6.32	ES-	1
184	PE 16:1-18:3	710.5	50	277.3	25	6.32	ES-	2
185	PE 16:1-18:4	708.5	50	253.3	25	6.32	ES-	1
186	PE 16:1-18:4	708.5	50	275.3	25	6.32	ES-	2
187	PE 16:1-20:0	744.6	50	253.3	25	6.32	ES-	1
188	PE 16:1-20:0	744.6	50	311.2	25	6.32	ES-	2

189	PE 16:1-20:1	742.5	50	253.3	25	6.32	ES-	1
190	PE 16:1-20:1	742.5	50	309.2	25	6.32	ES-	2
191	PE 16:1-20:2	740.5	50	253.3	25	6.32	ES-	1
192	PE 16:1-20:2	740.5	50	307.2	25	6.32	ES-	2
193	PE 16:1-20:3	738.5	50	253.3	25	6.32	ES-	1
194	PE 16:1-20:3	738.5	50	305.2	25	6.32	ES-	2
195	PE 16:1-20:4	736.5	50	253.3	25	6.32	ES-	1
196	PE 16:1-20:4	736.5	50	303.2	25	6.32	ES-	2
197	PE 16:1-20:5	734.5	50	253.3	25	6.32	ES-	1
198	PE 16:1-20:5	734.5	50	301.2	25	6.32	ES-	2
199	PE 16:1-22:0	772.6	50	253.3	25	6.32	ES-	1
200	PE 16:1-22:0	772.6	50	339.2	25	6.32	ES-	2
201	PE 16:1-22:1	770.6	50	253.3	25	6.32	ES-	1
202	PE 16:1-22:1	770.6	50	337.2	25	6.32	ES-	2
203	PE 16:1-22:2	768.6	50	253.3	25	6.32	ES-	1
204	PE 16:1-22:2	768.6	50	335.2	25	6.32	ES-	2
205	PE 16:1-22:3	766.5	50	253.3	25	6.32	ES-	1
206	PE 16:1-22:3	766.5	50	333.2	25	6.32	ES-	2
207	PE 16:1-22:4	764.5	50	253.3	25	6.32	ES-	1
208	PE 16:1-22:4	764.5	50	331.2	25	6.32	ES-	2
209	PE 16:1-22:5	762.5	50	253.3	25	6.32	ES-	1
210	PE 16:1-22:5	762.5	50	329.2	25	6.32	ES-	2
211	PE 16:1-22:6	760.5	50	253.3	25	6.32	ES-	1
212	PE 16:1-22:6	760.5	50	327.2	25	6.32	ES-	2
213	PE 17:0-17:0	718.5	50	269.3	25	6.32	ES-	1
214	PE 18:0-18:0	746.6	50	283.3	25	6.32	ES-	1
215	PE 18:0-18:1	744.6	50	281.3	25	6.32	ES-	1
216	PE 18:0-18:1	744.6	50	283.3	25	6.32	ES-	2
217	PE 18:0-18:2	742.5	50	279.3	25	6.32	ES-	1
218	PE 18:0-18:2	742.5	50	283.3	25	6.32	ES-	2
219	PE 18:0-18:3	740.5	50	277.3	25	6.32	ES-	1
220	PE 18:0-18:3	740.5	50	283.3	25	6.32	ES-	2
221	PE 18:0-18:4	738.5	50	275.3	25	6.32	ES-	1
222	PE 18:0-18:4	738.5	50	283.3	25	6.32	ES-	2
223	PE 18:0-20:0	774.6	50	283.3	25	6.32	ES-	1

224	PE 18:0-20:0	774.6	50	311.2	25	6.32	ES-	2
225	PE 18:0-20:1	772.6	50	283.3	25	6.32	ES-	1
226	PE 18:0-20:1	772.6	50	309.2	25	6.32	ES-	2
227	PE 18:0-20:2	770.6	50	283.3	25	6.32	ES-	1
228	PE 18:0-20:2	770.6	50	307.2	25	6.32	ES-	2
229	PE 18:0-20:3	768.6	50	283.3	25	6.32	ES-	1
230	PE 18:0-20:3	768.6	50	305.2	25	6.32	ES-	2
231	PE 18:0-20:4	766.5	50	283.3	25	6.32	ES-	1
232	PE 18:0-20:4	766.5	50	303.2	25	6.32	ES-	2
233	PE 18:0-20:5	764.5	50	283.3	25	6.32	ES-	1
234	PE 18:0-20:5	764.5	50	301.2	25	6.32	ES-	2
235	PE 18:0-22:0	802.6	50	283.3	25	6.32	ES-	1
236	PE 18:0-22:0	802.6	50	339.2	25	6.32	ES-	2
237	PE 18:0-22:1	800.6	50	283.3	25	6.32	ES-	1
238	PE 18:0-22:1	800.6	50	337.2	25	6.32	ES-	2
239	PE 18:0-22:2	798.6	50	283.3	25	6.32	ES-	1
240	PE 18:0-22:2	798.6	50	335.2	25	6.32	ES-	2
241	PE 18:0-22:3	796.6	50	283.3	25	6.32	ES-	1
242	PE 18:0-22:3	796.6	50	333.2	25	6.32	ES-	2
243	PE 18:0-22:4	794.6	50	283.3	25	6.32	ES-	1
244	PE 18:0-22:4	794.6	50	331.2	25	6.32	ES-	2
245	PE 18:0-22:5	792.6	50	283.3	25	6.32	ES-	1
246	PE 18:0-22:5	792.6	50	329.2	25	6.32	ES-	2
247	PE 18:0-22:6	790.5	50	283.3	25	6.32	ES-	1
248	PE 18:0-22:6	790.5	50	327.2	25	6.32	ES-	2
249	PE 18:1-18:1	742.5	50	281.3	25	6.32	ES-	1
250	PE 18:1-18:2	740.5	50	279.3	25	6.32	ES-	1
251	PE 18:1-18:2	740.5	50	281.3	25	6.32	ES-	2
252	PE 18:1-18:3	738.5	50	277.3	25	6.32	ES-	1
253	PE 18:1-18:3	738.5	50	281.3	25	6.32	ES-	2
254	PE 18:1-18:4	736.5	50	275.3	25	6.32	ES-	1
255	PE 18:1-18:4	736.5	50	281.3	25	6.32	ES-	2
256	PE 18:1-20:0	772.6	50	281.3	25	6.32	ES-	1
257	PE 18:1-20:0	772.6	50	311.2	25	6.32	ES-	2
258	PE 18:1-20:1	770.6	50	281.3	25	6.32	ES-	1

259	PE 18:1-20:1	770.6	50	309.2	25	6.32	ES-	2
260	PE 18:1-20:2	768.6	50	281.3	25	6.32	ES-	1
261	PE 18:1-20:2	768.6	50	307.2	25	6.32	ES-	2
262	PE 18:1-20:3	766.5	50	281.3	25	6.32	ES-	1
263	PE 18:1-20:3	766.5	50	305.2	25	6.32	ES-	2
264	PE 18:1-20:4	764.5	50	281.3	25	6.32	ES-	1
265	PE 18:1-20:4	764.5	50	303.2	25	6.32	ES-	2
266	PE 18:1-20:5	762.5	50	281.3	25	6.32	ES-	1
267	PE 18:1-20:5	762.5	50	301.2	25	6.32	ES-	2
268	PE 18:1-22:0	800.6	50	281.3	25	6.32	ES-	1
269	PE 18:1-22:0	800.6	50	339.2	25	6.32	ES-	2
270	PE 18:1-22:1	798.6	50	281.3	25	6.32	ES-	1
271	PE 18:1-22:1	798.6	50	337.2	25	6.32	ES-	2
272	PE 18:1-22:2	796.6	50	281.3	25	6.32	ES-	1
273	PE 18:1-22:2	796.6	50	335.2	25	6.32	ES-	2
274	PE 18:1-22:3	794.6	50	281.3	25	6.32	ES-	1
275	PE 18:1-22:3	794.6	50	333.2	25	6.32	ES-	2
276	PE 18:1-22:4	792.6	50	281.3	25	6.32	ES-	1
277	PE 18:1-22:4	792.6	50	331.2	25	6.32	ES-	2
278	PE 18:1-22:5	790.5	50	281.3	25	6.32	ES-	1
279	PE 18:1-22:5	790.5	50	329.2	25	6.32	ES-	2
280	PE 18:1-22:6	788.5	50	281.3	25	6.32	ES-	1
281	PE 18:1-22:6	788.5	50	327.2	25	6.32	ES-	2
282	PE 18:2-18:2	738.5	50	279.3	25	6.32	ES-	1
283	PE 18:2-18:3	736.5	50	277.3	25	6.32	ES-	1
284	PE 18:2-18:3	736.5	50	279.3	25	6.32	ES-	2
285	PE 18:2-18:4	734.5	50	275.3	25	6.32	ES-	1
286	PE 18:2-18:4	734.5	50	279.3	25	6.32	ES-	2
287	PE 18:2-20:0	770.6	50	279.3	25	6.32	ES-	1
288	PE 18:2-20:0	770.6	50	311.2	25	6.32	ES-	2
289	PE 18:2-20:1	768.6	50	279.3	25	6.32	ES-	1
290	PE 18:2-20:1	768.6	50	309.2	25	6.32	ES-	2
291	PE 18:2-20:2	766.5	50	279.3	25	6.32	ES-	1
292	PE 18:2-20:2	766.5	50	307.2	25	6.32	ES-	2
293	PE 18:2-20:3	764.5	50	279.3	25	6.32	ES-	1

294	PE 18:2-20:3	764.5	50	305.2	25	6.32	ES-	2
295	PE 18:2-20:4	762.5	50	279.3	25	6.32	ES-	1
296	PE 18:2-20:4	762.5	50	303.2	25	6.32	ES-	2
297	PE 18:2-20:5	760.5	50	279.3	25	6.32	ES-	1
298	PE 18:2-20:5	760.5	50	301.2	25	6.32	ES-	2
299	PG 16:0-20:0	777.6	30	255.3	40	8.99	ES-	1
300	PG 16:0-20:0	777.6	30	311.2	40	8.99	ES-	2
301	PG 16:0-20:1	775.5	30	255.3	40	8.99	ES-	1
302	PG 16:0-20:1	775.5	30	309.2	40	8.99	ES-	2
303	PG 16:0-20:2	773.5	30	255.3	40	8.99	ES-	1
304	PG 16:0-20:2	773.5	30	307.2	40	8.99	ES-	2
305	PG 16:0-20:3	771.5	30	255.3	40	8.99	ES-	1
306	PG 16:0-20:3	771.5	30	305.2	40	8.99	ES-	2
307	PG 16:0-20:4	769.5	30	255.3	40	8.99	ES-	1
308	PG 16:0-20:4	769.5	30	303.2	40	8.99	ES-	2
309	PG 16:0-20:5	767.5	30	255.3	40	8.99	ES-	1
310	PG 16:0-20:5	767.5	30	301.2	40	8.99	ES-	2
311	PG 16:0-22:0	805.6	30	255.3	40	8.99	ES-	1
312	PG 16:0-22:0	805.6	30	339.2	40	8.99	ES-	2
313	PG 16:0-22:1	803.6	30	255.3	40	8.99	ES-	1
314	PG 16:0-22:1	803.6	30	337.2	40	8.99	ES-	2
315	PG 16:0-22:2	801.6	30	255.3	40	8.99	ES-	1
316	PG 16:0-22:2	801.6	30	335.2	40	8.99	ES-	2
317	PG 16:0-22:3	799.5	30	255.3	40	8.99	ES-	1
318	PG 16:0-22:3	799.5	30	333.2	40	8.99	ES-	2
319	PG 16:0-22:4	797.5	30	255.3	40	8.99	ES-	1
320	PG 16:0-22:4	797.5	30	331.2	40	8.99	ES-	2
321	PG 16:0-22:5	795.5	30	255.3	40	8.99	ES-	1
322	PG 16:0-22:5	795.5	30	329.2	40	8.99	ES-	2
323	PG 16:0-22:6	793.5	30	255.3	40	8.99	ES-	1
324	PG 16:0-22:6	793.5	30	327.2	40	8.99	ES-	2
325	PG 16:1-16:1	717.5	30	253.3	40	8.99	ES-	1
326	PG 16:1-18:0	747.5	30	253.3	40	8.99	ES-	1
327	PG 16:1-18:0	747.5	30	283.3	40	8.99	ES-	2
328	PG 16:1-18:1	745.5	30	253.3	40	8.99	ES-	1

329	PG 16:1-18:1	745.5	30	281.3	40	8.99	ES-	2
330	PG 16:1-18:2	743.5	30	253.3	40	8.99	ES-	1
331	PG 16:1-18:2	743.5	30	279.3	40	8.99	ES-	2
332	PG 16:1-18:3	741.5	30	253.3	40	8.99	ES-	1
333	PG 16:1-18:3	741.5	30	277.3	40	8.99	ES-	2
334	PG 16:1-18:4	739.5	30	253.3	40	8.99	ES-	1
335	PG 16:1-18:4	739.5	30	275.3	40	8.99	ES-	2
336	PG 16:1-20:0	775.5	30	253.3	40	8.99	ES-	1
337	PG 16:1-20:0	775.5	30	311.2	40	8.99	ES-	2
338	PG 16:1-20:1	773.5	30	253.3	40	8.99	ES-	1
339	PG 16:1-20:1	773.5	30	309.2	40	8.99	ES-	2
340	PG 16:1-20:2	771.5	30	253.3	40	8.99	ES-	1
341	PG 16:1-20:2	771.5	30	307.2	40	8.99	ES-	2
342	PG 16:1-20:3	769.5	30	253.3	40	8.99	ES-	1
343	PG 16:1-20:3	769.5	30	305.2	40	8.99	ES-	2
344	PG 16:1-20:4	767.5	30	253.3	40	8.99	ES-	1
345	PG 16:1-20:4	767.5	30	303.2	40	8.99	ES-	2
346	PG 16:1-20:5	765.5	30	253.3	40	8.99	ES-	1
347	PG 16:1-20:5	765.5	30	301.2	40	8.99	ES-	2
348	PG 16:1-22:0	803.6	30	253.3	40	8.99	ES-	1
349	PG 16:1-22:0	803.6	30	339.2	40	8.99	ES-	2
350	PG 16:1-22:1	801.6	30	253.3	40	8.99	ES-	1
351	PG 16:1-22:1	801.6	30	337.2	40	8.99	ES-	2
352	PG 16:1-22:2	799.5	30	253.3	40	8.99	ES-	1
353	PG 16:1-22:2	799.5	30	335.2	40	8.99	ES-	2
354	PG 16:1-22:3	797.5	30	253.3	40	8.99	ES-	1
355	PG 16:1-22:3	797.5	30	333.2	40	8.99	ES-	2
356	PG 16:1-22:4	795.5	30	253.3	40	8.99	ES-	1
357	PG 16:1-22:4	795.5	30	331.2	40	8.99	ES-	2
358	PG 16:1-22:5	793.5	30	253.3	40	8.99	ES-	1
359	PG 16:1-22:5	793.5	30	329.2	40	8.99	ES-	2
360	PG 16:1-22:6	791.5	30	253.3	40	8.99	ES-	1
361	PG 16:1-22:6	791.5	30	327.2	40	8.99	ES-	2
362	PG 17:0-17:0	749.5	30	269.3	40	8.99	ES-	1
363	PG 18:0-18:0	777.6	30	283.3	40	8.99	ES-	1

364	PG 18:0-18:1	775.5	30	281.3	40	8.99	ES-	1
365	PG 18:0-18:1	775.5	30	283.3	40	8.99	ES-	2
366	PG 18:0-18:2	773.5	30	279.3	40	8.99	ES-	1
367	PG 18:0-18:2	773.5	30	283.3	40	8.99	ES-	2
368	PG 18:0-18:3	771.5	30	277.3	40	8.99	ES-	1
369	PG 18:0-18:3	771.5	30	283.3	40	8.99	ES-	2
370	PG 18:0-18:4	769.5	30	275.3	40	8.99	ES-	1
371	PG 18:0-18:4	769.5	30	283.3	40	8.99	ES-	2
372	PG 18:0-20:0	805.6	30	283.3	40	8.99	ES-	1
373	PG 18:0-20:0	805.6	30	311.2	40	8.99	ES-	2
374	PG 18:0-20:1	803.6	30	283.3	40	8.99	ES-	1
375	PG 18:0-20:1	803.6	30	309.2	40	8.99	ES-	2
376	PG 18:0-20:2	801.6	30	283.3	40	8.99	ES-	1
377	PG 18:0-20:2	801.6	30	307.2	40	8.99	ES-	2
378	PG 18:0-20:3	799.5	30	283.3	40	8.99	ES-	1
379	PG 18:0-20:3	799.5	30	305.2	40	8.99	ES-	2
380	PG 18:0-20:4	797.5	30	283.3	40	8.99	ES-	1
381	PG 18:0-20:4	797.5	30	303.2	40	8.99	ES-	2
382	PG 18:0-20:5	795.5	30	283.3	40	8.99	ES-	1
383	PG 18:0-20:5	795.5	30	301.2	40	8.99	ES-	2
384	PG 18:0-22:0	833.6	30	283.3	40	8.99	ES-	1
385	PG 18:0-22:0	833.6	30	339.2	40	8.99	ES-	2
386	PG 18:0-22:1	831.6	30	283.3	40	8.99	ES-	1
387	PG 18:0-22:1	831.6	30	337.2	40	8.99	ES-	2
388	PG 18:0-22:2	829.6	30	283.3	40	8.99	ES-	1
389	PG 18:0-22:2	829.6	30	335.2	40	8.99	ES-	2
390	PG 18:0-22:3	827.6	30	283.3	40	8.99	ES-	1
391	PG 18:0-22:3	827.6	30	333.2	40	8.99	ES-	2
392	PG 18:0-22:4	825.6	30	283.3	40	8.99	ES-	1
393	PG 18:0-22:4	825.6	30	331.2	40	8.99	ES-	2
394	PG 18:0-22:5	823.5	30	283.3	40	8.99	ES-	1
395	PG 18:0-22:5	823.5	30	329.2	40	8.99	ES-	2
396	PG 18:0-22:6	821.5	30	283.3	40	8.99	ES-	1
397	PG 18:0-22:6	821.5	30	327.2	40	8.99	ES-	2
398	PG 18:1-18:1	773.5	30	281.3	40	8.99	ES-	1

399	PG 18:1-18:2	771.5	30	279.3	40	8.99	ES-	1
400	PG 18:1-18:2	771.5	30	281.3	40	8.99	ES-	2
401	PG 18:1-18:3	769.5	30	277.3	40	8.99	ES-	1
402	PG 18:1-18:3	769.5	30	281.3	40	8.99	ES-	2
403	PG 18:1-18:4	767.5	30	275.3	40	8.99	ES-	1
404	PG 18:1-18:4	767.5	30	281.3	40	8.99	ES-	2
405	PG 18:1-20:0	803.6	30	281.3	40	8.99	ES-	1
406	PG 18:1-20:0	803.6	30	311.2	40	8.99	ES-	2
407	PG 18:1-20:1	801.6	30	281.3	40	8.99	ES-	1
408	PG 18:1-20:1	801.6	30	309.2	40	8.99	ES-	2
409	PG 18:1-20:2	799.5	30	281.3	40	8.99	ES-	1
410	PG 18:1-20:2	799.5	30	307.2	40	8.99	ES-	2
411	PG 18:1-20:3	797.5	30	281.3	40	8.99	ES-	1
412	PG 18:1-20:3	797.5	30	305.2	40	8.99	ES-	2
413	PG 18:1-20:4	795.5	30	281.3	40	8.99	ES-	1
414	PG 18:1-20:4	795.5	30	303.2	40	8.99	ES-	2
415	PG 18:1-20:5	793.5	30	281.3	40	8.99	ES-	1
416	PG 18:1-20:5	793.5	30	301.2	40	8.99	ES-	2
417	PG 18:1-22:0	831.6	30	281.3	40	8.99	ES-	1
418	PG 18:1-22:0	831.6	30	339.2	40	8.99	ES-	2
419	PG 18:1-22:1	829.6	30	281.3	40	8.99	ES-	1
420	PG 18:1-22:1	829.6	30	337.2	40	8.99	ES-	2
421	PG 18:1-22:2	827.6	30	281.3	40	8.99	ES-	1
422	PG 18:1-22:2	827.6	30	335.2	40	8.99	ES-	2
423	PG 18:1-22:3	825.6	30	281.3	40	8.99	ES-	1
424	PG 18:1-22:3	825.6	30	333.2	40	8.99	ES-	2
425	PG 18:1-22:4	823.5	30	281.3	40	8.99	ES-	1
426	PG 18:1-22:4	823.5	30	331.2	40	8.99	ES-	2
427	PG 18:1-22:5	821.5	30	281.3	40	8.99	ES-	1
428	PG 18:1-22:5	821.5	30	329.2	40	8.99	ES-	2
429	PG 18:1-22:6	819.5	30	281.3	40	8.99	ES-	1
430	PG 18:1-22:6	819.5	30	327.2	40	8.99	ES-	2
431	PG 18:2-18:2	769.5	30	279.3	40	8.99	ES-	1
432	PG 18:2-18:3	767.5	30	277.3	40	8.99	ES-	1
433	PG 18:2-18:3	767.5	30	279.3	40	8.99	ES-	2

434	PG 18:2-18:4	765.5	30	275.3	40	8.99	ES-	1
435	PG 18:2-18:4	765.5	30	279.3	40	8.99	ES-	2
436	PG 18:2-20:0	801.6	30	279.3	40	8.99	ES-	1
437	PG 18:2-20:0	801.6	30	311.2	40	8.99	ES-	2
438	PG 18:2-20:1	799.5	30	279.3	40	8.99	ES-	1
439	PG 18:2-20:1	799.5	30	309.2	40	8.99	ES-	2
440	PG 18:2-20:2	797.5	30	279.3	40	8.99	ES-	1
441	PG 18:2-20:2	797.5	30	307.2	40	8.99	ES-	2
442	PG 18:2-20:3	795.5	30	279.3	40	8.99	ES-	1
443	PG 18:2-20:3	795.5	30	305.2	40	8.99	ES-	2
444	PG 18:2-20:4	793.5	30	279.3	40	8.99	ES-	1
445	PG 18:2-20:4	793.5	30	303.2	40	8.99	ES-	2
446	PG 18:2-20:5	791.5	30	279.3	40	8.99	ES-	1
447	PG 18:2-20:5	791.5	30	301.2	40	8.99	ES-	2
448	PS 16:0-20:0	790.6	30	255.3	50	12.23	ES-	1
449	PS 16:0-20:0	790.6	30	311.2	50	12.23	ES-	2
450	PS 16:0-20:1	788.5	30	255.3	50	12.23	ES-	1
451	PS 16:0-20:1	788.5	30	309.2	50	12.23	ES-	2
452	PS 16:0-20:2	786.5	30	255.3	50	12.23	ES-	1
453	PS 16:0-20:2	786.5	30	307.2	50	12.23	ES-	2
454	PS 16:0-20:3	784.5	30	255.3	50	12.23	ES-	1
455	PS 16:0-20:3	784.5	30	305.2	50	12.23	ES-	2
456	PS 16:0-20:4	782.5	30	255.3	50	12.23	ES-	1
457	PS 16:0-20:4	782.5	30	303.2	50	12.23	ES-	2
458	PS 16:0-20:5	780.5	30	255.3	50	12.23	ES-	1
459	PS 16:0-20:5	780.5	30	301.2	50	12.23	ES-	2
460	PS 16:0-22:0	818.6	30	255.3	50	12.23	ES-	1
461	PS 16:0-22:0	818.6	30	339.2	50	12.23	ES-	2
462	PS 16:0-22:1	816.6	30	255.3	50	12.23	ES-	1
463	PS 16:0-22:1	816.6	30	337.2	50	12.23	ES-	2
464	PS 16:0-22:2	814.6	30	255.3	50	12.23	ES-	1
465	PS 16:0-22:2	814.6	30	335.2	50	12.23	ES-	2
466	PS 16:0-22:3	812.5	30	255.3	50	12.23	ES-	1
467	PS 16:0-22:3	812.5	30	333.2	50	12.23	ES-	2
468	PS 16:0-22:4	810.5	30	255.3	50	12.23	ES-	1

469	PS 16:0-22:4	810.5	30	331.2	50	12.23	ES-	2
470	PS 16:0-22:5	808.5	30	255.3	50	12.23	ES-	1
471	PS 16:0-22:5	808.5	30	329.2	50	12.23	ES-	2
472	PS 16:0-22:6	806.5	30	255.3	50	12.23	ES-	1
473	PS 16:0-22:6	806.5	30	327.2	50	12.23	ES-	2
474	PS 16:1-16:1	730.5	30	253.3	50	12.23	ES-	1
475	PS 16:1-18:0	760.5	30	253.3	50	12.23	ES-	1
476	PS 16:1-18:0	760.5	30	283.3	50	12.23	ES-	2
477	PS 16:1-18:1	758.5	30	253.3	50	12.23	ES-	1
478	PS 16:1-18:1	758.5	30	281.3	50	12.23	ES-	2
479	PS 16:1-18:2	756.5	30	253.3	50	12.23	ES-	1
480	PS 16:1-18:2	756.5	30	279.3	50	12.23	ES-	2
481	PS 16:1-18:3	754.5	30	253.3	50	12.23	ES-	1
482	PS 16:1-18:3	754.5	30	277.3	50	12.23	ES-	2
483	PS 16:1-18:4	752.5	30	253.3	50	12.23	ES-	1
484	PS 16:1-18:4	752.5	30	275.3	50	12.23	ES-	2
485	PS 16:1-20:0	788.5	30	253.3	50	12.23	ES-	1
486	PS 16:1-20:0	788.5	30	311.2	50	12.23	ES-	2
487	PS 16:1-20:1	786.5	30	253.3	50	12.23	ES-	1
488	PS 16:1-20:1	786.5	30	309.2	50	12.23	ES-	2
489	PS 16:1-20:2	784.5	30	253.3	50	12.23	ES-	1
490	PS 16:1-20:2	784.5	30	307.2	50	12.23	ES-	2
491	PS 16:1-20:3	782.5	30	253.3	50	12.23	ES-	1
492	PS 16:1-20:3	782.5	30	305.2	50	12.23	ES-	2
493	PS 16:1-20:4	780.5	30	253.3	50	12.23	ES-	1
494	PS 16:1-20:4	780.5	30	303.2	50	12.23	ES-	2
495	PS 16:1-20:5	778.5	30	253.3	50	12.23	ES-	1
496	PS 16:1-20:5	778.5	30	301.2	50	12.23	ES-	2
497	PS 16:1-22:0	816.6	30	253.3	50	12.23	ES-	1
498	PS 16:1-22:0	816.6	30	339.2	50	12.23	ES-	2
499	PS 16:1-22:1	814.6	30	253.3	50	12.23	ES-	1
500	PS 16:1-22:1	814.6	30	337.2	50	12.23	ES-	2
501	PS 16:1-22:2	812.5	30	253.3	50	12.23	ES-	1
502	PS 16:1-22:2	812.5	30	335.2	50	12.23	ES-	2
503	PS 16:1-22:3	810.5	30	253.3	50	12.23	ES-	1

504	PS 16:1-22:3	810.5	30	333.2	50	12.23	ES-	2
505	PS 16:1-22:4	808.5	30	253.3	50	12.23	ES-	1
506	PS 16:1-22:4	808.5	30	331.2	50	12.23	ES-	2
507	PS 16:1-22:5	806.5	30	253.3	50	12.23	ES-	1
508	PS 16:1-22:5	806.5	30	329.2	50	12.23	ES-	2
509	PS 16:1-22:6	804.5	30	253.3	50	12.23	ES-	1
510	PS 16:1-22:6	804.5	30	327.2	50	12.23	ES-	2
511	PS 17:0-17:0	762.5	30	269.3	50	12.23	ES-	1
512	PS 18:0-18:0	790.6	30	283.3	50	12.23	ES-	1
513	PS 18:0-18:1	788.5	30	281.3	50	12.23	ES-	1
514	PS 18:0-18:1	788.5	30	283.3	50	12.23	ES-	2
515	PS 18:0-18:2	786.5	30	279.3	50	12.23	ES-	1
516	PS 18:0-18:2	786.5	30	283.3	50	12.23	ES-	2
517	PS 18:0-18:3	784.5	30	277.3	50	12.23	ES-	1
518	PS 18:0-18:3	784.5	30	283.3	50	12.23	ES-	2
519	PS 18:0-18:4	782.5	30	275.3	50	12.23	ES-	1
520	PS 18:0-18:4	782.5	30	283.3	50	12.23	ES-	2
521	PS 18:0-20:0	818.6	30	283.3	50	12.23	ES-	1
522	PS 18:0-20:0	818.6	30	311.2	50	12.23	ES-	2
523	PS 18:0-20:1	816.6	30	283.3	50	12.23	ES-	1
524	PS 18:0-20:1	816.6	30	309.2	50	12.23	ES-	2
525	PS 18:0-20:2	814.6	30	283.3	50	12.23	ES-	1
526	PS 18:0-20:2	814.6	30	307.2	50	12.23	ES-	2
527	PS 18:0-20:3	812.5	30	283.3	50	12.23	ES-	1
528	PS 18:0-20:3	812.5	30	305.2	50	12.23	ES-	2
529	PS 18:0-20:4	810.5	30	283.3	50	12.23	ES-	1
530	PS 18:0-20:4	810.5	30	303.2	50	12.23	ES-	2
531	PS 18:0-20:5	808.5	30	283.3	50	12.23	ES-	1
532	PS 18:0-20:5	808.5	30	301.2	50	12.23	ES-	2
533	PS 18:0-22:0	846.6	30	283.3	50	12.23	ES-	1
534	PS 18:0-22:0	846.6	30	339.2	50	12.23	ES-	2
535	PS 18:0-22:1	844.6	30	283.3	50	12.23	ES-	1
536	PS 18:0-22:1	844.6	30	337.2	50	12.23	ES-	2
537	PS 18:0-22:2	842.6	30	283.3	50	12.23	ES-	1
538	PS 18:0-22:2	842.6	30	335.2	50	12.23	ES-	2

539	PS 18:0-22:3	840.6	30	283.3	50	12.23	ES-	1
540	PS 18:0-22:3	840.6	30	333.2	50	12.23	ES-	2
541	PS 18:0-22:4	838.6	30	283.3	50	12.23	ES-	1
542	PS 18:0-22:4	838.6	30	331.2	50	12.23	ES-	2
543	PS 18:0-22:5	836.5	30	283.3	50	12.23	ES-	1
544	PS 18:0-22:5	836.5	30	329.2	50	12.23	ES-	2
545	PS 18:0-22:6	834.5	30	283.3	50	12.23	ES-	1
546	PS 18:0-22:6	834.5	30	327.2	50	12.23	ES-	2
547	PS 18:1-18:1	786.5	30	281.3	50	12.23	ES-	1
548	PS 18:1-18:2	784.5	30	279.3	50	12.23	ES-	1
549	PS 18:1-18:2	784.5	30	281.3	50	12.23	ES-	2
550	PS 18:1-18:3	782.5	30	277.3	50	12.23	ES-	1
551	PS 18:1-18:3	782.5	30	281.3	50	12.23	ES-	2
552	PS 18:1-18:4	780.5	30	275.3	50	12.23	ES-	1
553	PS 18:1-18:4	780.5	30	281.3	50	12.23	ES-	2
554	PS 18:1-20:0	816.6	30	281.3	50	12.23	ES-	1
555	PS 18:1-20:0	816.6	30	311.2	50	12.23	ES-	2
556	PS 18:1-20:1	814.6	30	281.3	50	12.23	ES-	1
557	PS 18:1-20:1	814.6	30	309.2	50	12.23	ES-	2
558	PS 18:1-20:2	812.5	30	281.3	50	12.23	ES-	1
559	PS 18:1-20:2	812.5	30	307.2	50	12.23	ES-	2
560	PS 18:1-20:3	810.5	30	281.3	50	12.23	ES-	1
561	PS 18:1-20:3	810.5	30	305.2	50	12.23	ES-	2
562	PS 18:1-20:4	808.5	30	281.3	50	12.23	ES-	1
563	PS 18:1-20:4	808.5	30	303.2	50	12.23	ES-	2
564	PS 18:1-20:5	806.5	30	281.3	50	12.23	ES-	1
565	PS 18:1-20:5	806.5	30	301.2	50	12.23	ES-	2
566	PS 18:1-22:0	844.6	30	281.3	50	12.23	ES-	1
567	PS 18:1-22:0	844.6	30	339.2	50	12.23	ES-	2
568	PS 18:1-22:1	842.6	30	281.3	50	12.23	ES-	1
569	PS 18:1-22:1	842.6	30	337.2	50	12.23	ES-	2
570	PS 18:1-22:2	840.6	30	281.3	50	12.23	ES-	1
571	PS 18:1-22:2	840.6	30	335.2	50	12.23	ES-	2
572	PS 18:1-22:3	838.6	30	281.3	50	12.23	ES-	1
573	PS 18:1-22:3	838.6	30	333.2	50	12.23	ES-	2

574	PS 18:1-22:4	836.5	30	281.3	50	12.23	ES-	1
575	PS 18:1-22:4	836.5	30	331.2	50	12.23	ES-	2
576	PS 18:1-22:5	834.5	30	281.3	50	12.23	ES-	1
577	PS 18:1-22:5	834.5	30	329.2	50	12.23	ES-	2
578	PS 18:1-22:6	832.5	30	281.3	50	12.23	ES-	1
579	PS 18:1-22:6	832.5	30	327.2	50	12.23	ES-	2
580	PS 18:2-18:2	782.5	30	279.3	50	12.23	ES-	1
581	PS 18:2-18:3	780.5	30	277.3	50	12.23	ES-	1
582	PS 18:2-18:3	780.5	30	279.3	50	12.23	ES-	2
583	PS 18:2-18:4	778.5	30	275.3	50	12.23	ES-	1
584	PS 18:2-18:4	778.5	30	279.3	50	12.23	ES-	2
585	PS 18:2-20:0	814.6	30	279.3	50	12.23	ES-	1
586	PS 18:2-20:0	814.6	30	311.2	50	12.23	ES-	2
587	PS 18:2-20:1	812.5	30	279.3	50	12.23	ES-	1
588	PS 18:2-20:1	812.5	30	309.2	50	12.23	ES-	2
589	PS 18:2-20:2	810.5	30	279.3	50	12.23	ES-	1
590	PS 18:2-20:2	810.5	30	307.2	50	12.23	ES-	2
591	PS 18:2-20:3	808.5	30	279.3	50	12.23	ES-	1
592	PS 18:2-20:3	808.5	30	305.2	50	12.23	ES-	2
593	PS 18:2-20:4	806.5	30	279.3	50	12.23	ES-	1
594	PS 18:2-20:4	806.5	30	303.2	50	12.23	ES-	2
595	PS 18:2-20:5	804.5	30	279.3	50	12.23	ES-	1
596	PS 18:2-20:5	804.5	30	301.2	50	12.23	ES-	2

Method 11: PC, PE, PG, and PS (3)

No	Name	Precursor	CV (V)	Product	CE (V)	RT setting (min)	IonMode	Ion
1	PC 18:2-22:0	900.7	15	279.3	40	5.46	ES-	1
2	PC 18:2-22:0	900.7	15	339.2	40	5.46	ES-	2
3	PC 18:2-22:1	898.7	15	279.3	40	5.46	ES-	1
4	PC 18:2-22:1	898.7	15	337.2	40	5.46	ES-	2
5	PC 18:2-22:2	896.6	15	279.3	40	5.46	ES-	1
6	PC 18:2-22:2	896.6	15	335.2	40	5.46	ES-	2
7	PC 18:2-22:3	894.6	15	279.3	40	5.46	ES-	1
8	PC 18:2-22:3	894.6	15	333.2	40	5.46	ES-	2
9	PC 18:2-22:4	892.6	15	279.3	40	5.46	ES-	1
10	PC 18:2-22:4	892.6	15	331.2	40	5.46	ES-	2

11	PC 18:2-22:5	890.6	15	279.3	40	5.46	ES-	1
12	PC 18:2-22:5	890.6	15	329.2	40	5.46	ES-	2
13	PC 18:2-22:6	888.6	15	279.3	40	5.46	ES-	1
14	PC 18:2-22:6	888.6	15	327.2	40	5.46	ES-	2
15	PC 18:3-18:3	836.5	15	277.3	40	5.46	ES-	1
16	PC 18:3-18:4	834.5	15	275.3	40	5.46	ES-	1
17	PC 18:3-18:4	834.5	15	277.3	40	5.46	ES-	2
18	PC 18:3-20:0	870.6	15	277.3	40	5.46	ES-	1
19	PC 18:3-20:0	870.6	15	311.2	40	5.46	ES-	2
20	PC 18:3-20:1	868.6	15	277.3	40	5.46	ES-	1
21	PC 18:3-20:1	868.6	15	309.2	40	5.46	ES-	2
22	PC 18:3-20:2	866.6	15	277.3	40	5.46	ES-	1
23	PC 18:3-20:2	866.6	15	307.2	40	5.46	ES-	2
24	PC 18:3-20:3	864.6	15	277.3	40	5.46	ES-	1
25	PC 18:3-20:3	864.6	15	305.2	40	5.46	ES-	2
26	PC 18:3-20:4	862.6	15	277.3	40	5.46	ES-	1
27	PC 18:3-20:4	862.6	15	303.2	40	5.46	ES-	2
28	PC 18:3-20:5	860.5	15	277.3	40	5.46	ES-	1
29	PC 18:3-20:5	860.5	15	301.2	40	5.46	ES-	2
30	PC 18:3-22:0	898.7	15	277.3	40	5.46	ES-	1
31	PC 18:3-22:0	898.7	15	339.2	40	5.46	ES-	2
32	PC 18:3-22:1	896.6	15	277.3	40	5.46	ES-	1
33	PC 18:3-22:1	896.6	15	337.2	40	5.46	ES-	2
34	PC 18:3-22:2	894.6	15	277.3	40	5.46	ES-	1
35	PC 18:3-22:2	894.6	15	335.2	40	5.46	ES-	2
36	PC 18:3-22:3	892.6	15	277.3	40	5.46	ES-	1
37	PC 18:3-22:3	892.6	15	333.2	40	5.46	ES-	2
38	PC 18:3-22:4	890.6	15	277.3	40	5.46	ES-	1
39	PC 18:3-22:4	890.6	15	331.2	40	5.46	ES-	2
40	PC 18:3-22:5	888.6	15	277.3	40	5.46	ES-	1
41	PC 18:3-22:5	888.6	15	329.2	40	5.46	ES-	2
42	PC 18:3-22:6	886.6	15	277.3	40	5.46	ES-	1
43	PC 18:3-22:6	886.6	15	327.2	40	5.46	ES-	2
44	PC 18:4-18:4	832.5	15	275.3	40	5.46	ES-	1
45	PC 18:4-20:0	868.6	15	275.3	40	5.46	ES-	1

46	PC 18:4-20:0	868.6	15	311.2	40	5.46	ES-	2
47	PC 18:4-20:1	866.6	15	275.3	40	5.46	ES-	1
48	PC 18:4-20:1	866.6	15	309.2	40	5.46	ES-	2
49	PC 18:4-20:2	864.6	15	275.3	40	5.46	ES-	1
50	PC 18:4-20:2	864.6	15	307.2	40	5.46	ES-	2
51	PC 18:4-20:3	862.6	15	275.3	40	5.46	ES-	1
52	PC 18:4-20:3	862.6	15	305.2	40	5.46	ES-	2
53	PC 18:4-20:4	860.5	15	275.3	40	5.46	ES-	1
54	PC 18:4-20:4	860.5	15	303.2	40	5.46	ES-	2
55	PC 18:4-20:5	858.5	15	275.3	40	5.46	ES-	1
56	PC 18:4-20:5	858.5	15	301.2	40	5.46	ES-	2
57	PC 18:4-22:0	896.6	15	275.3	40	5.46	ES-	1
58	PC 18:4-22:0	896.6	15	339.2	40	5.46	ES-	2
59	PC 18:4-22:1	894.6	15	275.3	40	5.46	ES-	1
60	PC 18:4-22:1	894.6	15	337.2	40	5.46	ES-	2
61	PC 18:4-22:2	892.6	15	275.3	40	5.46	ES-	1
62	PC 18:4-22:2	892.6	15	335.2	40	5.46	ES-	2
63	PC 18:4-22:3	890.6	15	275.3	40	5.46	ES-	1
64	PC 18:4-22:3	890.6	15	333.2	40	5.46	ES-	2
65	PC 18:4-22:4	888.6	15	275.3	40	5.46	ES-	1
66	PC 18:4-22:4	888.6	15	331.2	40	5.46	ES-	2
67	PC 18:4-22:5	886.6	15	275.3	40	5.46	ES-	1
68	PC 18:4-22:5	886.6	15	329.2	40	5.46	ES-	2
69	PC 18:4-22:6	884.5	15	275.3	40	5.46	ES-	1
70	PC 18:4-22:6	884.5	15	327.2	40	5.46	ES-	2
71	PC 20:0-20:0	904.7	15	311.2	40	5.46	ES-	1
72	PC 20:0-20:1	902.7	15	309.2	40	5.46	ES-	1
73	PC 20:0-20:1	902.7	15	311.2	40	5.46	ES-	2
74	PC 20:0-20:2	900.7	15	307.2	40	5.46	ES-	1
75	PC 20:0-20:2	900.7	15	311.2	40	5.46	ES-	2
76	PC 20:0-20:3	898.7	15	305.2	40	5.46	ES-	1
77	PC 20:0-20:3	898.7	15	311.2	40	5.46	ES-	2
78	PC 20:0-20:4	896.6	15	303.2	40	5.46	ES-	1
79	PC 20:0-20:4	896.6	15	311.2	40	5.46	ES-	2
80	PC 20:0-20:5	894.6	15	301.2	40	5.46	ES-	1

81	PC 20:0-20:5	894.6	15	311.2	40	5.46	ES-	2
82	PC 20:0-22:0	932.7	15	311.2	40	5.46	ES-	1
83	PC 20:0-22:0	932.7	15	339.2	40	5.46	ES-	2
84	PC 20:0-22:1	930.7	15	311.2	40	5.46	ES-	1
85	PC 20:0-22:1	930.7	15	337.2	40	5.46	ES-	2
86	PC 20:0-22:2	928.7	15	311.2	40	5.46	ES-	1
87	PC 20:0-22:2	928.7	15	335.2	40	5.46	ES-	2
88	PC 20:0-22:3	926.7	15	311.2	40	5.46	ES-	1
89	PC 20:0-22:3	926.7	15	333.2	40	5.46	ES-	2
90	PC 20:0-22:4	924.7	15	311.2	40	5.46	ES-	1
91	PC 20:0-22:4	924.7	15	331.2	40	5.46	ES-	2
92	PC 20:0-22:5	922.7	15	311.2	40	5.46	ES-	1
93	PC 20:0-22:5	922.7	15	329.2	40	5.46	ES-	2
94	PC 20:0-22:6	920.6	15	311.2	40	5.46	ES-	1
95	PC 20:0-22:6	920.6	15	327.2	40	5.46	ES-	2
96	PC 20:1-20:1	900.7	15	309.2	40	5.46	ES-	1
97	PC 20:1-20:2	898.7	15	307.2	40	5.46	ES-	1
98	PC 20:1-20:2	898.7	15	309.2	40	5.46	ES-	2
99	PC 20:1-20:3	896.6	15	305.2	40	5.46	ES-	1
100	PC 20:1-20:3	896.6	15	309.2	40	5.46	ES-	2
101	PC 20:1-20:4	894.6	15	303.2	40	5.46	ES-	1
102	PC 20:1-20:4	894.6	15	309.2	40	5.46	ES-	2
103	PC 20:1-20:5	892.6	15	301.2	40	5.46	ES-	1
104	PC 20:1-20:5	892.6	15	309.2	40	5.46	ES-	2
105	PC 20:1-22:0	930.7	15	309.2	40	5.46	ES-	1
106	PC 20:1-22:0	930.7	15	339.2	40	5.46	ES-	2
107	PC 20:1-22:1	928.7	15	309.2	40	5.46	ES-	1
108	PC 20:1-22:1	928.7	15	337.2	40	5.46	ES-	2
109	PC 20:1-22:2	926.7	15	309.2	40	5.46	ES-	1
110	PC 20:1-22:2	926.7	15	335.2	40	5.46	ES-	2
111	PC 20:1-22:3	924.7	15	309.2	40	5.46	ES-	1
112	PC 20:1-22:3	924.7	15	333.2	40	5.46	ES-	2
113	PC 20:1-22:4	922.7	15	309.2	40	5.46	ES-	1
114	PC 20:1-22:4	922.7	15	331.2	40	5.46	ES-	2
115	PC 20:1-22:5	920.6	15	309.2	40	5.46	ES-	1

116	PC 20:1-22:5	920.6	15	329.2	40	5.46	ES-	2
117	PC 20:1-22:6	918.6	15	309.2	40	5.46	ES-	1
118	PC 20:1-22:6	918.6	15	327.2	40	5.46	ES-	2
119	PC 20:2-20:2	896.6	15	307.2	40	5.46	ES-	1
120	PC 20:2-20:3	894.6	15	305.2	40	5.46	ES-	1
121	PC 20:2-20:3	894.6	15	307.2	40	5.46	ES-	2
122	PC 20:2-20:4	892.6	15	303.2	40	5.46	ES-	1
123	PC 20:2-20:4	892.6	15	307.2	40	5.46	ES-	2
124	PC 20:2-20:5	890.6	15	301.2	40	5.46	ES-	1
125	PC 20:2-20:5	890.6	15	307.2	40	5.46	ES-	2
126	PC 20:2-22:0	928.7	15	307.2	40	5.46	ES-	1
127	PC 20:2-22:0	928.7	15	339.2	40	5.46	ES-	2
128	PC 20:2-22:1	926.7	15	307.2	40	5.46	ES-	1
129	PC 20:2-22:1	926.7	15	337.2	40	5.46	ES-	2
130	PC 20:2-22:2	924.7	15	307.2	40	5.46	ES-	1
131	PC 20:2-22:2	924.7	15	335.2	40	5.46	ES-	2
132	PC 20:2-22:3	922.7	15	307.2	40	5.46	ES-	1
133	PC 20:2-22:3	922.7	15	333.2	40	5.46	ES-	2
134	PC 20:2-22:4	920.6	15	307.2	40	5.46	ES-	1
135	PC 20:2-22:4	920.6	15	331.2	40	5.46	ES-	2
136	PC 20:2-22:5	918.6	15	307.2	40	5.46	ES-	1
137	PC 20:2-22:5	918.6	15	329.2	40	5.46	ES-	2
138	PC 20:2-22:6	916.6	15	307.2	40	5.46	ES-	1
139	PC 20:2-22:6	916.6	15	327.2	40	5.46	ES-	2
140	PC 20:3-20:3	892.6	15	305.2	40	5.46	ES-	1
141	PC 20:3-20:4	890.6	15	303.2	40	5.46	ES-	1
142	PC 20:3-20:4	890.6	15	305.2	40	5.46	ES-	2
143	PC 20:3-20:5	888.6	15	301.2	40	5.46	ES-	1
144	PC 20:3-20:5	888.6	15	305.2	40	5.46	ES-	2
145	PE 18:2-22:0	798.6	50	279.3	25	6.32	ES-	1
146	PE 18:2-22:0	798.6	50	339.2	25	6.32	ES-	2
147	PE 18:2-22:1	796.6	50	279.3	25	6.32	ES-	1
148	PE 18:2-22:1	796.6	50	337.2	25	6.32	ES-	2
149	PE 18:2-22:2	794.6	50	279.3	25	6.32	ES-	1
150	PE 18:2-22:2	794.6	50	335.2	25	6.32	ES-	2

151	PE 18:2-22:3	792.6	50	279.3	25	6.32	ES-	1
152	PE 18:2-22:3	792.6	50	333.2	25	6.32	ES-	2
153	PE 18:2-22:4	790.5	50	279.3	25	6.32	ES-	1
154	PE 18:2-22:4	790.5	50	331.2	25	6.32	ES-	2
155	PE 18:2-22:5	788.5	50	279.3	25	6.32	ES-	1
156	PE 18:2-22:5	788.5	50	329.2	25	6.32	ES-	2
157	PE 18:2-22:6	786.5	50	279.3	25	6.32	ES-	1
158	PE 18:2-22:6	786.5	50	327.2	25	6.32	ES-	2
159	PE 18:3-18:3	734.5	50	277.3	25	6.32	ES-	1
160	PE 18:3-18:4	732.5	50	275.3	25	6.32	ES-	1
161	PE 18:3-18:4	732.5	50	277.3	25	6.32	ES-	2
162	PE 18:3-20:0	768.6	50	277.3	25	6.32	ES-	1
163	PE 18:3-20:0	768.6	50	311.2	25	6.32	ES-	2
164	PE 18:3-20:1	766.5	50	277.3	25	6.32	ES-	1
165	PE 18:3-20:1	766.5	50	309.2	25	6.32	ES-	2
166	PE 18:3-20:2	764.5	50	277.3	25	6.32	ES-	1
167	PE 18:3-20:2	764.5	50	307.2	25	6.32	ES-	2
168	PE 18:3-20:3	762.5	50	277.3	25	6.32	ES-	1
169	PE 18:3-20:3	762.5	50	305.2	25	6.32	ES-	2
170	PE 18:3-20:4	760.5	50	277.3	25	6.32	ES-	1
171	PE 18:3-20:4	760.5	50	303.2	25	6.32	ES-	2
172	PE 18:3-20:5	758.5	50	277.3	25	6.32	ES-	1
173	PE 18:3-20:5	758.5	50	301.2	25	6.32	ES-	2
174	PE 18:3-22:0	796.6	50	277.3	25	6.32	ES-	1
175	PE 18:3-22:0	796.6	50	339.2	25	6.32	ES-	2
176	PE 18:3-22:1	794.6	50	277.3	25	6.32	ES-	1
177	PE 18:3-22:1	794.6	50	337.2	25	6.32	ES-	2
178	PE 18:3-22:2	792.6	50	277.3	25	6.32	ES-	1
179	PE 18:3-22:2	792.6	50	335.2	25	6.32	ES-	2
180	PE 18:3-22:3	790.5	50	277.3	25	6.32	ES-	1
181	PE 18:3-22:3	790.5	50	333.2	25	6.32	ES-	2
182	PE 18:3-22:4	788.5	50	277.3	25	6.32	ES-	1
183	PE 18:3-22:4	788.5	50	331.2	25	6.32	ES-	2
184	PE 18:3-22:5	786.5	50	277.3	25	6.32	ES-	1
185	PE 18:3-22:5	786.5	50	329.2	25	6.32	ES-	2

186	PE 18:3-22:6	784.5	50	277.3	25	6.32	ES-	1
187	PE 18:3-22:6	784.5	50	327.2	25	6.32	ES-	2
188	PE 18:4-18:4	730.4	50	275.3	25	6.32	ES-	1
189	PE 18:4-20:0	766.5	50	275.3	25	6.32	ES-	1
190	PE 18:4-20:0	766.5	50	311.2	25	6.32	ES-	2
191	PE 18:4-20:1	764.5	50	275.3	25	6.32	ES-	1
192	PE 18:4-20:1	764.5	50	309.2	25	6.32	ES-	2
193	PE 18:4-20:2	762.5	50	275.3	25	6.32	ES-	1
194	PE 18:4-20:2	762.5	50	307.2	25	6.32	ES-	2
195	PE 18:4-20:3	760.5	50	275.3	25	6.32	ES-	1
196	PE 18:4-20:3	760.5	50	305.2	25	6.32	ES-	2
197	PE 18:4-20:4	758.5	50	275.3	25	6.32	ES-	1
198	PE 18:4-20:4	758.5	50	303.2	25	6.32	ES-	2
199	PE 18:4-20:5	756.5	50	275.3	25	6.32	ES-	1
200	PE 18:4-20:5	756.5	50	301.2	25	6.32	ES-	2
201	PE 18:4-22:0	794.6	50	275.3	25	6.32	ES-	1
202	PE 18:4-22:0	794.6	50	339.2	25	6.32	ES-	2
203	PE 18:4-22:1	792.6	50	275.3	25	6.32	ES-	1
204	PE 18:4-22:1	792.6	50	337.2	25	6.32	ES-	2
205	PE 18:4-22:2	790.5	50	275.3	25	6.32	ES-	1
206	PE 18:4-22:2	790.5	50	335.2	25	6.32	ES-	2
207	PE 18:4-22:3	788.5	50	275.3	25	6.32	ES-	1
208	PE 18:4-22:3	788.5	50	333.2	25	6.32	ES-	2
209	PE 18:4-22:4	786.5	50	275.3	25	6.32	ES-	1
210	PE 18:4-22:4	786.5	50	331.2	25	6.32	ES-	2
211	PE 18:4-22:5	784.5	50	275.3	25	6.32	ES-	1
212	PE 18:4-22:5	784.5	50	329.2	25	6.32	ES-	2
213	PE 18:4-22:6	782.5	50	275.3	25	6.32	ES-	1
214	PE 18:4-22:6	782.5	50	327.2	25	6.32	ES-	2
215	PE 20:0-20:0	802.6	50	311.2	25	6.32	ES-	1
216	PE 20:0-20:1	800.6	50	309.2	25	6.32	ES-	1
217	PE 20:0-20:1	800.6	50	311.2	25	6.32	ES-	2
218	PE 20:0-20:2	798.6	50	307.2	25	6.32	ES-	1
219	PE 20:0-20:2	798.6	50	311.2	25	6.32	ES-	2
220	PE 20:0-20:3	796.6	50	305.2	25	6.32	ES-	1

221	PE 20:0-20:3	796.6	50	311.2	25	6.32	ES-	2
222	PE 20:0-20:4	794.6	50	303.2	25	6.32	ES-	1
223	PE 20:0-20:4	794.6	50	311.2	25	6.32	ES-	2
224	PE 20:0-20:5	792.6	50	301.2	25	6.32	ES-	1
225	PE 20:0-20:5	792.6	50	311.2	25	6.32	ES-	2
226	PE 20:0-22:0	830.7	50	311.2	25	6.32	ES-	1
227	PE 20:0-22:0	830.7	50	339.2	25	6.32	ES-	2
228	PE 20:0-22:1	828.6	50	311.2	25	6.32	ES-	1
229	PE 20:0-22:1	828.6	50	337.2	25	6.32	ES-	2
230	PE 20:0-22:2	826.6	50	311.2	25	6.32	ES-	1
231	PE 20:0-22:2	826.6	50	335.2	25	6.32	ES-	2
232	PE 20:0-22:3	824.6	50	311.2	25	6.32	ES-	1
233	PE 20:0-22:3	824.6	50	333.2	25	6.32	ES-	2
234	PE 20:0-22:4	822.6	50	311.2	25	6.32	ES-	1
235	PE 20:0-22:4	822.6	50	331.2	25	6.32	ES-	2
236	PE 20:0-22:5	820.6	50	311.2	25	6.32	ES-	1
237	PE 20:0-22:5	820.6	50	329.2	25	6.32	ES-	2
238	PE 20:0-22:6	818.6	50	311.2	25	6.32	ES-	1
239	PE 20:0-22:6	818.6	50	327.2	25	6.32	ES-	2
240	PE 20:1-20:1	798.6	50	309.2	25	6.32	ES-	1
241	PE 20:1-20:2	796.6	50	307.2	25	6.32	ES-	1
242	PE 20:1-20:2	796.6	50	309.2	25	6.32	ES-	2
243	PE 20:1-20:3	794.6	50	305.2	25	6.32	ES-	1
244	PE 20:1-20:3	794.6	50	309.2	25	6.32	ES-	2
245	PE 20:1-20:4	792.6	50	303.2	25	6.32	ES-	1
246	PE 20:1-20:4	792.6	50	309.2	25	6.32	ES-	2
247	PE 20:1-20:5	790.5	50	301.2	25	6.32	ES-	1
248	PE 20:1-20:5	790.5	50	309.2	25	6.32	ES-	2
249	PE 20:1-22:0	828.6	50	309.2	25	6.32	ES-	1
250	PE 20:1-22:0	828.6	50	339.2	25	6.32	ES-	2
251	PE 20:1-22:1	826.6	50	309.2	25	6.32	ES-	1
252	PE 20:1-22:1	826.6	50	337.2	25	6.32	ES-	2
253	PE 20:1-22:2	824.6	50	309.2	25	6.32	ES-	1
254	PE 20:1-22:2	824.6	50	335.2	25	6.32	ES-	2
255	PE 20:1-22:3	822.6	50	309.2	25	6.32	ES-	1

256	PE 20:1-22:3	822.6	50	333.2	25	6.32	ES-	2
257	PE 20:1-22:4	820.6	50	309.2	25	6.32	ES-	1
258	PE 20:1-22:4	820.6	50	331.2	25	6.32	ES-	2
259	PE 20:1-22:5	818.6	50	309.2	25	6.32	ES-	1
260	PE 20:1-22:5	818.6	50	329.2	25	6.32	ES-	2
261	PE 20:1-22:6	816.6	50	309.2	25	6.32	ES-	1
262	PE 20:1-22:6	816.6	50	327.2	25	6.32	ES-	2
263	PE 20:2-20:2	794.6	50	307.2	25	6.32	ES-	1
264	PE 20:2-20:3	792.6	50	305.2	25	6.32	ES-	1
265	PE 20:2-20:3	792.6	50	307.2	25	6.32	ES-	2
266	PE 20:2-20:4	790.5	50	303.2	25	6.32	ES-	1
267	PE 20:2-20:4	790.5	50	307.2	25	6.32	ES-	2
268	PE 20:2-20:5	788.5	50	301.2	25	6.32	ES-	1
269	PE 20:2-20:5	788.5	50	307.2	25	6.32	ES-	2
270	PE 20:2-22:0	826.6	50	307.2	25	6.32	ES-	1
271	PE 20:2-22:0	826.6	50	339.2	25	6.32	ES-	2
272	PE 20:2-22:1	824.6	50	307.2	25	6.32	ES-	1
273	PE 20:2-22:1	824.6	50	337.2	25	6.32	ES-	2
274	PE 20:2-22:2	822.6	50	307.2	25	6.32	ES-	1
275	PE 20:2-22:2	822.6	50	335.2	25	6.32	ES-	2
276	PE 20:2-22:3	820.6	50	307.2	25	6.32	ES-	1
277	PE 20:2-22:3	820.6	50	333.2	25	6.32	ES-	2
278	PE 20:2-22:4	818.6	50	307.2	25	6.32	ES-	1
279	PE 20:2-22:4	818.6	50	331.2	25	6.32	ES-	2
280	PE 20:2-22:5	816.6	50	307.2	25	6.32	ES-	1
281	PE 20:2-22:5	816.6	50	329.2	25	6.32	ES-	2
282	PE 20:2-22:6	814.5	50	307.2	25	6.32	ES-	1
283	PE 20:2-22:6	814.5	50	327.2	25	6.32	ES-	2
284	PE 20:3-20:3	790.5	50	305.2	25	6.32	ES-	1
285	PE 20:3-20:4	788.5	50	303.2	25	6.32	ES-	1
286	PE 20:3-20:4	788.5	50	305.2	25	6.32	ES-	2
287	PE 20:3-20:5	786.5	50	301.2	25	6.32	ES-	1
288	PE 20:3-20:5	786.5	50	305.2	25	6.32	ES-	2
289	PG 18:2-22:0	829.6	30	279.3	40	8.99	ES-	1
290	PG 18:2-22:0	829.6	30	339.2	40	8.99	ES-	2

291	PG 18:2-22:1	827.6	30	279.3	40	8.99	ES-	1
292	PG 18:2-22:1	827.6	30	337.2	40	8.99	ES-	2
293	PG 18:2-22:2	825.6	30	279.3	40	8.99	ES-	1
294	PG 18:2-22:2	825.6	30	335.2	40	8.99	ES-	2
295	PG 18:2-22:3	823.5	30	279.3	40	8.99	ES-	1
296	PG 18:2-22:3	823.5	30	333.2	40	8.99	ES-	2
297	PG 18:2-22:4	821.5	30	279.3	40	8.99	ES-	1
298	PG 18:2-22:4	821.5	30	331.2	40	8.99	ES-	2
299	PG 18:2-22:5	819.5	30	279.3	40	8.99	ES-	1
300	PG 18:2-22:5	819.5	30	329.2	40	8.99	ES-	2
301	PG 18:2-22:6	817.5	30	279.3	40	8.99	ES-	1
302	PG 18:2-22:6	817.5	30	327.2	40	8.99	ES-	2
303	PG 18:3-18:3	765.5	30	277.3	40	8.99	ES-	1
304	PG 18:3-18:4	763.5	30	275.3	40	8.99	ES-	1
305	PG 18:3-18:4	763.5	30	277.3	40	8.99	ES-	2
306	PG 18:3-20:0	799.5	30	277.3	40	8.99	ES-	1
307	PG 18:3-20:0	799.5	30	311.2	40	8.99	ES-	2
308	PG 18:3-20:1	797.5	30	277.3	40	8.99	ES-	1
309	PG 18:3-20:1	797.5	30	309.2	40	8.99	ES-	2
310	PG 18:3-20:2	795.5	30	277.3	40	8.99	ES-	1
311	PG 18:3-20:2	795.5	30	307.2	40	8.99	ES-	2
312	PG 18:3-20:3	793.5	30	277.3	40	8.99	ES-	1
313	PG 18:3-20:3	793.5	30	305.2	40	8.99	ES-	2
314	PG 18:3-20:4	791.5	30	277.3	40	8.99	ES-	1
315	PG 18:3-20:4	791.5	30	303.2	40	8.99	ES-	2
316	PG 18:3-20:5	789.5	30	277.3	40	8.99	ES-	1
317	PG 18:3-20:5	789.5	30	301.2	40	8.99	ES-	2
318	PG 18:3-22:0	827.6	30	277.3	40	8.99	ES-	1
319	PG 18:3-22:0	827.6	30	339.2	40	8.99	ES-	2
320	PG 18:3-22:1	825.6	30	277.3	40	8.99	ES-	1
321	PG 18:3-22:1	825.6	30	337.2	40	8.99	ES-	2
322	PG 18:3-22:2	823.5	30	277.3	40	8.99	ES-	1
323	PG 18:3-22:2	823.5	30	335.2	40	8.99	ES-	2
324	PG 18:3-22:3	821.5	30	277.3	40	8.99	ES-	1
325	PG 18:3-22:3	821.5	30	333.2	40	8.99	ES-	2

326	PG 18:3-22:4	819.5	30	277.3	40	8.99	ES-	1
327	PG 18:3-22:4	819.5	30	331.2	40	8.99	ES-	2
328	PG 18:3-22:5	817.5	30	277.3	40	8.99	ES-	1
329	PG 18:3-22:5	817.5	30	329.2	40	8.99	ES-	2
330	PG 18:3-22:6	815.5	30	277.3	40	8.99	ES-	1
331	PG 18:3-22:6	815.5	30	327.2	40	8.99	ES-	2
332	PG 18:4-18:4	761.4	30	275.3	40	8.99	ES-	1
333	PG 18:4-20:0	797.5	30	275.3	40	8.99	ES-	1
334	PG 18:4-20:0	797.5	30	311.2	40	8.99	ES-	2
335	PG 18:4-20:1	795.5	30	275.3	40	8.99	ES-	1
336	PG 18:4-20:1	795.5	30	309.2	40	8.99	ES-	2
337	PG 18:4-20:2	793.5	30	275.3	40	8.99	ES-	1
338	PG 18:4-20:2	793.5	30	307.2	40	8.99	ES-	2
339	PG 18:4-20:3	791.5	30	275.3	40	8.99	ES-	1
340	PG 18:4-20:3	791.5	30	305.2	40	8.99	ES-	2
341	PG 18:4-20:4	789.5	30	275.3	40	8.99	ES-	1
342	PG 18:4-20:4	789.5	30	303.2	40	8.99	ES-	2
343	PG 18:4-20:5	787.5	30	275.3	40	8.99	ES-	1
344	PG 18:4-20:5	787.5	30	301.2	40	8.99	ES-	2
345	PG 18:4-22:0	825.6	30	275.3	40	8.99	ES-	1
346	PG 18:4-22:0	825.6	30	339.2	40	8.99	ES-	2
347	PG 18:4-22:1	823.5	30	275.3	40	8.99	ES-	1
348	PG 18:4-22:1	823.5	30	337.2	40	8.99	ES-	2
349	PG 18:4-22:2	821.5	30	275.3	40	8.99	ES-	1
350	PG 18:4-22:2	821.5	30	335.2	40	8.99	ES-	2
351	PG 18:4-22:3	819.5	30	275.3	40	8.99	ES-	1
352	PG 18:4-22:3	819.5	30	333.2	40	8.99	ES-	2
353	PG 18:4-22:4	817.5	30	275.3	40	8.99	ES-	1
354	PG 18:4-22:4	817.5	30	331.2	40	8.99	ES-	2
355	PG 18:4-22:5	815.5	30	275.3	40	8.99	ES-	1
356	PG 18:4-22:5	815.5	30	329.2	40	8.99	ES-	2
357	PG 18:4-22:6	813.5	30	275.3	40	8.99	ES-	1
358	PG 18:4-22:6	813.5	30	327.2	40	8.99	ES-	2
359	PG 20:0-20:0	833.6	30	311.2	40	8.99	ES-	1
360	PG 20:0-20:1	831.6	30	309.2	40	8.99	ES-	1

361	PG 20:0-20:1	831.6	30	311.2	40	8.99	ES-	2
362	PG 20:0-20:2	829.6	30	307.2	40	8.99	ES-	1
363	PG 20:0-20:2	829.6	30	311.2	40	8.99	ES-	2
364	PG 20:0-20:3	827.6	30	305.2	40	8.99	ES-	1
365	PG 20:0-20:3	827.6	30	311.2	40	8.99	ES-	2
366	PG 20:0-20:4	825.6	30	303.2	40	8.99	ES-	1
367	PG 20:0-20:4	825.6	30	311.2	40	8.99	ES-	2
368	PG 20:0-20:5	823.5	30	301.2	40	8.99	ES-	1
369	PG 20:0-20:5	823.5	30	311.2	40	8.99	ES-	2
370	PG 20:0-22:0	861.7	30	311.2	40	8.99	ES-	1
371	PG 20:0-22:0	861.7	30	339.2	40	8.99	ES-	2
372	PG 20:0-22:1	859.6	30	311.2	40	8.99	ES-	1
373	PG 20:0-22:1	859.6	30	337.2	40	8.99	ES-	2
374	PG 20:0-22:2	857.6	30	311.2	40	8.99	ES-	1
375	PG 20:0-22:2	857.6	30	335.2	40	8.99	ES-	2
376	PG 20:0-22:3	855.6	30	311.2	40	8.99	ES-	1
377	PG 20:0-22:3	855.6	30	333.2	40	8.99	ES-	2
378	PG 20:0-22:4	853.6	30	311.2	40	8.99	ES-	1
379	PG 20:0-22:4	853.6	30	331.2	40	8.99	ES-	2
380	PG 20:0-22:5	851.6	30	311.2	40	8.99	ES-	1
381	PG 20:0-22:5	851.6	30	329.2	40	8.99	ES-	2
382	PG 20:0-22:6	849.6	30	311.2	40	8.99	ES-	1
383	PG 20:0-22:6	849.6	30	327.2	40	8.99	ES-	2
384	PG 20:1-20:1	829.6	30	309.2	40	8.99	ES-	1
385	PG 20:1-20:2	827.6	30	307.2	40	8.99	ES-	1
386	PG 20:1-20:2	827.6	30	309.2	40	8.99	ES-	2
387	PG 20:1-20:3	825.6	30	305.2	40	8.99	ES-	1
388	PG 20:1-20:3	825.6	30	309.2	40	8.99	ES-	2
389	PG 20:1-20:4	823.5	30	303.2	40	8.99	ES-	1
390	PG 20:1-20:4	823.5	30	309.2	40	8.99	ES-	2
391	PG 20:1-20:5	821.5	30	301.2	40	8.99	ES-	1
392	PG 20:1-20:5	821.5	30	309.2	40	8.99	ES-	2
393	PG 20:1-22:0	859.6	30	309.2	40	8.99	ES-	1
394	PG 20:1-22:0	859.6	30	339.2	40	8.99	ES-	2
395	PG 20:1-22:1	857.6	30	309.2	40	8.99	ES-	1

396	PG 20:1-22:1	857.6	30	337.2	40	8.99	ES-	2
397	PG 20:1-22:2	855.6	30	309.2	40	8.99	ES-	1
398	PG 20:1-22:2	855.6	30	335.2	40	8.99	ES-	2
399	PG 20:1-22:3	853.6	30	309.2	40	8.99	ES-	1
400	PG 20:1-22:3	853.6	30	333.2	40	8.99	ES-	2
401	PG 20:1-22:4	851.6	30	309.2	40	8.99	ES-	1
402	PG 20:1-22:4	851.6	30	331.2	40	8.99	ES-	2
403	PG 20:1-22:5	849.6	30	309.2	40	8.99	ES-	1
404	PG 20:1-22:5	849.6	30	329.2	40	8.99	ES-	2
405	PG 20:1-22:6	847.5	30	309.2	40	8.99	ES-	1
406	PG 20:1-22:6	847.5	30	327.2	40	8.99	ES-	2
407	PG 20:2-20:2	825.6	30	307.2	40	8.99	ES-	1
408	PG 20:2-20:3	823.5	30	305.2	40	8.99	ES-	1
409	PG 20:2-20:3	823.5	30	307.2	40	8.99	ES-	2
410	PG 20:2-20:4	821.5	30	303.2	40	8.99	ES-	1
411	PG 20:2-20:4	821.5	30	307.2	40	8.99	ES-	2
412	PG 20:2-20:5	819.5	30	301.2	40	8.99	ES-	1
413	PG 20:2-20:5	819.5	30	307.2	40	8.99	ES-	2
414	PG 20:2-22:0	857.6	30	307.2	40	8.99	ES-	1
415	PG 20:2-22:0	857.6	30	339.2	40	8.99	ES-	2
416	PG 20:2-22:1	855.6	30	307.2	40	8.99	ES-	1
417	PG 20:2-22:1	855.6	30	337.2	40	8.99	ES-	2
418	PG 20:2-22:2	853.6	30	307.2	40	8.99	ES-	1
419	PG 20:2-22:2	853.6	30	335.2	40	8.99	ES-	2
420	PG 20:2-22:3	851.6	30	307.2	40	8.99	ES-	1
421	PG 20:2-22:3	851.6	30	333.2	40	8.99	ES-	2
422	PG 20:2-22:4	849.6	30	307.2	40	8.99	ES-	1
423	PG 20:2-22:4	849.6	30	331.2	40	8.99	ES-	2
424	PG 20:2-22:5	847.5	30	307.2	40	8.99	ES-	1
425	PG 20:2-22:5	847.5	30	329.2	40	8.99	ES-	2
426	PG 20:2-22:6	845.5	30	307.2	40	8.99	ES-	1
427	PG 20:2-22:6	845.5	30	327.2	40	8.99	ES-	2
428	PG 20:3-20:3	821.5	30	305.2	40	8.99	ES-	1
429	PG 20:3-20:4	819.5	30	303.2	40	8.99	ES-	1
430	PG 20:3-20:4	819.5	30	305.2	40	8.99	ES-	2

431	PG 20:3-20:5	817.5	30	301.2	40	8.99	ES-	1
432	PG 20:3-20:5	817.5	30	305.2	40	8.99	ES-	2
433	PS 18:2-22:0	842.6	30	279.3	50	12.23	ES-	1
434	PS 18:2-22:0	842.6	30	339.2	50	12.23	ES-	2
435	PS 18:2-22:1	840.6	30	279.3	50	12.23	ES-	1
436	PS 18:2-22:1	840.6	30	337.2	50	12.23	ES-	2
437	PS 18:2-22:2	838.6	30	279.3	50	12.23	ES-	1
438	PS 18:2-22:2	838.6	30	335.2	50	12.23	ES-	2
439	PS 18:2-22:3	836.5	30	279.3	50	12.23	ES-	1
440	PS 18:2-22:3	836.5	30	333.2	50	12.23	ES-	2
441	PS 18:2-22:4	834.5	30	279.3	50	12.23	ES-	1
442	PS 18:2-22:4	834.5	30	331.2	50	12.23	ES-	2
443	PS 18:2-22:5	832.5	30	279.3	50	12.23	ES-	1
444	PS 18:2-22:5	832.5	30	329.2	50	12.23	ES-	2
445	PS 18:2-22:6	830.5	30	279.3	50	12.23	ES-	1
446	PS 18:2-22:6	830.5	30	327.2	50	12.23	ES-	2
447	PS 18:3-18:3	778.5	30	277.3	50	12.23	ES-	1
448	PS 18:3-18:4	776.5	30	275.3	50	12.23	ES-	1
449	PS 18:3-18:4	776.5	30	277.3	50	12.23	ES-	2
450	PS 18:3-20:0	812.5	30	277.3	50	12.23	ES-	1
451	PS 18:3-20:0	812.5	30	311.2	50	12.23	ES-	2
452	PS 18:3-20:1	810.5	30	277.3	50	12.23	ES-	1
453	PS 18:3-20:1	810.5	30	309.2	50	12.23	ES-	2
454	PS 18:3-20:2	808.5	30	277.3	50	12.23	ES-	1
455	PS 18:3-20:2	808.5	30	307.2	50	12.23	ES-	2
456	PS 18:3-20:3	806.5	30	277.3	50	12.23	ES-	1
457	PS 18:3-20:3	806.5	30	305.2	50	12.23	ES-	2
458	PS 18:3-20:4	804.5	30	277.3	50	12.23	ES-	1
459	PS 18:3-20:4	804.5	30	303.2	50	12.23	ES-	2
460	PS 18:3-20:5	802.5	30	277.3	50	12.23	ES-	1
461	PS 18:3-20:5	802.5	30	301.2	50	12.23	ES-	2
462	PS 18:3-22:0	840.6	30	277.3	50	12.23	ES-	1
463	PS 18:3-22:0	840.6	30	339.2	50	12.23	ES-	2
464	PS 18:3-22:1	838.6	30	277.3	50	12.23	ES-	1
465	PS 18:3-22:1	838.6	30	337.2	50	12.23	ES-	2

466	PS 18:3-22:2	836.5	30	277.3	50	12.23	ES-	1
467	PS 18:3-22:2	836.5	30	335.2	50	12.23	ES-	2
468	PS 18:3-22:3	834.5	30	277.3	50	12.23	ES-	1
469	PS 18:3-22:3	834.5	30	333.2	50	12.23	ES-	2
470	PS 18:3-22:4	832.5	30	277.3	50	12.23	ES-	1
471	PS 18:3-22:4	832.5	30	331.2	50	12.23	ES-	2
472	PS 18:3-22:5	830.5	30	277.3	50	12.23	ES-	1
473	PS 18:3-22:5	830.5	30	329.2	50	12.23	ES-	2
474	PS 18:3-22:6	828.5	30	277.3	50	12.23	ES-	1
475	PS 18:3-22:6	828.5	30	327.2	50	12.23	ES-	2
476	PS 18:4-18:4	774.4	30	275.3	50	12.23	ES-	1
477	PS 18:4-20:0	810.5	30	275.3	50	12.23	ES-	1
478	PS 18:4-20:0	810.5	30	311.2	50	12.23	ES-	2
479	PS 18:4-20:1	808.5	30	275.3	50	12.23	ES-	1
480	PS 18:4-20:1	808.5	30	309.2	50	12.23	ES-	2
481	PS 18:4-20:2	806.5	30	275.3	50	12.23	ES-	1
482	PS 18:4-20:2	806.5	30	307.2	50	12.23	ES-	2
483	PS 18:4-20:3	804.5	30	275.3	50	12.23	ES-	1
484	PS 18:4-20:3	804.5	30	305.2	50	12.23	ES-	2
485	PS 18:4-20:4	802.5	30	275.3	50	12.23	ES-	1
486	PS 18:4-20:4	802.5	30	303.2	50	12.23	ES-	2
487	PS 18:4-20:5	800.5	30	275.3	50	12.23	ES-	1
488	PS 18:4-20:5	800.5	30	301.2	50	12.23	ES-	2
489	PS 18:4-22:0	838.6	30	275.3	50	12.23	ES-	1
490	PS 18:4-22:0	838.6	30	339.2	50	12.23	ES-	2
491	PS 18:4-22:1	836.5	30	275.3	50	12.23	ES-	1
492	PS 18:4-22:1	836.5	30	337.2	50	12.23	ES-	2
493	PS 18:4-22:2	834.5	30	275.3	50	12.23	ES-	1
494	PS 18:4-22:2	834.5	30	335.2	50	12.23	ES-	2
495	PS 18:4-22:3	832.5	30	275.3	50	12.23	ES-	1
496	PS 18:4-22:3	832.5	30	333.2	50	12.23	ES-	2
497	PS 18:4-22:4	830.5	30	275.3	50	12.23	ES-	1
498	PS 18:4-22:4	830.5	30	331.2	50	12.23	ES-	2
499	PS 18:4-22:5	828.5	30	275.3	50	12.23	ES-	1
500	PS 18:4-22:5	828.5	30	329.2	50	12.23	ES-	2

501	PS 18:4-22:6	826.5	30	275.3	50	12.23	ES-	1
502	PS 18:4-22:6	826.5	30	327.2	50	12.23	ES-	2
503	PS 20:0-20:0	846.6	30	311.2	50	12.23	ES-	1
504	PS 20:0-20:1	844.6	30	309.2	50	12.23	ES-	1
505	PS 20:0-20:1	844.6	30	311.2	50	12.23	ES-	2
506	PS 20:0-20:2	842.6	30	307.2	50	12.23	ES-	1
507	PS 20:0-20:2	842.6	30	311.2	50	12.23	ES-	2
508	PS 20:0-20:3	840.6	30	305.2	50	12.23	ES-	1
509	PS 20:0-20:3	840.6	30	311.2	50	12.23	ES-	2
510	PS 20:0-20:4	838.6	30	303.2	50	12.23	ES-	1
511	PS 20:0-20:4	838.6	30	311.2	50	12.23	ES-	2
512	PS 20:0-20:5	836.5	30	301.2	50	12.23	ES-	1
513	PS 20:0-20:5	836.5	30	311.2	50	12.23	ES-	2
514	PS 20:0-22:0	874.7	30	311.2	50	12.23	ES-	1
515	PS 20:0-22:0	874.7	30	339.2	50	12.23	ES-	2
516	PS 20:0-22:1	872.6	30	311.2	50	12.23	ES-	1
517	PS 20:0-22:1	872.6	30	337.2	50	12.23	ES-	2
518	PS 20:0-22:2	870.6	30	311.2	50	12.23	ES-	1
519	PS 20:0-22:2	870.6	30	335.2	50	12.23	ES-	2
520	PS 20:0-22:3	868.6	30	311.2	50	12.23	ES-	1
521	PS 20:0-22:3	868.6	30	333.2	50	12.23	ES-	2
522	PS 20:0-22:4	866.6	30	311.2	50	12.23	ES-	1
523	PS 20:0-22:4	866.6	30	331.2	50	12.23	ES-	2
524	PS 20:0-22:5	864.6	30	311.2	50	12.23	ES-	1
525	PS 20:0-22:5	864.6	30	329.2	50	12.23	ES-	2
526	PS 20:0-22:6	862.6	30	311.2	50	12.23	ES-	1
527	PS 20:0-22:6	862.6	30	327.2	50	12.23	ES-	2
528	PS 20:1-20:1	842.6	30	309.2	50	12.23	ES-	1
529	PS 20:1-20:2	840.6	30	307.2	50	12.23	ES-	1
530	PS 20:1-20:2	840.6	30	309.2	50	12.23	ES-	2
531	PS 20:1-20:3	838.6	30	305.2	50	12.23	ES-	1
532	PS 20:1-20:3	838.6	30	309.2	50	12.23	ES-	2
533	PS 20:1-20:4	836.5	30	303.2	50	12.23	ES-	1
534	PS 20:1-20:4	836.5	30	309.2	50	12.23	ES-	2
535	PS 20:1-20:5	834.5	30	301.2	50	12.23	ES-	1

536	PS 20:1-20:5	834.5	30	309.2	50	12.23	ES-	2
537	PS 20:1-22:0	872.6	30	309.2	50	12.23	ES-	1
538	PS 20:1-22:0	872.6	30	339.2	50	12.23	ES-	2
539	PS 20:1-22:1	870.6	30	309.2	50	12.23	ES-	1
540	PS 20:1-22:1	870.6	30	337.2	50	12.23	ES-	2
541	PS 20:1-22:2	868.6	30	309.2	50	12.23	ES-	1
542	PS 20:1-22:2	868.6	30	335.2	50	12.23	ES-	2
543	PS 20:1-22:3	866.6	30	309.2	50	12.23	ES-	1
544	PS 20:1-22:3	866.6	30	333.2	50	12.23	ES-	2
545	PS 20:1-22:4	864.6	30	309.2	50	12.23	ES-	1
546	PS 20:1-22:4	864.6	30	331.2	50	12.23	ES-	2
547	PS 20:1-22:5	862.6	30	309.2	50	12.23	ES-	1
548	PS 20:1-22:5	862.6	30	329.2	50	12.23	ES-	2
549	PS 20:1-22:6	860.5	30	309.2	50	12.23	ES-	1
550	PS 20:1-22:6	860.5	30	327.2	50	12.23	ES-	2
551	PS 20:2-20:2	838.6	30	307.2	50	12.23	ES-	1
552	PS 20:2-20:3	836.5	30	305.2	50	12.23	ES-	1
553	PS 20:2-20:3	836.5	30	307.2	50	12.23	ES-	2
554	PS 20:2-20:4	834.5	30	303.2	50	12.23	ES-	1
555	PS 20:2-20:4	834.5	30	307.2	50	12.23	ES-	2
556	PS 20:2-20:5	832.5	30	301.2	50	12.23	ES-	1
557	PS 20:2-20:5	832.5	30	307.2	50	12.23	ES-	2
558	PS 20:2-22:0	870.6	30	307.2	50	12.23	ES-	1
559	PS 20:2-22:0	870.6	30	339.2	50	12.23	ES-	2
560	PS 20:2-22:1	868.6	30	307.2	50	12.23	ES-	1
561	PS 20:2-22:1	868.6	30	337.2	50	12.23	ES-	2
562	PS 20:2-22:2	866.6	30	307.2	50	12.23	ES-	1
563	PS 20:2-22:2	866.6	30	335.2	50	12.23	ES-	2
564	PS 20:2-22:3	864.6	30	307.2	50	12.23	ES-	1
565	PS 20:2-22:3	864.6	30	333.2	50	12.23	ES-	2
566	PS 20:2-22:4	862.6	30	307.2	50	12.23	ES-	1
567	PS 20:2-22:4	862.6	30	331.2	50	12.23	ES-	2
568	PS 20:2-22:5	860.5	30	307.2	50	12.23	ES-	1
569	PS 20:2-22:5	860.5	30	329.2	50	12.23	ES-	2
570	PS 20:2-22:6	858.5	30	307.2	50	12.23	ES-	1

571	PS 20:2-22:6	858.5	30	327.2	50	12.23	ES-	2
572	PS 20:3-20:3	834.5	30	305.2	50	12.23	ES-	1
573	PS 20:3-20:4	832.5	30	303.2	50	12.23	ES-	1
574	PS 20:3-20:4	832.5	30	305.2	50	12.23	ES-	2
575	PS 20:3-20:5	830.5	30	301.2	50	12.23	ES-	1
576	PS 20:3-20:5	830.5	30	305.2	50	12.23	ES-	2

Method 12: PC, PE, PG, and PS (4)

No	Name	Precursor	CV (V)	Product	CE (V)	RT setting (min)	IonMode	Ion
1	PC 20:3-22:0	926.7	15	305.2	40	5.46	ES-	1
2	PC 20:3-22:0	926.7	15	339.2	40	5.46	ES-	2
3	PC 20:3-22:1	924.7	15	305.2	40	5.46	ES-	1
4	PC 20:3-22:1	924.7	15	337.2	40	5.46	ES-	2
5	PC 20:3-22:2	922.7	15	305.2	40	5.46	ES-	1
6	PC 20:3-22:2	922.7	15	335.2	40	5.46	ES-	2
7	PC 20:3-22:3	920.6	15	305.2	40	5.46	ES-	1
8	PC 20:3-22:3	920.6	15	333.2	40	5.46	ES-	2
9	PC 20:3-22:4	918.6	15	305.2	40	5.46	ES-	1
10	PC 20:3-22:4	918.6	15	331.2	40	5.46	ES-	2
11	PC 20:3-22:5	916.6	15	305.2	40	5.46	ES-	1
12	PC 20:3-22:5	916.6	15	329.2	40	5.46	ES-	2
13	PC 20:3-22:6	914.6	15	305.2	40	5.46	ES-	1
14	PC 20:3-22:6	914.6	15	327.2	40	5.46	ES-	2
15	PC 20:4-20:4	888.6	15	303.2	40	5.46	ES-	1
16	PC 20:4-20:5	886.6	15	301.2	40	5.46	ES-	1
17	PC 20:4-20:5	886.6	15	303.2	40	5.46	ES-	2
18	PC 20:4-22:0	924.7	15	303.2	40	5.46	ES-	1
19	PC 20:4-22:0	924.7	15	339.2	40	5.46	ES-	2
20	PC 20:4-22:1	922.7	15	303.2	40	5.46	ES-	1
21	PC 20:4-22:1	922.7	15	337.2	40	5.46	ES-	2
22	PC 20:4-22:2	920.6	15	303.2	40	5.46	ES-	1
23	PC 20:4-22:2	920.6	15	335.2	40	5.46	ES-	2
24	PC 20:4-22:3	918.6	15	303.2	40	5.46	ES-	1
25	PC 20:4-22:3	918.6	15	333.2	40	5.46	ES-	2
26	PC 20:4-22:4	916.6	15	303.2	40	5.46	ES-	1
27	PC 20:4-22:4	916.6	15	331.2	40	5.46	ES-	2

28	PC 20:4-22:5	914.6	15	303.2	40	5.46	ES-	1
29	PC 20:4-22:5	914.6	15	329.2	40	5.46	ES-	2
30	PC 20:4-22:6	912.6	15	303.2	40	5.46	ES-	1
31	PC 20:4-22:6	912.6	15	327.2	40	5.46	ES-	2
32	PC 20:5-20:5	884.5	15	301.2	40	5.46	ES-	1
33	PC 20:5-22:0	922.7	15	301.2	40	5.46	ES-	1
34	PC 20:5-22:0	922.7	15	339.2	40	5.46	ES-	2
35	PC 20:5-22:1	920.6	15	301.2	40	5.46	ES-	1
36	PC 20:5-22:1	920.6	15	337.2	40	5.46	ES-	2
37	PC 20:5-22:2	918.6	15	301.2	40	5.46	ES-	1
38	PC 20:5-22:2	918.6	15	335.2	40	5.46	ES-	2
39	PC 20:5-22:3	916.6	15	301.2	40	5.46	ES-	1
40	PC 20:5-22:3	916.6	15	333.2	40	5.46	ES-	2
41	PC 20:5-22:4	914.6	15	301.2	40	5.46	ES-	1
42	PC 20:5-22:4	914.6	15	331.2	40	5.46	ES-	2
43	PC 20:5-22:5	912.6	15	301.2	40	5.46	ES-	1
44	PC 20:5-22:5	912.6	15	329.2	40	5.46	ES-	2
45	PC 20:5-22:6	910.6	15	301.2	40	5.46	ES-	1
46	PC 20:5-22:6	910.6	15	327.2	40	5.46	ES-	2
47	PC 22:0-22:0	960.8	15	339.2	40	5.46	ES-	1
48	PC 22:0-22:1	958.7	15	337.2	40	5.46	ES-	1
49	PC 22:0-22:1	958.7	15	339.2	40	5.46	ES-	2
50	PC 22:0-22:2	956.7	15	335.2	40	5.46	ES-	1
51	PC 22:0-22:2	956.7	15	339.2	40	5.46	ES-	2
52	PC 22:0-22:3	954.7	15	333.2	40	5.46	ES-	1
53	PC 22:0-22:3	954.7	15	339.2	40	5.46	ES-	2
54	PC 22:0-22:4	952.7	15	331.2	40	5.46	ES-	1
55	PC 22:0-22:4	952.7	15	339.2	40	5.46	ES-	2
56	PC 22:0-22:5	950.7	15	329.2	40	5.46	ES-	1
57	PC 22:0-22:5	950.7	15	339.2	40	5.46	ES-	2
58	PC 22:0-22:6	948.7	15	327.2	40	5.46	ES-	1
59	PC 22:0-22:6	948.7	15	339.2	40	5.46	ES-	2
60	PC 22:1-22:1	956.7	15	337.2	40	5.46	ES-	1
61	PC 22:1-22:2	954.7	15	335.2	40	5.46	ES-	1
62	PC 22:1-22:2	954.7	15	337.2	40	5.46	ES-	2

63	PC 22:1-22:3	952.7	15	333.2	40	5.46	ES-	1
64	PC 22:1-22:3	952.7	15	337.2	40	5.46	ES-	2
65	PC 22:1-22:4	950.7	15	331.2	40	5.46	ES-	1
66	PC 22:1-22:4	950.7	15	337.2	40	5.46	ES-	2
67	PC 22:1-22:5	948.7	15	329.2	40	5.46	ES-	1
68	PC 22:1-22:5	948.7	15	337.2	40	5.46	ES-	2
69	PC 22:1-22:6	946.7	15	327.2	40	5.46	ES-	1
70	PC 22:1-22:6	946.7	15	337.2	40	5.46	ES-	2
71	PC 22:2-22:2	952.7	15	335.2	40	5.46	ES-	1
72	PC 22:2-22:3	950.7	15	333.2	40	5.46	ES-	1
73	PC 22:2-22:3	950.7	15	335.2	40	5.46	ES-	2
74	PC 22:2-22:4	948.7	15	331.2	40	5.46	ES-	1
75	PC 22:2-22:4	948.7	15	335.2	40	5.46	ES-	2
76	PC 22:2-22:5	946.7	15	329.2	40	5.46	ES-	1
77	PC 22:2-22:5	946.7	15	335.2	40	5.46	ES-	2
78	PC 22:2-22:6	944.6	15	327.2	40	5.46	ES-	1
79	PC 22:2-22:6	944.6	15	335.2	40	5.46	ES-	2
80	PC 22:3-22:3	948.7	15	333.2	40	5.46	ES-	1
81	PC 22:3-22:4	946.7	15	331.2	40	5.46	ES-	1
82	PC 22:3-22:4	946.7	15	333.2	40	5.46	ES-	2
83	PC 22:3-22:5	944.6	15	329.2	40	5.46	ES-	1
84	PC 22:3-22:5	944.6	15	333.2	40	5.46	ES-	2
85	PC 22:3-22:6	942.6	15	327.2	40	5.46	ES-	1
86	PC 22:3-22:6	942.6	15	333.2	40	5.46	ES-	2
87	PC 22:4-22:4	944.6	15	331.2	40	5.46	ES-	1
88	PC 22:4-22:5	942.6	15	329.2	40	5.46	ES-	1
89	PC 22:4-22:5	942.6	15	331.2	40	5.46	ES-	2
90	PC 22:4-22:6	940.6	15	327.2	40	5.46	ES-	1
91	PC 22:4-22:6	940.6	15	331.2	40	5.46	ES-	2
92	PC 22:5-22:5	940.6	15	329.2	40	5.46	ES-	1
93	PC 22:5-22:6	938.6	15	327.2	40	5.46	ES-	1
94	PC 22:5-22:6	938.6	15	329.2	40	5.46	ES-	2
95	PC 22:6-22:6	936.6	15	327.2	40	5.46	ES-	1
96	PE 20:3-22:0	824.6	50	305.2	25	6.32	ES-	1
97	PE 20:3-22:0	824.6	50	339.2	25	6.32	ES-	2

98	PE 20:3-22:1	822.6	50	305.2	25	6.32	ES-	1
99	PE 20:3-22:1	822.6	50	337.2	25	6.32	ES-	2
100	PE 20:3-22:2	820.6	50	305.2	25	6.32	ES-	1
101	PE 20:3-22:2	820.6	50	335.2	25	6.32	ES-	2
102	PE 20:3-22:3	818.6	50	305.2	25	6.32	ES-	1
103	PE 20:3-22:3	818.6	50	333.2	25	6.32	ES-	2
104	PE 20:3-22:4	816.6	50	305.2	25	6.32	ES-	1
105	PE 20:3-22:4	816.6	50	331.2	25	6.32	ES-	2
106	PE 20:3-22:5	814.5	50	305.2	25	6.32	ES-	1
107	PE 20:3-22:5	814.5	50	329.2	25	6.32	ES-	2
108	PE 20:3-22:6	812.5	50	305.2	25	6.32	ES-	1
109	PE 20:3-22:6	812.5	50	327.2	25	6.32	ES-	2
110	PE 20:4-20:4	786.5	50	303.2	25	6.32	ES-	1
111	PE 20:4-20:5	784.5	50	301.2	25	6.32	ES-	1
112	PE 20:4-20:5	784.5	50	303.2	25	6.32	ES-	2
113	PE 20:4-22:0	822.6	50	303.2	25	6.32	ES-	1
114	PE 20:4-22:0	822.6	50	339.2	25	6.32	ES-	2
115	PE 20:4-22:1	820.6	50	303.2	25	6.32	ES-	1
116	PE 20:4-22:1	820.6	50	337.2	25	6.32	ES-	2
117	PE 20:4-22:2	818.6	50	303.2	25	6.32	ES-	1
118	PE 20:4-22:2	818.6	50	335.2	25	6.32	ES-	2
119	PE 20:4-22:3	816.6	50	303.2	25	6.32	ES-	1
120	PE 20:4-22:3	816.6	50	333.2	25	6.32	ES-	2
121	PE 20:4-22:4	814.5	50	303.2	25	6.32	ES-	1
122	PE 20:4-22:4	814.5	50	331.2	25	6.32	ES-	2
123	PE 20:4-22:5	812.5	50	303.2	25	6.32	ES-	1
124	PE 20:4-22:5	812.5	50	329.2	25	6.32	ES-	2
125	PE 20:4-22:6	810.5	50	303.2	25	6.32	ES-	1
126	PE 20:4-22:6	810.5	50	327.2	25	6.32	ES-	2
127	PE 20:5-20:5	782.5	50	301.2	25	6.32	ES-	1
128	PE 20:5-22:0	820.6	50	301.2	25	6.32	ES-	1
129	PE 20:5-22:0	820.6	50	339.2	25	6.32	ES-	2
130	PE 20:5-22:1	818.6	50	301.2	25	6.32	ES-	1
131	PE 20:5-22:1	818.6	50	337.2	25	6.32	ES-	2
132	PE 20:5-22:2	816.6	50	301.2	25	6.32	ES-	1

133	PE 20:5-22:2	816.6	50	335.2	25	6.32	ES-	2
134	PE 20:5-22:3	814.5	50	301.2	25	6.32	ES-	1
135	PE 20:5-22:3	814.5	50	333.2	25	6.32	ES-	2
136	PE 20:5-22:4	812.5	50	301.2	25	6.32	ES-	1
137	PE 20:5-22:4	812.5	50	331.2	25	6.32	ES-	2
138	PE 20:5-22:5	810.5	50	301.2	25	6.32	ES-	1
139	PE 20:5-22:5	810.5	50	329.2	25	6.32	ES-	2
140	PE 20:5-22:6	808.5	50	301.2	25	6.32	ES-	1
141	PE 20:5-22:6	808.5	50	327.2	25	6.32	ES-	2
142	PE 22:0-22:0	858.7	50	339.2	25	6.32	ES-	1
143	PE 22:0-22:1	856.7	50	337.2	25	6.32	ES-	1
144	PE 22:0-22:1	856.7	50	339.2	25	6.32	ES-	2
145	PE 22:0-22:2	854.7	50	335.2	25	6.32	ES-	1
146	PE 22:0-22:2	854.7	50	339.2	25	6.32	ES-	2
147	PE 22:0-22:3	852.6	50	333.2	25	6.32	ES-	1
148	PE 22:0-22:3	852.6	50	339.2	25	6.32	ES-	2
149	PE 22:0-22:4	850.6	50	331.2	25	6.32	ES-	1
150	PE 22:0-22:4	850.6	50	339.2	25	6.32	ES-	2
151	PE 22:0-22:5	848.6	50	329.2	25	6.32	ES-	1
152	PE 22:0-22:5	848.6	50	339.2	25	6.32	ES-	2
153	PE 22:0-22:6	846.6	50	327.2	25	6.32	ES-	1
154	PE 22:0-22:6	846.6	50	339.2	25	6.32	ES-	2
155	PE 22:1-22:1	854.7	50	337.2	25	6.32	ES-	1
156	PE 22:1-22:2	852.6	50	335.2	25	6.32	ES-	1
157	PE 22:1-22:2	852.6	50	337.2	25	6.32	ES-	2
158	PE 22:1-22:3	850.6	50	333.2	25	6.32	ES-	1
159	PE 22:1-22:3	850.6	50	337.2	25	6.32	ES-	2
160	PE 22:1-22:4	848.6	50	331.2	25	6.32	ES-	1
161	PE 22:1-22:4	848.6	50	337.2	25	6.32	ES-	2
162	PE 22:1-22:5	846.6	50	329.2	25	6.32	ES-	1
163	PE 22:1-22:5	846.6	50	337.2	25	6.32	ES-	2
164	PE 22:1-22:6	844.6	50	327.2	25	6.32	ES-	1
165	PE 22:1-22:6	844.6	50	337.2	25	6.32	ES-	2
166	PE 22:2-22:2	850.6	50	335.2	25	6.32	ES-	1
167	PE 22:2-22:3	848.6	50	333.2	25	6.32	ES-	1

168	PE 22:2-22:3	848.6	50	335.2	25	6.32	ES-	2
169	PE 22:2-22:4	846.6	50	331.2	25	6.32	ES-	1
170	PE 22:2-22:4	846.6	50	335.2	25	6.32	ES-	2
171	PE 22:2-22:5	844.6	50	329.2	25	6.32	ES-	1
172	PE 22:2-22:5	844.6	50	335.2	25	6.32	ES-	2
173	PE 22:2-22:6	842.6	50	327.2	25	6.32	ES-	1
174	PE 22:2-22:6	842.6	50	335.2	25	6.32	ES-	2
175	PE 22:3-22:3	846.6	50	333.2	25	6.32	ES-	1
176	PE 22:3-22:4	844.6	50	331.2	25	6.32	ES-	1
177	PE 22:3-22:4	844.6	50	333.2	25	6.32	ES-	2
178	PE 22:3-22:5	842.6	50	329.2	25	6.32	ES-	1
179	PE 22:3-22:5	842.6	50	333.2	25	6.32	ES-	2
180	PE 22:3-22:6	840.6	50	327.2	25	6.32	ES-	1
181	PE 22:3-22:6	840.6	50	333.2	25	6.32	ES-	2
182	PE 22:4-22:4	842.6	50	331.2	25	6.32	ES-	1
183	PE 22:4-22:5	840.6	50	329.2	25	6.32	ES-	1
184	PE 22:4-22:5	840.6	50	331.2	25	6.32	ES-	2
185	PE 22:4-22:6	838.5	50	327.2	25	6.32	ES-	1
186	PE 22:4-22:6	838.5	50	331.2	25	6.32	ES-	2
187	PE 22:5-22:5	838.5	50	329.2	25	6.32	ES-	1
188	PE 22:5-22:6	836.5	50	327.2	25	6.32	ES-	1
189	PE 22:5-22:6	836.5	50	329.2	25	6.32	ES-	2
190	PE 22:6-22:6	834.5	50	327.2	25	6.32	ES-	1
191	PG 20:3-22:0	855.6	30	305.2	40	8.99	ES-	1
192	PG 20:3-22:0	855.6	30	339.2	40	8.99	ES-	2
193	PG 20:3-22:1	853.6	30	305.2	40	8.99	ES-	1
194	PG 20:3-22:1	853.6	30	337.2	40	8.99	ES-	2
195	PG 20:3-22:2	851.6	30	305.2	40	8.99	ES-	1
196	PG 20:3-22:2	851.6	30	335.2	40	8.99	ES-	2
197	PG 20:3-22:3	849.6	30	305.2	40	8.99	ES-	1
198	PG 20:3-22:3	849.6	30	333.2	40	8.99	ES-	2
199	PG 20:3-22:4	847.5	30	305.2	40	8.99	ES-	1
200	PG 20:3-22:4	847.5	30	331.2	40	8.99	ES-	2
201	PG 20:3-22:5	845.5	30	305.2	40	8.99	ES-	1
202	PG 20:3-22:5	845.5	30	329.2	40	8.99	ES-	2

203	PG 20:3-22:6	843.5	30	305.2	40	8.99	ES-	1
204	PG 20:3-22:6	843.5	30	327.2	40	8.99	ES-	2
205	PG 20:4-20:4	817.5	30	303.2	40	8.99	ES-	1
206	PG 20:4-20:5	815.5	30	301.2	40	8.99	ES-	1
207	PG 20:4-20:5	815.5	30	303.2	40	8.99	ES-	2
208	PG 20:4-22:0	853.6	30	303.2	40	8.99	ES-	1
209	PG 20:4-22:0	853.6	30	339.2	40	8.99	ES-	2
210	PG 20:4-22:1	851.6	30	303.2	40	8.99	ES-	1
211	PG 20:4-22:1	851.6	30	337.2	40	8.99	ES-	2
212	PG 20:4-22:2	849.6	30	303.2	40	8.99	ES-	1
213	PG 20:4-22:2	849.6	30	335.2	40	8.99	ES-	2
214	PG 20:4-22:3	847.5	30	303.2	40	8.99	ES-	1
215	PG 20:4-22:3	847.5	30	333.2	40	8.99	ES-	2
216	PG 20:4-22:4	845.5	30	303.2	40	8.99	ES-	1
217	PG 20:4-22:4	845.5	30	331.2	40	8.99	ES-	2
218	PG 20:4-22:5	843.5	30	303.2	40	8.99	ES-	1
219	PG 20:4-22:5	843.5	30	329.2	40	8.99	ES-	2
220	PG 20:4-22:6	841.5	30	303.2	40	8.99	ES-	1
221	PG 20:4-22:6	841.5	30	327.2	40	8.99	ES-	2
222	PG 20:5-20:5	813.5	30	301.2	40	8.99	ES-	1
223	PG 20:5-22:0	851.6	30	301.2	40	8.99	ES-	1
224	PG 20:5-22:0	851.6	30	339.2	40	8.99	ES-	2
225	PG 20:5-22:1	849.6	30	301.2	40	8.99	ES-	1
226	PG 20:5-22:1	849.6	30	337.2	40	8.99	ES-	2
227	PG 20:5-22:2	847.5	30	301.2	40	8.99	ES-	1
228	PG 20:5-22:2	847.5	30	335.2	40	8.99	ES-	2
229	PG 20:5-22:3	845.5	30	301.2	40	8.99	ES-	1
230	PG 20:5-22:3	845.5	30	333.2	40	8.99	ES-	2
231	PG 20:5-22:4	843.5	30	301.2	40	8.99	ES-	1
232	PG 20:5-22:4	843.5	30	331.2	40	8.99	ES-	2
233	PG 20:5-22:5	841.5	30	301.2	40	8.99	ES-	1
234	PG 20:5-22:5	841.5	30	329.2	40	8.99	ES-	2
235	PG 20:5-22:6	839.5	30	301.2	40	8.99	ES-	1
236	PG 20:5-22:6	839.5	30	327.2	40	8.99	ES-	2
237	PG 22:0-22:0	889.7	30	339.2	40	8.99	ES-	1

238	PG 22:0-22:1	887.7	30	337.2	40	8.99	ES-	1
239	PG 22:0-22:1	887.7	30	339.2	40	8.99	ES-	2
240	PG 22:0-22:2	885.7	30	335.2	40	8.99	ES-	1
241	PG 22:0-22:2	885.7	30	339.2	40	8.99	ES-	2
242	PG 22:0-22:3	883.6	30	333.2	40	8.99	ES-	1
243	PG 22:0-22:3	883.6	30	339.2	40	8.99	ES-	2
244	PG 22:0-22:4	881.6	30	331.2	40	8.99	ES-	1
245	PG 22:0-22:4	881.6	30	339.2	40	8.99	ES-	2
246	PG 22:0-22:5	879.6	30	329.2	40	8.99	ES-	1
247	PG 22:0-22:5	879.6	30	339.2	40	8.99	ES-	2
248	PG 22:0-22:6	877.6	30	327.2	40	8.99	ES-	1
249	PG 22:0-22:6	877.6	30	339.2	40	8.99	ES-	2
250	PG 22:1-22:1	885.7	30	337.2	40	8.99	ES-	1
251	PG 22:1-22:2	883.6	30	335.2	40	8.99	ES-	1
252	PG 22:1-22:2	883.6	30	337.2	40	8.99	ES-	2
253	PG 22:1-22:3	881.6	30	333.2	40	8.99	ES-	1
254	PG 22:1-22:3	881.6	30	337.2	40	8.99	ES-	2
255	PG 22:1-22:4	879.6	30	331.2	40	8.99	ES-	1
256	PG 22:1-22:4	879.6	30	337.2	40	8.99	ES-	2
257	PG 22:1-22:5	877.6	30	329.2	40	8.99	ES-	1
258	PG 22:1-22:5	877.6	30	337.2	40	8.99	ES-	2
259	PG 22:1-22:6	875.6	30	327.2	40	8.99	ES-	1
260	PG 22:1-22:6	875.6	30	337.2	40	8.99	ES-	2
261	PG 22:2-22:2	881.6	30	335.2	40	8.99	ES-	1
262	PG 22:2-22:3	879.6	30	333.2	40	8.99	ES-	1
263	PG 22:2-22:3	879.6	30	335.2	40	8.99	ES-	2
264	PG 22:2-22:4	877.6	30	331.2	40	8.99	ES-	1
265	PG 22:2-22:4	877.6	30	335.2	40	8.99	ES-	2
266	PG 22:2-22:5	875.6	30	329.2	40	8.99	ES-	1
267	PG 22:2-22:5	875.6	30	335.2	40	8.99	ES-	2
268	PG 22:2-22:6	873.6	30	327.2	40	8.99	ES-	1
269	PG 22:2-22:6	873.6	30	335.2	40	8.99	ES-	2
270	PG 22:3-22:3	877.6	30	333.2	40	8.99	ES-	1
271	PG 22:3-22:4	875.6	30	331.2	40	8.99	ES-	1
272	PG 22:3-22:4	875.6	30	333.2	40	8.99	ES-	2

273	PG 22:3-22:5	873.6	30	329.2	40	8.99	ES-	1
274	PG 22:3-22:5	873.6	30	333.2	40	8.99	ES-	2
275	PG 22:3-22:6	871.5	30	327.2	40	8.99	ES-	1
276	PG 22:3-22:6	871.5	30	333.2	40	8.99	ES-	2
277	PG 22:4-22:4	873.6	30	331.2	40	8.99	ES-	1
278	PG 22:4-22:5	871.5	30	329.2	40	8.99	ES-	1
279	PG 22:4-22:5	871.5	30	331.2	40	8.99	ES-	2
280	PG 22:4-22:6	869.5	30	327.2	40	8.99	ES-	1
281	PG 22:4-22:6	869.5	30	331.2	40	8.99	ES-	2
282	PG 22:5-22:5	869.5	30	329.2	40	8.99	ES-	1
283	PG 22:5-22:6	867.5	30	327.2	40	8.99	ES-	1
284	PG 22:5-22:6	867.5	30	329.2	40	8.99	ES-	2
285	PG 22:6-22:6	865.5	30	327.2	40	8.99	ES-	1
286	PS 20:3-22:0	868.6	30	305.2	50	12.23	ES-	1
287	PS 20:3-22:0	868.6	30	339.2	50	12.23	ES-	2
288	PS 20:3-22:1	866.6	30	305.2	50	12.23	ES-	1
289	PS 20:3-22:1	866.6	30	337.2	50	12.23	ES-	2
290	PS 20:3-22:2	864.6	30	305.2	50	12.23	ES-	1
291	PS 20:3-22:2	864.6	30	335.2	50	12.23	ES-	2
292	PS 20:3-22:3	862.6	30	305.2	50	12.23	ES-	1
293	PS 20:3-22:3	862.6	30	333.2	50	12.23	ES-	2
294	PS 20:3-22:4	860.5	30	305.2	50	12.23	ES-	1
295	PS 20:3-22:4	860.5	30	331.2	50	12.23	ES-	2
296	PS 20:3-22:5	858.5	30	305.2	50	12.23	ES-	1
297	PS 20:3-22:5	858.5	30	329.2	50	12.23	ES-	2
298	PS 20:3-22:6	856.5	30	305.2	50	12.23	ES-	1
299	PS 20:3-22:6	856.5	30	327.2	50	12.23	ES-	2
300	PS 20:4-20:4	830.5	30	303.2	50	12.23	ES-	1
301	PS 20:4-20:5	828.5	30	301.2	50	12.23	ES-	1
302	PS 20:4-20:5	828.5	30	303.2	50	12.23	ES-	2
303	PS 20:4-22:0	866.6	30	303.2	50	12.23	ES-	1
304	PS 20:4-22:0	866.6	30	339.2	50	12.23	ES-	2
305	PS 20:4-22:1	864.6	30	303.2	50	12.23	ES-	1
306	PS 20:4-22:1	864.6	30	337.2	50	12.23	ES-	2
307	PS 20:4-22:2	862.6	30	303.2	50	12.23	ES-	1

308	PS 20:4-22:2	862.6	30	335.2	50	12.23	ES-	2
309	PS 20:4-22:3	860.5	30	303.2	50	12.23	ES-	1
310	PS 20:4-22:3	860.5	30	333.2	50	12.23	ES-	2
311	PS 20:4-22:4	858.5	30	303.2	50	12.23	ES-	1
312	PS 20:4-22:4	858.5	30	331.2	50	12.23	ES-	2
313	PS 20:4-22:5	856.5	30	303.2	50	12.23	ES-	1
314	PS 20:4-22:5	856.5	30	329.2	50	12.23	ES-	2
315	PS 20:4-22:6	854.5	30	303.2	50	12.23	ES-	1
316	PS 20:4-22:6	854.5	30	327.2	50	12.23	ES-	2
317	PS 20:5-20:5	826.5	30	301.2	50	12.23	ES-	1
318	PS 20:5-22:0	864.6	30	301.2	50	12.23	ES-	1
319	PS 20:5-22:0	864.6	30	339.2	50	12.23	ES-	2
320	PS 20:5-22:1	862.6	30	301.2	50	12.23	ES-	1
321	PS 20:5-22:1	862.6	30	337.2	50	12.23	ES-	2
322	PS 20:5-22:2	860.5	30	301.2	50	12.23	ES-	1
323	PS 20:5-22:2	860.5	30	335.2	50	12.23	ES-	2
324	PS 20:5-22:3	858.5	30	301.2	50	12.23	ES-	1
325	PS 20:5-22:3	858.5	30	333.2	50	12.23	ES-	2
326	PS 20:5-22:4	856.5	30	301.2	50	12.23	ES-	1
327	PS 20:5-22:4	856.5	30	331.2	50	12.23	ES-	2
328	PS 20:5-22:5	854.5	30	301.2	50	12.23	ES-	1
329	PS 20:5-22:5	854.5	30	329.2	50	12.23	ES-	2
330	PS 20:5-22:6	852.5	30	301.2	50	12.23	ES-	1
331	PS 20:5-22:6	852.5	30	327.2	50	12.23	ES-	2
332	PS 22:0-22:0	902.7	30	339.2	50	12.23	ES-	1
333	PS 22:0-22:1	900.7	30	337.2	50	12.23	ES-	1
334	PS 22:0-22:1	900.7	30	339.2	50	12.23	ES-	2
335	PS 22:0-22:2	898.7	30	335.2	50	12.23	ES-	1
336	PS 22:0-22:2	898.7	30	339.2	50	12.23	ES-	2
337	PS 22:0-22:3	896.6	30	333.2	50	12.23	ES-	1
338	PS 22:0-22:3	896.6	30	339.2	50	12.23	ES-	2
339	PS 22:0-22:4	894.6	30	331.2	50	12.23	ES-	1
340	PS 22:0-22:4	894.6	30	339.2	50	12.23	ES-	2
341	PS 22:0-22:5	892.6	30	329.2	50	12.23	ES-	1
342	PS 22:0-22:5	892.6	30	339.2	50	12.23	ES-	2

343	PS 22:0-22:6	890.6	30	327.2	50	12.23	ES-	1
344	PS 22:0-22:6	890.6	30	339.2	50	12.23	ES-	2
345	PS 22:1-22:1	898.7	30	337.2	50	12.23	ES-	1
346	PS 22:1-22:2	896.6	30	335.2	50	12.23	ES-	1
347	PS 22:1-22:2	896.6	30	337.2	50	12.23	ES-	2
348	PS 22:1-22:3	894.6	30	333.2	50	12.23	ES-	1
349	PS 22:1-22:3	894.6	30	337.2	50	12.23	ES-	2
350	PS 22:1-22:4	892.6	30	331.2	50	12.23	ES-	1
351	PS 22:1-22:4	892.6	30	337.2	50	12.23	ES-	2
352	PS 22:1-22:5	890.6	30	329.2	50	12.23	ES-	1
353	PS 22:1-22:5	890.6	30	337.2	50	12.23	ES-	2
354	PS 22:1-22:6	888.6	30	327.2	50	12.23	ES-	1
355	PS 22:1-22:6	888.6	30	337.2	50	12.23	ES-	2
356	PS 22:2-22:2	894.6	30	335.2	50	12.23	ES-	1
357	PS 22:2-22:3	892.6	30	333.2	50	12.23	ES-	1
358	PS 22:2-22:3	892.6	30	335.2	50	12.23	ES-	2
359	PS 22:2-22:4	890.6	30	331.2	50	12.23	ES-	1
360	PS 22:2-22:4	890.6	30	335.2	50	12.23	ES-	2
361	PS 22:2-22:5	888.6	30	329.2	50	12.23	ES-	1
362	PS 22:2-22:5	888.6	30	335.2	50	12.23	ES-	2
363	PS 22:2-22:6	886.6	30	327.2	50	12.23	ES-	1
364	PS 22:2-22:6	886.6	30	335.2	50	12.23	ES-	2
365	PS 22:3-22:3	890.6	30	333.2	50	12.23	ES-	1
366	PS 22:3-22:4	888.6	30	331.2	50	12.23	ES-	1
367	PS 22:3-22:4	888.6	30	333.2	50	12.23	ES-	2
368	PS 22:3-22:5	886.6	30	329.2	50	12.23	ES-	1
369	PS 22:3-22:5	886.6	30	333.2	50	12.23	ES-	2
370	PS 22:3-22:6	884.5	30	327.2	50	12.23	ES-	1
371	PS 22:3-22:6	884.5	30	333.2	50	12.23	ES-	2
372	PS 22:4-22:4	886.6	30	331.2	50	12.23	ES-	1
373	PS 22:4-22:5	884.5	30	329.2	50	12.23	ES-	1
374	PS 22:4-22:5	884.5	30	331.2	50	12.23	ES-	2
375	PS 22:4-22:6	882.5	30	327.2	50	12.23	ES-	1
376	PS 22:4-22:6	882.5	30	331.2	50	12.23	ES-	2
377	PS 22:5-22:5	882.5	30	329.2	50	12.23	ES-	1

378	PS 22:5-22:6	880.5	30	327.2	50	12.23	ES-	1
379	PS 22:5-22:6	880.5	30	329.2	50	12.23	ES-	2
380	PS 22:6-22:6	878.5	30	327.2	50	12.23	ES-	1

Method 13: PCp and PEp (1)

No	Name	Precursor	CV (V)	Product	CE (V)	RT setting (min)	IonMode	Ion
1	PC 16:0p-12:0	662.5	20	422.3	30	5.45	ES+	1
2	PC 16:0p-12:0	662.5	20	480.4	30	5.45	ES+	2
3	PC 16:0p-14:0	690.5	20	450.3	30	5.45	ES+	1
4	PC 16:0p-14:0	690.5	20	480.4	30	5.45	ES+	2
5	PC 16:0p-14:1	688.5	20	448.3	30	5.45	ES+	1
6	PC 16:0p-14:1	688.5	20	480.4	30	5.45	ES+	2
7	PC 16:0p-16:0	718.6	20	478.3	30	5.45	ES+	1
8	PC 16:0p-16:0	718.6	20	480.4	30	5.45	ES+	2
9	PC 16:0p-16:1	716.6	20	476.3	30	5.45	ES+	1
10	PC 16:0p-16:1	716.6	20	480.4	30	5.45	ES+	2
11	PC 16:0p-18:0	746.6	20	480.4	30	5.45	ES+	1
12	PC 16:0p-18:0	746.6	20	506.3	30	5.45	ES+	2
13	PC 16:0p-18:1	744.6	20	480.4	30	5.45	ES+	1
14	PC 16:0p-18:1	744.6	20	504.3	30	5.45	ES+	2
15	PC 16:0p-18:2	742.6	20	480.4	30	5.45	ES+	1
16	PC 16:0p-18:2	742.6	20	502.3	30	5.45	ES+	2
17	PC 16:0p-18:3	740.6	20	480.4	30	5.45	ES+	1
18	PC 16:0p-18:3	740.6	20	500.3	30	5.45	ES+	2
19	PC 16:0p-18:4	738.5	20	480.4	30	5.45	ES+	1
20	PC 16:0p-18:4	738.5	20	498.3	30	5.45	ES+	2
21	PC 16:0p-20:0	774.6	20	480.4	30	5.45	ES+	1
22	PC 16:0p-20:0	774.6	20	534.3	30	5.45	ES+	2
23	PC 16:0p-20:1	772.6	20	480.4	30	5.45	ES+	1
24	PC 16:0p-20:1	772.6	20	532.3	30	5.45	ES+	2
25	PC 16:0p-20:2	770.6	20	480.4	30	5.45	ES+	1
26	PC 16:0p-20:2	770.6	20	530.3	30	5.45	ES+	2
27	PC 16:0p-20:3	768.6	20	480.4	30	5.45	ES+	1
28	PC 16:0p-20:3	768.6	20	528.3	30	5.45	ES+	2
29	PC 16:0p-20:4	766.6	20	480.4	30	5.45	ES+	1
30	PC 16:0p-20:4	766.6	20	526.3	30	5.45	ES+	2

31	PC 16:0p-20:5	764.6	20	480.4	30	5.45	ES+	1
32	PC 16:0p-20:5	764.6	20	524.3	30	5.45	ES+	2
33	PC 16:0p-22:0	802.7	20	480.4	30	5.45	ES+	1
34	PC 16:0p-22:0	802.7	20	562.3	30	5.45	ES+	2
35	PC 16:0p-22:1	800.7	20	480.4	30	5.45	ES+	1
36	PC 16:0p-22:1	800.7	20	560.3	30	5.45	ES+	2
37	PC 16:0p-22:2	798.6	20	480.4	30	5.45	ES+	1
38	PC 16:0p-22:2	798.6	20	558.3	30	5.45	ES+	2
39	PC 16:0p-22:3	796.6	20	480.4	30	5.45	ES+	1
40	PC 16:0p-22:3	796.6	20	556.3	30	5.45	ES+	2
41	PC 16:0p-22:4	794.6	20	480.4	30	5.45	ES+	1
42	PC 16:0p-22:4	794.6	20	554.3	30	5.45	ES+	2
43	PC 16:0p-22:5	792.6	20	480.4	30	5.45	ES+	1
44	PC 16:0p-22:5	792.6	20	552.3	30	5.45	ES+	2
45	PC 16:0p-22:6	790.6	20	480.4	30	5.45	ES+	1
46	PC 16:0p-22:6	790.6	20	550.3	30	5.45	ES+	2
47	PC 16:1p-12:0	660.5	20	422.3	30	5.45	ES+	1
48	PC 16:1p-12:0	660.5	20	478.4	30	5.45	ES+	2
49	PC 16:1p-14:0	688.5	20	450.3	30	5.45	ES+	1
50	PC 16:1p-14:0	688.5	20	478.4	30	5.45	ES+	2
51	PC 16:1p-14:1	686.5	20	448.3	30	5.45	ES+	1
52	PC 16:1p-14:1	686.5	20	478.4	30	5.45	ES+	2
53	PC 16:1p-16:0	716.6	20	478.3	30	5.45	ES+	1
54	PC 16:1p-16:1	714.5	20	476.3	30	5.45	ES+	1
55	PC 16:1p-16:1	714.5	20	478.4	30	5.45	ES+	2
56	PC 16:1p-18:0	744.6	20	478.4	30	5.45	ES+	1
57	PC 16:1p-18:0	744.6	20	506.3	30	5.45	ES+	2
58	PC 16:1p-18:1	742.6	20	478.4	30	5.45	ES+	1
59	PC 16:1p-18:1	742.6	20	504.3	30	5.45	ES+	2
60	PC 16:1p-18:2	740.6	20	478.4	30	5.45	ES+	1
61	PC 16:1p-18:2	740.6	20	502.3	30	5.45	ES+	2
62	PC 16:1p-18:3	738.5	20	478.4	30	5.45	ES+	1
63	PC 16:1p-18:3	738.5	20	500.3	30	5.45	ES+	2
64	PC 16:1p-18:4	736.5	20	478.4	30	5.45	ES+	1
65	PC 16:1p-18:4	736.5	20	498.3	30	5.45	ES+	2

66	PC 16:1p-20:0	772.6	20	478.4	30	5.45	ES+	1
67	PC 16:1p-20:0	772.6	20	534.3	30	5.45	ES+	2
68	PC 16:1p-20:1	770.6	20	478.4	30	5.45	ES+	1
69	PC 16:1p-20:1	770.6	20	532.3	30	5.45	ES+	2
70	PC 16:1p-20:2	768.6	20	478.4	30	5.45	ES+	1
71	PC 16:1p-20:2	768.6	20	530.3	30	5.45	ES+	2
72	PC 16:1p-20:3	766.6	20	478.4	30	5.45	ES+	1
73	PC 16:1p-20:3	766.6	20	528.3	30	5.45	ES+	2
74	PC 16:1p-20:4	764.6	20	478.4	30	5.45	ES+	1
75	PC 16:1p-20:4	764.6	20	526.3	30	5.45	ES+	2
76	PC 16:1p-20:5	762.5	20	478.4	30	5.45	ES+	1
77	PC 16:1p-20:5	762.5	20	524.3	30	5.45	ES+	2
78	PE 16:0p-12:0	620.5	55	257.3	20	6.22	ES+	1
79	PE 16:0p-12:0	620.5	55	364.2	20	6.22	ES+	2
80	PE 16:0p-14:0	648.5	55	285.3	20	6.22	ES+	1
81	PE 16:0p-14:0	648.5	55	364.2	20	6.22	ES+	2
82	PE 16:0p-14:1	646.5	55	283.3	20	6.22	ES+	1
83	PE 16:0p-14:1	646.5	55	364.2	20	6.22	ES+	2
84	PE 16:0p-16:0	676.5	55	313.3	20	6.22	ES+	1
85	PE 16:0p-16:0	676.5	55	364.2	20	6.22	ES+	2
86	PE 16:0p-16:1	674.5	55	311.3	20	6.22	ES+	1
87	PE 16:0p-16:1	674.5	55	364.2	20	6.22	ES+	2
88	PE 16:0p-18:0	704.6	55	341.3	20	6.22	ES+	1
89	PE 16:0p-18:0	704.6	55	364.2	20	6.22	ES+	2
90	PE 16:0p-18:1	702.5	55	339.3	20	6.22	ES+	1
91	PE 16:0p-18:1	702.5	55	364.2	20	6.22	ES+	2
92	PE 16:0p-18:2	700.5	55	337.3	20	6.22	ES+	1
93	PE 16:0p-18:2	700.5	55	364.2	20	6.22	ES+	2
94	PE 16:0p-18:3	698.5	55	335.3	20	6.22	ES+	1
95	PE 16:0p-18:3	698.5	55	364.2	20	6.22	ES+	2
96	PE 16:0p-18:4	696.5	55	333.3	20	6.22	ES+	1
97	PE 16:0p-18:4	696.5	55	364.2	20	6.22	ES+	2
98	PE 16:0p-20:0	732.6	55	364.2	20	6.22	ES+	1
99	PE 16:0p-20:0	732.6	55	369.3	20	6.22	ES+	2
100	PE 16:0p-20:1	730.6	55	364.2	20	6.22	ES+	1

101	PE 16:0p-20:1	730.6	55	367.3	20	6.22	ES+	2
102	PE 16:0p-20:2	728.6	55	364.2	20	6.22	ES+	1
103	PE 16:0p-20:2	728.6	55	365.3	20	6.22	ES+	2
104	PE 16:0p-20:3	726.5	55	363.3	20	6.22	ES+	1
105	PE 16:0p-20:3	726.5	55	364.2	20	6.22	ES+	2
106	PE 16:0p-20:4	724.5	55	361.3	20	6.22	ES+	1
107	PE 16:0p-20:4	724.5	55	364.2	20	6.22	ES+	2
108	PE 16:0p-20:5	722.5	55	359.3	20	6.22	ES+	1
109	PE 16:0p-20:5	722.5	55	364.2	20	6.22	ES+	2
110	PE 16:0p-22:0	760.6	55	364.2	20	6.22	ES+	1
111	PE 16:0p-22:0	760.6	55	397.3	20	6.22	ES+	2
112	PE 16:0p-22:1	758.6	55	364.2	20	6.22	ES+	1
113	PE 16:0p-22:1	758.6	55	395.3	20	6.22	ES+	2
114	PE 16:0p-22:2	756.6	55	364.2	20	6.22	ES+	1
115	PE 16:0p-22:2	756.6	55	393.3	20	6.22	ES+	2
116	PE 16:0p-22:3	754.6	55	364.2	20	6.22	ES+	1
117	PE 16:0p-22:3	754.6	55	391.3	20	6.22	ES+	2
118	PE 16:0p-22:4	752.6	55	364.2	20	6.22	ES+	1
119	PE 16:0p-22:4	752.6	55	389.3	20	6.22	ES+	2
120	PE 16:0p-22:5	750.5	55	364.2	20	6.22	ES+	1
121	PE 16:0p-22:5	750.5	55	387.3	20	6.22	ES+	2
122	PE 16:0p-22:6	748.5	55	364.2	20	6.22	ES+	1
123	PE 16:0p-22:6	748.5	55	385.3	20	6.22	ES+	2
124	PE 16:1p-12:0	618.4	55	257.3	20	6.22	ES+	1
125	PE 16:1p-12:0	618.4	55	362.2	20	6.22	ES+	2
126	PE 16:1p-14:0	646.5	55	285.3	20	6.22	ES+	1
127	PE 16:1p-14:0	646.5	55	362.2	20	6.22	ES+	2
128	PE 16:1p-14:1	644.5	55	283.3	20	6.22	ES+	1
129	PE 16:1p-14:1	644.5	55	362.2	20	6.22	ES+	2
130	PE 16:1p-16:0	674.5	55	313.3	20	6.22	ES+	1
131	PE 16:1p-16:0	674.5	55	362.2	20	6.22	ES+	2
132	PE 16:1p-16:1	672.5	55	311.3	20	6.22	ES+	1
133	PE 16:1p-16:1	672.5	55	362.2	20	6.22	ES+	2
134	PE 16:1p-18:0	702.5	55	341.3	20	6.22	ES+	1
135	PE 16:1p-18:0	702.5	55	362.2	20	6.22	ES+	2

136	PE 16:1p-18:1	698.5	55	339.3	20	6.22	ES+	1
137	PE 16:1p-18:1	698.5	55	362.2	20	6.22	ES+	2
138	PE 16:1p-18:2	698.5	55	337.3	20	6.22	ES+	1
139	PE 16:1p-18:2	698.5	55	362.2	20	6.22	ES+	2
140	PE 16:1p-18:3	696.5	55	335.3	20	6.22	ES+	1
141	PE 16:1p-18:3	696.5	55	362.2	20	6.22	ES+	2
142	PE 16:1p-18:4	694.5	55	333.3	20	6.22	ES+	1
143	PE 16:1p-18:4	694.5	55	362.2	20	6.22	ES+	2
144	PE 16:1p-20:0	730.6	55	362.2	20	6.22	ES+	1
145	PE 16:1p-20:0	730.6	55	369.3	20	6.22	ES+	2
146	PE 16:1p-20:1	728.6	55	362.2	20	6.22	ES+	1
147	PE 16:1p-20:1	728.6	55	367.3	20	6.22	ES+	2
148	PE 16:1p-20:2	726.5	55	362.2	20	6.22	ES+	1
149	PE 16:1p-20:2	726.5	55	365.3	20	6.22	ES+	2
150	PE 16:1p-20:3	724.5	55	362.2	20	6.22	ES+	1
151	PE 16:1p-20:3	724.5	55	363.3	20	6.22	ES+	2
152	PE 16:1p-20:4	722.5	55	361.3	20	6.22	ES+	1
153	PE 16:1p-20:4	722.5	55	362.2	20	6.22	ES+	2
154	PE 16:1p-20:5	720.5	55	359.3	20	6.22	ES+	1
155	PE 16:1p-20:5	720.5	55	362.2	20	6.22	ES+	2

Method 14: PCp and PEp (2)

No	Name	Precursor	CV (V)	Product	CE (V)	RT setting (min)	IonMode	Ion
1	PC 16:1p-22:0	800.7	20	478.4	30	5.45	ES+	1
2	PC 16:1p-22:0	800.7	20	562.3	30	5.45	ES+	2
3	PC 16:1p-22:1	798.6	20	478.4	30	5.45	ES+	1
4	PC 16:1p-22:1	798.6	20	560.3	30	5.45	ES+	2
5	PC 16:1p-22:2	796.6	20	478.4	30	5.45	ES+	1
6	PC 16:1p-22:2	796.6	20	558.3	30	5.45	ES+	2
7	PC 16:1p-22:3	794.6	20	478.4	30	5.45	ES+	1
8	PC 16:1p-22:3	794.6	20	556.3	30	5.45	ES+	2
9	PC 16:1p-22:4	792.6	20	478.4	30	5.45	ES+	1
10	PC 16:1p-22:4	792.6	20	554.3	30	5.45	ES+	2
11	PC 16:1p-22:5	790.6	20	478.4	30	5.45	ES+	1
12	PC 16:1p-22:5	790.6	20	552.3	30	5.45	ES+	2
13	PC 16:1p-22:6	788.6	20	478.4	30	5.45	ES+	1

14	PC 16:1p-22:6	788.6	20	550.3	30	5.45	ES+	2
15	PC 18:0p-12:0	690.5	20	422.3	30	5.45	ES+	1
16	PC 18:0p-12:0	690.5	20	508.4	30	5.45	ES+	2
17	PC 18:0p-14:0	718.6	20	450.3	30	5.45	ES+	1
18	PC 18:0p-14:0	718.6	20	508.4	30	5.45	ES+	2
19	PC 18:0p-14:1	716.6	20	448.3	30	5.45	ES+	1
20	PC 18:0p-14:1	716.6	20	508.4	30	5.45	ES+	2
21	PC 18:0p-16:0	746.6	20	478.3	30	5.45	ES+	1
22	PC 18:0p-16:0	746.6	20	508.4	30	5.45	ES+	2
23	PC 18:0p-16:1	744.6	20	476.3	30	5.45	ES+	1
24	PC 18:0p-16:1	744.6	20	508.4	30	5.45	ES+	2
25	PC 18:0p-18:0	774.6	20	506.3	30	5.45	ES+	1
26	PC 18:0p-18:0	774.6	20	508.4	30	5.45	ES+	2
27	PC 18:0p-18:1	772.6	20	504.3	30	5.45	ES+	1
28	PC 18:0p-18:1	772.6	20	508.4	30	5.45	ES+	2
29	PC 18:0p-18:2	770.6	20	502.3	30	5.45	ES+	1
30	PC 18:0p-18:2	770.6	20	508.4	30	5.45	ES+	2
31	PC 18:0p-18:3	768.6	20	500.3	30	5.45	ES+	1
32	PC 18:0p-18:3	768.6	20	508.4	30	5.45	ES+	2
33	PC 18:0p-18:4	766.6	20	498.3	30	5.45	ES+	1
34	PC 18:0p-18:4	766.6	20	508.4	30	5.45	ES+	2
35	PC 18:0p-20:0	802.7	20	508.4	30	5.45	ES+	1
36	PC 18:0p-20:0	802.7	20	534.3	30	5.45	ES+	2
37	PC 18:0p-20:1	800.7	20	508.4	30	5.45	ES+	1
38	PC 18:0p-20:1	800.7	20	532.3	30	5.45	ES+	2
39	PC 18:0p-20:2	798.6	20	508.4	30	5.45	ES+	1
40	PC 18:0p-20:2	798.6	20	530.3	30	5.45	ES+	2
41	PC 18:0p-20:3	796.6	20	508.4	30	5.45	ES+	1
42	PC 18:0p-20:3	796.6	20	528.3	30	5.45	ES+	2
43	PC 18:0p-20:4	794.6	20	508.4	30	5.45	ES+	1
44	PC 18:0p-20:4	794.6	20	526.3	30	5.45	ES+	2
45	PC 18:0p-20:5	792.6	20	508.4	30	5.45	ES+	1
46	PC 18:0p-20:5	792.6	20	524.3	30	5.45	ES+	2
47	PC 18:0p-22:0	830.7	20	508.4	30	5.45	ES+	1
48	PC 18:0p-22:0	830.7	20	562.3	30	5.45	ES+	2

49	PC 18:0p-22:1	828.7	20	508.4	30	5.45	ES+	1
50	PC 18:0p-22:1	828.7	20	560.3	30	5.45	ES+	2
51	PC 18:0p-22:2	826.7	20	508.4	30	5.45	ES+	1
52	PC 18:0p-22:2	826.7	20	558.3	30	5.45	ES+	2
53	PC 18:0p-22:3	824.7	20	508.4	30	5.45	ES+	1
54	PC 18:0p-22:3	824.7	20	556.3	30	5.45	ES+	2
55	PC 18:0p-22:4	822.6	20	508.4	30	5.45	ES+	1
56	PC 18:0p-22:4	822.6	20	554.3	30	5.45	ES+	2
57	PC 18:0p-22:5	820.6	20	508.4	30	5.45	ES+	1
58	PC 18:0p-22:5	820.6	20	552.3	30	5.45	ES+	2
59	PC 18:0p-22:6	818.6	20	508.4	30	5.45	ES+	1
60	PC 18:0p-22:6	818.6	20	550.3	30	5.45	ES+	2
61	PC 18:1p-12:0	688.5	20	422.3	30	5.45	ES+	1
62	PC 18:1p-12:0	688.5	20	506.4	30	5.45	ES+	2
63	PC 18:1p-14:0	716.6	20	450.3	30	5.45	ES+	1
64	PC 18:1p-14:0	716.6	20	506.4	30	5.45	ES+	2
65	PC 18:1p-14:1	714.5	20	448.3	30	5.45	ES+	1
66	PC 18:1p-14:1	714.5	20	506.4	30	5.45	ES+	2
67	PC 18:1p-16:0	744.6	20	478.3	30	5.45	ES+	1
68	PC 18:1p-16:0	744.6	20	506.4	30	5.45	ES+	2
69	PC 18:1p-16:1	740.6	20	476.3	30	5.45	ES+	1
70	PC 18:1p-16:1	740.6	20	506.4	30	5.45	ES+	2
71	PC 18:1p-18:0	772.6	20	506.3	30	5.45	ES+	1
72	PC 18:1p-18:1	770.6	20	504.3	30	5.45	ES+	1
73	PC 18:1p-18:1	770.6	20	506.4	30	5.45	ES+	2
74	PC 18:1p-18:2	768.6	20	502.3	30	5.45	ES+	1
75	PC 18:1p-18:2	768.6	20	506.4	30	5.45	ES+	2
76	PC 18:1p-18:3	766.6	20	500.3	30	5.45	ES+	1
77	PC 18:1p-18:3	766.6	20	506.4	30	5.45	ES+	2
78	PC 18:1p-18:4	764.6	20	498.3	30	5.45	ES+	1
79	PC 18:1p-18:4	764.6	20	506.4	30	5.45	ES+	2
80	PE 16:1p-22:0	758.6	55	362.2	20	6.22	ES+	1
81	PE 16:1p-22:0	758.6	55	397.3	20	6.22	ES+	2
82	PE 16:1p-22:1	756.6	55	362.2	20	6.22	ES+	1
83	PE 16:1p-22:1	756.6	55	395.3	20	6.22	ES+	2

84	PE 16:1p-22:2	754.6	55	362.2	20	6.22	ES+	1
85	PE 16:1p-22:2	754.6	55	393.3	20	6.22	ES+	2
86	PE 16:1p-22:3	752.6	55	362.2	20	6.22	ES+	1
87	PE 16:1p-22:3	752.6	55	391.3	20	6.22	ES+	2
88	PE 16:1p-22:4	750.5	55	362.2	20	6.22	ES+	1
89	PE 16:1p-22:4	750.5	55	389.3	20	6.22	ES+	2
90	PE 16:1p-22:5	748.5	55	362.2	20	6.22	ES+	1
91	PE 16:1p-22:5	748.5	55	387.3	20	6.22	ES+	2
92	PE 16:1p-22:6	746.5	55	362.2	20	6.22	ES+	1
93	PE 16:1p-22:6	746.5	55	385.3	20	6.22	ES+	2
94	PE 18:0p-12:0	648.5	55	257.3	20	6.22	ES+	1
95	PE 18:0p-12:0	648.5	55	392.3	20	6.22	ES+	2
96	PE 18:0p-14:0	676.5	55	285.3	20	6.22	ES+	1
97	PE 18:0p-14:0	676.5	55	392.3	20	6.22	ES+	2
98	PE 18:0p-14:1	674.5	55	283.3	20	6.22	ES+	1
99	PE 18:0p-14:1	674.5	55	392.3	20	6.22	ES+	2
100	PE 18:0p-16:0	704.6	55	313.3	20	6.22	ES+	1
101	PE 18:0p-16:0	704.6	55	392.3	20	6.22	ES+	2
102	PE 18:0p-16:1	702.5	55	311.3	20	6.22	ES+	1
103	PE 18:0p-16:1	702.5	55	392.3	20	6.22	ES+	2
104	PE 18:0p-18:0	732.6	55	341.3	20	6.22	ES+	1
105	PE 18:0p-18:0	732.6	55	392.3	20	6.22	ES+	2
106	PE 18:0p-18:1	730.6	55	339.3	20	6.22	ES+	1
107	PE 18:0p-18:1	730.6	55	392.3	20	6.22	ES+	2
108	PE 18:0p-18:2	728.6	55	337.3	20	6.22	ES+	1
109	PE 18:0p-18:2	728.6	55	392.3	20	6.22	ES+	2
110	PE 18:0p-18:3	726.5	55	335.3	20	6.22	ES+	1
111	PE 18:0p-18:3	726.5	55	392.3	20	6.22	ES+	2
112	PE 18:0p-18:4	724.5	55	333.3	20	6.22	ES+	1
113	PE 18:0p-18:4	724.5	55	392.3	20	6.22	ES+	2
114	PE 18:0p-20:0	760.6	55	369.3	20	6.22	ES+	1
115	PE 18:0p-20:0	760.6	55	392.3	20	6.22	ES+	2
116	PE 18:0p-20:1	758.6	55	367.3	20	6.22	ES+	1
117	PE 18:0p-20:1	758.6	55	392.3	20	6.22	ES+	2
118	PE 18:0p-20:2	756.6	55	365.3	20	6.22	ES+	1

119	PE 18:0p-20:2	756.6	55	392.3	20	6.22	ES+	2
120	PE 18:0p-20:3	754.6	55	363.3	20	6.22	ES+	1
121	PE 18:0p-20:3	754.6	55	392.3	20	6.22	ES+	2
122	PE 18:0p-20:4	752.6	55	361.3	20	6.22	ES+	1
123	PE 18:0p-20:4	752.6	55	392.3	20	6.22	ES+	2
124	PE 18:0p-20:5	750.5	55	359.3	20	6.22	ES+	1
125	PE 18:0p-20:5	750.5	55	392.3	20	6.22	ES+	2
126	PE 18:0p-22:0	788.7	55	392.3	20	6.22	ES+	1
127	PE 18:0p-22:0	788.7	55	397.3	20	6.22	ES+	2
128	PE 18:0p-22:1	786.6	55	392.3	20	6.22	ES+	1
129	PE 18:0p-22:1	786.6	55	395.3	20	6.22	ES+	2
130	PE 18:0p-22:2	784.6	55	392.3	20	6.22	ES+	1
131	PE 18:0p-22:2	784.6	55	393.3	20	6.22	ES+	2
132	PE 18:0p-22:3	782.6	55	391.3	20	6.22	ES+	1
133	PE 18:0p-22:3	782.6	55	392.3	20	6.22	ES+	2
134	PE 18:0p-22:4	780.6	55	389.3	20	6.22	ES+	1
135	PE 18:0p-22:4	780.6	55	392.3	20	6.22	ES+	2
136	PE 18:0p-22:5	778.6	55	387.3	20	6.22	ES+	1
137	PE 18:0p-22:5	778.6	55	392.3	20	6.22	ES+	2
138	PE 18:0p-22:6	776.6	55	385.3	20	6.22	ES+	1
139	PE 18:0p-22:6	776.6	55	392.3	20	6.22	ES+	2
140	PE 18:1p-12:0	646.5	55	257.3	20	6.22	ES+	1
141	PE 18:1p-12:0	646.5	55	390.3	20	6.22	ES+	2
142	PE 18:1p-14:0	674.5	55	285.3	20	6.22	ES+	1
143	PE 18:1p-14:0	674.5	55	390.3	20	6.22	ES+	2
144	PE 18:1p-14:1	672.5	55	283.3	20	6.22	ES+	1
145	PE 18:1p-14:1	672.5	55	390.3	20	6.22	ES+	2
146	PE 18:1p-16:0	702.5	55	313.3	20	6.22	ES+	1
147	PE 18:1p-16:0	702.5	55	390.3	20	6.22	ES+	2
148	PE 18:1p-16:1	698.5	55	311.3	20	6.22	ES+	1
149	PE 18:1p-16:1	698.5	55	390.3	20	6.22	ES+	2
150	PE 18:1p-18:0	730.6	55	341.3	20	6.22	ES+	1
151	PE 18:1p-18:0	730.6	55	390.3	20	6.22	ES+	2
152	PE 18:1p-18:1	728.6	55	339.3	20	6.22	ES+	1
153	PE 18:1p-18:1	728.6	55	390.3	20	6.22	ES+	2

154	PE 18:1p-18:2	726.5	55	337.3	20	6.22	ES+	1
155	PE 18:1p-18:2	726.5	55	390.3	20	6.22	ES+	2
156	PE 18:1p-18:3	724.5	55	335.3	20	6.22	ES+	1
157	PE 18:1p-18:3	724.5	55	390.3	20	6.22	ES+	2
158	PE 18:1p-18:4	722.5	55	333.3	20	6.22	ES+	1
159	PE 18:1p-18:4	722.5	55	390.3	20	6.22	ES+	2

Method 15: PCp and PEp (3)

No	Name	Precursor	CV (V)	Product	CE (V)	RT setting (min)	IonMode	Ion
1	PC 18:1p-20:0	800.7	20	506.4	30	5.45	ES+	1
2	PC 18:1p-20:0	800.7	20	534.3	30	5.45	ES+	2
3	PC 18:1p-20:1	798.6	20	506.4	30	5.45	ES+	1
4	PC 18:1p-20:1	798.6	20	532.3	30	5.45	ES+	2
5	PC 18:1p-20:2	796.6	20	506.4	30	5.45	ES+	1
6	PC 18:1p-20:2	796.6	20	530.3	30	5.45	ES+	2
7	PC 18:1p-20:3	794.6	20	506.4	30	5.45	ES+	1
8	PC 18:1p-20:3	794.6	20	528.3	30	5.45	ES+	2
9	PC 18:1p-20:4	792.6	20	506.4	30	5.45	ES+	1
10	PC 18:1p-20:4	792.6	20	526.3	30	5.45	ES+	2
11	PC 18:1p-20:5	790.6	20	506.4	30	5.45	ES+	1
12	PC 18:1p-20:5	790.6	20	524.3	30	5.45	ES+	2
13	PC 18:1p-22:0	828.7	20	506.4	30	5.45	ES+	1
14	PC 18:1p-22:0	828.7	20	562.3	30	5.45	ES+	2
15	PC 18:1p-22:1	826.7	20	506.4	30	5.45	ES+	1
16	PC 18:1p-22:1	826.7	20	560.3	30	5.45	ES+	2
17	PC 18:1p-22:2	824.7	20	506.4	30	5.45	ES+	1
18	PC 18:1p-22:2	824.7	20	558.3	30	5.45	ES+	2
19	PC 18:1p-22:3	822.6	20	506.4	30	5.45	ES+	1
20	PC 18:1p-22:3	822.6	20	556.3	30	5.45	ES+	2
21	PC 18:1p-22:4	820.6	20	506.4	30	5.45	ES+	1
22	PC 18:1p-22:4	820.6	20	554.3	30	5.45	ES+	2
23	PC 18:1p-22:5	818.6	20	506.4	30	5.45	ES+	1
24	PC 18:1p-22:5	818.6	20	552.3	30	5.45	ES+	2
25	PC 18:1p-22:6	816.6	20	506.4	30	5.45	ES+	1
26	PC 18:1p-22:6	816.6	20	550.3	30	5.45	ES+	2
27	PC 18:2p-12:0	684.5	20	422.3	30	5.45	ES+	1

28	PC 18:2p-12:0	684.5	20	504.4	30	5.45	ES+	2
29	PC 18:2p-14:0	712.5	20	450.3	30	5.45	ES+	1
30	PC 18:2p-14:0	712.5	20	504.4	30	5.45	ES+	2
31	PC 18:2p-14:1	710.5	20	448.3	30	5.45	ES+	1
32	PC 18:2p-14:1	710.5	20	504.4	30	5.45	ES+	2
33	PC 18:2p-16:0	740.6	20	478.3	30	5.45	ES+	1
34	PC 18:2p-16:0	740.6	20	504.4	30	5.45	ES+	2
35	PC 18:2p-16:1	740.6	20	476.3	30	5.45	ES+	1
36	PC 18:2p-16:1	740.6	20	504.4	30	5.45	ES+	2
37	PC 18:2p-18:0	770.6	20	504.4	30	5.45	ES+	1
38	PC 18:2p-18:0	770.6	20	506.3	30	5.45	ES+	2
39	PC 18:2p-18:1	768.6	20	504.3	30	5.45	ES+	1
40	PC 18:2p-18:2	766.6	20	502.3	30	5.45	ES+	1
41	PC 18:2p-18:2	766.6	20	504.4	30	5.45	ES+	2
42	PC 18:2p-18:3	764.6	20	500.3	30	5.45	ES+	1
43	PC 18:2p-18:3	764.6	20	504.4	30	5.45	ES+	2
44	PC 18:2p-18:4	762.5	20	498.3	30	5.45	ES+	1
45	PC 18:2p-18:4	762.5	20	504.4	30	5.45	ES+	2
46	PC 18:2p-20:0	798.6	20	504.4	30	5.45	ES+	1
47	PC 18:2p-20:0	798.6	20	534.3	30	5.45	ES+	2
48	PC 18:2p-20:1	796.6	20	504.4	30	5.45	ES+	1
49	PC 18:2p-20:1	796.6	20	532.3	30	5.45	ES+	2
50	PC 18:2p-20:2	794.6	20	504.4	30	5.45	ES+	1
51	PC 18:2p-20:2	794.6	20	530.3	30	5.45	ES+	2
52	PC 18:2p-20:3	792.6	20	504.4	30	5.45	ES+	1
53	PC 18:2p-20:3	792.6	20	528.3	30	5.45	ES+	2
54	PC 18:2p-20:4	790.6	20	504.4	30	5.45	ES+	1
55	PC 18:2p-20:4	790.6	20	526.3	30	5.45	ES+	2
56	PC 18:2p-20:5	788.6	20	504.4	30	5.45	ES+	1
57	PC 18:2p-20:5	788.6	20	524.3	30	5.45	ES+	2
58	PC 18:2p-22:0	826.7	20	504.4	30	5.45	ES+	1
59	PC 18:2p-22:0	826.7	20	562.3	30	5.45	ES+	2
60	PC 18:2p-22:1	824.7	20	504.4	30	5.45	ES+	1
61	PC 18:2p-22:1	824.7	20	560.3	30	5.45	ES+	2
62	PC 18:2p-22:2	822.6	20	504.4	30	5.45	ES+	1

63	PC 18:2p-22:2	822.6	20	558.3	30	5.45	ES+	2
64	PC 18:2p-22:3	820.6	20	504.4	30	5.45	ES+	1
65	PC 18:2p-22:3	820.6	20	556.3	30	5.45	ES+	2
66	PC 18:2p-22:4	818.6	20	504.4	30	5.45	ES+	1
67	PC 18:2p-22:4	818.6	20	554.3	30	5.45	ES+	2
68	PC 18:2p-22:5	816.6	20	504.4	30	5.45	ES+	1
69	PC 18:2p-22:5	816.6	20	552.3	30	5.45	ES+	2
70	PC 18:2p-22:6	814.6	20	504.4	30	5.45	ES+	1
71	PC 18:2p-22:6	814.6	20	550.3	30	5.45	ES+	2
72	PE 18:1p-20:0	758.6	55	369.3	20	6.22	ES+	1
73	PE 18:1p-20:0	758.6	55	390.3	20	6.22	ES+	2
74	PE 18:1p-20:1	756.6	55	367.3	20	6.22	ES+	1
75	PE 18:1p-20:1	756.6	55	390.3	20	6.22	ES+	2
76	PE 18:1p-20:2	754.6	55	365.3	20	6.22	ES+	1
77	PE 18:1p-20:2	754.6	55	390.3	20	6.22	ES+	2
78	PE 18:1p-20:3	752.6	55	363.3	20	6.22	ES+	1
79	PE 18:1p-20:3	752.6	55	390.3	20	6.22	ES+	2
80	PE 18:1p-20:4	750.5	55	361.3	20	6.22	ES+	1
81	PE 18:1p-20:4	750.5	55	390.3	20	6.22	ES+	2
82	PE 18:1p-20:5	748.5	55	359.3	20	6.22	ES+	1
83	PE 18:1p-20:5	748.5	55	390.3	20	6.22	ES+	2
84	PE 18:1p-22:0	786.6	55	390.3	20	6.22	ES+	1
85	PE 18:1p-22:0	786.6	55	397.3	20	6.22	ES+	2
86	PE 18:1p-22:1	784.6	55	390.3	20	6.22	ES+	1
87	PE 18:1p-22:1	784.6	55	395.3	20	6.22	ES+	2
88	PE 18:1p-22:2	782.6	55	390.3	20	6.22	ES+	1
89	PE 18:1p-22:2	782.6	55	393.3	20	6.22	ES+	2
90	PE 18:1p-22:3	780.6	55	390.3	20	6.22	ES+	1
91	PE 18:1p-22:3	780.6	55	391.3	20	6.22	ES+	2
92	PE 18:1p-22:4	778.6	55	389.3	20	6.22	ES+	1
93	PE 18:1p-22:4	778.6	55	390.3	20	6.22	ES+	2
94	PE 18:1p-22:5	776.6	55	387.3	20	6.22	ES+	1
95	PE 18:1p-22:5	776.6	55	390.3	20	6.22	ES+	2
96	PE 18:1p-22:6	774.5	55	385.3	20	6.22	ES+	1
97	PE 18:1p-22:6	774.5	55	390.3	20	6.22	ES+	2

98	PE 18:2p-12:0	642.4	55	257.3	20	6.22	ES+	1
99	PE 18:2p-12:0	642.4	55	388.3	20	6.22	ES+	2
100	PE 18:2p-14:0	670.5	55	285.3	20	6.22	ES+	1
101	PE 18:2p-14:0	670.5	55	388.3	20	6.22	ES+	2
102	PE 18:2p-14:1	668.5	55	283.3	20	6.22	ES+	1
103	PE 18:2p-14:1	668.5	55	388.3	20	6.22	ES+	2
104	PE 18:2p-16:0	698.5	55	313.3	20	6.22	ES+	1
105	PE 18:2p-16:0	698.5	55	388.3	20	6.22	ES+	2
106	PE 18:2p-16:1	698.5	55	311.3	20	6.22	ES+	1
107	PE 18:2p-16:1	698.5	55	388.3	20	6.22	ES+	2
108	PE 18:2p-18:0	728.6	55	341.3	20	6.22	ES+	1
109	PE 18:2p-18:0	728.6	55	388.3	20	6.22	ES+	2
110	PE 18:2p-18:1	726.5	55	339.3	20	6.22	ES+	1
111	PE 18:2p-18:1	726.5	55	388.3	20	6.22	ES+	2
112	PE 18:2p-18:2	724.5	55	337.3	20	6.22	ES+	1
113	PE 18:2p-18:2	724.5	55	388.3	20	6.22	ES+	2
114	PE 18:2p-18:3	722.5	55	335.3	20	6.22	ES+	1
115	PE 18:2p-18:3	722.5	55	388.3	20	6.22	ES+	2
116	PE 18:2p-18:4	720.5	55	333.3	20	6.22	ES+	1
117	PE 18:2p-18:4	720.5	55	388.3	20	6.22	ES+	2
118	PE 18:2p-20:0	756.6	55	369.3	20	6.22	ES+	1
119	PE 18:2p-20:0	756.6	55	388.3	20	6.22	ES+	2
120	PE 18:2p-20:1	754.6	55	367.3	20	6.22	ES+	1
121	PE 18:2p-20:1	754.6	55	388.3	20	6.22	ES+	2
122	PE 18:2p-20:2	752.6	55	365.3	20	6.22	ES+	1
123	PE 18:2p-20:2	752.6	55	388.3	20	6.22	ES+	2
124	PE 18:2p-20:3	750.5	55	363.3	20	6.22	ES+	1
125	PE 18:2p-20:3	750.5	55	388.3	20	6.22	ES+	2
126	PE 18:2p-20:4	748.5	55	361.3	20	6.22	ES+	1
127	PE 18:2p-20:4	748.5	55	388.3	20	6.22	ES+	2
128	PE 18:2p-20:5	746.5	55	359.3	20	6.22	ES+	1
129	PE 18:2p-20:5	746.5	55	388.3	20	6.22	ES+	2
130	PE 18:2p-22:0	784.6	55	388.3	20	6.22	ES+	1
131	PE 18:2p-22:0	784.6	55	397.3	20	6.22	ES+	2
132	PE 18:2p-22:1	782.6	55	388.3	20	6.22	ES+	1

133	PE 18:2p-22:1	782.6	55	395.3	20	6.22	ES+	2
134	PE 18:2p-22:2	780.6	55	388.3	20	6.22	ES+	1
135	PE 18:2p-22:2	780.6	55	393.3	20	6.22	ES+	2
136	PE 18:2p-22:3	778.6	55	388.3	20	6.22	ES+	1
137	PE 18:2p-22:3	778.6	55	391.3	20	6.22	ES+	2
138	PE 18:2p-22:4	776.6	55	388.3	20	6.22	ES+	1
139	PE 18:2p-22:4	776.6	55	389.3	20	6.22	ES+	2
140	PE 18:2p-22:5	774.5	55	387.3	20	6.22	ES+	1
141	PE 18:2p-22:5	774.5	55	388.3	20	6.22	ES+	2
142	PE 18:2p-22:6	772.5	55	385.3	20	6.22	ES+	1
143	PE 18:2p-22:6	772.5	55	388.3	20	6.22	ES+	2

Method 16: TAG and PI

No	Name	Precursor	CV (V)	Product	CE (V)	RT setting (min)	IonMode	Ion
1	TAG 36:0	656.6	10	656.6	10	1.61	ES+	1
2	TAG 38:1	682.6	10	682.6	10	1.61	ES+	1
3	TAG 38:0	684.6	10	684.6	10	1.61	ES+	1
4	TAG 40:2	708.6	10	708.6	10	1.61	ES+	1
5	TAG 40:1	710.6	10	710.6	10	1.61	ES+	1
6	TAG 40:0	712.6	10	712.6	10	1.61	ES+	1
7	TAG 42:4	732.6	10	732.6	10	1.61	ES+	1
8	TAG 42:3	734.6	10	734.6	10	1.61	ES+	1
9	TAG 42:2	736.6	10	736.6	10	1.61	ES+	1
10	TAG 42:1	738.7	10	738.7	10	1.61	ES+	1
11	TAG 42:0	740.7	10	740.7	10	1.61	ES+	1
12	TAG 44:5	758.6	10	758.6	10	1.61	ES+	1
13	TAG 44:4	760.6	10	760.6	10	1.61	ES+	1
14	TAG 44:3	762.7	10	762.7	10	1.61	ES+	1
15	TAG 44:2	764.7	10	764.7	10	1.61	ES+	1
16	TAG 44:1	766.7	10	766.7	10	1.61	ES+	1
17	TAG 44:0	768.7	10	768.7	10	1.61	ES+	1
18	TAG 46:6	784.6	10	784.6	10	1.61	ES+	1
19	TAG 46:5	786.7	10	786.7	10	1.61	ES+	1
20	TAG 46:4	788.7	10	788.7	10	1.61	ES+	1
21	TAG 46:3	790.7	10	790.7	10	1.61	ES+	1
22	TAG 46:2	792.7	10	792.7	10	1.61	ES+	1

23	TAG 46:1	794.7	10	794.7	10	1.61	ES+	1
24	TAG 46:0	796.7	10	796.7	10	1.61	ES+	1
25	TAG 48:8	808.6	10	808.6	10	1.61	ES+	1
26	TAG 48:7	810.7	10	810.7	10	1.61	ES+	1
27	TAG 48:6	812.7	10	812.7	10	1.61	ES+	1
28	TAG 48:5	814.7	10	814.7	10	1.61	ES+	1
29	TAG 48:4	816.7	10	816.7	10	1.61	ES+	1
30	TAG 48:3	818.7	10	818.7	10	1.61	ES+	1
31	TAG 48:2	820.7	10	820.7	10	1.61	ES+	1
32	TAG 48:1	822.8	10	822.8	10	1.61	ES+	1
33	TAG 48:0	824.8	10	824.8	10	1.61	ES+	1
34	TAG 50:9	834.7	10	834.7	10	1.61	ES+	1
35	TAG 50:8	836.7	10	836.7	10	1.61	ES+	1
36	TAG 50:7	838.7	10	838.7	10	1.61	ES+	1
37	TAG 50:6	840.7	10	840.7	10	1.61	ES+	1
38	TAG 50:5	842.7	10	842.7	10	1.61	ES+	1
39	TAG 50:4	844.7	10	844.7	10	1.61	ES+	1
40	TAG 50:3	846.8	10	846.8	10	1.61	ES+	1
41	TAG 50:2	848.8	10	848.8	10	1.61	ES+	1
42	TAG 50:1	850.8	10	850.8	10	1.61	ES+	1
43	TAG 50:0	852.8	10	852.8	10	1.61	ES+	1
44	TAG 51:0	866.8	10	866.8	10	1.61	ES+	1
45	TAG 52:10	860.7	10	860.7	10	1.61	ES+	1
46	TAG 52:9	862.7	10	862.7	10	1.61	ES+	1
47	TAG 52:8	864.7	10	864.7	10	1.61	ES+	1
48	TAG 52:7	866.7	10	866.7	10	1.61	ES+	1
49	TAG 52:6	868.7	10	868.7	10	1.61	ES+	1
50	TAG 52:5	870.8	10	870.8	10	1.61	ES+	1
51	TAG 52:4	872.8	10	872.8	10	1.61	ES+	1
52	TAG 52:3	874.8	10	874.8	10	1.61	ES+	1
53	TAG 52:2	876.8	10	876.8	10	1.61	ES+	1
54	TAG 52:1	878.8	10	878.8	10	1.61	ES+	1
55	TAG 52:0	880.8	10	880.8	10	1.61	ES+	1
56	TAG 54:12	884.7	10	884.7	10	1.61	ES+	1
57	TAG 54:11	886.7	10	886.7	10	1.61	ES+	1

58	TAG 54:10	888.7	10	888.7	10	1.61	ES+	1
59	TAG 54:9	890.7	10	890.7	10	1.61	ES+	1
60	TAG 54:8	892.7	10	892.7	10	1.61	ES+	1
61	TAG 54:7	894.8	10	894.8	10	1.61	ES+	1
62	TAG 54:6	896.8	10	896.8	10	1.61	ES+	1
63	TAG 54:5	898.8	10	898.8	10	1.61	ES+	1
64	TAG 54:4	900.8	10	900.8	10	1.61	ES+	1
65	TAG 54:3	902.8	10	902.8	10	1.61	ES+	1
66	TAG 54:2	904.8	10	904.8	10	1.61	ES+	1
67	TAG 54:1	906.8	10	906.8	10	1.61	ES+	1
68	TAG 54:0	908.9	10	908.9	10	1.61	ES+	1
69	TAG 56:13	910.7	10	910.7	10	1.61	ES+	1
70	TAG 56:12	912.7	10	912.7	10	1.61	ES+	1
71	TAG 56:11	914.7	10	914.7	10	1.61	ES+	1
72	TAG 56:10	916.7	10	916.7	10	1.61	ES+	1
73	TAG 56:9	918.8	10	918.8	10	1.61	ES+	1
74	TAG 56:8	920.8	10	920.8	10	1.61	ES+	1
75	TAG 56:7	922.8	10	922.8	10	1.61	ES+	1
76	TAG 56:6	924.8	10	924.8	10	1.61	ES+	1
77	TAG 56:5	926.8	10	926.8	10	1.61	ES+	1
78	TAG 56:4	928.8	10	928.8	10	1.61	ES+	1
79	TAG 56:3	930.8	10	930.8	10	1.61	ES+	1
80	TAG 56:2	932.9	10	932.9	10	1.61	ES+	1
81	TAG 56:1	934.9	10	934.9	10	1.61	ES+	1
82	TAG 58:14	936.7	10	936.7	10	1.61	ES+	1
83	TAG 56:0	936.9	10	936.9	10	1.61	ES+	1
84	TAG 58:13	938.7	10	938.7	10	1.61	ES+	1
85	TAG 58:12	940.7	10	940.7	10	1.61	ES+	1
86	TAG 58:11	942.8	10	942.8	10	1.61	ES+	1
87	TAG 58:10	944.8	10	944.8	10	1.61	ES+	1
88	TAG 58:9	946.8	10	946.8	10	1.61	ES+	1
89	TAG 58:8	948.8	10	948.8	10	1.61	ES+	1
90	TAG 58:7	950.8	10	950.8	10	1.61	ES+	1
91	TAG 58:6	952.8	10	952.8	10	1.61	ES+	1
92	TAG 58:5	954.8	10	954.8	10	1.61	ES+	1

93	TAG 58:4	956.9	10	956.9	10	1.61	ES+	1
94	TAG 58:3	958.9	10	958.9	10	1.61	ES+	1
95	TAG 58:2	960.9	10	960.9	10	1.61	ES+	1
96	TAG 60:15	962.7	10	962.7	10	1.61	ES+	1
97	TAG 58:1	962.9	10	962.9	10	1.61	ES+	1
98	TAG 60:14	964.7	10	964.7	10	1.61	ES+	1
99	TAG 58:0	964.9	10	964.9	10	1.61	ES+	1
100	TAG 60:13	966.8	10	966.8	10	1.61	ES+	1
101	TAG 60:12	968.8	10	968.8	10	1.61	ES+	1
102	TAG 60:11	970.8	10	970.8	10	1.61	ES+	1
103	TAG 60:10	972.8	10	972.8	10	1.61	ES+	1
104	TAG 60:9	974.8	10	974.8	10	1.61	ES+	1
105	TAG 60:8	976.8	10	976.8	10	1.61	ES+	1
106	TAG 60:7	978.8	10	978.8	10	1.61	ES+	1
107	TAG 60:6	980.9	10	980.9	10	1.61	ES+	1
108	TAG 60:5	982.9	10	982.9	10	1.61	ES+	1
109	TAG 60:4	984.9	10	984.9	10	1.61	ES+	1
110	TAG 60:3	986.9	10	986.9	10	1.61	ES+	1
111	TAG 62:16	988.7	10	988.7	10	1.61	ES+	1
112	TAG 60:2	988.9	10	988.9	10	1.61	ES+	1
113	TAG 62:15	990.8	10	990.8	10	1.61	ES+	1
114	TAG 60:1	990.9	10	990.9	10	1.61	ES+	1
115	TAG 62:14	992.8	10	992.8	10	1.61	ES+	1
116	TAG 60:0	993.0	10	993.0	10	1.61	ES+	1
117	TAG 62:13	994.8	10	994.8	10	1.61	ES+	1
118	TAG 62:12	996.8	10	996.8	10	1.61	ES+	1
119	TAG 62:11	998.8	10	998.8	10	1.61	ES+	1
120	TAG 62:10	1000.8	10	1000.8	10	1.61	ES+	1
121	TAG 62:9	1002.8	10	1002.8	10	1.61	ES+	1
122	TAG 62:8	1004.9	10	1004.9	10	1.61	ES+	1
123	TAG 62:7	1006.9	10	1006.9	10	1.61	ES+	1
124	TAG 62:6	1008.9	10	1008.9	10	1.61	ES+	1
125	TAG 62:5	1010.9	10	1010.9	10	1.61	ES+	1
126	TAG 62:4	1012.9	10	1012.9	10	1.61	ES+	1
127	TAG 64:17	1014.8	10	1014.8	10	1.61	ES+	1

128	TAG 62:3	1014.9	10	1014.9	10	1.61	ES+	1
129	TAG 64:16	1016.8	10	1016.8	10	1.61	ES+	1
130	TAG 62:2	1017.0	10	1017.0	10	1.61	ES+	1
131	TAG 64:15	1018.8	10	1018.8	10	1.61	ES+	1
132	TAG 62:1	1019.0	10	1019.0	10	1.61	ES+	1
133	TAG 64:14	1020.8	10	1020.8	10	1.61	ES+	1
134	TAG 62:0	1021.0	10	1021.0	10	1.61	ES+	1
135	TAG 64:13	1022.8	10	1022.8	10	1.61	ES+	1
136	TAG 64:12	1024.8	10	1024.8	10	1.61	ES+	1
137	TAG 64:11	1026.8	10	1026.8	10	1.61	ES+	1
138	TAG 64:10	1028.9	10	1028.9	10	1.61	ES+	1
139	TAG 64:9	1030.9	10	1030.9	10	1.61	ES+	1
140	TAG 64:8	1032.9	10	1032.9	10	1.61	ES+	1
141	TAG 64:7	1034.9	10	1034.9	10	1.61	ES+	1
142	TAG 64:6	1036.9	10	1036.9	10	1.61	ES+	1
143	TAG 64:5	1038.9	10	1038.9	10	1.61	ES+	1
144	TAG 66:18	1040.8	10	1040.8	10	1.61	ES+	1
145	TAG 64:4	1041.0	10	1041.0	10	1.61	ES+	1
146	TAG 66:17	1042.8	10	1042.8	10	1.61	ES+	1
147	TAG 64:3	1043.0	10	1043.0	10	1.61	ES+	1
148	TAG 66:16	1044.8	10	1044.8	10	1.61	ES+	1
149	TAG 64:2	1045.0	10	1045.0	10	1.61	ES+	1
150	TAG 66:15	1046.8	10	1046.8	10	1.61	ES+	1
151	TAG 64:1	1047.0	10	1047.0	10	1.61	ES+	1
152	TAG 66:14	1048.8	10	1048.8	10	1.61	ES+	1
153	TAG 64:0	1049.0	10	1049.0	10	1.61	ES+	1
154	TAG 66:13	1050.8	10	1050.8	10	1.61	ES+	1
155	TAG 66:12	1052.9	10	1052.9	10	1.61	ES+	1
156	TAG 66:11	1054.9	10	1054.9	10	1.61	ES+	1
157	TAG 66:10	1056.9	10	1056.9	10	1.61	ES+	1
158	TAG 66:9	1058.9	10	1058.9	10	1.61	ES+	1
159	TAG 66:8	1060.9	10	1060.9	10	1.61	ES+	1
160	TAG 66:7	1062.9	10	1062.9	10	1.61	ES+	1
161	TAG 66:6	1065.0	10	1065.0	10	1.61	ES+	1
162	TAG 66:5	1067.0	10	1067.0	10	1.61	ES+	1

163	TAG 66:4	1069.0	10	1069.0	10	1.61	ES+	1
164	TAG 66:3	1071.0	10	1071.0	10	1.61	ES+	1
165	TAG 66:2	1073.0	10	1073.0	10	1.61	ES+	1
166	TAG 66:1	1075.0	10	1075.0	10	1.61	ES+	1
167	TAG 66:0	1077.1	10	1077.1	10	1.61	ES+	1
168	PI 20:3-22:0	943.6	50	305.2	50	12.06	ES-	1
169	PI 20:3-22:0	943.6	50	339.2	50	12.06	ES-	2
170	PI 20:3-22:1	941.6	50	305.2	50	12.06	ES-	1
171	PI 20:3-22:1	941.6	50	337.2	50	12.06	ES-	2
172	PI 20:3-22:2	939.6	50	305.2	50	12.06	ES-	1
173	PI 20:3-22:2	939.6	50	335.2	50	12.06	ES-	2
174	PI 20:3-22:3	937.6	50	305.2	50	12.06	ES-	1
175	PI 20:3-22:3	937.6	50	333.2	50	12.06	ES-	2
176	PI 20:3-22:4	935.6	50	305.2	50	12.06	ES-	1
177	PI 20:3-22:4	935.6	50	331.2	50	12.06	ES-	2
178	PI 20:3-22:5	933.5	50	305.2	50	12.06	ES-	1
179	PI 20:3-22:5	933.5	50	329.2	50	12.06	ES-	2
180	PI 20:3-22:6	931.5	50	305.2	50	12.06	ES-	1
181	PI 20:3-22:6	931.5	50	327.2	50	12.06	ES-	2
182	PI 20:4-20:4	905.5	50	303.2	50	12.06	ES-	1
183	PI 20:4-20:5	903.5	50	301.2	50	12.06	ES-	1
184	PI 20:4-20:5	903.5	50	303.2	50	12.06	ES-	2
185	PI 20:4-22:0	941.6	50	303.2	50	12.06	ES-	1
186	PI 20:4-22:0	941.6	50	339.2	50	12.06	ES-	2
187	PI 20:4-22:1	939.6	50	303.2	50	12.06	ES-	1
188	PI 20:4-22:1	939.6	50	337.2	50	12.06	ES-	2
189	PI 20:4-22:2	937.6	50	303.2	50	12.06	ES-	1
190	PI 20:4-22:2	937.6	50	335.2	50	12.06	ES-	2
191	PI 20:4-22:3	935.6	50	303.2	50	12.06	ES-	1
192	PI 20:4-22:3	935.6	50	333.2	50	12.06	ES-	2
193	PI 20:4-22:4	933.5	50	303.2	50	12.06	ES-	1
194	PI 20:4-22:4	933.5	50	331.2	50	12.06	ES-	2
195	PI 20:4-22:5	931.5	50	303.2	50	12.06	ES-	1
196	PI 20:4-22:5	931.5	50	329.2	50	12.06	ES-	2
197	PI 20:4-22:6	929.5	50	303.2	50	12.06	ES-	1

198	PI 20:4-22:6	929.5	50	327.2	50	12.06	ES-	2
199	PI 20:5-20:5	901.5	50	301.2	50	12.06	ES-	1
200	PI 20:5-22:0	939.6	50	301.2	50	12.06	ES-	1
201	PI 20:5-22:0	939.6	50	339.2	50	12.06	ES-	2
202	PI 20:5-22:1	937.6	50	301.2	50	12.06	ES-	1
203	PI 20:5-22:1	937.6	50	337.2	50	12.06	ES-	2
204	PI 20:5-22:2	935.6	50	301.2	50	12.06	ES-	1
205	PI 20:5-22:2	935.6	50	335.2	50	12.06	ES-	2
206	PI 20:5-22:3	933.5	50	301.2	50	12.06	ES-	1
207	PI 20:5-22:3	933.5	50	333.2	50	12.06	ES-	2
208	PI 20:5-22:4	931.5	50	301.2	50	12.06	ES-	1
209	PI 20:5-22:4	931.5	50	331.2	50	12.06	ES-	2
210	PI 20:5-22:5	929.5	50	301.2	50	12.06	ES-	1
211	PI 20:5-22:5	929.5	50	329.2	50	12.06	ES-	2
212	PI 20:5-22:6	927.5	50	301.2	50	12.06	ES-	1
213	PI 20:5-22:6	927.5	50	327.2	50	12.06	ES-	2
214	PI 22:0-22:0	977.7	50	339.2	50	12.06	ES-	1
215	PI 22:0-22:1	975.7	50	337.2	50	12.06	ES-	1
216	PI 22:0-22:1	975.7	50	339.2	50	12.06	ES-	2
217	PI 22:0-22:2	973.7	50	335.2	50	12.06	ES-	1
218	PI 22:0-22:2	973.7	50	339.2	50	12.06	ES-	2
219	PI 22:0-22:3	971.7	50	333.2	50	12.06	ES-	1
220	PI 22:0-22:3	971.7	50	339.2	50	12.06	ES-	2
221	PI 22:0-22:4	969.6	50	331.2	50	12.06	ES-	1
222	PI 22:0-22:4	969.6	50	339.2	50	12.06	ES-	2
223	PI 22:0-22:5	967.6	50	329.2	50	12.06	ES-	1
224	PI 22:0-22:5	967.6	50	339.2	50	12.06	ES-	2
225	PI 22:0-22:6	965.6	50	327.2	50	12.06	ES-	1
226	PI 22:0-22:6	965.6	50	339.2	50	12.06	ES-	2
227	PI 22:1-22:1	973.7	50	337.2	50	12.06	ES-	1
228	PI 22:1-22:2	971.7	50	335.2	50	12.06	ES-	1
229	PI 22:1-22:2	971.7	50	337.2	50	12.06	ES-	2
230	PI 22:1-22:3	969.6	50	333.2	50	12.06	ES-	1
231	PI 22:1-22:3	969.6	50	337.2	50	12.06	ES-	2
232	PI 22:1-22:4	967.6	50	331.2	50	12.06	ES-	1

233	PI 22:1-22:4	967.6	50	337.2	50	12.06	ES-	2
234	PI 22:1-22:5	965.6	50	329.2	50	12.06	ES-	1
235	PI 22:1-22:5	965.6	50	337.2	50	12.06	ES-	2
236	PI 22:1-22:6	963.6	50	327.2	50	12.06	ES-	1
237	PI 22:1-22:6	963.6	50	337.2	50	12.06	ES-	2
238	PI 22:2-22:2	969.6	50	335.2	50	12.06	ES-	1
239	PI 22:2-22:3	967.6	50	333.2	50	12.06	ES-	1
240	PI 22:2-22:3	967.6	50	335.2	50	12.06	ES-	2
241	PI 22:2-22:4	965.6	50	331.2	50	12.06	ES-	1
242	PI 22:2-22:4	965.6	50	335.2	50	12.06	ES-	2
243	PI 22:2-22:5	963.6	50	329.2	50	12.06	ES-	1
244	PI 22:2-22:5	963.6	50	335.2	50	12.06	ES-	2
245	PI 22:2-22:6	961.6	50	327.2	50	12.06	ES-	1
246	PI 22:2-22:6	961.6	50	335.2	50	12.06	ES-	2
247	PI 22:3-22:3	965.6	50	333.2	50	12.06	ES-	1
248	PI 22:3-22:4	963.6	50	331.2	50	12.06	ES-	1
249	PI 22:3-22:4	963.6	50	333.2	50	12.06	ES-	2
250	PI 22:3-22:5	961.6	50	329.2	50	12.06	ES-	1
251	PI 22:3-22:5	961.6	50	333.2	50	12.06	ES-	2
252	PI 22:3-22:6	959.6	50	327.2	50	12.06	ES-	1
253	PI 22:3-22:6	959.6	50	333.2	50	12.06	ES-	2
254	PI 22:4-22:4	961.6	50	331.2	50	12.06	ES-	1
255	PI 22:4-22:5	959.6	50	329.2	50	12.06	ES-	1
256	PI 22:4-22:5	959.6	50	331.2	50	12.06	ES-	2
257	PI 22:4-22:6	957.5	50	327.2	50	12.06	ES-	1
258	PI 22:4-22:6	957.5	50	331.2	50	12.06	ES-	2
259	PI 22:5-22:5	957.5	50	329.2	50	12.06	ES-	1
260	PI 22:5-22:6	955.5	50	327.2	50	12.06	ES-	1
261	PI 22:5-22:6	955.5	50	329.2	50	12.06	ES-	2
262	PI 22:6-22:6	953.5	50	327.2	50	12.06	ES-	1

Supplemental Table S6: Repeatability of retention time on five different days.

Lipid class	RT (min)					RSD (%) [a]
	Day 1	Day 2	Day 3	Day 4	Day 5	
LPC 17:0	6.22 ± 0.01	6.21 ± 0.01	6.17 ± 0.01	6.19 ± 0.00	6.21 ± 0.00	0.3
LPE 17:1	7.66 ± 0.01	7.64 ± 0.01	7.58 ± 0.02	7.62 ± 0.01	7.63 ± 0.00	0.4
PC 17:0-17:0	5.53 ± 0.01	5.52 ± 0.01	5.46 ± 0.01	5.49 ± 0.01	5.51 ± 0.00	0.5
PE 17:0-17:0	6.41 ± 0.01	6.38 ± 0.00	6.31 ± 0.02	6.37 ± 0.00	6.37 ± 0.00	0.6
PS 17:0-17:0	12.44 ± 0.01	12.39 ± 0.01	12.36 ± 0.02	12.40 ± 0.01	12.38 ± 0.01	0.2
SM d18:1-17:0	5.93 ± 0.01	5.92 ± 0.00	5.88 ± 0.01	5.90 ± 0.01	5.92 ± 0.00	0.3
Cer d18:1-17:0	4.40 ± 0.02	4.40 ± 0.01	4.47 ± 0.02	4.44 ± 0.02	4.42 ± 0.00	0.7
CE 17:0	1.17 ± 0.05	1.13 ± 0.05	1.02 ± 0.03	1.06 ± 0.02	1.09 ± 0.01	5.4
MAG 17:0	3.92 ± 0.01	3.93 ± 0.01	3.98 ± 0.02	3.95 ± 0.01	3.94 ± 0.01	0.6
DAG 12:0-12:0	3.07 ± 0.01	3.08 ± 0.01	3.08 ± 0.00	3.09 ± 0.01	3.09 ± 0.01	0.3
TAG 17:0-17:0-17:0	1.56 ± 0.01	1.58 ± 0.01	1.44 ± 0.13	1.56 ± 0.09	1.61 ± 0.02	4.2
FFA 17:0	4.04 ± 0.01	4.05 ± 0.01	4.09 ± 0.02	4.07 ± 0.01	4.06 ± 0.01	0.5

[a] Relative standard deviation (RSD) observed by the analysis of internal standards in rabbit plasama samples on five different measurement days.

Supplemental Table S7: Sensitivity of SFC/QTOFMS system.

Lipid class	Ion mode	Adduct ion	MS^1 (*m/z*)	LOD [a] (μM)
LPC 17:0	ESI＋	$[M + H]^+$	510.3554	0.1
LPE 17:1	ESI＋	$[M + H]^+$	466.2928	0.1
LPG 17:1	ESI＋	$[M + H]^+$	497.2874	50
LPA 17:0	ESI－	$[M - H]^-$	423.2517	1
LPI 17:1	ESI－	$[M - H]^-$	583.2889	1
LPS 17:1	ESI＋	$[M + H]^+$	498.3874	n.d.
PC 17:0-17:0	ESI－	$[M + CH_3COO]^-$	820.6073	1
PE 17:0-17:0	ESI－	$[M - H]^-$	718.5392	1
PG 17:0-17:0	ESI－	$[M - H]^-$	749.5338	0.1
PA 17:0-17:0	ESI－	$[M - H]^-$	675.497	1
PS 17:0-17:0	ESI－	$[M - H]^-$	762.5291	1
SM d18:1-17:0	ESI＋	$[M + H]^+$	717.5905	0.1
Cer d18:1-17:0	ESI＋	$[M + H]^+$	552.535	0.1
CE 17:0	ESI＋	$[M + NH_4]^+$	656.634	n.d.
MAG 17:0	ESI＋	$[M + H]^+$	245.2999	1
DAG 12:0-12:0	ESI＋	$[M + NH_4]^+$	474.4153	1
TAG 17:0-17:0-17:0	ESI＋	$[M + NH_4]^+$	866.8171	0.1
FFA 17:0	ESI－	$[M - H]^-$	269.2486	0.1

[a] Limit of detection (*S/N* = 3).

Xevo G2-XS QTof MS analytical conditions were as follows: ion source mode, ESI mode; capillary voltage, 3.0 kV; sampling cone, 40; source offset, 80; source temperature, 150 ˚C; desolvation temperature, 500 ˚C; cone gas flow rate, 50 L h–1; desolvation gas flow rate, 1000 L h^{-1}. Mass range of MSe acquisition was set to 50－1200 Da, and scan time was set to 0.1 sec. Low-energy of collision energy was off, and its high-energy was set to 10－30 V.

Supplemental Table S8: Characteristics of WHHLMI rabbits by EPA administration.

	Placebo group (n = 6)		EPA group (n = 6)	
Age (month)	14 ± 1		14 ± 1	
Sex (% female)	100		100	
	Before administration	5 weeks after administration	Before administration	5 weeks after administration
Body weight (kg)	3.5 ± 0.4	3.5 ± 0.4	3.5 ± 0.2	3.5 ± 0.2
Total Cho (mg dL^{-1})	1196 ± 118	1110 ± 135	1171 ± 68	840 ± 113*

Values are mean ± standard deviation. Statistical significance was determined using Paired t-test (*P < 0.001).

Supplemental Table S9: Concentration of each lipid molecule in the WHHLMI rabbit plasma.

Lipid	Ion mode	MS[1]	RT	Lipid concentration (nmol mL^{-1} in plasma)					
				Placebo group (n = 6)			EPA group (n = 6)		
				Administration period (weeks)		p-value	Administration period (weeks)		p-value
		(m/z)	(min)	0	5	0 week (placebo) vs. 5 week (placebo)	0	5	0 week (EPA) vs. 5 week (EPA)
LPC 14:0 (*sn*-1 and *sn*-2)	Positive	468.3	6.15 ± 0.01	0.54 ± 0.12	0.63 ± 0.11	0.22148808	0.45 ± 0.13	0.39 ± 0.10	0.33877507
LPC 16:0 (*sn*-1)	Positive	496.3	6.10 ± 0.01	188 ± 18	200 ± 16	0.23905348	189 ± 13	185 ± 14	0.57573889
LPC 16:0 (*sn*-2)	Positive	496.3	6.17 ± 0.01	24.3 ± 2.4	26.5 ± 2.6	0.14970214	23.6 ± 2.0	23.9 ± 1.8	0.79923921
LPC 16:1 (*sn*-1)	Positive	494.3	6.15 ± 0.01	4.6 ± 0.6	4.6 ± 0.8	0.91760713	5.1 ± 0.4	3.6 ± 0.5 ***	0.00016648
LPC 16:1 (*sn*-2)	Positive	494.3	6.22 ± 0.01	0.62 ± 0.07	0.63 ± 0.17	0.88980424	0.59 ± 0.10	0.43 ± 0.02 *	0.00451377
LPC 18:0 (*sn*-1)	Positive	524.4	6.06 ± 0.01	258 ± 24	271 ± 15	0.29437566	267 ± 33	253 ± 29	0.42671344
LPC 18:0 (*sn*-2)	Positive	524.4	6.12 ± 0.01	43.9 ± 4.3	45.8 ± 3.7	0.41606963	43.3 ± 4.4	42.3 ± 2.8	0.63502556
LPC 18:1 (*sn*-1)	Positive	522.4	6.10 ± 0.01	67.9 ± 4.2	76.4 ± 5.1 *	0.01053796	69.4 ± 7.8	49.2 ± 2.3 ***	0.00011010
LPC 18:1 (*sn*-2)	Positive	522.4	6.17 ± 0.01	15.8 ± 1.6	18.5 ± 1.1 **	0.00708809	16.0 ± 1.2	11.3 ± 0.4 ***	0.00000388
LPC 18:2 (*sn*-1)	Positive	520.3	6.16 ± 0.01	142 ± 14	150 ± 8	0.24644059	145 ± 7	88.5 ± 5.5 ***	0.00000002
LPC 18:2 (*sn*-2)	Positive	520.3	6.23 ± 0.01	25.6 ± 2.2	27.3 ± 2.0	0.19420385	26.9 ± 1.9	17.0 ± 1.0 ***	0.00000063
LPC 18:3 (*sn*-1)	Positive	518.3	6.22 ± 0.01	5.6 ± 0.6	6.4 ± 1.1	0.18936881	6.1 ± 0.9	3.3 ± 0.7 ***	0.00018714
LPC 18:3 (*sn*-2)	Positive	518.3	6.28 ± 0.01	1.1 ± 0.2	1.3 ± 0.3	0.16672866	1.1 ± 0.2	0.66 ± 0.18 **	0.00127981
LPC 20:0 (*sn*-1)	Positive	552.4	6.03 ± 0.01	1.6 ± 0.4	1.3 ± 0.2	0.19577715	1.5 ± 0.2	1.3 ± 0.3	0.11637590
LPC 20:0 (*sn*-2)	Positive	552.4	6.07 ± 0.01	0.33 ± 0.08	0.28 ± 0.06	0.24779310	0.33 ± 0.12	0.19 ± 0.11	0.06873377
LPC 20:1 (*sn*-1)	Positive	550.4	6.07 ± 0.01	1.4 ± 0.1	1.2 ± 0.3	0.15983041	1.4 ± 0.2	0.87 ± 0.20 **	0.00115289
LPC 20:1 (*sn*-2)	Positive	550.4	6.12 ± 0.01	0.29 ± 0.05	0.24 ± 0.05	0.12458244	0.22 ± 0.06	0.12 ± 0.04 *	0.01160282

LPC 20:2 (*sn*-1)	Positive	548.4	6.12 ± 0.01	1.8 ± 0.4	2.1 ± 0.4	0.14499747	1.7 ± 0.3	1.1 ± 0.2 ***	0.00091420
LPC 20:2 (*sn*-2)	Positive	548.4	6.18 ± 0.02	0.27 ± 0.08	0.32 ± 0.09	0.34059388	0.19 ± 0.06	0.17 ± 0.05	0.52889817
LPC 20:3 (*sn*-1)	Positive	546.4	6.15 ± 0.01	2.6 ± 0.5	2.9 ± 0.4	0.24152064	2.5 ± 0.5	1.8 ± 0.2 **	0.00926394
LPC 20:3 (*sn*-2)	Positive	546.4	6.22 ± 0.02	0.41 ± 0.09	0.48 ± 0.11	0.27679075	0.37 ± 0.10	0.28 ± 0.13	0.19549735
LPC 20:4 (*sn*-1)	Positive	544.3	6.18 ± 0.01	7.8 ± 0.9	8.5 ± 0.9	0.28097577	8.3 ± 0.7	8.0 ± 0.8	0.47120068
LPC 20:4 (*sn*-2)	Positive	544.3	6.24 ± 0.01	1.8 ± 0.3	1.9 ± 0.5	0.76103297	1.9 ± 0.1	2.7 ± 0.2 ***	0.00000654
LPC 20:5 (*sn*-1)	Positive	542.3	6.24 ± 0.01	0.21 ± 0.09	0.25 ± 0.06	0.48549756	0.18 ± 0.07	12.3 ± 2.8 ***	0.00000103
LPC 20:5 (*sn*-2)	Positive	542.3	6.30 ± 0.02	$(3.9 \pm 2.3) \times 10^{-2}$	$(3.2 \pm 1.7) \times 10^{-2}$	0.58734440	$(3.7 \pm 2.4) \times 10^{-2}$	3.0 ± 0.6 ***	0.00000012
LPC 22:0 (*sn*-1)	Positive	580.4	6.00 ± 0.01	0.44 ± 0.15	0.34 ± 0.06	0.16518053	0.48 ± 0.08	0.31 ± 0.06 **	0.00262235
LPC 22:0 (*sn*-2)	Positive	580.4	6.05 ± 0.01	$(8.7 \pm 6.1) \times 10^{-2}$	$(8.9 \pm 5.2) \times 10^{-2}$	0.96308750	0.16 ± 0.07	0.10 ± 0.03	0.08467982
LPC 22:1 (*sn*-1 and *sn*-2)	Positive	578.4	6.04 ± 0.02	0.14 ± 0.06	0.12 ± 0.03	0.36450327	0.10 ± 0.06	$(8.8 \pm 3.7) \times 10^{-2}$	0.74824637
LPC 22:4 (*sn*-1)	Positive	572.4	6.15 ± 0.01	0.76 ± 0.12	0.84 ± 0.21	0.40600317	0.76 ± 0.15	0.21 ± 0.08 ***	0.00001235
LPC 22:4 (*sn*-2)	Positive	572.4	6.21 ± 0.02	0.18 ± 0.09	0.18 ± 0.04	0.97806787	0.13 ± 0.02	0.38 ± 0.13 **	0.00081991
LPC 22:5 (*sn*-1)	Positive	570.4	6.20 ± 0.01	1.1 ± 0.2	1.1 ± 0.2	0.48229559	1.2 ± 0.2	7.1 ± 1.5 ***	0.00000224
LPC 22:5 (*sn*-2)	Positive	570.4	6.26 ± 0.01	0.20 ± 0.06	0.23 ± 0.05	0.31246450	0.21 ± 0.02	1.4 ± 0.2 ***	0.00000009
LPC 22:6 (*sn*-1)	Positive	568.3	6.23 ± 0.01	0.46 ± 0.09	0.43 ± 0.12	0.61821187	0.48 ± 0.12	0.66 ± 0.12 *	0.02561064
LPC 22:6 (*sn*-2)	Positive	568.3	6.29 ± 0.02	0.10 ± 0.02	$(9.3 \pm 3.0) \times 10^{-2}$	0.54877074	0.10 ± 0.03	0.16 ± 0.03 **	0.00576482
LPC total				799 ± 64	852 ± 47	0.13648069	816 ± 66	720 ± 52 *	0.01811988
LPE 16:0 (*sn*-1 and *sn*-2)	Positive	454.3	7.39 ± 0.02	2.2 ± 0.5	2.0 ± 0.4	0.32685007	2.0 ± 0.9	2.0 ± 0.5	0.96212421
LPE 18:0 (*sn*-1)	Positive	482.3	7.32 ± 0.02	7.5 ± 1.6	6.5 ± 0.8	0.19495173	7.6 ± 1.2	6.6 ± 1.7	0.24268167
LPE 18:0 (*sn*-2)	Positive	482.3	7.42 ± 0.02	1.6 ± 0.3	1.3 ± 0.3	0.14916369	1.6 ± 0.5	1.3 ± 0.4	0.20804767
LPE 18:1 (*sn*-1)	Positive	480.3	7.39 ± 0.02	2.5 ± 0.6	2.2 ± 0.4	0.40533490	2.2 ± 0.6	0.55 ± 0.25 ***	0.00008198

LPE 18:1 (*sn*-2)	Positive	480.3	7.48 ± 0.02	0.66 ± 0.33	1.1 ± 0.6	0.13859435	0.63 ± 0.38	0.16 ± 0.12 *	0.02669492
LPE 18:2 (*sn*-1)	Positive	478.3	7.46 ± 0.02	7.4 ± 0.4	7.9 ± 0.6	0.20697592	7.3 ± 1.1	2.6 ± 0.6 ***	0.00000276
LPE 18:2 (*sn*-2)	Positive	478.3	7.56 ± 0.02	3.1 ± 1.0	4.1 ± 2.6	0.38546636	2.9 ± 0.8	1.5 ± 0.5 **	0.00492525
LPE total				24.9 ± 3.8	25.0 ± 4.5	0.98994330	24.3 ± 3.2	14.6 ± 3.1	0.00030335
PC 14:0-18:2	Negative	788.5	5.44 ± 0.04	8.2 ± 3.7	5.8 ± 3.4	0.27174462	9.4 ± 3.3	1.3 ± 1.3 ***	0.00022528
PC 14:1-18:0	Negative	790.6	5.41 ± 0.02	11.4 ± 4.1	12.2 ± 3.9	0.75674876	10.8 ± 2.7	6.2 ± 2.9 *	0.01651469
PC 14:1-18:2	Negative	786.5	5.41 ± 0.02	20.0 ± 1.7	21.4 ± 3.7	0.44053005	19.9 ± 6.8	8.0 ± 2.6 **	0.00246465
PC 16:0-16:0	Negative	792.6	5.39 ± 0.02	92.4 ± 13.4	79.2 ± 8.4	0.06751446	100 ± 15	73.6 ± 15.2 *	0.01230531
PC 16:0-16:1	Negative	790.6	5.43 ± 0.03	18.7 ± 6.2	15.7 ± 4.9	0.36557151	14.7 ± 5.5	7.4 ± 2.0 *	0.01227847
PC 16:0-18:0	Negative	820.6	5.39 ± 0.02	232 ± 19	235 ± 26	0.81861941	206 ± 38	153 ± 12 *	0.00830681
PC 16:0-18:1	Negative	818.6	5.39 ± 0.02	979 ± 126	1072 ± 105	0.19315254	969 ± 125	572 ± 44 ***	0.00002534
PC 16:0-18:2	Negative	816.6	5.43 ± 0.02	1655 ± 124	1633 ± 126	0.77270848	1743 ± 113	877 ± 48 ***	0.00000001
PC 16:0-18:3	Negative	814.6	5.46 ± 0.01	113 ± 21	131 ± 23	0.17287984	124 ± 21	51.4 ± 9.3 ***	0.00001302
PC 16:0-20:2	Negative	844.6	5.43 ± 0.02	16.9 ± 6.4	15.7 ± 4.6	0.71545429	11.9 ± 5.1	10.7 ± 3.6	0.65944274
PC 16:0-20:3	Negative	842.6	5.43 ± 0.02	60.8 ± 10.3	67.3 ± 11.0	0.31434810	55.6 ± 8.2	50.5 ± 6.8	0.26714577
PC 16:0-20:4	Negative	840.6	5.43 ± 0.02	86.3 ± 9.5	94.6 ± 5.5	0.09487941	86.3 ± 9.8	169 ± 35 **	0.00025413
PC 16:0-20:5	Negative	838.6	5.47 ± 0.02	2.8 ± 1.5	2.4 ± 0.9	0.60833019	2.8 ± 0.7	168 ± 43 ***	0.00000274
PC 16:0-22:3	Negative	870.6	5.44 ± 0.02	2.0 ± 1.1	2.7 ± 1.6	0.37295445	2.8 ± 1.4	4.6 ± 2.9	0.22292745
PC 16:0-22:4	Negative	868.6	5.45 ± 0.01	11.9 ± 5.0	17.3 ± 4.8	0.08570088	11.8 ± 4.7	48.5 ± 12.2 ***	0.00004411
PC 16:0-22:5	Negative	866.6	5.46 ± 0.02	18.3 ± 6.4	21.1 ± 6.9	0.48601220	20.6 ± 4.8	126 ± 18 ***	0.00000008
PC 16:0-22:6	Negative	864.6	5.47 ± 0.02	4.2 ± 3.3	3.6 ± 1.9	0.71757771	3.3 ± 1.5	4.2 ± 3.1	0.50744920
PC 16:1-18:0	Negative	818.6	5.41 ± 0.02	7.7 ± 3.0	8.7 ± 2.8	0.56395417	8.3 ± 2.0	5.9 ± 2.9	0.12990525

PC 16:1-18:1	Negative	816.6	5.42 ± 0.02	23.7 ± 4.4	23.7 ± 5.3	0.98884101	25.4 ± 3.8	10.3 ± 2.7 ***	0.00001155
PC 16:1-18:2	Negative	814.6	5.46 ± 0.02	56.9 ± 7.5	48.9 ± 10.4	0.15867805	61.1 ± 9.3	21.9 ± 4.1 ***	0.00000263
PC 16:1-18:3	Negative	812.5	5.49 ± 0.02	2.0 ± 1.4	2.0 ± 1.4	0.99853909	2.5 ± 1.9	1.3 ± 0.8	0.27002098
PC 16:1-20:4	Negative	838.6	5.43 ± 0.04	2.7 ± 2.5	1.2 ± 0.9	0.23850895	1.9 ± 1.3	0.79 ± 0.44	0.08732020
PC 18:0-18:0	Negative	848.6	5.38 ± 0.02	103 ± 9	108 ± 13	0.40112188	89.7 ± 14.2	55.7 ± 5.8 ***	0.00028450
PC 18:0-18:1	Negative	846.6	5.41 ± 0.02	829 ± 63	848 ± 54	0.59408985	755 ± 100	429 ± 17 ***	0.00001320
PC 18:0-18:2	Negative	844.6	5.41 ± 0.02	1847 ± 127	1758 ± 104	0.21521337	1822 ± 111	1044 ± 53 ***	0.00000003
PC 18:0-18:3	Negative	842.6	5.44 ± 0.02	77.3 ± 13.5	96.2 ± 19.7	0.08232542	87.8 ± 20.9	32.1 ± 3.3 **	0.00007224
PC 18:0-18:4	Negative	840.6	5.42 ± 0.02	5.9 ± 4.0	5.4 ± 3.0	0.80156875	4.3 ± 3.3	6.7 ± 2.4	0.17462174
PC 18:0-20:0	Negative	876.7	5.41 ± 0.02	2.4 ± 2.1	2.0 ± 1.2	0.65058929	2.2 ± 1.0	2.0 ± 1.6	0.79443415
PC 18:0-20:2	Negative	872.6	5.41 ± 0.02	15.4 ± 6.3	25.1 ± 8.9	0.05519947	12.9 ± 5.7	8.3 ± 2.8	0.10676947
PC 18:0-20:3	Negative	870.6	5.41 ± 0.02	77.4 ± 17.1	79.1 ± 13.7	0.85501946	68.1 ± 9.0	68.5 ± 16.4	0.95444824
PC 18:0-20:4	Negative	868.6	5.41 ± 0.02	121 ± 18	127 ± 25	0.66643549	123 ± 25	217 ± 41 ***	0.00066549
PC 18:0-20:5	Negative	866.6	5.44 ± 0.02	3.4 ± 1.6	3.2 ± 0.9	0.87533855	3.7 ± 1.3	183 ± 39 ***	0.00000057
PC 18:0-22:3	Negative	898.7	5.41 ± 0.02	2.0 ± 1.6	2.6 ± 1.6	0.59676237	0.63 ± 0.19	4.5 ± 1.6 **	0.00044667
PC 18:0-22:4	Negative	896.6	5.43 ± 0.03	11.4 ± 3.2	13.3 ± 2.0	0.24750042	8.4 ± 4.0	34.6 ± 5.3 ***	0.00000222
PC 18:0-22:5	Negative	894.6	5.44 ± 0.02	14.1 ± 4.3	12.5 ± 4.7	0.55079901	12.6 ± 3.5	83.5 ± 15.0 ***	0.00000053
PC 18:0-22:6	Negative	892.6	5.44 ± 0.02	2.9 ± 2.8	3.5 ± 2.7	0.72522735	2.1 ± 1.1	4.9 ± 3.2	0.06488521
PC 18:1-18:1	Negative	844.6	5.44 ± 0.02	117 ± 17	123 ± 19	0.59299950	105 ± 15	45.5 ± 4.9 ***	0.00000369
PC 18:1-18:2	Negative	842.6	5.46 ± 0.02	529 ± 20	538 ± 49	0.71093423	514 ± 59	162 ± 9 ***	0.00000005
PC 18:1-18:3	Negative	840.6	5.48 ± 0.02	36.3 ± 11.2	45.4 ± 4.2	0.08813838	40.1 ± 12.8	9.1 ± 3.4 **	0.00018610
PC 18:1-20:4	Negative	866.6	5.46 ± 0.02	19.8 ± 7.9	19.9 ± 5.2	0.97783133	15.8 ± 6.2	20.5 ± 6.3	0.21847039

PC 18:1-20:5	Negative	864.6	5.48 ± 0.01	n.d.	n.d.		n.d.	21.6 ± 7.8	
PC 18:2-18:2	Negative	840.6	5.47 ± 0.02	399 ± 16	376 ± 30	0.12655587	394 ± 47	102 ± 14 ***	0.00000005
PC 18:2-18:3	Negative	838.6	5.50 ± 0.01	74.1 ± 9.6	69.9 ± 14.5	0.57205125	71.3 ± 9.0	23.6 ± 7.8 ***	0.00000188
PC 18:2-20:0	Negative	872.6	5.33 ± 0.02	44.4 ± 5.3	24.3 ± 7.0 ***	2.3×10^{-4}	37.2 ± 11.2	8.6 ± 4.1 ***	0.00015270
PC 18:2-20:1	Negative	870.6	5.45 ± 0.02	7.4 ± 1.8	8.2 ± 2.8	0.53998873	4.8 ± 3.8	2.4 ± 0.8	0.15951241
PC 18:2-20:2	Negative	868.6	5.45 ± 0.02	14.0 ± 3.7	15.7 ± 5.6	0.53830320	9.2 ± 1.7	2.9 ± 1.7 ***	0.00008349
PC 18:2-20:3	Negative	866.6	5.48 ± 0.02	22.3 ± 5.4	22.7 ± 3.1	0.87188556	21.4 ± 5.3	6.7 ± 3.2 ***	0.00017362
PC 18:2-20:4	Negative	864.6	5.49 ± 0.02	33.9 ± 9.3	33.7 ± 7.8	0.96567153	35.1 ± 8.4	22.8 ± 3.6 **	0.00778687
PC 18:2-20:5	Negative	862.6	5.51 ± 0.01	n.d.	n.d.		n.d.	25.7 ± 4.1	
PC total				7834 ± 400	7874 ± 510	0.88187082	7730 ± 697	4998 ± 315 ***	0.00000531
PC 16:0e-16:0	Positive	720.6	5.33 ± 0.01	6.8 ± 1.3	3.3 ± 2.3 *	0.01232171	3.5 ± 2.9	2.4 ± 1.6	0.57511892
PC 16:0e-18:2	Positive	744.6	5.37 ± 0.02	37.9 ± 4.7	25.9 ± 3.6 ***	0.00059851	33.8 ± 7.5	14.1 ± 4.0 ***	0.00020513
PC 16:0e-20:4	Positive	768.6	5.38 ± 0.01	14.3 ± 3.4	11.1 ± 2.1	0.08045555	11.2 ± 4.3	5.4 ± 2.6 *	0.01707430
PC 16:1e-16:0 / PC 16:0p-16:0	Positive	718.6	5.38 ± 0.02	30.6 ± 3.9	25.4 ± 6.2	0.11330472	25.0 ± 4.3	17.2 ± 2.4 **	0.00319235
PC 16:1e-18:1 / PC 16:0p-18:1	Positive	744.6	5.38 ± 0.01	122 ± 20	103 ± 14	0.07738251	113 ± 11	103 ± 13	0.16954039
PC 16:1e-18:2 / PC 16:0p-18:2	Positive	742.6	5.41 ± 0.01	66.3 ± 14.1	56.9 ± 12.1	0.24309863	76.2 ± 9.9	60.5 ± 8.9 *	0.01604548
PC 16:1e-20:4 / PC 16:0p-20:4	Positive	766.6	5.42 ± 0.01	64.7 ± 7.3	52.5 ± 6.1 *	0.01067697	71.6 ± 11.9	51.1 ± 10.8 *	0.01066177
PC 16:1e-20:5 / PC	Positive	764.6	5.45 ± 0.02	1.0 ± 0.8	1.2 ± 0.5	0.80510977	n.d.	26.4 ± 4.6	

16:0p-20:5									
PC 16:1e-22:5 / PC 16:0p-22:5	Positive	792.6	5.44 ± 0.01	10.4 ± 1.2	9.1 ± 4.0	0.47727123	8.8 ± 3.4	28.9 ± 8.6 ***	0.00034153
PC 16:1p-20:5	Positive	762.5	5.38 ± 0.01	16.2 ± 2.6	18.2 ± 7.0	0.53326057	16.0 ± 5.8	13.9 ± 4.2	0.47684892
PC 18:0e-18:1	Positive	774.6	5.39 ± 0.02	7.0 ± 3.6	7.1 ± 1.1	0.94775622	10.1 ± 4.3	3.8 ± 2.2 **	0.00932371
PC 18:0e-18:2	Positive	772.6	5.42 ± 0.02	38.3 ± 6.8	26.6 ± 6.0 **	0.00953999	44.7 ± 8.0	20.3 ± 4.5 ***	0.00006795
PC 18:0e-20:4	Positive	796.6	5.38 ± 0.04	7.6 ± 1.8	6.9 ± 2.5	0.61074487	7.4 ± 4.8	3.7 ± 2.0	0.11067120
PC 18:1e-18:2 / PC 18:0p-18:2	Positive	770.6	5.38 ± 0.01	24.8 ± 4.7	24.7 ± 6.1	0.96196844	25.2 ± 5.3	13.3 ± 4.1 **	0.00134970
PC 18:1e-20:4 / PC 18:0p-20:4	Positive	794.6	5.39 ± 0.02	32.9 ± 5.6	28.0 ± 5.4	0.15468492	31.8 ± 10.4	17.2 ± 4.8 *	0.01033804
PC 18:1e-20:5 / PC 18:0p-20:5	Positive	792.6	5.41 ± 0.01	2.3 ± 0.3	1.9 ± 1.3	0.63049349	1.9 ± 1.2	13.5 ± 3.6 ***	0.00001719
PC 18:2p-20:5	Positive	788.6	5.38 ± 0.01	192 ± 10	206 ± 20	0.17474175	178 ± 31	107 ± 17 ***	0.00057831
PC 18:2p-20:4	Positive	790.6	5.39 ± 0.03	5.6 ± 0.9	5.3 ± 2.0	0.76060697	5.9 ± 2.3	1.6 ± 1.4 **	0.00279858
Ether PC total				679 ± 50	612 ± 61	0.06317305	664 ± 57	501 ± 28 ***	0.00009909
PE 16:0-18:1	Negative	716.5	6.10 ± 0.02	8.1 ± 4.3	11.4 ± 4.8	0.23758867	7.1 ± 4.1	1.7 ± 1.2 *	0.01001288
PE 16:0-18:2	Negative	714.5	6.21 ± 0.06	47.6 ± 14.4	43.1 ± 10.2	0.54305981	37.6 ± 9.6	11.2 ± 3.8 ***	0.00009157
PE 16:0-20:4	Negative	738.5	6.22 ± 0.06	11.1 ± 3.3	8.4 ± 1.8	0.10564726	9.0 ± 2.7	3.0 ± 1.1 ***	0.00041539
PE 16:0-22:5	Negative	764.5	6.27 ± 0.07	1.7 ± 0.8	1.5 ± 0.4	0.48216659	1.7 ± 1.8	13.0 ± 3.4 ***	0.00002970
PE 16:1-18:1	Negative	714.5	6.07 ± 0.01	4.7 ± 2.0	5.1 ± 0.5	0.58099482	4.0 ± 1.2	2.0 ± 0.8 **	0.00635496
PE 16:1-18:2	Negative	712.5	6.09 ± 0.01	32.9 ± 11.2	31.4 ± 9.0	0.80610791	24.7 ± 5.6	13.5 ± 6.0 **	0.00727000

PE 16:1-20:4	Negative	736.5	6.10 ± 0.02	6.4 ± 1.5	6.1 ± 1.7	0.75448708	5.6 ± 1.8	2.6 ± 1.3 **	0.00796482
PE 16:1-20:5	Negative	734.5	5.80 ± 0.00	n.d.	n.d.		n.d.	5.2 ± 2.9	
PE 18:0-18:1	Negative	744.6	6.08 ± 0.01	18.4 ± 7.0	17.7 ± 4.7	0.83952450	16.3 ± 4.7	5.1 ± 1.1 **	0.00019928
PE 18:0-18:2	Negative	742.5	6.13 ± 0.04	180 ± 39	159 ± 22	0.27429388	164 ± 38	49 ± 14 ***	0.00004052
PE 18:0-18:3	Negative	740.5	6.23 ± 0.05	9.3 ± 3.7	6.1 ± 1.5	0.07573067	8.2 ± 2.0	2.2 ± 0.7 ***	0.00003597
PE 18:0-20:4	Negative	766.5	6.14 ± 0.05	61.3 ± 11.0	63.3 ± 6.6	0.70810785	54.2 ± 12.5	23.4 ± 2.7 **	0.00015010
PE 18:0-20:5	Negative	764.5	6.08 ± 0.23	n.d.	n.d.		n.d.	26.8 ± 5.6	
PE 18:0-22:5	Negative	792.6	6.20 ± 0.07	1.5 ± 0.5	1.8 ± 0.9	0.47449296	0.74 ± 0.40	15.6 ± 6.8 **	0.00034741
PE 18:1-18:1	Negative	742.5	6.11 ± 0.04	5.5 ± 1.9	7.3 ± 1.1	0.06629617	4.4 ± 3.1	0.60 ± 0.43 *	0.01420862
PE 18:1-18:2	Negative	740.5	6.21 ± 0.08	26.7 ± 6.6	32.3 ± 6.9	0.17962900	21.3 ± 7.5	3.9 ± 1.2 **	0.00022113
PE 18:1-20:4	Negative	764.5	6.21 ± 0.08	3.6 ± 0.8	4.4 ± 1.3	0.21025078	3.2 ± 1.6	0.8 ± 0.3 *	0.00853859
PE 18:1-20:5	Negative	762.5	6.32 ± 0.03	n.d.	n.d.		n.d.	1.2 ± 0.7	
PE 18:2-18:2	Negative	738.5	6.30 ± 0.03	10.3 ± 2.4	8.2 ± 2.3	0.15045940	10.4 ± 2.6	1.2 ± 0.8 ***	0.00000900
PE total				429 ± 97	407 ± 64	0.65082500	372 ± 82	182 ± 28 **	0.00031262
PE 16:0p-16:0	Positive	676.5	6.07 ± 0.01	3.9 ± 3.1	4.4 ± 3.2	0.79721858	3.1 ± 2.1	3.5 ± 2.3	0.74549000
PE 16:0p-16:1	Positive	674.5	6.10 ± 0.02	0.86 ± 0.67	1.5 ± 1.0	0.23066412	0.61 ± 0.34	0.48 ± 0.29	0.51270055
PE 16:0p-18:1	Positive	702.5	6.08 ± 0.01	40.2 ± 13.8	38.0 ± 8.1	0.74046184	37.9 ± 10.8	29.4 ± 8.3	0.15540169
PE 16:0p-18:2	Positive	700.5	6.10 ± 0.01	229 ± 110	219 ± 75	0.84813862	197 ± 71	143 ± 65	0.20120678
PE 16:0p-18:3	Positive	698.5	6.21 ± 0.05	13.2 ± 7.1	12.3 ± 5.1	0.80333280	12.2 ± 5.6	7.6 ± 4.1	0.13027391
PE 16:0p-20:3	Positive	726.5	6.10 ± 0.01	2.6 ± 0.7	3.3 ± 0.8	0.10210550	2.7 ± 1.2	1.9 ± 1.2	0.23276333
PE 16:0p-20:4	Positive	724.5	6.11 ± 0.01	40.4 ± 8.3	41.6 ± 2.7	0.74359460	42.6 ± 7.9	32.8 ± 5.6 *	0.03164516
PE 16:0p-20:5	Positive	722.5	6.23 ± 0.04	1.5 ± 1.0	0.64 ± 0.31	0.11137937	1.3 ± 0.9	91.6 ± 31.2 ***	0.00003348

PE 16:0p-22:4	Positive	752.6	6.12 ± 0.05	8.4 ± 2.1	8.2 ± 1.6	0.87365841	8.3 ± 1.3	1.4 ± 0.8 ***	0.00000063
PE 16:0p-22:5	Positive	750.5	6.17 ± 0.07	22.1 ± 2.4	21.7 ± 2.1	0.72972907	20.4 ± 3.6	31.0 ± 6.5 **	0.00574274
PE 16:0p-22:6	Positive	748.5	6.22 ± 0.05	10.4 ± 1.4	8.0 ± 0.8 **	0.00403605	10.0 ± 2.4	13.3 ± 3.0	0.05790982
PE 16:1p-20:2	Positive	726.5	6.11 ± 0.03	1.2 ± 0.7	1.4 ± 0.5	0.49438540	1.4 ± 0.6	0.68 ± 0.54	0.07058813
PE 16:1p-22:2	Positive	754.6	6.08 ± 0.01	3.6 ± 1.2	2.7 ± 1.0	0.20742569	2.9 ± 1.2	1.2 ± 0.5 *	0.01103157
PE 16:1p-22:3	Positive	752.6	6.14 ± 0.04	0.84 ± 0.36	1.0 ± 0.4	0.37347474	0.82 ± 0.33	0.37 ± 0.24	0.05010158
PE 18:0p-16:0	Positive	704.6	6.05 ± 0.01	3.8 ± 2.6	4.7 ± 1.7	0.50065082	3.3 ± 1.2	3.7 ± 1.3	0.56717442
PE 18:0p-16:1	Positive	702.5	6.08 ± 0.01	2.4 ± 0.8	2.5 ± 0.9	0.91640323	1.9 ± 0.4	1.1 ± 0.9	0.10516347
PE 18:0p-18:1	Positive	730.6	6.07 ± 0.01	59.7 ± 14.2	63.7 ± 9.7	0.57632563	52.9 ± 9.0	33.4 ± 7.0 **	0.00182286
PE 18:0p-18:2	Positive	728.6	6.08 ± 0.01	502 ± 103	513 ± 67	0.82824433	417 ± 43	236 ± 38 ***	0.00001646
PE 18:0p-18:3	Positive	726.5	6.12 ± 0.02	31.4 ± 6.2	34.7 ± 3.9	0.29841190	27.6 ± 5.3	14.6 ± 3.8 ***	0.00065315
PE 18:0p-20:3	Positive	754.6	6.08 ± 0.01	5.9 ± 1.1	7.3 ± 0.5 *	0.02251702	4.6 ± 1.0	3.2 ± 1.1 *	0.04227053
PE 18:0p-20:4	Positive	752.6	6.08 ± 0.01	71.5 ± 7.3	67.8 ± 6.6	0.38423331	62.9 ± 5.2	53.9 ± 11.4	0.10793482
PE 18:0p-20:5	Positive	750.5	6.14 ± 0.04	2.9 ± 1.2	2.9 ± 0.7	0.96264458	2.6 ± 1.1	162 ± 41 ***	0.00000221
PE 18:0p-22:4	Positive	780.6	6.08 ± 0.01	6.3 ± 1.5	5.4 ± 0.7	0.20807198	5.0 ± 1.3	1.4 ± 0.7 ***	0.00011897
PE 18:0p-22:5	Positive	778.6	6.10 ± 0.01	19.0 ± 1.6	17.6 ± 1.8	0.19229091	17.4 ± 1.4	32.2 ± 4.7 ***	0.00002183
PE 18:0p-22:6	Positive	776.6	6.12 ± 0.03	10.0 ± 1.7	10.4 ± 0.7	0.66494360	8.3 ± 2.2	12.9 ± 2.7 **	0.00818941
PE 18:1p-16:0	Positive	702.5	6.08 ± 0.01	11.4 ± 7.5	12.6 ± 3.4	0.72308601	7.7 ± 2.9	7.0 ± 2.8	0.64998373
PE 18:1p-18:1	Positive	728.6	6.08 ± 0.01	36.7 ± 12.8	45.0 ± 7.1	0.19266056	30.2 ± 8.9	22.6 ± 4.0	0.08396482
PE 18:1p-18:2	Positive	726.5	6.11 ± 0.02	203 ± 85	220 ± 43	0.67869194	151 ± 26	92.5 ± 17.8 **	0.00109398
PE 18:1p-18:3	Positive	724.5	6.25 ± 0.03	12.5 ± 6.9	11.5 ± 2.9	0.73696610	8.2 ± 3.3	4.7 ± 1.9 *	0.04781206
PE 18:1p-20:3	Positive	752.6	6.13 ± 0.05	2.2 ± 1.2	2.9 ± 0.5	0.23217977	1.5 ± 0.9	0.88 ± 0.33	0.17863784

PE 18:1p-20:4	Positive	750.5	6.14 ± 0.04	32.8 ± 4.6	36.9 ± 6.0	0.20708319	29.6 ± 3.8	21.9 ± 5.0 *	0.01381148
PE 18:1p-20:5	Positive	748.5	6.26 ± 0.03	1.0 ± 0.4	0.63 ± 0.38	0.14225214	0.69 ± 0.45	82.1 ± 17.0 ***	0.00000036
PE 18:1p-22:4	Positive	778.6	6.13 ± 0.05	1.9 ± 0.4	2.5 ± 0.7	0.09598330	2.2 ± 0.6	0.32 ± 0.26 ***	0.00048165
PE 18:1p-22:5	Positive	776.6	6.20 ± 0.07	7.6 ± 1.7	7.5 ± 1.9	0.89524307	6.5 ± 2.3	14.7 ± 1.6 ***	0.00002480
PE 18:1p-22:6	Positive	774.5	6.26 ± 0.04	5.4 ± 1.0	4.1 ± 0.5 *	0.01734112	3.9 ± 1.3	6.9 ± 2.2 *	0.01529133
PE 18:2p-18:1	Positive	726.5	6.12 ± 0.04	1.5 ± 0.7	2.0 ± 0.4	0.19202386	1.3 ± 0.8	0.46 ± 0.28 *	0.03441169
PE 18:2p-18:2	Positive	724.5	6.24 ± 0.04	13.9 ± 3.2	11.4 ± 3.2	0.22096573	10.4 ± 2.6	3.9 ± 1.0 ***	0.00023135
PE 18:2p-20:4	Positive	748.5	6.25 ± 0.02	2.7 ± 1.4	1.7 ± 0.4	0.13324558	2.1 ± 0.8	1.1 ± 0.6 *	0.02750428
PE 18:2p-20:5	Positive	746.5	6.33 ± 0.02	n.d.	n.d.		n.d.	2.5 ± 0.7	
PE 18:2p-22:2	Positive	780.6	6.10 ± 0.02	0.31 ± 0.30	0.66 ± 0.39	0.11193746	0.57 ± 0.39	0.75 ± 0.39	0.49730270
PEpln total				1426 ± 378	1452 ± 212	0.88393090	1200 ± 163	1175 ± 179	0.80717449
PI 16:0-18:2	Negative	833.5	11.98 ± 0.02	5011 ± 1263	3444 ± 726 *	0.02495163	2501 ± 549	1125 ± 259 ***	0.00024328
PI 18:0-18:1	Negative	863.6	11.84 ± 0.03	7588 ± 1783	7083 ± 1809	0.63675600	3434 ± 681	1448 ± 242 ***	0.00005160
PI 18:0-18:2	Negative	861.5	11.89 ± 0.02	27810 ± 4795	21272 ± 4290 *	0.03204158	14029 ± 1504	7267 ± 595 ***	0.00000128
PI 18:0-20:2	Negative	889.6	11.84 ± 0.02	1133 ± 371	1262 ± 434	0.59063144	367 ± 54	78.5 ± 36.1 ***	0.00000077
PI 18:0-20:3	Negative	887.6	11.88 ± 0.03	1902 ± 315	1642 ± 534	0.32747006	789 ± 148	394 ± 66 ***	0.00013996
PI 18:0-20:4	Negative	885.5	11.90 ± 0.02	8710 ± 1324	6973 ± 1506	0.05997466	4624 ± 509	3527 ± 511 **	0.00395214
PI 18:0-20:5	Negative	883.5	11.94 ± 0.04	66.2 ± 46.0	54.0 ± 23.0	0.57352684	16.0 ± 16.4	1754 ± 541 ***	0.00001361
PI 18:1-18:1	Negative	861.5	11.89 ± 0.02	581 ± 173	492 ± 164	0.37978571	260 ± 88	45.8 ± 14.7 **	0.00015221
PI total				52800 ± 8755	42221 ± 9044	0.06652109	26019 ± 3072	15639 ± 1745 ***	0.00002939
SM d18:1-14:0	Positive	675.5	5.84 ± 0.01	0.68 ± 0.05	0.59 ± 0.04 **	0.00537244	0.60 ± 0.10	0.66 ± 0.09	0.28374626
SM d18:1-14:1	Positive	673.5	5.88 ± 0.01	$(3.2 \pm 0.9) \times 10^{-2}$	$(3.5 \pm 0.6) \times 10^{-2}$	0.46658906	$(3.3 \pm 0.9) \times 10^{-2}$	$(3.7 \pm 0.7) \times 10^{-2}$	0.45387791

SM d18:1-16:0	Positive	703.6	5.81 ± 0.01	58.1 ± 4.9	59.3 ± 1.7	0.57836898	54.8 ± 4.0	64.0 ± 5.6 **	0.00854087
SM d18:1-16:1	Positive	701.6	5.85 ± 0.01	3.7 ± 0.3	3.1 ± 0.2 **	0.00395563	3.1 ± 0.6	3.9 ± 0.4 *	0.02112991
SM d18:1-18:0	Positive	731.6	5.78 ± 0.01	14.2 ± 0.5	16.2 ± 1.2 **	0.00435569	13.4 ± 1.6	15.5 ± 0.9 *	0.01565729
SM d18:1-18:1	Positive	729.6	5.82 ± 0.01	3.8 ± 0.4	3.9 ± 0.3	0.81579107	3.4 ± 0.6	4.1 ± 0.3 *	0.01606589
SM d18:1-18:2	Positive	727.6	5.84 ± 0.01	$(7.3 \pm 1.3) \times 10^{-2}$	$(6.0 \pm 1.1) \times 10^{-2}$	0.08513545	$(6.2 \pm 1.5) \times 10^{-2}$	$(8.1 \pm 1.5) \times 10^{-2}$	0.05414837
SM d18:1-18:3	Positive	725.6	5.87 ± 0.01	$(6.1 \pm 1.9) \times 10^{-3}$	$(5.0 \pm 1.3) \times 10^{-3}$	0.26272716	$(6.1 \pm 2.4) \times 10^{-3}$	$(7.2 \pm 5.2) \times 10^{-3}$	0.64618746
SM d18:1-20:0	Positive	759.6	5.76 ± 0.01	5.8 ± 0.3	5.5 ± 0.5	0.11270202	5.3 ± 0.6	6.4 ± 0.3 **	0.00309547
SM d18:1-20:1	Positive	757.6	5.79 ± 0.01	2.9 ± 0.2	3.4 ± 0.4 *	0.02409410	2.9 ± 0.3	3.4 ± 0.2 *	0.01123738
SM d18:1-20:2	Positive	755.6	5.82 ± 0.01	0.11 ± 0.02	0.11 ± 0.01	0.86857156	$(8.7 \pm 2.0) \times 10^{-2}$	0.14 ± 0.02 **	0.00249765
SM d18:1-20:3	Positive	753.6	5.86 ± 0.02	$(9.8 \pm 2.4) \times 10^{-3}$	$(1.4 \pm 0.4) \times 10^{-2}$	0.06180254	$(7.2 \pm 4.4) \times 10^{-3}$	$(3.5 \pm 1.1) \times 10^{-2}$ ***	0.00015977
SM d18:1-20:5	Positive	749.6	5.92 ± 0.01	0.14 ± 0.02	0.11 ± 0.01 **	0.00975825	0.13 ± 0.02	0.13 ± 0.01	0.94669517
SM d18:1-22:0	Positive	787.7	5.74 ± 0.01	7.2 ± 0.4	6.6 ± 0.5	0.05859460	6.4 ± 0.7	8.2 ± 0.6 **	0.00107512
SM d18:1-22:1	Positive	785.7	5.77 ± 0.01	4.8 ± 0.2	4.7 ± 0.4	0.70009811	4.4 ± 0.6	5.4 ± 0.1 **	0.00285852
SM d18:1-22:2	Positive	783.6	5.81 ± 0.01	0.83 ± 0.08	0.87 ± 0.07	0.40769600	0.76 ± 0.06	0.80 ± 0.05	0.23881982
SM d18:1-22:3	Positive	781.6	5.84 ± 0.01	0.18 ± 0.01	0.16 ± 0.01	0.13136862	0.15 ± 0.03	0.19 ± 0.01 **	0.00776457
SM total				103 ± 7	105 ± 4	0.55430453	95.5 ± 8.3	113 ± 7 **	0.00262727
Cer d18:1-16:0	Positive	538.5	4.48 ± 0.01	3.9 ± 1.0	4.1 ± 0.7	0.71621552	4.6 ± 0.7	4.1 ± 0.8	0.35565524
Cer d18:1-16:1	Positive	536.5	4.48 ± 0.01	1.1 ± 0.1	0.96 ± 0.05	0.07948242	1.1 ± 0.1	1.1 ± 0.1	0.72846614
Cer d18:1-18:0	Positive	566.6	4.48 ± 0.01	3.4 ± 1.1	4.2 ± 1.2	0.24417604	3.5 ± 0.7	3.4 ± 0.9	0.77891585
Cer d18:1-18:1	Positive	564.5	4.49 ± 0.01	$(2.7 \pm 1.4) \times 10^{-2}$	$(4.3 \pm 2.3) \times 10^{-2}$	0.17654222	$(2.5 \pm 0.7) \times 10^{-2}$	$(2.5 \pm 1.1) \times 10^{-2}$	0.93010042
Cer d18:1-18:2	Positive	562.5	4.48 ± 0.01	0.65 ± 0.18	0.62 ± 0.10	0.76428123	0.70 ± 0.08	0.62 ± 0.09	0.15508199
Cer d18:1-18:4	Positive	558.5	4.49 ± 0.01	$(5.6 \pm 2.4) \times 10^{-2}$	$(4.5 \pm 1.2) \times 10^{-2}$	0.31610197	$(4.9 \pm 2.0) \times 10^{-2}$	$(4.8 \pm 1.6) \times 10^{-2}$	0.93347253

Cer d18:1-20:0	Positive	594.6	4.49 ± 0.01	3.4 ± 0.8	4.1 ± 1.2	0.28732697	4.0 ± 0.6	4.1 ± 0.6	0.82780066
Cer d18:1-20:1	Positive	592.6	4.49 ± 0.01	$(4.4 \pm 1.4) \times 10^{-2}$	$(5.2 \pm 1.6) \times 10^{-2}$	0.37094215	$(4.5 \pm 2.0) \times 10^{-2}$	$(7.7 \pm 2.2) \times 10^{-2}$ *	0.02436778
Cer d18:1-20:2	Positive	590.6	4.49 ± 0.01	1.3 ± 0.3	1.3 ± 0.2	0.96100796	1.6 ± 0.2	1.5 ± 0.2	0.52084745
Cer d18:1-20:4	Positive	586.5	4.49 ± 0.01	0.17 ± 0.04	0.19 ± 0.06	0.41760884	0.20 ± 0.05	0.19 ± 0.04	0.74765773
Cer d18:1-22:0	Positive	622.6	4.49 ± 0.01	16.0 ± 4.1	19.5 ± 4.6	0.20151153	18.0 ± 2.3	18.4 ± 3.1	0.78878230
Cer d18:1-22:1	Positive	620.6	4.49 ± 0.01	0.77 ± 0.19	0.75 ± 0.17	0.84585287	0.83 ± 0.09	0.81 ± 0.17	0.81526479
Cer d18:1-22:2	Positive	618.6	4.49 ± 0.01	17.3 ± 3.7	17.3 ± 3.0	0.99849283	20.6 ± 2.7	19.1 ± 2.6	0.34112238
Cer d18:1-22:3	Positive	616.6	4.51 ± 0.01	0.16 ± 0.04	0.19 ± 0.04	0.25992105	0.15 ± 0.05	0.19 ± 0.05	0.14657820
Cer d18:1-22:4	Positive	614.6	4.49 ± 0.01	0.20 ± 0.03	0.20 ± 0.02	0.89009714	0.22 ± 0.06	0.20 ± 0.03	0.43188454
Cer d18:1-22:5	Positive	612.5	4.51 ± 0.01	$(7.0 \pm 3.1) \times 10^{-2}$	$(9.7 \pm 3.1) \times 10^{-2}$	0.16594838	$(8.6 \pm 3.1) \times 10^{-2}$	$(7.0 \pm 1.8) \times 10^{-2}$	0.30618184
Cer total				48.6 ± 11.1	53.7 ± 10.6	0.43730987	55.6 ± 6.4	53.9 ± 7.6	0.68453246
CE 16:0	Positive	642.6	1.12 ± 0.03	4962 ± 1780	4018 ± 889	0.27230393	2918 ± 477	3983 ± 896 *	0.02797415
CE 16:1	Positive	640.6	1.14 ± 0.03	3401 ± 1347	5105 ± 1347	0.05325902	4469 ± 946	3470 ± 520 *	0.04685439
CE 18:0	Positive	670.6	1.15 ± 0.03	750 ± 321	1796 ± 608 **	0.00393517	932 ± 230	734 ± 344	0.26822021
CE 18:1	Positive	668.6	1.16 ± 0.03	8480 ± 3084	14896 ± 7618	0.08490389	12525 ± 7407	12700 ± 3337	0.95886372
CE 18:2	Positive	666.6	1.22 ± 0.02	144420 ± 42213	88095 ± 32425 *	0.02685993	141666 ± 46886	147395 ± 68857	0.86957658
CE 18:3	Positive	664.6	1.23 ± 0.02	76925 ± 29235	57531 ± 21453	0.21948448	66024 ± 19954	50780 ± 27404	0.29647685
CE 18:4	Positive	662.6	1.24 ± 0.03	605 ± 217	451 ± 217	0.24690662	407 ± 145	728 ± 456	0.13145019
CE 20:0	Positive	698.7	1.21 ± 0.07	20.5 ± 21.4	12.0 ± 11.3	0.40798744	n.d.	4.6 ± 3.3	
CE 20:1	Positive	696.7	1.23 ± 0.03	57.6 ± 24.6	31.6 ± 15.0	0.05209412	37.2 ± 18.1	25.4 ± 7.0	0.16678409
CE 20:2	Positive	694.6	1.24 ± 0.02	473 ± 168	372 ± 155	0.30582783	301 ± 115	218 ± 75	0.16734244
CE 20:3	Positive	692.6	1.24 ± 0.02	4071 ± 1600	3634 ± 1697	0.65549931	2624 ± 1181	2547 ± 1199	0.91216733

CE 20:4	Positive	690.6	1.24 ± 0.03	58081 ± 23440	45887 ± 18565	0.34140786	38878 ± 25507	42460 ± 19887.86	0.79167655
CE 20:5	Positive	688.6	1.25 ± 0.03	5520 ± 2637	5096 ± 2239	0.77030501	2890 ± 1470	179812 ± 96689 **	0.00117616
CE 22:0	Positive	726.7	1.25 ± 0.03	33.0 ± 19.9	28.2 ± 17.8	0.66829809	20.8 ± 14.7	11.3 ± 5.7	0.16706474
CE 22:1	Positive	724.7	1.24 ± 0.03	25.8 ± 12.9	18.3 ± 10.0	0.28264121	15.9 ± 7.9	10.2 ± 4.6	0.16135876
CE 22:2	Positive	722.7	1.24 ± 0.02	51.3 ± 28.0	31.5 ± 13.1	0.14959675	27.5 ± 15.6	13.5 ± 6.7	0.07268283
CE 22:3	Positive	720.7	1.24 ± 0.03	81.7 ± 33.9	61.7 ± 26.2	0.28063154	44.3 ± 33.9	20.5 ± 8.3	0.12534406
CE 22:4	Positive	718.6	1.26 ± 0.03	669 ± 274	511 ± 227	0.30168430	341 ± 268	245 ± 126	0.44319203
CE 22:5	Positive	716.6	1.27 ± 0.04	1359 ± 649	1158 ± 538	0.57246231	728 ± 536	3283 ± 1854 *	0.00883452
CE 22:6	Positive	714.6	1.30 ± 0.04	1495 ± 743	1375 ± 607	0.76654771	806 ± 578	1353 ± 700	0.17066330
CE total				311478 ± 103097	230108 ± 78259	0.15460699	275654 ± 82839	449791 ± 205639	0.08325502
MAG 14:0	Positive	303.3	4.02 ± 0.03	2.3 ± 1.0	1.8 ± 0.6	0.29348623	2.8 ± 0.8	1.4 ± 0.4 **	0.00183486
MAG 16:0	Positive	331.3	4.04 ± 0.02	57.2 ± 17.2	45.8 ± 10.9	0.19822634	63.5 ± 17.5	45.7 ± 6.6	0.04178279
MAG 16:1	Positive	329.3	4.09 ± 0.02	1.0 ± 0.5	0.58 ± 0.31	0.09833084	1.4 ± 0.6	0.54 ± 0.30 *	0.01445036
MAG 18:0	Positive	359.3	4.06 ± 0.02	29.0 ± 2.8	34.1 ± 12.5	0.34783936	37.0 ± 10.7	41.2 ± 26.2	0.72505312
MAG 18:1	Positive	357.3	4.10 ± 0.02	15.0 ± 6.3	11.1 ± 3.8	0.22405664	16.9 ± 5.5	6.9 ± 1.8 **	0.00169292
MAG 18:2	Positive	355.3	4.15 ± 0.02	5.4 ± 2.2	2.9 ± 0.8 *	0.02636887	6.9 ± 2.4	3.1 ± 0.9 **	0.00417467
MAG total				110 ± 29	96.2 ± 23.0	0.39130388	128 ± 31	98.8 ± 24.9	0.09781030
DAG 14:0-16:0	Positive	558.5	3.14 ± 0.01	0.14 ± 0.05	0.18 ± 0.06	0.20702950	0.13 ± 0.03	$(6.6 \pm 3.5) \times 10^{-2}$ *	0.01212783
DAG 14:0-16:1	Positive	556.5	3.16 ± 0.02	$(3.1 \pm 1.1) \times 10^{-2}$	$(3.5 \pm 1.9) \times 10^{-2}$	0.68951346	$(2.5 \pm 1.4) \times 10^{-2}$	$(1.5 \pm 1.2) \times 10^{-2}$	0.20772814
DAG 14:0-18:1	Positive	584.5	3.17 ± 0.01	0.25 ± 0.08	0.34 ± 0.13	0.19154994	0.30 ± 0.16	0.10 ± 0.05 *	0.01397408
DAG 14:0-18:2	Positive	582.5	3.19 ± 0.01	0.26 ± 0.11	0.31 ± 0.12	0.51715991	0.34 ± 0.15	0.12 ± 0.07 *	0.01061967
DAG 14:0-18:3	Positive	580.5	3.23 ± 0.01	$(3.7 \pm 1.7) \times 10^{-2}$	$(3.1 \pm 1.6) \times 10^{-2}$	0.57950489	$(4.8 \pm 1.9) \times 10^{-2}$	$(1.4 \pm 1.4) \times 10^{-2}$ **	0.00501591

DAG 14:0-20:5	Positive	604.5	3.26 ± 0.01	n.d.	n.d.		n.d.	$(2.9 \pm 0.9) \times 10^{-2}$	
DAG 14:0-22:5	Positive	632.5	3.28 ± 0.02	$(2.4 \pm 3.1) \times 10^{-3}$	$(1.6 \pm 0.7) \times 10^{-3}$	0.64488739	$(1.8 \pm 1.8) \times 10^{-3}$	$(4.3 \pm 1.1) \times 10^{-2}$ ***	0.00051769
DAG 14:1-18:2	Positive	580.5	3.22 ± 0.01	$(2.0 \pm 0.7) \times 10^{-2}$	$(1.8 \pm 1.2) \times 10^{-2}$	0.77552917	$(2.6 \pm 1.5) \times 10^{-2}$	$(1.3 \pm 1.2) \times 10^{-2}$	0.13916559
DAG 14:1-22:2	Positive	636.6	3.25 ± 0.02	$(1.3 \pm 0.6) \times 10^{-2}$	$(8.9 \pm 5.1) \times 10^{-3}$	0.18815580	$(1.6 \pm 0.6) \times 10^{-2}$	$(3.8 \pm 2.1) \times 10^{-3}$ **	0.00106726
DAG 16:0-16:0	Positive	586.5	3.16 ± 0.01	0.86 ± 0.24	0.87 ± 0.28	0.92221028	0.72 ± 0.14	0.34 ± 0.11 ***	0.00031598
DAG 16:0-16:1	Positive	584.5	3.18 ± 0.01	0.49 ± 0.13	0.45 ± 0.23	0.71447544	0.53 ± 0.18	0.22 ± 0.14 **	0.00743974
DAG 16:0-18:0	Positive	614.6	3.18 ± 0.01	0.44 ± 0.10	0.45 ± 0.12	0.90194702	0.36 ± 0.09	0.13 ± 0.05 ***	0.00027325
DAG 16:0-18:1	Positive	612.6	3.20 ± 0.01	3.1 ± 0.7	3.0 ± 1.0	0.89798438	2.7 ± 1.0	1.2 ± 0.5 **	0.00533238
DAG 16:0-18:2	Positive	610.5	3.22 ± 0.01	4.0 ± 0.9	3.7 ± 1.3	0.67382038	3.9 ± 1.0	1.7 ± 0.7 **	0.00149741
DAG 16:0-18:3	Positive	608.5	3.24 ± 0.01	0.62 ± 0.20	0.56 ± 0.19	0.56068908	0.66 ± 0.14	0.27 ± 0.13 ***	0.00050278
DAG 16:0-20:2	Positive	638.6	3.24 ± 0.02	$(2.2 \pm 1.4) \times 10^{-2}$	$(2.1 \pm 1.8) \times 10^{-2}$	0.87148124	$(1.9 \pm 2.3) \times 10^{-2}$	$(7.5 \pm 5.4) \times 10^{-3}$	0.24075785
DAG 16:0-20:3	Positive	636.6	3.25 ± 0.01	$(3.3 \pm 1.4) \times 10^{-2}$	$(2.8 \pm 1.4) \times 10^{-2}$	0.52435497	$(2.6 \pm 1.2) \times 10^{-2}$	$(2.0 \pm 0.8) \times 10^{-2}$	0.37191297
DAG 16:0-20:4	Positive	634.5	3.25 ± 0.02	$(4.2 \pm 1.1) \times 10^{-2}$	$(3.7 \pm 0.9) \times 10^{-2}$	0.45048744	$(4.9 \pm 2.6) \times 10^{-2}$	$(6.6 \pm 1.9) \times 10^{-2}$	0.24466220
DAG 16:0-20:5	Positive	632.5	3.28 ± 0.01	$(3.7 \pm 3.6) \times 10^{-3}$	$(3.0 \pm 3.2) \times 10^{-3}$	0.70955164	$(4.1 \pm 2.0) \times 10^{-3}$	0.39 ± 0.12 ***	0.00005910
DAG 16:1-16:1	Positive	582.5	3.19 ± 0.01	$(4.7 \pm 1.2) \times 10^{-2}$	$(5.3 \pm 2.6) \times 10^{-2}$	0.63098731	$(5.2 \pm 1.0) \times 10^{-2}$	$(2.6 \pm 1.6) \times 10^{-2}$ **	0.00627238
DAG 16:1-18:0	Positive	612.6	3.20 ± 0.01	$(7.3 \pm 2.0) \times 10^{-2}$	$(6.6 \pm 2.7) \times 10^{-2}$	0.62095644	$(6.8 \pm 3.0) \times 10^{-2}$	$(2.5 \pm 1.5) \times 10^{-2}$ **	0.00971542
DAG 16:1-18:1	Positive	610.5	3.21 ± 0.01	0.66 ± 0.21	0.75 ± 0.37	0.59377620	0.79 ± 0.23	0.34 ± 0.17 **	0.00352561
DAG 16:1-18:2	Positive	608.5	3.24 ± 0.01	0.82 ± 0.22	0.75 ± 0.31	0.67275486	0.96 ± 0.25	0.57 ± 0.28 *	0.03015742
DAG 16:1-18:3	Positive	606.5	3.26 ± 0.01	0.12 ± 0.04	$(8.7 \pm 5.3) \times 10^{-2}$	0.24187825	0.17 ± 0.07	$(7.7 \pm 5.7) \times 10^{-2}$ *	0.02748192
DAG 16:1-20:2	Positive	636.6	3.25 ± 0.02	$(2.1 \pm 0.8) \times 10^{-2}$	$(1.5 \pm 0.5) \times 10^{-2}$	0.14049913	$(2.5 \pm 1.5) \times 10^{-2}$	$(6.0 \pm 3.4) \times 10^{-3}$ *	0.01414243
DAG 16:1-20:3	Positive	634.5	3.27 ± 0.01	$(2.0 \pm 1.0) \times 10^{-2}$	$(1.5 \pm 0.6) \times 10^{-2}$	0.28448612	$(2.1 \pm 1.1) \times 10^{-2}$	$(1.0 \pm 0.5) \times 10^{-2}$	0.05034798
DAG 16:1-20:4	Positive	632.5	3.27 ± 0.02	$(1.2 \pm 0.5) \times 10^{-2}$	$(1.0 \pm 0.5) \times 10^{-2}$	0.41976876	$(1.6 \pm 1.0) \times 10^{-2}$	$(2.2 \pm 1.0) \times 10^{-2}$	0.38317153

DAG 16:1-20:5	Positive	630.5	3.29 ± 0.02	n.d.	n.d.		n.d.	$(8.1 \pm 2.4) \times 10^{-2}$	
DAG 18:0-18:0	Positive	642.6	3.21 ± 0.01	$(6.1 \pm 2.5) \times 10^{-2}$	$(6.4 \pm 2.6) \times 10^{-2}$	0.86235379	$(5.0 \pm 2.2) \times 10^{-2}$	$(2.3 \pm 1.6) \times 10^{-2}$ *	0.03075030
DAG 18:0-18:1	Positive	640.6	3.22 ± 0.01	0.63 ± 0.13	0.66 ± 0.21	0.80028306	0.58 ± 0.18	0.17 ± 0.09 ***	0.00051060
DAG 18:0-18:2	Positive	638.6	3.24 ± 0.01	1.3 ± 0.3	1.1 ± 0.2	0.16705264	1.3 ± 0.3	0.39 ± 0.17 ***	0.00014791
DAG 18:0-18:3	Positive	636.6	3.26 ± 0.02	0.15 ± 0.04	0.12 ± 0.05	0.19755193	0.16 ± 0.06	$(5.2 \pm 3.3) \times 10^{-2}$ **	0.00181955
DAG 18:0-18:4	Positive	634.5	3.26 ± 0.01	$(4.1 \pm 2.6) \times 10^{-3}$	$(2.4 \pm 1.4) \times 10^{-3}$	0.27827884	$(3.4 \pm 2.8) \times 10^{-3}$	$(1.6 \pm 1.4) \times 10^{-3}$	0.27314492
DAG 18:0-20:4	Positive	662.6	3.28 ± 0.02	$(2.3 \pm 0.4) \times 10^{-2}$	$(1.6 \pm 0.5) \times 10^{-2}$ *	0.01835844	$(1.9 \pm 0.5) \times 10^{-2}$	$(1.2 \pm 0.7) \times 10^{-2}$ *	0.10224676
DAG 18:0-20:5	Positive	660.6	3.31 ± 0.02	n.d.	n.d.		n.d.	$(3.7 \pm 1.5) \times 10^{-2}$	
DAG 18:1-18:1	Positive	638.6	3.23 ± 0.01	2.7 ± 0.7	2.8 ± 0.9	0.81719753	2.8 ± 0.8	1.1 ± 0.5 ***	0.00082304
DAG 18:1-18:2	Positive	636.6	3.25 ± 0.02	6.7 ± 1.6	6.1 ± 1.8	0.55614795	7.9 ± 2.5	3.5 ± 1.4 **	0.00401720
DAG 18:1-18:3	Positive	634.5	3.27 ± 0.02	1.0 ± 0.3	0.82 ± 0.24	0.26410352	1.4 ± 0.4	0.54 ± 0.21 **	0.00107849
DAG 18:1-18:4	Positive	632.5	3.30 ± 0.02	$(2.0 \pm 1.0) \times 10^{-2}$	$(1.3 \pm 0.8) \times 10^{-2}$	0.24377871	$(2.6 \pm 1.8) \times 10^{-2}$	$(1.6 \pm 0.3) \times 10^{-2}$	0.28427552
DAG 18:1-20:1	Positive	666.6	3.24 ± 0.03	$(3.1 \pm 0.9) \times 10^{-2}$	$(4.1 \pm 2.0) \times 10^{-2}$	0.26860246	$(3.3 \pm 2.1) \times 10^{-2}$	$(2.5 \pm 1.3) \times 10^{-3}$ *	0.00519172
DAG 18:1-20:2	Positive	664.6	3.27 ± 0.02	$(3.2 \pm 1.2) \times 10^{-2}$	$(3.0 \pm 1.4) \times 10^{-2}$	0.78038666	$(3.6 \pm 1.7) \times 10^{-2}$	$(9.2 \pm 6.3) \times 10^{-3}$ **	0.00997239
DAG 18:1-20:4	Positive	660.6	3.29 ± 0.02	$(9.4 \pm 1.8) \times 10^{-2}$	$(8.3 \pm 3.1) \times 10^{-2}$	0.46832426	0.12 ± 0.05	0.10 ± 0.03	0.35562919
DAG 18:1-20:5	Positive	658.5	3.32 ± 0.02	$(5.0 \pm 4.4) \times 10^{-3}$	$(2.3 \pm 2.5) \times 10^{-3}$	0.22369677	$(8.3 \pm 5.6) \times 10^{-3}$	0.48 ± 0.15 ***	0.00001397
DAG 18:1-22:4	Positive	688.6	3.31 ± 0.02	$(7.2 \pm 3.6) \times 10^{-3}$	$(4.4 \pm 2.8) \times 10^{-3}$	0.17505181	$(7.6 \pm 4.9) \times 10^{-3}$	$(2.9 \pm 4.4) \times 10^{-3}$	0.17421491
DAG 18:1-22:5	Positive	686.6	3.34 ± 0.03	$(7.5 \pm 4.1) \times 10^{-3}$	$(5.5 \pm 3.6) \times 10^{-3}$	0.38385246	$(9.4 \pm 7.5) \times 10^{-3}$	$(7.0 \pm 4.0) \times 10^{-2}$ *	0.00467176
DAG 18:2-18:2	Positive	634.5	3.27 ± 0.02	2.7 ± 0.8	1.9 ± 0.7	0.11494759	3.3 ± 0.7	1.5 ± 0.6 ***	0.00050715
DAG 18:2-18:3	Positive	632.5	3.30 ± 0.02	0.53 ± 0.19	0.41 ± 0.16	0.23423457	0.74 ± 0.28	0.26 ± 0.11 **	0.00275656
DAG 18:2-20:4	Positive	658.5	3.32 ± 0.02	$(5.6 \pm 1.2) \times 10^{-2}$	$(4.1 \pm 1.2) \times 10^{-2}$	0.05039565	$(7.3 \pm 4.1) \times 10^{-2}$	0.10 ± 0.03	0.17654246
DAG 18:2-20:5	Positive	656.5	3.35 ± 0.02	$(3.5 \pm 2.1) \times 10^{-3}$	$(1.3 \pm 1.1) \times 10^{-3}$ *	0.04155523	$(2.6 \pm 1.5) \times 10^{-3}$	0.60 ± 0.14 ***	0.00000072

DAG 18:2-22:4	Positive	686.6	3.34 ± 0.03	$(2.3 \pm 1.8) \times 10^{-3}$	$(2.6 \pm 1.5) \times 10^{-3}$	0.77147079	$(4.8 \pm 3.1) \times 10^{-3}$	$(1.4 \pm 1.7) \times 10^{-3}$	0.06810799
DAG 18:2-22:5	Positive	684.6	3.36 ± 0.03	$(5.0 \pm 3.0) \times 10^{-3}$	$(3.8 \pm 2.0) \times 10^{-3}$	0.48927801	$(6.2 \pm 6.1) \times 10^{-3}$	$(5.3 \pm 2.9) \times 10^{-2}$ *	0.00706365
DAG 18:3-20:4	Positive	656.5	3.35 ± 0.02	$(2.0 \pm 2.0) \times 10^{-3}$	$(2.6 \pm 3.5) \times 10^{-3}$	0.78318074	$(3.7 \pm 2.7) \times 10^{-3}$	$(5.8 \pm 2.5) \times 10^{-3}$	0.22489440
DAG 18:3-20:5	Positive	654.5	3.40 ± 0.01	n.d.	n.d.		n.d.	$(4.1 \pm 2.0) \times 10^{-2}$	
DAG total				28.1 ± 6.8	26.0 ± 8.1	0.63055436	30.4 ± 8.1	14.8 ± 5.5 **	0.00290913
TAG 40:0	Positive	712.6	1.19 ± 0.04	51.6 ± 12.8	44.7 ± 7.2	0.27245601	69.9 ± 14.8	94.7 ± 28.7	0.08910160
TAG 40:1	Positive	710.6	1.09 ± 0.13	45.0 ± 13.2	39.4 ± 7.8	0.39112738	59.6 ± 10.8	211 ± 71 **	0.00040821
TAG 40:2	Positive	708.6	1.06 ± 0.02	168 ± 55	162 ± 26	0.80157852	275 ± 96	254 ± 38	0.62491177
TAG 42:0	Positive	740.7	1.02 ± 0.04	34.5 ± 11.0	35.2 ± 8.0	0.90042043	36.6 ± 8.7	27.4 ± 4.1 *	0.04082777
TAG 42:1	Positive	738.7	1.01 ± 0.04	106 ± 18	95.8 ± 8.9	0.23307827	111 ± 10	83.0 ± 8.0 ***	0.00036976
TAG 42:2	Positive	736.6	1.12 ± 0.03	215 ± 75	216 ± 46	0.98289714	361 ± 131	324 ± 55	0.52957929
TAG 42:3	Positive	734.6	0.97 ± 0.02	31.4 ± 3.9	32.9 ± 10.5	0.75044870	41.4 ± 4.7	38.4 ± 3.0	0.21058542
TAG 42:4	Positive	732.6	0.99 ± 0.02	118 ± 26	103 ± 24	0.34066073	150 ± 26	117 ± 11 *	0.01655077
TAG 44:0	Positive	768.7	1.07 ± 0.05	116 ± 55	188 ± 65	0.06377608	169 ± 72	89.8 ± 31.1 *	0.03295966
TAG 44:1	Positive	766.7	1.10 ± 0.04	74.3 ± 36.2	103 ± 41	0.21965904	121 ± 46	66.4 ± 23.3 *	0.02601978
TAG 44:2	Positive	764.7	1.17 ± 0.04	137 ± 47	146 ± 28	0.69592282	216 ± 75	174 ± 23	0.22732924
TAG 44:3	Positive	762.7	1.01 ± 0.02	39.0 ± 9.0	33.6 ± 6.5	0.26798354	52.6 ± 5.6	41.5 ± 3.9 **	0.00260638
TAG 44:4	Positive	760.6	1.02 ± 0.02	467 ± 70	411 ± 67	0.18931512	607 ± 81	487 ± 81 *	0.02833085
TAG 44:5	Positive	758.6	1.08 ± 0.04	2594 ± 520	2198 ± 332	0.14753318	3595 ± 626	3100 ± 632	0.20335209
TAG 46:0	Positive	796.7	1.11 ± 0.03	624 ± 329	1177 ± 412 *	0.02789043	849 ± 419	379 ± 217 *	0.03473659
TAG 46:1	Positive	794.7	1.15 ± 0.05	603 ± 303	1001 ± 426	0.09214586	960 ± 444	425 ± 246 *	0.02721232
TAG 46:2	Positive	792.7	1.20 ± 0.04	361 ± 168	484 ± 176	0.24281001	583 ± 202	357 ± 106 *	0.03632193

TAG 46:3	Positive	790.7	1.22 ± 0.03	76.5 ± 36.5	104 ± 42	0.26064935	131 ± 59	69.6 ± 36.9	0.05702088
TAG 46:4	Positive	788.7	1.23 ± 0.03	22.5 ± 8.7	23.5 ± 9.1	0.84878670	31.1 ± 10.6	23.8 ± 9.1	0.22728593
TAG 46:5	Positive	786.7	1.17 ± 0.03	21.7 ± 6.3	19.3 ± 2.8	0.41203251	28.0 ± 4.4	23.4 ± 5.1	0.12169241
TAG 46:6	Positive	784.6	1.19 ± 0.03	144 ± 24	135 ± 19	0.48745084	177 ± 21	137 ± 25 *	0.01229923
TAG 48:0	Positive	824.8	1.18 ± 0.05	2192 ± 939	3533 ± 1078 *	0.04442981	2689 ± 965	1233 ± 690 *	0.01325689
TAG 48:1	Positive	822.8	1.20 ± 0.03	4138 ± 1706	6288 ± 1933	0.06837398	5669 ± 2191	2411 ± 1401 *	0.01187460
TAG 48:2	Positive	820.7	1.22 ± 0.03	3119 ± 1281	4119 ± 1323	0.21328643	4478 ± 1753	2058 ± 1114 *	0.01714136
TAG 48:3	Positive	818.7	1.23 ± 0.03	932 ± 395	1175 ± 427	0.33090144	1461 ± 589	728 ± 432 *	0.03379169
TAG 48:4	Positive	816.7	1.25 ± 0.03	219 ± 93	260 ± 105	0.49630047	365 ± 132	197 ± 113 *	0.04013274
TAG 48:5	Positive	814.7	1.28 ± 0.04	55.8 ± 19.8	64.6 ± 20.8	0.47014797	82.9 ± 28.3	64.0 ± 27.2	0.26417671
TAG 48:6	Positive	812.7	1.17 ± 0.04	87.8 ± 46.2	120 ± 34	0.20599444	106 ± 38	44.4 ± 16.4 **	0.00438595
TAG 48:7	Positive	810.7	1.15 ± 0.05	463 ± 228	638 ± 220	0.20549543	585 ± 227	218 ± 85 **	0.00407282
TAG 48:8	Positive	808.6	1.19 ± 0.09	409 ± 164	505 ± 155	0.32119178	511 ± 162	324 ± 63 *	0.02503009
TAG 50:0	Positive	852.8	1.22 ± 0.03	2796 ± 938	3902 ± 840	0.05703776	3228 ± 982	1361 ± 570 **	0.00240699
TAG 50:1	Positive	850.8	1.22 ± 0.03	11993 ± 3635	16824 ± 3496 *	0.04089984	14523 ± 4724	6676 ± 3081 **	0.00667753
TAG 50:2	Positive	848.8	1.24 ± 0.03	15469 ± 4569	17937 ± 4108	0.34842507	20387 ± 6247	10425 ± 5349 *	0.01411310
TAG 50:3	Positive	846.8	1.26 ± 0.03	6857 ± 2115	7755 ± 2209	0.48852259	10376 ± 3691	5513 ± 3207 *	0.03507881
TAG 50:4	Positive	844.7	1.29 ± 0.04	2173 ± 737	2486 ± 795	0.49535073	3445 ± 1371	1779 ± 1040 *	0.03910477
TAG 50:5	Positive	842.7	1.35 ± 0.09	533 ± 193	588 ± 189	0.63028039	864 ± 345	553 ± 265	0.11015620
TAG 50:6	Positive	840.7	1.25 ± 0.11	210 ± 79	248 ± 65	0.38749588	284 ± 96	206 ± 80	0.15846787
TAG 50:7	Positive	838.7	1.21 ± 0.03	688 ± 297	908 ± 256	0.19999501	792 ± 269	278 ± 95 **	0.00132625
TAG 50:8	Positive	836.7	1.22 ± 0.03	1617 ± 587	1995 ± 497	0.25711466	1979 ± 664	730 ± 276 **	0.00167835

TAG 50:9	Positive	834.7	1.22 ± 0.03	1750 ± 619	1800 ± 404	0.87317461	2209 ± 713	895 ± 353 **	0.00234792
TAG 52:0	Positive	880.8	1.22 ± 0.06	1856 ± 414	1694 ± 287	0.45106897	2045 ± 353	904 ± 212 ***	0.00004820
TAG 52:1	Positive	878.8	1.26 ± 0.03	5251 ± 1168	6686 ± 1253	0.06722400	6549 ± 1935	2617 ± 1027 **	0.00134348
TAG 52:2	Positive	876.8	1.27 ± 0.03	17633 ± 3692	21365 ± 4258	0.13585276	23749 ± 7446	10592 ± 4386 **	0.00391422
TAG 52:3	Positive	874.8	1.31 ± 0.08	25914 ± 5856	27323 ± 5818	0.68465582	36275 ± 11590	17911 ± 8159 **	0.00992771
TAG 52:4	Positive	872.8	1.38 ± 0.11	18246 ± 4955	17793 ± 4048	0.86573012	26282 ± 9137	13337 ± 6589 *	0.01832237
TAG 52:5	Positive	870.8	1.49 ± 0.13	5678 ± 1690	5500 ± 1317	0.84275059	8737 ± 3267	4890 ± 2499 *	0.04492959
TAG 52:6	Positive	868.7	1.53 ± 0.15	1253 ± 307	1226 ± 245	0.87364824	1810 ± 600	1570 ± 646	0.52025167
TAG 52:8	Positive	864.7	1.24 ± 0.03	1397 ± 380	1651 ± 304	0.23007336	1594 ± 450	661 ± 212 **	0.00100095
TAG 52:9	Positive	862.7	1.25 ± 0.03	2241 ± 656	2445 ± 473	0.54986044	2819 ± 901	1065 ± 384 **	0.00136902
TAG 52:10	Positive	860.7	1.28 ± 0.04	1844 ± 523	1839 ± 376	0.98707446	2487 ± 815	1018 ± 426 **	0.00288529
TAG 54:0	Positive	908.9	1.22 ± 0.10	567 ± 121	397 ± 77 *	0.01567108	602 ± 73	305 ± 54 ***	0.00001149
TAG 54:1	Positive	906.8	1.22 ± 0.03	1867 ± 328	1544 ± 251	0.08504040	2015 ± 316	672 ± 135 ***	0.00000238
TAG 54:2	Positive	904.8	1.27 ± 0.08	4334 ± 763	4119 ± 677	0.61801355	5137 ± 1163	1624 ± 440 ***	0.00004091
TAG 54:3	Positive	902.8	1.42 ± 0.13	7031 ± 1406	7583 ± 1426	0.51454007	9456 ± 2710	3159 ± 1187 ***	0.00039320
TAG 54:4	Positive	900.8	1.51 ± 0.13	8168 ± 2082	8541 ± 1852	0.74970338	12015 ± 4041	4713 ± 2129 **	0.00288940
TAG 54:5	Positive	898.8	1.56 ± 0.11	6426 ± 1945	6191 ± 1408	0.81585427	9889 ± 3473	5577 ± 2669 *	0.03657973
TAG 54:6	Positive	896.8	1.62 ± 0.03	3682 ± 1335	3188 ± 744	0.44646718	5810 ± 2101	4589 ± 1761	0.30091075
TAG 54:7	Positive	894.8	1.66 ± 0.04	1498 ± 523	1221 ± 261	0.27299647	2228 ± 717	3133 ± 894	0.08210057
TAG 54:8	Positive	892.7	1.39 ± 0.22	775 ± 181	731 ± 118	0.63081156	994 ± 270	973 ± 248	0.89101680
TAG 54:9	Positive	890.7	1.29 ± 0.04	1156 ± 179	1194 ± 164	0.70795365	1370 ± 333	508 ± 108 ***	0.00012762
TAG 54:10	Positive	888.7	1.34 ± 0.09	1418 ± 241	1393 ± 205	0.84592540	1780 ± 466	691 ± 220 ***	0.00041071

TAG 54:11	Positive	886.7	1.44 ± 0.13	1022 ± 214	947 ± 154	0.50266934	1341 ± 384	600 ± 203 **	0.00188092
TAG 54:12	Positive	884.7	1.53 ± 0.13	489 ± 104	449 ± 74	0.46696724	664 ± 196	471 ± 164	0.09476384
TAG 56:1	Positive	934.9	1.24 ± 0.03	226 ± 41	160 ± 36 *	0.01464455	254 ± 38	116 ± 22 ***	0.00001734
TAG 56:2	Positive	932.9	1.25 ± 0.03	554 ± 112	366 ± 84 **	0.00816609	628 ± 98	208 ± 41 ***	0.00000219
TAG 56:3	Positive	930.8	1.28 ± 0.08	982 ± 218	640 ± 142 **	0.00929751	1091 ± 189	429 ± 93 ***	0.00001658
TAG 56:4	Positive	928.8	1.35 ± 0.13	1120 ± 243	758 ± 142 *	0.01037069	1275 ± 226	517 ± 109 ***	0.00002323
TAG 56:5	Positive	926.8	1.57 ± 0.13	851 ± 158	711 ± 113	0.10605482	1063 ± 244	1102 ± 346	0.82792026
TAG 56:6	Positive	924.8	1.65 ± 0.04	674 ± 137	628 ± 97	0.51777724	935 ± 270	2671 ± 1184 *	0.00570745
TAG 56:7	Positive	922.8	1.68 ± 0.04	478 ± 98	467 ± 64	0.82560489	682 ± 174	3046 ± 1211 **	0.00079891
TAG 56:8	Positive	920.8	1.46 ± 0.27	419 ± 80	342 ± 49	0.07169493	541 ± 97	1848 ± 437 ***	0.00003083
TAG 56:9	Positive	918.8	1.43 ± 0.33	433 ± 62	351 ± 64 *	0.04904593	541 ± 91	1387 ± 217 ***	0.00000513
TAG 56:10	Positive	916.7	1.51 ± 0.39	331 ± 50	286 ± 42	0.11680018	405 ± 88	1280 ± 155 ***	0.00000028
TAG 56:11	Positive	914.7	1.49 ± 0.16	275 ± 46	246 ± 34	0.24838127	351 ± 82	167 ± 39 ***	0.00056849
TAG 56:12	Positive	912.7	1.56 ± 0.12	201 ± 40	182 ± 29	0.37007845	266 ± 64	245 ± 47	0.52979636
TAG 56:13	Positive	910.7	1.32 ± 0.20	202 ± 34	174 ± 28	0.14240388	251 ± 49	265 ± 69	0.68238490
TAG 58:2	Positive	960.9	1.52 ± 0.12	138 ± 26	94.7 ± 21.7 *	0.01098611	191 ± 44	107 ± 32 **	0.00315013
TAG 58:3	Positive	958.9	1.57 ± 0.14	78.3 ± 14.8	56.3 ± 10.9 *	0.01517915	104 ± 24	63.6 ± 9.3 **	0.00325850
TAG 58:4	Positive	956.9	1.62 ± 0.09	63.8 ± 12.5	47.7 ± 7.6 *	0.02229952	87.2 ± 16.3	48.7 ± 11.0 ***	0.00073515
TAG 58:5	Positive	954.8	1.62 ± 0.15	87.4 ± 16.2	71.8 ± 10.5	0.07512194	110 ± 24	116 ± 24	0.66771445
TAG 58:6	Positive	952.8	1.49 ± 0.23	134 ± 19	106 ± 15 *	0.02140328	180 ± 30	285 ± 65 **	0.00507973
TAG 58:7	Positive	950.8	1.20 ± 0.18	261 ± 44	192 ± 28 **	0.00847024	429 ± 81	558 ± 96 *	0.02996315
TAG 58:8	Positive	948.8	1.52 ± 0.32	127 ± 21	102 ± 15 *	0.03990968	175 ± 29	322 ± 107 *	0.00855050

TAG 58:9	Positive	946.8	1.57 ± 0.38	122 ± 20	94.2 ± 11.5 *	0.01500399	160 ± 29	429 ± 111 **	0.00018699
TAG 58:10	Positive	944.8	1.65 ± 0.42	94.7 ± 15.9	78.1 ± 10.9	0.06054119	122 ± 16	854 ± 118 ***	0.00000003
TAG 58:11	Positive	942.8	1.62 ± 0.44	86.5 ± 12.0	79.4 ± 12.7	0.34473941	111 ± 19	1355 ± 187 ***	0.00000002
TAG 58:12	Positive	940.7	1.50 ± 0.48	180 ± 41	183 ± 36	0.88864150	245 ± 61	1504 ± 157 ***	0.00000001
TAG 58:13	Positive	938.7	1.41 ± 0.41	300 ± 63	277 ± 61	0.52466988	420 ± 100	367 ± 88	0.35668502
TAG 58:14	Positive	936.7	1.29 ± 0.06	320 ± 65	270 ± 55	0.17905152	439 ± 93	313 ± 111	0.05874272
TAG 60:3	Positive	986.9	1.65 ± 0.04	119 ± 43	87.4 ± 26.0	0.15460406	184 ± 44	146 ± 38	0.13590073
TAG 60:4	Positive	984.9	1.68 ± 0.06	49.5 ± 13.1	35.1 ± 9.0	0.05068809	69.9 ± 17.1	68.5 ± 20.5	0.90421247
TAG 60:5	Positive	982.9	1.67 ± 0.16	29.1 ± 7.8	22.1 ± 4.5	0.08270878	35.8 ± 7.6	28.4 ± 5.2	0.07547040
TAG 60:6	Positive	980.9	1.42 ± 0.16	30.8 ± 3.9	22.1 ± 4.4 **	0.00491508	42.9 ± 8.6	29.0 ± 5.1 **	0.00672795
TAG 60:7	Positive	978.8	1.22 ± 0.04	156 ± 29	104 ± 14 **	0.00279711	241 ± 41	151 ± 15 ***	0.00049772
TAG 60:8	Positive	976.8	1.48 ± 0.11	81.8 ± 16.1	65.5 ± 9.1	0.05616898	107 ± 17	75.9 ± 18.9 *	0.01367412
TAG 60:9	Positive	974.8	1.55 ± 0.12	59.4 ± 8.6	48.0 ± 5.0 *	0.01890040	77.9 ± 12.1	90.8 ± 12.5	0.09768329
TAG 60:10	Positive	972.8	1.66 ± 0.26	43.5 ± 6.7	34.2 ± 4.9 *	0.02124692	55.6 ± 11.1	148 ± 12 ***	0.00000009
TAG 60:11	Positive	970.8	1.42 ± 0.20	34.7 ± 4.8	31.0 ± 4.9	0.21780308	48.5 ± 10.3	36.1 ± 6.1 *	0.03015715
TAG 60:12	Positive	968.8	1.29 ± 0.06	127 ± 20	123 ± 21	0.71800837	175 ± 37	80.5 ± 24.0 ***	0.00036886
TAG 60:13	Positive	966.8	1.33 ± 0.08	504 ± 89	426 ± 96	0.17234821	676 ± 132	315 ± 120 ***	0.00058472
TAG 60:14	Positive	964.7	1.37 ± 0.08	1590 ± 278	1315 ± 277	0.11655080	2043 ± 414	1112 ± 413 **	0.00295290
TAG 60:15	Positive	962.7	1.44 ± 0.11	1520 ± 299	1266 ± 262	0.14844625	2013 ± 419	1160 ± 411 **	0.00517557
TAG 62:4	Positive	1012.9	1.72 ± 0.06	30.3 ± 6.0	20.9 ± 5.3 *	0.01637455	40.9 ± 9.2	196 ± 64 **	0.00015905
TAG 62:5	Positive	1010.9	1.76 ± 0.16	19.1 ± 3.1	15.2 ± 3.1	0.05301551	25.3 ± 5.2	97.0 ± 19.0 ***	0.00000444
TAG 62:6	Positive	1008.9	1.52 ± 0.35	14.2 ± 1.6	10.5 ± 2.8 *	0.02066313	19.6 ± 3.5	57.3 ± 11.1 ***	0.00001292

TAG 62:7	Positive	1006.9	1.25 ± 0.04	34.3 ± 7.1	21.1 ± 4.3 **	0.00288988	58.6 ± 10.6	55.5 ± 9.0	0.59845080
TAG 62:8	Positive	1004.9	1.47 ± 0.13	22.0 ± 4.5	16.1 ± 3.0 *	0.02561916	28.3 ± 4.8	24.0 ± 3.6	0.11110034
TAG 62:9	Positive	1002.8	1.58 ± 0.11	31.2 ± 5.2	27.3 ± 3.4	0.15239053	45.6 ± 10.1	55.2 ± 5.5	0.06815535
TAG 62:10	Positive	1000.8	1.63 ± 0.09	26.5 ± 4.5	21.3 ± 4.7	0.07793046	33.5 ± 8.2	50.2 ± 9.1 **	0.00738455
TAG 62:11	Positive	998.8	1.55 ± 0.21	20.8 ± 2.8	16.9 ± 3.3	0.05029285	24.9 ± 4.4	39.9 ± 7.5 **	0.00175951
TAG 62:12	Positive	996.8	1.40 ± 0.21	50.2 ± 8.5	40.3 ± 5.0 *	0.03398796	59.0 ± 10.3	38.9 ± 7.7 **	0.00333893
TAG 62:13	Positive	994.8	1.43 ± 0.12	177 ± 26	152 ± 22	0.09673189	222 ± 44	102 ± 22 ***	0.00014552
TAG 62:14	Positive	992.8	1.50 ± 0.12	481 ± 90	437 ± 80	0.39490576	633 ± 115	279 ± 75 ***	0.00009044
TAG 62:15	Positive	990.8	1.56 ± 0.10	739 ± 169	707 ± 152	0.73145243	1030 ± 219	541 ± 179 **	0.00173628
TAG 62:16	Positive	988.7	1.61 ± 0.06	1100 ± 297	1070 ± 243	0.85435126	1514 ± 370	984 ± 301 *	0.02167489
TAG 64:17	Positive	1014.8	1.68 ± 0.05	126 ± 19	112 ± 17	0.19587354	164 ± 32	648 ± 210 **	0.00023194
TAG total				197453 ± 48984	216130 ± 45266	0.50835227	269026 ± 80862	150014 ± 58800 *	0.01541178
FFA 14:0	Negative	227.2	3.97 ± 0.03	12.4 ± 3.9	10.4 ± 3.0	0.35459489	13.2 ± 3.3	12.7 ± 2.3	0.77196738
FFA 16:0	Negative	255.2	4.00 ± 0.03	221 ± 75	183 ± 34	0.28632454	204 ± 30	195 ± 27	0.59281497
FFA 16:1	Negative	253.2	4.05 ± 0.03	52.5 ± 35.2	38.0 ± 16.2	0.38360317	47.1 ± 21.0	45.6 ± 16.7	0.89248600
FFA 18:0	Negative	283.3	4.04 ± 0.03	142 ± 21	125 ± 15	0.15183219	134 ± 21	140 ± 11	0.54594403
FFA 18:1	Negative	281.2	4.07 ± 0.03	271 ± 124	232 ± 60	0.50127856	247 ± 64	229 ± 38	0.57198682
FFA 18:2	Negative	279.2	4.15 ± 0.03	257 ± 101	199 ± 71	0.27456164	219 ± 61	185 ± 34	0.25276592
FFA 18:3	Negative	277.2	4.23 ± 0.02	56.9 ± 30.5	43.6 ± 15.6	0.36502695	53.9 ± 24.2	44.9 ± 10.7	0.42262107
FFA 20:4	Negative	303.2	4.35 ± 0.01	13.1 ± 2.2	9.0 ± 1.9 **	0.00563612	9.5 ± 2.5	8.2 ± 2.0	0.35335809
FFA 20:5	Negative	301.2	4.40 ± 0.01	0.79 ± 0.32	0.45 ± 0.31	0.09660903	0.68 ± 0.33	27.7 ± 7.5 ***	0.00000502
FFA 22:5	Negative	329.2	4.36 ± 0.01	3.1 ± 0.8	1.8 ± 0.7 *	0.01234242	2.4 ± 0.5	13.6 ± 2.3 ***	0.00000044

FFA total	1030 ± 388	843 ± 208	0.32231564	931 ± 216	902 ± 128	0.78010851

Values are mean ± standard deviation. Statistical significance was determined using Paired *t*–test ($^{*}P < 0.05$, $^{**}P < 0.01$, $^{***}P < 0.001$).