Supplementary Materials

Comprehensive Profiling of Platycodonis Radix in Different Growing Regions Using Liquid Chromatography Coupled with Mass Spectrometry: from Metabolome and Lipidome Aspects

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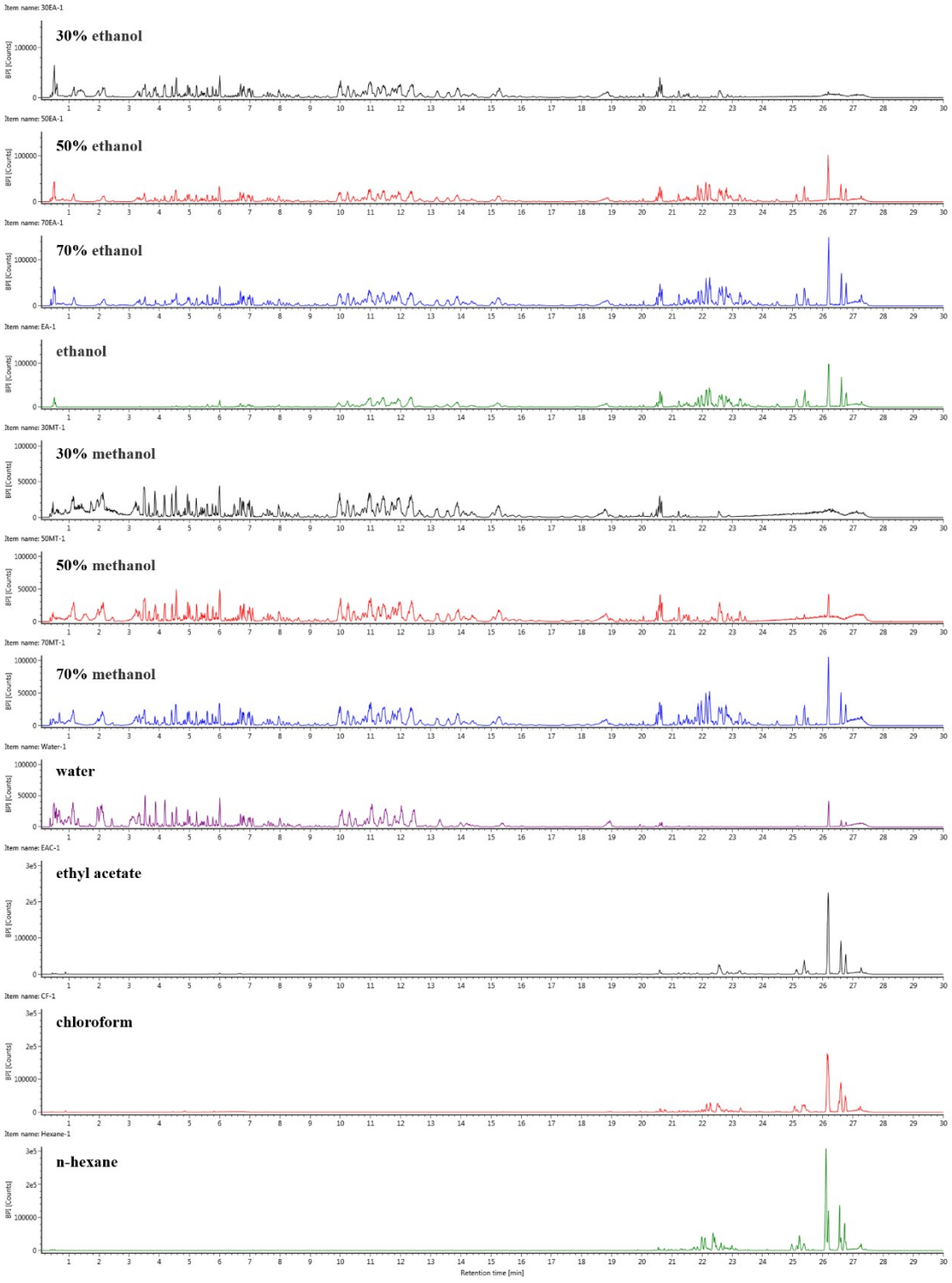

Figure S1. Representative chromatograms of different solvent extractions for metabolome sample.

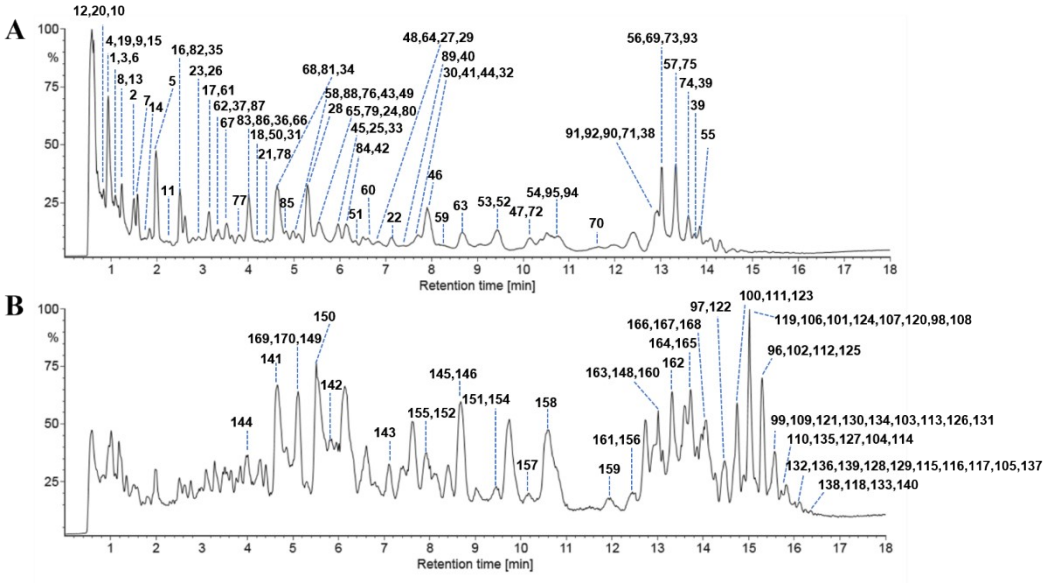

Figure S2. Representative chromatograms of lipid profiling via UPLC/IM-QTOF-HDMS^{E} analysis in negative (A) and positive (B)modes

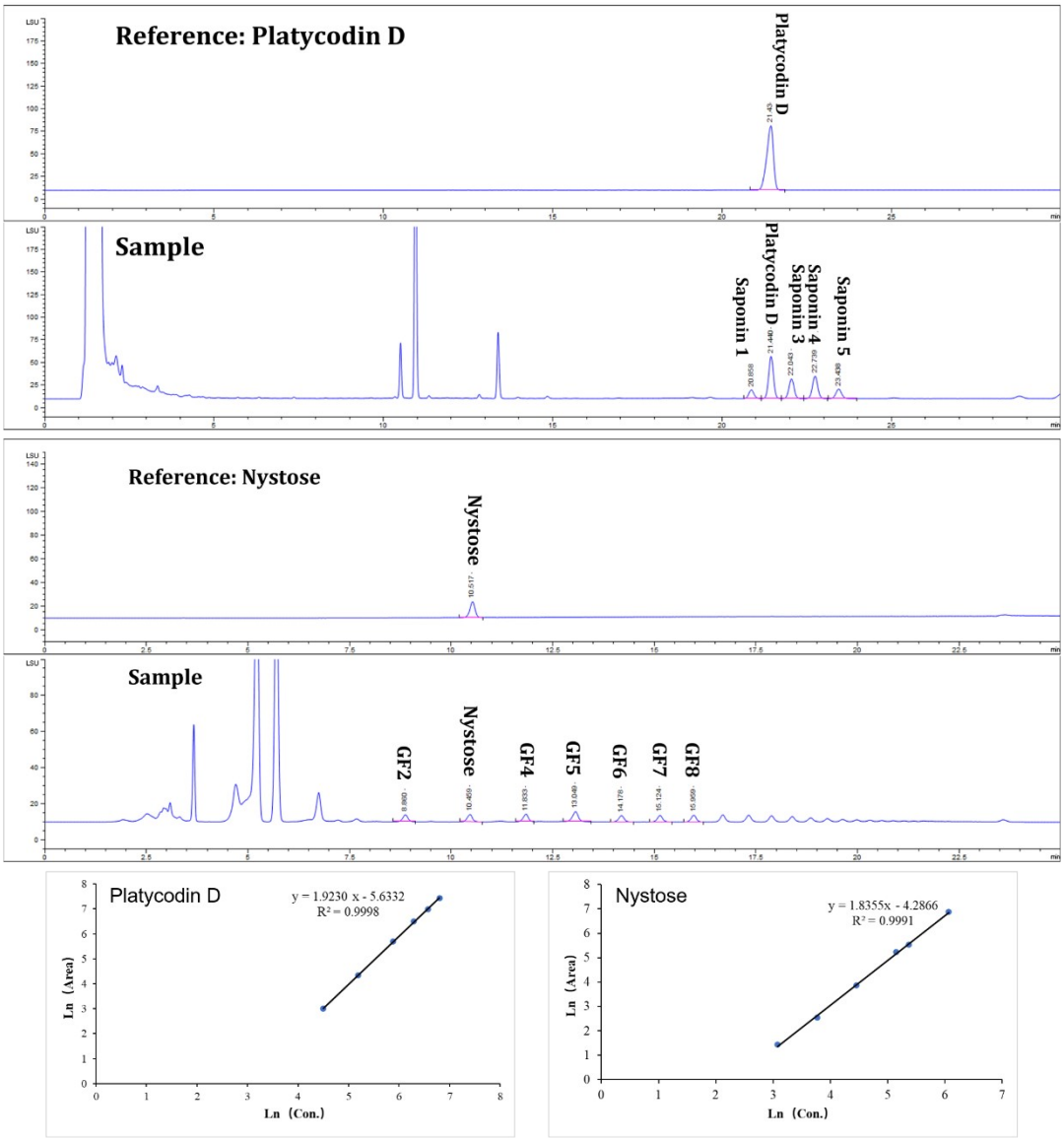

Figure S3. Representative chromatograms and linear calibration curves for assays on total saponins and oligosaccharides.

21 **Table S1 Detailed information of the samples**

NO.	Sample location	Growth year	Date for handpicking	Local weather
AH1 AH2 AH3 AH4	Lixing, Taihe county	2-3 years	2020.10.23	Sunny
AH5 AH6 AH7 AH8	Lixing, Taihe county	2-3 years	2020.10.24	Cloudy with breeze
AH9 AH10 AH11 AH12	Shuangmaio, Taihe county	2-3 years	2020.10.25	Cloudy with breeze
NM1 NM2 NM3 NM4 NM5 NM6 NM7 NM8 NM9 NM10 NM11 NM12	Harqin banner, Chifeng city	2-3 years	2020.09.16-2020.09.17	Cloudy to sunny

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23 **Table 2 Lipid molecular species identified in *Platycodonis Radix***

NO.	Lipid species	Adduct	Observed m/z	Mass error (ppm)	Formula	Retention time (min)
1	LPA 16:0	$[M-H]^-$	409.2361	0.13	C19H39O7P	1.12
2	LPA 18:0	$[M-H]^-$	437.2673	-0.1	C21H43O7P	1.56
3	LPA 18:1	$[M-H]^-$	435.2512	-1.21	C21H41O7P	1.17
4	LPA 18:2	$[M-H]^-$	433.2358	-0.64	C21H39O7P	0.96
5	LPA 18:2	$[M-H]^-$	433.2363	0.43	C21H39O7P	2.00
6	LPC 16:0/0:0	$[M+HCOO]^-$	540.3308	0.22	C24H50NO7P	1.19
7	LPC 18:0/0:0	$[M+HCOO]^-$	568.3622	0.33	C26H54NO7P	1.63
8	LPC 18:1/0:0	$[M+HCOO]^-$	566.3454	-1.76	C26H52NO7P	1.24
9	LPC 18:2/0:0	$[M+HCOO]^-$	564.3303	-0.64	C26H50NO7P	1.02
10	LPC 18:3	$[M+HCOO]^-$	562.3149	-0.29	C26H48NO7P	0.87
11	LPC 20:0/0:0	$[M+HCOO]^-$	596.3928	-0.87	C28H58NO7P	2.31
12	LPE 0:0/18:2	$[M-H]^-$	476.2786	0.41	C23H44NO7P	0.83
13	LPE 16:0/0:0	$[M-H]^-$	452.2785	0.6	C21H44NO7P	1.24
14	LPE 18:0/0:0	$[M-H]^-$	480.3105	1.98	C23H48NO7P	1.72
15	LPE 18:2/0:0	$[M-H]^-$	476.2785	-0.29	C23H44NO7P	1.06
16	LPE 20:0/0:0	$[M-H]^-$	508.3413	0.93	C25H52NO7P	2.46
17	LPE 22:0/0:0	$[M-H]^-$	536.3721	-0.15	C27H56NO7P	3.25
18	LPE 24:0/0:0	$[M-H]^-$	564.4044	1.66	C29H60NO7P	4.21
19	LPI 16:0	$[M-H]^-$	571.2881	-1.37	C25H49O12P	0.98
20	LPI 18:2	$[M-H]^-$	595.2883	-0.93	C27H49O12P	0.86
21	PA 14:0/18:2	$[M-H]^-$	643.4417	0.34	C35H65O8P	4.39
22	PA 16:0/18:1	$[M-H]^-$	673.4808	-0.93	C37H71O8P	7.14
23	PA 16:0/18:1(OH)	$[M-H]^-$	685.4449	0.12	C37H67O9P	2.95
24	PA 16:0/18:2	$[M-H]^-$	671.4661	0.53	C37H69O8P	5.59
25	PA 16:0/18:2	$[M-H]^-$	671.4653	-0.61	C37H69O8P	5.94
26	PA 16:0/18:2(OH)	$[M-H]^-$	687.4601	-0.82	C37H69O9P	3.01
27	PA 17:0/17:2	$[M-H]^-$	671.4655	-0.34	C37H69O8P	6.80
28	PA 17:1/15:0	$[M-H]^-$	645.4502	0.26	C35H67O8P	5.43
29	PA 17:1/18:1	$[M-H]^-$	685.4812	-0.3	C38H71O8P	6.80
30	PA 18:0/18:2	$[M-H]^-$	699.4966	-0.66	C39H73O8P	7.60
31	PA 18:2/15:1	$[M-H]^-$	655.4341	-0.51	C36H65O8P	4.36
32	PA 18:2/18:0	$[M-H]^-$	699.4966	-0.65	C39H73O8P	7.75
33	PA 18:2/18:1	$[M-H]^-$	697.4813	-0.18	C39H71O8P	5.94
34	PA 18:2/18:2	$[M-H]^-$	695.4655	-0.37	C39H69O8P	4.69
35	PA 18:2/18:2(OH)	$[M-H]^-$	711.4402	0.38	C39H69O9P	2.52
36	PA 18:2/18:3	$[M-H]^-$	693.4496	-0.47	C39H67O8P	4.02
37	PA 18:3/18:3	$[M-H]^-$	691.4347	0.34	C39H65O8P	3.42
38	PA 22:0/18:2	$[M-H]^-$	755.5591	-0.65	C43H81O8P	12.89
39	PA 24:0/18:2	$[M-H]^-$	783.5902	-0.9	C45H85O8P	13.71
40	PC 16:0/16:0	$[M+HCOO]^-$	778.5598	-0.76	C40H80NO8P	7.39
41	PC 16:0/18:1	$[M+HCOO]^-$	804.5753	-0.86	C42H82NO8P	7.62

42	PC 16:0/18:2	$[M+HCOO]^-$	802.5599	-0.56	C42H80NO8P	6.15
43	PC 16:0/18:3	$[M+HCOO]^-$	800.5448	0.11	C42H78NO8P	5.10
44	PC 17:0_18:2	$[M+HCOO]^-$	816.5746	-1.72	C43H82NO8P	7.70
45	PC 17:1_18:2	$[M+HCOO]^-$	814.5605	0.2	C43H80NO8P	5.91
46	PC 18:0/18:2	$[M+HCOO]^-$	830.5907	-1.17	C44H84NO8P	8.14
47	PC 18:0_18:1	$[M+HCOO]^-$	832.6057	-1.99	C44H86NO8P	10.07
48	PC 18:0_18:3	$[M+HCOO]^-$	828.5755	-0.67	C44H82NO8P	6.72
49	PC 18:2/18:2	$[M+HCOO]^-$	826.5676	-0.5	C44H80NO8P	5.12
50	PC 18:2/18:3	$[M+HCOO]^-$	824.5440	-0.85	C44H78NO8P	4.29
51	PC 18:2_18:1	$[M+HCOO]^-$	828.5766	-0.9	C44H82NO8P	6.30
52	PC 18:2_21:1	$[M+HCOO]^-$	870.6224	-0.68	C47H88NO8P	9.38
53	PC 19:0_18:2	$[M+HCOO]^-$	844.6060	-1.54	C45H86NO8P	9.33
54	PC 20:0/18:2	$[M+HCOO]^-$	858.6218	-1.31	C46H88NO8P	10.73
55	PC 20:0_18:1	$[M+HCOO]^-$	860.6385	-0.18	C46H90NO8P	13.84
56	PC 22:0_18:2	$[M+HCOO]^-$	886.6543	0.09	C48H92NO8P	12.99
57	PC 22:0_19:2	$[M+HCOO]^-$	900.6772	1.74	C49H94NO8P	13.28
58	PE 15:1/18:2	$[M-H]^-$	698.4839	-0.87	C38H70NO8P	4.98
59	PE 16:0/18:1	$[M-H]^-$	716.5227	-1.24	C39H76NO8P	8.25
60	PE 16:0/18:2	$[M-H]^-$	714.5075	-0.73	C39H74NO8P	6.64
61	PE 16:0/18:2(OH)	$[M-H]^-$	730.5014	-2	C39H74NO9P	3.27
62	PE 16:0/18:3(OH)	$[M-H]^-$	728.4861	0.34	C39H72NO9P	3.31
63	PE 18:0/18:2	$[M-H]^-$	742.5386	-0.89	C41H78NO8P	8.77
64	PE 18:1/18:2	$[M-H]^-$	740.5234	-0.39	C41H76NO8P	6.78
65	PE 18:1/18:3	$[M-H]^-$	738.5079	-0.1	C41H74NO8P	5.49
66	PE 18:2/16:0	$[M-H]^-$	714.5071	-1.1	C39H74NO8P	4.07
67	PE 18:2/18:2	$[M-H]^-$	738.5079	-1.47	C41H74NO8P	3.53
68	PE 18:3/18:2	$[M-H]^-$	736.4926	0.38	C41H72NO8P	4.57
69	PE 18:3/24:0	$[M-H]^-$	870.6261	3.61	C47H88NO8P	13.05
70	PE 20:0/18:2	$[M-H]^-$	770.5709	0.49	C43H82NO8P	11.59
71	PE 20:0/20:0	$[M-H]^-$	802.6324	-0.92	C45H90NO8P	12.86
72	PE 21:1_18:2	$[M-H]^-$	782.5703	-0.24	C44H82NO8P	10.11
73	PE 22:0/18:2	$[M-H]^-$	798.6007	-1.48	C45H86NO8P	13.15
74	PE 24:0/18:2	$[M-H]^-$	826.6326	-0.6	C47H90NO8P	13.67
75	PE 25:1/18:2	$[M-H]^-$	838.6320	-1.34	C48H89NO8P	13.38
76	PG 16:0/18:2	$[M-H]^-$	745.5019	-1.08	C40H75O10P	5.03
77	PG 18:2/18:2	$[M-H]^-$	769.5014	-1.52	C42H75O10P	3.82
78	PG 18:2/18:2	$[M-H]^-$	769.5025	-0.05	C42H75O10P	4.45
79	PI 16:0/16:0	$[M-H]^-$	809.5185	-0.08	C41H79O13P	5.55
80	PI 16:0/18:1	$[M-H]^-$	835.5343	0.35	C43H81O13P	5.75
81	PI 16:0/18:2	$[M-H]^-$	833.5183	-0.28	C43H79O13P	4.68
82	PI 16:0/18:2 (OH)	$[M-H]^-$	849.5119	-1.19	C43H80O14P	2.50
83	PI 16:0/18:3	$[M-H]^-$	831.5019	-1.23	C43H76O13P	3.98
84	PI 18:0/18:2	$[M-H]^-$	861.5494	-0.9	C45H83O13P	6.12
85	PI 18:0/18:3	$[M-H]^-$	859.5340	-0.78	C45H81O13P	4.83

86	PI 18:1/18:3	$[M-H]^-$	857.5175	-1.26	C45H79O13P	4.01
87	PI 18:3/18:2	$[M-H]^-$	855.5017	-1.41	C45H77O13P	3.43
88	PMeOH 15:0/17:2	$[M-H]^-$	657.4499	-0.25	C36H67O8P	5.01
89	PMeOH 18:0/18:2	$[M-H]^-$	713.5200	-0.78	C40H75O8P	7.38
90	PMeOH 21:0/18:2	$[M-H]^-$	755.5591	-1.1	C43H81O8P	12.85
91	PMeOH 22:0/18:2	$[M-H]^-$	769.5750	-0.33	C44H83O8P	12.73
92	PMeOH 23:1/18:2	$[M-H]^-$	781.5747	-0.76	C45H83O8P	12.82
93	PMeOH 24:1/18:2	$[M-H]^-$	795.5901	-0.16	C46H85O8P	13.15
94	PS 22:0/18:2	$[M-H]^-$	842.5911	-0.61	C46H86NO10P	10.99
95	PS 24:1/18:2	$[M-H]^-$	868.6067	-0.76	C48H88NO10P	10.87
96	TG 16:1/16:1/16:0	$[M+NH_4]^+$	820.7365	-2.86	C51H94O6	15.22
97	TG 16:0/16:0/18:3	$[M+H]^+$	829.7268	-1.37	C53H96O6	14.27
98	TG 14:0/18:2/17:1	$[M+NH_4]^+$	832.7368	-2.46	C52H94O6	15.19
99	TG 16:0/17:0/18:2	$[M+NH_4]^+$	834.7540	-0.64	C52H96O6	15.42
100	TG 16:1/18:2/16:2	$[M+NH_4]^+$	842.7228	-0.53	C53H92O6	14.69
101	TG 16:1/16:1/18:2	$[M+NH_4]^+$	844.7390	0.16	C53H94O6	14.95
102	TG 18:2/14:0/18:1	$[M+NH_4]^+$	846.7522	-2.68	C53H96O6	15.24
103	TG 16:0/18:2/16:0	$[M+NH_4]^+$	848.7686	-1.87	C53H98O6	15.56
104	TG 16:0/18:1/16:0	$[M+NH_4]^+$	850.7840	-2.19	C53H100O6	15.82
105	TG 16:0/18:0/16:0	$[M+NH_4]^+$	852.8003	-1.35	C53H102O6	16.11
106	TG 16:1/17:2/18:2	$[M+NH_4]^+$	856.7372	-1.99	C54H94O6	14.90
107	TG 16:1/17:1/18:2	$[M+NH_4]^+$	858.7522	-2.76	C54H96O6	15.15
108	TG 16:1/16:0/19:3	$[M+NH_4]^+$	858.7526	-2.46	C54H96O6	15.19
109	TG 16:0/17:1/18:2	$[M+NH_4]^+$	860.7689	-1.43	C54H98O6	15.44
110	TG 16:0/17:0/18:2	$[M+NH_4]^+$	862.7851	-0.8	C54H100O6	15.71
111	TG 18:2/16:1/18:3	$[M+NH_4]^+$	868.7365	-2.7	C55H94O6	14.70
112	TG 18:2/18:2/16:0	$[M+NH_4]^+$	872.7656	-2.93	C55H98O6	15.30
113	TG 18:1//18:2/16:0	$[M+NH_4]^+$	874.7845	-2.13	C55H100O6	15.56
114	TG 18:1/18:1/16:0	$[M+NH_4]^+$	876.7993	-2.49	C55H102O6	15.83
115	TG 16:0/16:0/20:1	$[M+NH_4]^+$	878.8157	-1.62	C55H104O6	16.10
116	TG 18:1/18:0/16:0	$[M+NH_4]^+$	878.8157	-1.62	C55H104O6	16.10
117	TG 18:0/18:0/16:1	$[M+NH_4]^+$	878.8157	-1.62	C55H104O6	16.10
118	TG 18:0/18:0/16:0	$[M+NH_4]^+$	880.8303	-2.8	C55H106O6	16.37
119	TG 18:2/15:1/20:3	$[M+NH_4]^+$	882.7527	-2.05	C56H96O6	14.88
120	TG 18:2/15:0/20:3	$[M+NH_4]^+$	884.7676	-2.96	C56H98O6	15.17
121	TG 18:1/15:0/20:3	$[M+NH_4]^+$	886.7838	-2.25	C56H100O6	15.45
122	TG 18:3/18:2/18:3	$[M+NH_4]^+$	892.7361	-3.09	C57H94O6	14.48
123	TG 18:2/18:2/18:3	$[M+NH_4]^+$	894.7528	-1.96	C57H96O6	14.75
124	TG 18:2/18:2/18:2	$[M+NH_4]^+$	896.7682	-2.16	C57H98O6	15.03
125	TG 20:3/16:1/18:1	$[M+NH_4]^+$	898.7829	-3.23	C57H100O6	15.30
126	TG 18:1/18:1/18:2	$[M+NH_4]^+$	900.7998	-1.18	C57H102O6	15.60
127	TG 18:1/18:1/18:1	$[M+NH_4]^+$	902.8150	-2.3	C57H104O6	15.81

128	TG 18:1/18:1/18:0	$[M+NH_4]^+$	904.8310	-1.96	C57H106O6	16.09
129	TG 18:0/18:0/18:2	$[M+NH_4]^+$	904.8310	-1.96	C57H106O6	16.09
130	TG 18:2/19:1/18:2	$[M+NH_4]^+$	910.7999	-1.73	C58H102O6	15.45
131	TG 18:2/20:1/18:2	$[M+NH_4]^+$	926.8157	-1.56	C59H104O6	15.60
132	TG 20:0/18:2/18:2	$[M+NH_4]^+$	928.8305	-2.48	C59H106O6	15.88
133	TG 22:0/16:0/18:2	$[M+NH_4]^+$	932.8598	-4.53	C59H110O6	16.37
134	TG 21:1/18:2/18:3	$[M+NH_4]^+$	938.8150	-2.28	C60H104O6	15.49
135	TG 18:2/21:1/18:2	$[M+NH_4]^+$	940.8312	-1.62	C60H106O6	15.73
136	TG 22:1/18:2/18:2	$[M+NH_4]^+$	954.8461	-2.44	C61H108O6	15.90
137	TG 22:0/18:2/18:2	$[M+NH_4]^+$	956.8625	-1.61	C61H110O6	16.15
138	TG 18:2/22:0/18:1	$[M+NH_4]^+$	958.8768	-3.07	C61H112O6	16.35
139	TG 18:2/21:1/20:2	$[M+NH_4]^+$	968.8612	-2.14	C62H110O6	15.99
140	TG 18:2/18:2/24:0	$[M+NH_4]^+$	984.8915	-3.93	C63H114O6	16.40
141	DG 18:3/16:0	$[M+H]^+$	591.4970	-2.23	C37H66O5	4.76
142	DG 18:3/18:3	$[M+H]^+$	613.4819	-1.23	C39H64O5	5.86
143	DG 18:3/18:2	$[M+H]^+$	615.4971	-1.94	C39H66O5	7.11
144	DG 18:3/18:2	$[M+H]^+$	615.4973	-1.58	C39H66O5	4.02
145	DG 18:2/18:2	$[M+H]^+$	617.5127	-1.98	C39H68O5	8.68
146	DG 18:1/18:3	$[M+H]^+$	617.5127	-1.98	C39H68O5	8.68
147	DG 18:2/18:1	$[M+H]^+$	619.5289	-1.18	C39H70O5	10.83
148	DG 18:2/18:0	$[M+H]^+$	621.5430	-3.57	C39H72O5	12.97
149	Cer d18:2/n16:1	$[M+H]^+$	534.4872	-1.69	C34H63NO3	4.98
150	Cer d18:1/h16:0	$[M+H]^+$	554.5130	-2.25	C34H67NO4	5.46
151	Cer t18:1/h20:0	$[M+H]^+$	626.5718	-0.04	C38H75NO5	9.35
152	Cer t18:1/n22:2	$[M+H]^+$	634.5759	-0.95	C40H75NO4	7.93
153	Cer t18:1/h21:0	$[M+H]^+$	640.5864	-1.6	C39H77NO5	10.80
154	Cer t18:1/h22:1	$[M+H]^+$	652.5863	2.2	C40H77NO5	9.45
155	Cer t18:1/h22:1	$[M+H]^+$	652.5868	2.3	C40H77NO5	7.92
156	Cer t18:1/h22:0	$[M+H]^+$	654.6020	-1.61	C40H79NO5	12.45
157	Cer t18:1/h22:0	$[M+H]^+$	654.6020	-1.69	C40H79NO5	10.17
158	Cer t18:1/h22:0	$[M+H]^+$	654.6021	-1.51	C40H79NO5	10.46
159	Cer t18:1/h23:0	$[M+H]^+$	668.6176	-1.7	C41H81NO5	11.99
160	Cer t18:1/h23:0	$[M+H]^+$	668.6179	-1.25	C41H81NO5	13.04
161	Cer t18:1/h24:1	$[M+H]^+$	680.6177	-1.06	C42H81NO5	12.39
162	Cer t18:1/h24:0	$[M+H]^+$	682.6334	-1.44	C42H83NO5	13.34
163	Cer t18:1/h24:0	$[M+H]^+$	682.6336	-1.12	C42H83NO5	12.91
164	Cer t18:0/h24:0	$[M+H]^+$	684.6491	-1.46	C42H85NO5	13.60
165	Cer t18:1/h25:0	$[M+H]^+$	696.6492	-1.2	C43H85NO5	13.60
166	Cer t18:1/h26:0	$[M+H]^+$	710.6652	-0.96	C44H87NO5	13.86
167	Cer t18:0/h26:0	$[M+H]^+$	712.6804	-1.39	C44H89NO5	14.10
168	Cer t18:1/h27:0	$[M+H]^+$	724.6802	-1.63	C45H89NO5	14.10
169	HexCer d18:3/n16:0	$[M+H]^+$	696.5394	1.24	C40H73NO8	4.84
170	HexCer d18:3/n16:0	$[M+H]^+$	696.5399	1.95	C40H73NO8	4.97

LPA: Lysosphosphatidic acid; LPC: Lysophosphatidylcholine; LPE: Lysophosphatidylethanolamine; LPI: Lysophosphatidylinositol; PA: Phosphatidic acid; PC: Phosphatidylcholine; PE: Phosphatidylethanolamine; PG: Phosphatidylglycerol; PI: Phosphatidylinositol; PMeOH: Phosphatidylmethanol; PS: Phosphatidylinositol; TG: Triacylglycerol; DG: Diacylglycerol; Cer: Ceramide; HexCer: Hexosylceramide.