

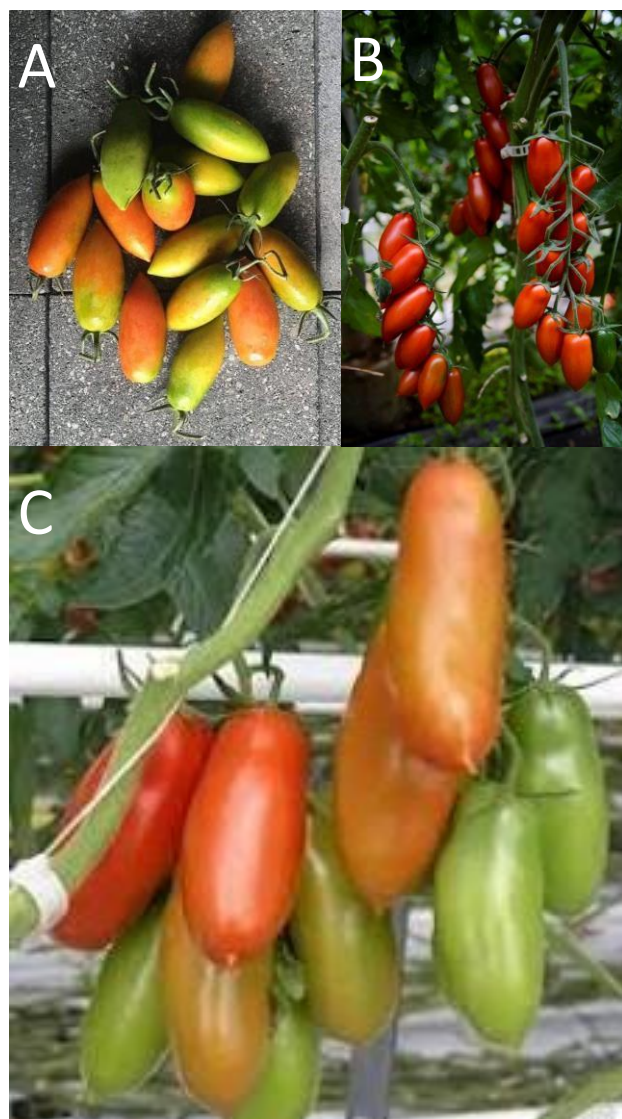


Figure 1. TF and SM tomato fruits from Fondi area (Lazio region): **A)** TF at pink ripening stage; **B)** TF at red ripening stage; **C)** SM at both pink and red ripening stages.

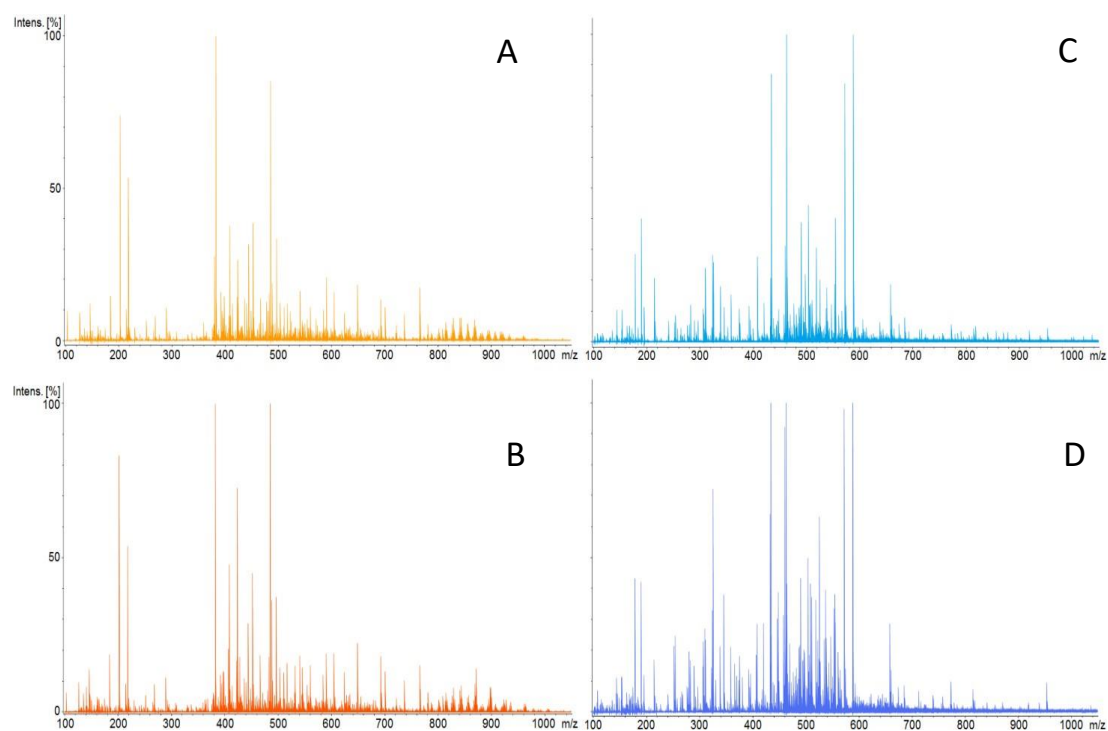


Figure 2. Raw ESI(+) FT-ICR MS spectra of hydroalcoholic extracts of **A)** SM_p (yellow profile) and **B)** SM_r (orange profile); raw ESI(-) FT-ICR MS spectra of hydroalcoholic extracts of **C)** SM_p (light blue profile) and **D)** SM_r (blue profile).

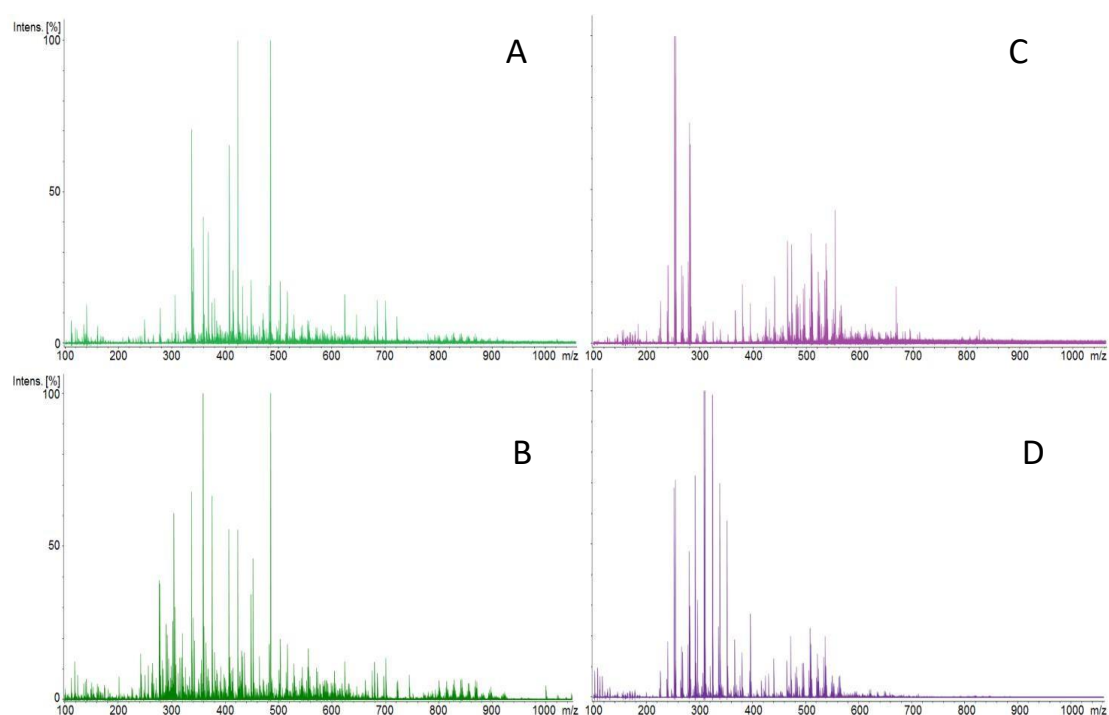


Figure 3. Raw ESI(+) FT-ICR MS spectra of organic extracts of **A)** SM_p (green profile), **B)** SM_r (dark green profile); raw ESI(-) FT-ICR MS spectra of organic extracts of **C)** SM_p (pink profile) and **D)** SM_r (violet profile).

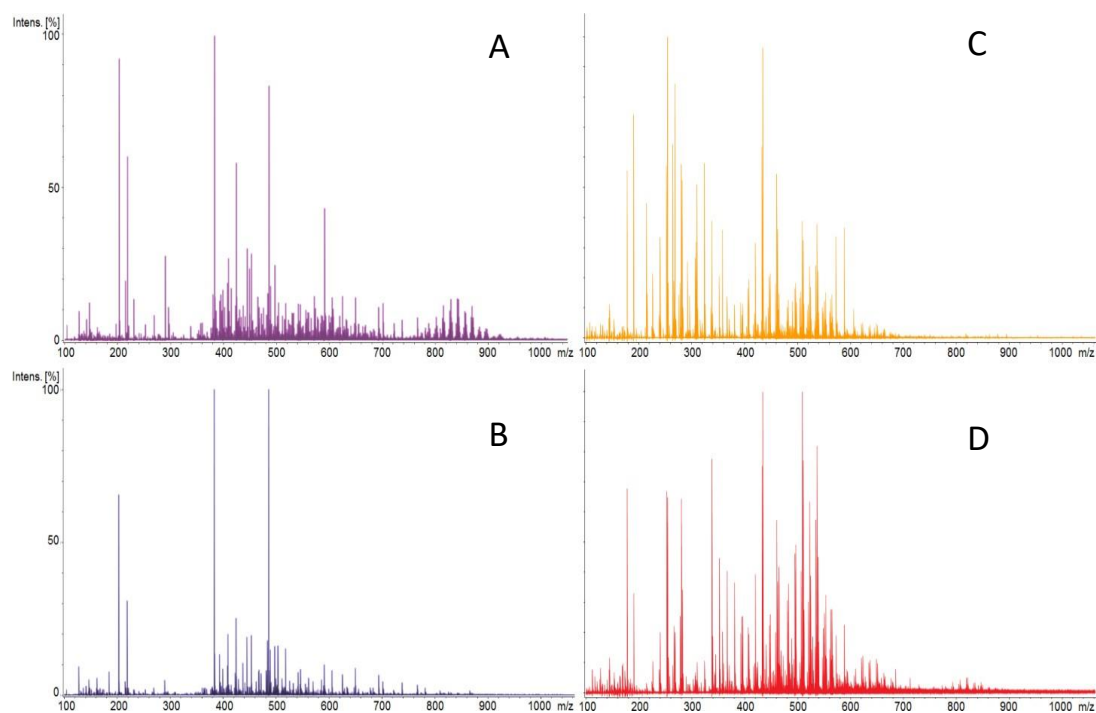


Figure 4. Raw ESI(+) FT-ICR MS spectra of hydroalcoholic extracts **A)** TFP (violet profile), **B)** TFR (blue profile); raw ESI(-) FT-ICR MS spectra of hydroalcoholic extracts **C)** TFP (orange profile) and **D)** TFR (red profile).

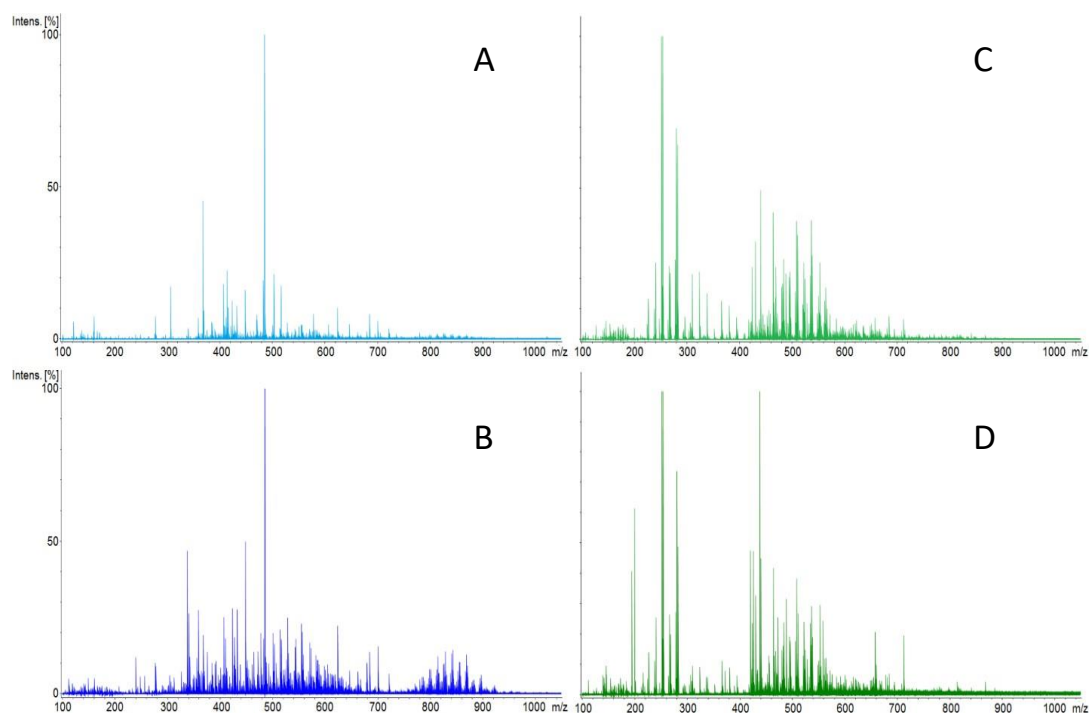


Figure 5. Raw ESI(+) FT-ICR MS spectra of organic extracts **A)** TFP (light blue profile) and **B)** TFR (blue profile); raw ESI(-) FT-ICR MS spectra of **C)** TFP (light green profile) and **D)** TFR (dark green profile).

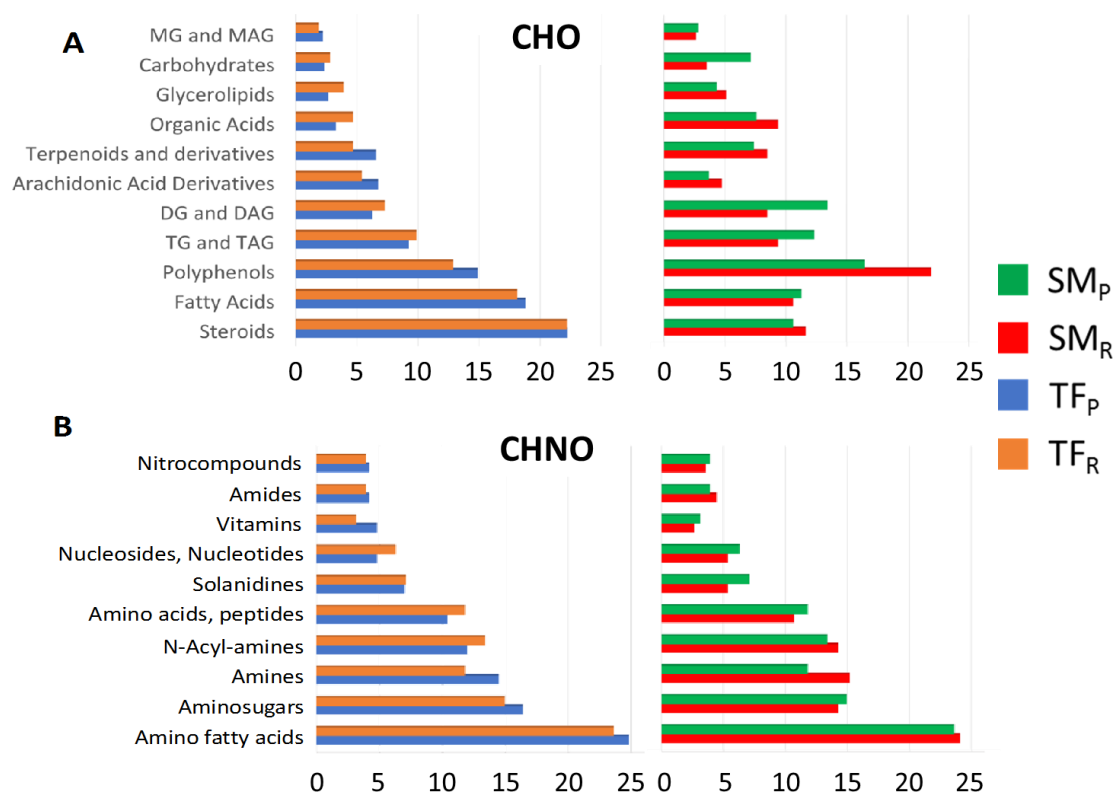


Figure 6. Comparison between TFP and TFR and SMP and SMR of number of possible A) CHO and B) CHNO metabolites assigned in the various metabolic pathways of *Solanum lycopersicum* var. Torpedino di Fondi and San Marzano.

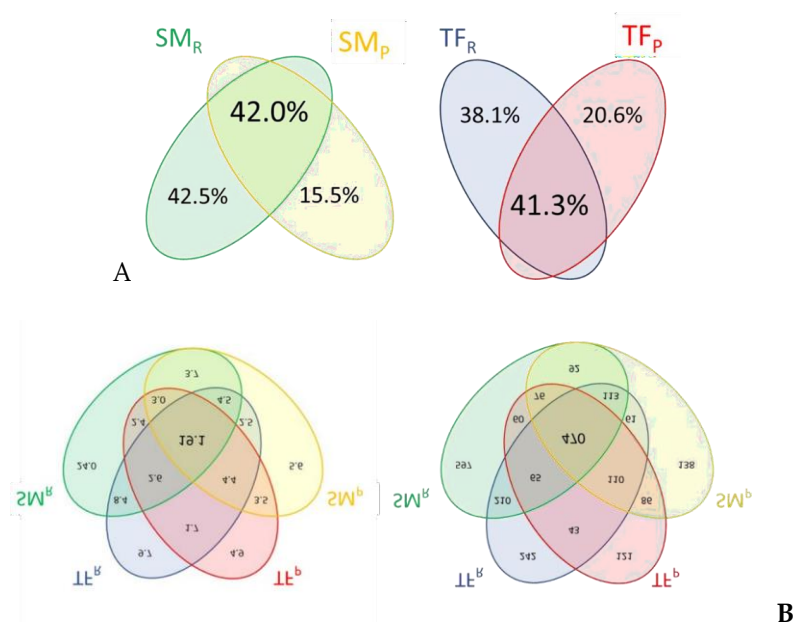


Figure 7. Common and uncommon features (in %) in the combined pattern of hydroalcoholic and organic extracts of A) SMR and SMP and TFR and TFP, shown in a two-way Venn diagram, and B) SMR and SMP and TFR and TFP, shown in a four-way Venn diagram. The results are reported as relative percentages (A and left B) or absolute numbers (right B) of total hits.

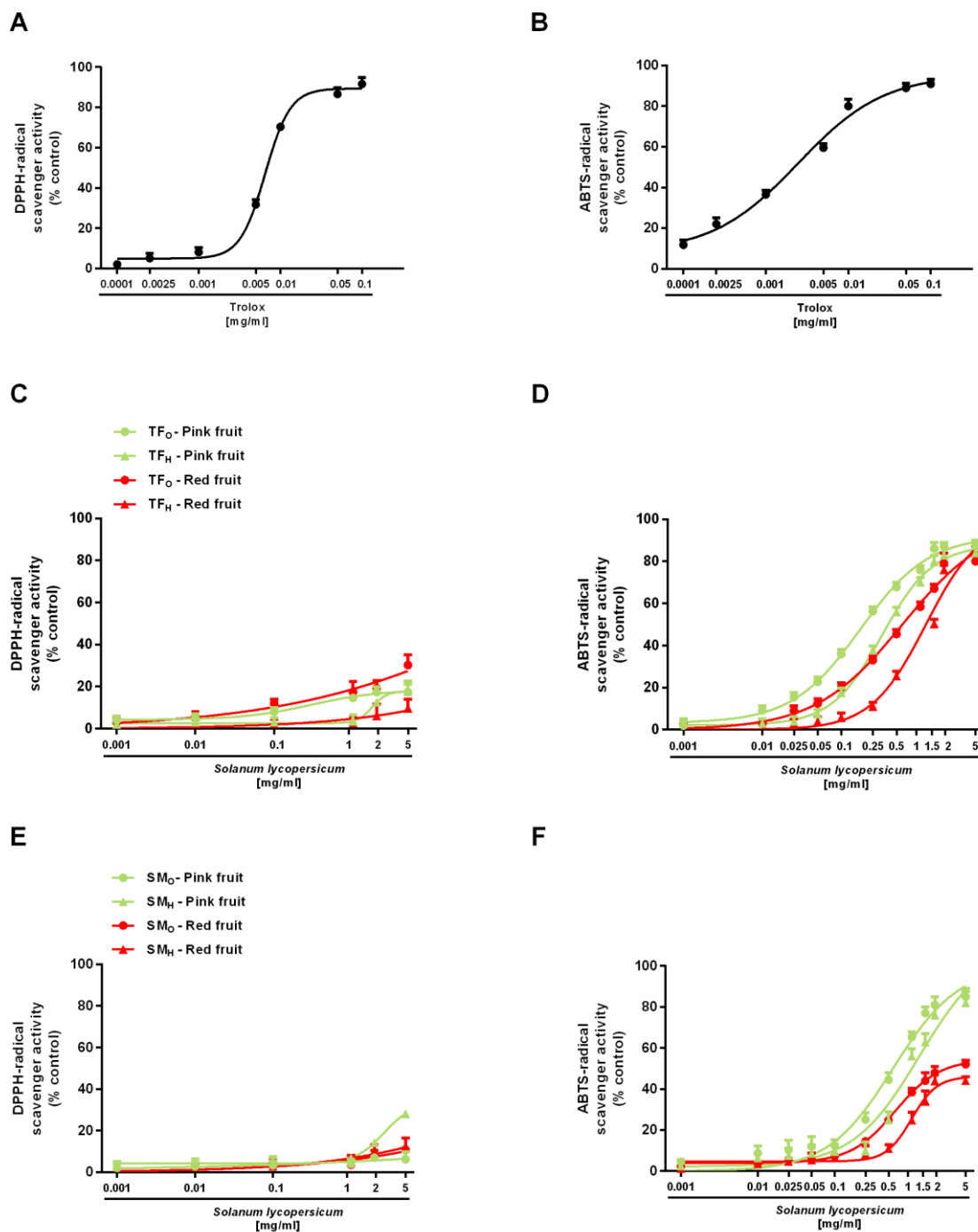


Figure 8. Concentration-response curves of the scavenging activity of TF and SM extracts and the positive control trolox towards DPPH and ABTS radicals. **A-B** Scavenging activity of trolox. **C-D** Scavenging activity of TF_P and TF_R hydroalcoholic (H) and organic (O) extracts. **E-F** Scavenging activity of SM_P and SM_R hydroalcoholic (H) and organic (O) extracts. Each value represents the mean $\pm$ SE of at least two experiments and at least three replicates for each experiment (n = 6).

Table 1. Amount of peel, pulp, seeds and juice in both pink and red *Solanum lycopersicum* var. TF and SM fruits.^a

Sample	Peel	Pulp	Seeds		Juice
	mg/g fruit	mg/g fruit	mg/g fruit	Number/ g fruit	g/g fruit
	% fruit w/w	% fruit w/w	(mg/seed) % fruit w/w		(pH) % fruit w/w
TF _P	15.1 ± 0.2	630.0 ± 10.1	17.0 ± 0.6	3.1 ± 0.2	0.34 ± 0.02
			(5.6 ± 0.6)		(4.1 ± 0.1)
	1.5	62.6	1.7		34.3
TF _R	37.9 ± 0.2 ^{§§}	820.0 ± 20.3 ^{§§}	15.7 ± 0.8 [§]	3.6 ± 0.1 [§]	0.13 ± 0.01 ^{§§}
			(4.4 ± 0.1) [§]		(4.0 ± 0.1)
	3.7	81.7	1.6		13.0
SM _P	8.2 ± 0.6 ^{**}	161.0 ± 11.0 ^{**}	3.9 ± 0.01 ^{**}	0.6 ± 0.02 ^{**}	0.83 ± 0.02 ^{**}
			(7.5 ± 0.5)		(4.2 ± 0.1)
	0.4	16.1	0.5		83.0
SM _R	4.0 ± 0.4 ^{§§**}	178.0 ± 10.4 ^{§§**}	4.4 ± 0.02 ^{**}	0.7 ± 0.02 ^{§**}	0.83 ± 0.03 ^{**}
			(5.9 ± 0.01) [§]		(4.0 ± 0.1)
	0.7	15.7	0.4		83.1

^a) ^{**}p < 0.01 denotes a statistically significant difference respect to TF tomato at the same stage of ripening (ANOVA followed by Bonferroni Multiple Comparison Post Test). [§] p < 0.05 and ^{§§} p < 0.01 denote a statistically significant difference respect to unripe stage within the same variety (ANOVA followed by Bonferroni Multiple Comparison Post Test).

Table S2: Comprehensive list of metabolites detected in hydroalcoholic and organic fractions of pink and red San Marzano (SM) and Torpedino di Fondi (TF) extracts using ESI(+) FT-ICR MS.

ESI(+) FT-ICR MS														
No.	Plausible Compound ^a	Molecular formula (M)	Ion	Theor m/z ^b	Exp. m/z ^c	Δ ppm _d	SM _{RH} ^e	SM _{RO} ^e	SM _{PH} ^e	SM _{PO} ^e	TF _{RH} ^e	TF _{RO} ^e	TF _{PH} ^e	TF _{PO} ^e
1	Gamma-Aminobutyric acid	C ₄ H ₉ NO ₂	[M+H] ⁺	104.07060	104.07065	-0.41	7.0E+07		1.1E+08		3.6E+07		3.8E+07	
2	L-Serine	C ₃ H ₇ NO ₃	[M+H] ⁺	106.04987	106.04992	-0.46	1.7E+06	7.9E+06	2.6E+06	1.7E+06		6.2E+06	2.4E+06	1.2E+06
3	Aminobutyraldehyde	C ₄ H ₉ NO	[M+Na] ⁺	110.05763	110.05768	-0.41		1.8E+06		8.8E+05		1.5E+06		1.3E+06
4	Lactic acid	C ₃ H ₆ O ₃	[M+Na] ⁺	113.02091	113.02097	-0.47		1.6E+07	9.6E+05	3.8E+06		8.9E+06	2.1E+06	2.6E+06
5	Butanediol	C ₄ H ₁₀ O ₂	[M+Na] ⁺	113.05730	113.05735	-0.44		4.1E+06		1.2E+06		1.6E+06		1.7E+06
6	Glycerol	C ₃ H ₈ O ₃	[M+Na] ⁺	115.03656	115.03662	-0.44		2.9E+06		1.1E+06		2.2E+06		2.7E+06
7	Amino-piperidone	C ₅ H ₁₀ N ₂ O	[M+H] ⁺	115.08659	115.08664	-0.44		2.6E+06					1.4E+06	
8	Proline	C ₅ H ₉ NO ₂	[M+H] ⁺	116.07060	116.07065	-0.40	1.0E+06	3.3E+06	1.4E+06			1.5E+06	1.7E+06	
9	L-Valine	C ₅ H ₁₁ NO ₂	[M+H] ⁺	118.08626	118.08631	-0.45	1.4E+06	4.8E+06	2.0E+06			1.9E+06	1.2E+06	
10	L-Threonine	C ₄ H ₉ NO ₃	[M+H] ⁺	120.06552	120.06558	-0.48	1.9E+06	3.4E+06	2.3E+06		1.4E+06	1.8E+06	1.2E+06	
11	Tromethamine	C ₄ H ₁₁ NO ₃	[M+H] ⁺	122.08117	122.08123	-0.49							1.1E+06	
12	Diethylene glycol	C ₄ H ₁₀ O ₃	[M+Na] ⁺	129.05221	129.05225	-0.27								1.0E+06
13	Pyroglutamic acid	C ₅ H ₇ NO ₃	[M+H] ⁺	130.04987	130.04993	-0.45	3.1E+06	4.0E+06	2.4E+06		2.0E+06	1.6E+06	1.6E+06	
14	Octylamine	C ₈ H ₁₉ N	[M+H] ⁺	130.15903	130.15909	-0.49								1.9E+06
15	Leucine	C ₆ H ₁₃ NO ₂	[M+H] ⁺	132.10191	132.10195	-0.37	2.7E+06	1.6E+07	4.3E+06		1.3E+06	3.4E+06	2.1E+06	1.1E+06
16	Hydroxy-hexanoic acid	C ₆ H ₁₂ O ₃	[M+H] ⁺	133.08592	133.08593	-0.07	1.0E+06							
17	Ornithine	C ₅ H ₁₂ N ₂ O ₂	[M+H] ⁺	133.09715	133.09721	-0.38	7.4E+06	1.1E+07	1.0E+07	5.6E+06	2.9E+06	8.1E+06	1.2E+07	2.1E+06
18	Aspartic acid	C ₄ H ₇ NO ₄	[M+H] ⁺	134.04478	134.04484	-0.42	5.6E+06	3.6E+06	3.2E+06	9.2E+05	3.0E+06	3.0E+06	3.5E+06	
19	p-Cymene	C ₁₀ H ₁₄	[M+H] ⁺	135.11683	135.11688	-0.39						1.1E+06		
20	Limonene	C ₁₀ H ₁₆	[M+H] ⁺	137.13248	137.13254	-0.42		1.4E+06				1.5E+06		
21	Trigonelline	C ₇ H ₇ NO ₂	[M+H] ⁺	138.05495	138.05500	-0.34	3.0E+06		3.1E+06		2.0E+06		2.6E+06	
22	Nicotinamide N-oxide	C ₆ H ₆ N ₂ O ₂	[M+H] ⁺	139.05020	139.05026	-0.38	3.3E+06	5.6E+07	6.2E+06	3.7E+06	1.1E+06	8.6E+06	7.5E+06	1.3E+06
23	Succinic acid	C ₄ H ₆ O ₄	[M+Na] ⁺	141.01583	141.01588	-0.36				4.6E+05		1.0E+06		
24	L-Histidinol	C ₆ H ₁₁ N ₃ O	[M+H] ⁺	142.09749	142.09743	0.41	1.1E+06							
25	Hydroxyisobutyric acid	C ₄ H ₈ O ₃	[M+H] ⁺	143.01050	143.01052	-0.08			1.3E+06				1.4E+06	
26	Ectoine	C ₆ H ₁₀ N ₂ O ₂	[M+H] ⁺	143.08150	143.08156	-0.39		1.4E+06						

ESI(+) FT-ICR MS														
No.	Plausible Compound ^a	Molecular formula (M)	Ion	Theor m/z ^b	Exp. m/z ^c	Δ ppm _d	SM _R H ^e	SM _R O ^e	SM _P H ^e	SM _P O ^e	TF _R H ^e	TF _R O ^e	TF _P H ^e	TF _P O ^e
27	Hexenyl acetate	C ₈ H ₁₄ O ₂	[M+H] ⁺	143.10666	143.10671	-0.38		1.4E+06						
28	Solerol	C ₆ H ₁₀ O ₄	[M+H] ⁺	147.06519	147.06511	0.55	1.1E+06					1.1E+06		
29	Glutamine	C ₅ H ₁₀ N ₂ O ₃	[M+H] ⁺	147.07642	147.07648	-0.42	2.0E+08	7.1E+06	1.5E+08		1.1E+08	1.5E+06	7.8E+07	
30	Lysine	C ₆ H ₁₄ N ₂ O ₂	[M+H] ⁺	147.11280	147.11286	-0.39	7.2E+06	1.1E+07	6.8E+06	2.1E+06	5.5E+06	4.5E+06	5.1E+06	1.5E+06
31	Glutamic acid	C ₅ H ₉ NO ₄	[M+H] ⁺	148.06043	148.06049	-0.35	8.4E+07	1.0E+07	2.5E+07	8.3E+05	4.8E+07	3.2E+06	2.3E+07	7.8E+05
32	Thymine	C ₅ H ₆ N ₂ O ₂	[M+Na] ⁺	149.03215	149.03220	-0.31	1.2E+06				1.7E+06			
33	Cinnamic acid	C ₉ H ₈ O ₂	[M+H] ⁺	149.05971	149.05975	-0.30				4.5E+05				2.0E+06
34	Mevalonic acid	C ₆ H ₁₂ O ₄	[M+H] ⁺	149.08084	149.08072	0.75	2.1E+06		1.6E+06		1.5E+06			
35	Ectocarpin	C ₁₁ H ₁₆	[M+H] ⁺	149.13248	149.13254	-0.42		3.0E+06				1.7E+06		
36	Creatinine	C ₄ H ₇ N ₃ O	[M+K] ⁺	152.02207	152.02213	-0.39				1.3E+06				
37	Oxoproline	C ₅ H ₇ NO ₃	[M+Na] ⁺	152.03181	152.03188	-0.40				2.5E+06				1.7E+06
38	Ketoleucine	C ₆ H ₁₀ O ₃	[M+Na] ⁺	153.05221	153.05228	-0.43		2.1E+06						
39	Histidine	C ₆ H ₉ N ₃ O ₂	[M+H] ⁺	156.07675	156.07681	-0.36	1.3E+07	2.2E+07	1.2E+07	2.6E+06	7.9E+06	4.8E+06	1.1E+07	1.2E+06
40	Dimethyl-heptenoic acid	C ₉ H ₁₆ O ₂	[M+H] ⁺	157.12231	157.12238	-0.47		1.2E+06						
41	Methylnicotinamide	C ₇ H ₈ N ₂ O	[M+Na] ⁺	159.05288	159.05273	0.97								8.2E+05
42	Trigonelline	C ₇ H ₇ NO ₂	[M+Na] ⁺	160.03690	160.03694	-0.26			1.5E+06					
43	Valerylglycine	C ₇ H ₁₃ NO ₃	[M+H] ⁺	160.09682	160.09686	-0.25	1.1E+06							
44	Pargyline	C ₁₁ H ₁₃ N	[M+H] ⁺	160.11208	160.11206	0.10			1.5E+06					
45	Alanyl-alanine	C ₆ H ₁₂ N ₂ O ₃	[M+H] ⁺	161.09207	161.09215	-0.50			1.0E+06					
46	Tryptamine	C ₁₀ H ₁₂ N ₂	[M+H] ⁺	161.10732	161.10739	-0.40							1.1E+06	
47	Dimethylmalic acid	C ₆ H ₁₀ O ₅	[M+H] ⁺	163.06010	163.06015	-0.29	1.9E+06		2.1E+06		1.6E+06		3.2E+06	
48	Nicotine	C ₁₀ H ₁₄ N ₂	[M+H] ⁺	163.12297	163.12303	-0.33	2.1E+06	1.8E+07	3.9E+06	1.1E+06	1.2E+06	4.8E+06	4.0E+06	1.3E+06
49	S-(carboxypropyl)-Cysteamine	C ₆ H ₁₃ NO ₂ S	[M+H] ⁺	164.07398	164.07403	-0.31	1.4E+06		1.7E+06		1.2E+06		1.1E+06	
50	L-Phenylalanine	C ₉ H ₁₁ NO ₂	[M+H] ⁺	166.08626	166.08631	-0.34	5.9E+06	2.7E+07	5.6E+06		3.1E+06	2.5E+06	3.6E+06	
51	Dihydrothymine	C ₅ H ₈ N ₂ O ₂	[M+K] ⁺	167.02174	167.02179	-0.32	1.9E+06		2.9E+06		2.0E+06			
52	Formylsalicylic acid	C ₈ H ₆ O ₄	[M+H] ⁺	167.03389	167.03395	-0.36	9.9E+05	1.9E+06		9.9E+05		1.3E+06	1.3E+06	1.0E+06
53	Hydroxy-methyl-oxopentanoic acid	C ₆ H ₁₀ O ₄	[M+Na] ⁺	169.04713	169.04719	-0.33				1.5E+06				1.3E+06
54	Creatine	C ₄ H ₉ N ₃ O ₂	[M+K] ⁺	170.03264	170.03271	-0.44				1.1E+06				
55	Ectocarpin	C ₁₁ H ₁₆	[M+Na] ⁺	171.11442	171.11434	0.47			1.3E+06					

ESI(+) FT-ICR MS														
No.	Plausible Compound ^a	Molecular formula (M)	Ion	Theor m/z ^b	Exp m/z ^c	Δ ppm ^d	SM _R H ^e	SM _R O ^e	SM _P H ^e	SM _P O ^e	TF _R H ^e	TF _R O ^e	TF _P H ^e	TF _P O ^e
56	Limonene-1,2-diol	C ₁₀ H ₁₈ O ₂	[M+H] ⁺	171.13796	171.13802	-0.37		1.4E+06						
57	Glycylproline	C ₇ H ₁₂ N ₂ O ₃	[M+H] ⁺	173.09207	173.09214	-0.41		7.8E+06						
58	Propylglutaric acid	C ₈ H ₁₄ O ₄	[M+H] ⁺	175.09649	175.09657	-0.48	1.1E+06							
59	Arginine	C ₆ H ₁₄ N ₄ O ₂	[M+H] ⁺	175.11895	175.11901	-0.30	4.0E+07	4.9E+07	4.6E+07	3.5E+06	3.5E+07	8.5E+06	1.4E+07	2.7E+06
60	Dimethyl-2-aminoethylphosphonate	C ₄ H ₁₂ NO ₃ P	[M+Na] ⁺	176.04470	176.04477	-0.41	1.5E+06		1.2E+06		1.8E+06			
61	Citrulline	C ₆ H ₁₃ N ₃ O ₃	[M+H] ⁺	176.10297	176.10302	-0.32	4.0E+06	3.5E+07	3.5E+06	1.0E+06	1.8E+06	4.1E+06	4.9E+06	9.0E+05
62	Serotonin	C ₁₀ H ₁₂ N ₂ O	[M+H] ⁺	177.10224	177.10230	-0.34	1.8E+06		1.7E+06		1.3E+06		1.8E+06	
63	Hydroxy-methylglutamate	C ₆ H ₁₁ NO ₅	[M+H] ⁺	178.07100	178.07105	-0.29	2.9E+06				2.2E+06		3.2E+06	
64	Methoxycinnamic acid	C ₁₀ H ₁₀ O ₃	[M+H] ⁺	179.07027	179.07033	-0.33		1.2E+06						
65	Hexylphenol	C ₁₂ H ₁₈ O	[M+H] ⁺	179.14304	179.14299	0.27		1.1E+06				1.2E+06		1.1E+06
66	Glucosamine	C ₆ H ₁₃ NO ₅	[M+H] ⁺	180.08665	180.08671	-0.32			1.3E+06		1.2E+06		1.8E+06	
67	Oxooctanoic acid	C ₈ H ₁₄ O ₃	[M+Na] ⁺	181.08352	181.08357	-0.30						1.3E+06		
68	Methyl-hydroxy-formylpyridine-carboxylate	C ₈ H ₇ NO ₄	[M+H] ⁺	182.04478	182.04485	-0.33	9.6E+05				1.6E+06			
69	Tyrosine	C ₉ H ₁₁ NO ₃	[M+H] ⁺	182.08117	182.08122	-0.29	2.4E+06	3.1E+07	2.7E+06	1.2E+06	1.6E+06	3.6E+06	2.0E+06	
70	Dimethylglutaric acid	C ₇ H ₁₂ O ₄	[M+Na] ⁺	183.06278	183.06283	-0.25				1.3E+06	1.1E+06	2.9E+06		2.0E+06
71	Oxo-campholide	C ₁₀ H ₁₄ O ₃	[M+H] ⁺	183.10157	183.10173	-0.87			1.5E+06		1.9E+06			
72	Indole-ethanol	C ₁₀ H ₁₁ NO	[M+Na] ⁺	184.07328	184.07339	-0.57	1.1E+06							
73	Solerol	C ₆ H ₁₀ O ₄	[M+K] ⁺	185.02107	185.02113	-0.33		1.5E+07						
74	beta-L-Oleandropyranose;Oleandrose ([M+Na] ⁺)	C ₇ H ₁₄ O ₄	[M+Na] ⁺	185.07843	185.07849	-0.33				9.4E+05		1.3E+06		
75	Citronellyl formate	C ₁₁ H ₂₀ O ₂	[M+H] ⁺	185.15361	185.15367	-0.34		1.8E+06						
76	D-O-Phosphoserine	C ₃ H ₈ NO ₆ P	[M+H] ⁺	186.01620	186.01638	-0.94	2.2E+07		8.3E+06		2.0E+07		3.5E+06	
77	Hydroxycinnamic acid	C ₉ H ₈ O ₃	[M+Na] ⁺	187.03656	187.03656	0.01	1.4E+06		1.7E+06		1.5E+06			
78	Mevalonic acid	C ₆ H ₁₂ O ₄	[M+K] ⁺	187.03672	187.03659	0.71			1.7E+06		1.5E+06			
79	Methyl-decanoic acid	C ₁₁ H ₂₂ O ₂	[M+H] ⁺	187.16926	187.16920	0.30		9.9E+05						
80	Monomethyl-arginine	C ₇ H ₁₆ N ₄ O ₂	[M+H] ⁺	189.13460	189.13466	-0.28	1.1E+06		9.6E+05					
81	Citric acid	C ₆ H ₈ O ₇	[M+H] ⁺	193.03428	193.03433	-0.28	1.1E+06		1.1E+06				2.2E+06	
82	Tridecatrienal	C ₁₃ H ₂₀ O	[M+H] ⁺	193.15869	193.15876	-0.35		3.0E+06						
83	Oxononanoic acid	C ₉ H ₁₆ O ₃	[M+Na] ⁺	195.09917	195.09924	-0.36		3.4E+06				1.6E+06		
84	Allantoin	C ₄ H ₆ N ₄ O ₃	[M+K] ⁺	197.00715	197.00722	-0.36			1.4E+06		1.2E+06			

ESI(+) FT-ICR MS														
No.	Plausible Compound ^a	Molecular formula (M)	Ion	Theor m/z ^b	Exp. m/z ^c	Δ ppm _d	SM _R H ^e	SM _R O ^e	SM _P H ^e	SM _P O ^e	TF _R H ^e	TF _R O ^e	TF _P H ^e	TF _P O ^e
85	Suberic acid	C ₈ H ₁₄ O ₄	[M+Na] ⁺	197.07843	197.07849	-0.31				1.2E+06		3.2E+06		1.7E+06
86	N-Acetylornithine	C ₇ H ₁₄ N ₂ O ₃	[M+Na] ⁺	197.08966	197.08975	-0.42				9.4E+05				1.0E+06
87	Hydroxy pelargonic acid	C ₉ H ₁₈ O ₃	[M+Na] ⁺	197.11482	197.11488	-0.33						1.2E+06		
88	Terpinyl acetate	C ₁₂ H ₂₀ O ₂	[M+H] ⁺	197.15361	197.15367	-0.32		2.0E+06						
89	Ascorbic acid	C ₆ H ₈ O ₆	[M+Na] ⁺	199.02131	199.02137	-0.28				7.0E+05				3.0E+06
90	Lauroleic acid	C ₁₂ H ₂₂ O ₂	[M+H] ⁺	199.16926	199.16931	-0.27		2.2E+06						
91	D-galacto-Hexodialdose	C ₆ H ₁₀ O ₆	[M+Na] ⁺	201.03696	201.03704	-0.40					1.1E+06			
92	Sulfobenzoate	C ₇ H ₆ O ₅ S	[M+H] ⁺	203.00087	203.00087	0.00	1.8E+06				2.7E+06		2.4E+06	
93	Aldohexose	C ₆ H ₁₂ O ₆	[M+Na] ⁺	203.05261	203.05267	-0.32	8.3E+08	1.3E+07	1.2E+09	1.6E+06	1.2E+09	2.4E+06	1.1E+09	3.8E+06
94	Metamitron	C ₁₀ H ₁₀ N ₄ O	[M+H] ⁺	203.09274	203.09278	-0.21							3.0E+06	
95	alpha-Curcumene	C ₁₅ H ₂₂	[M+H] ⁺	203.17943	203.17946	-0.18	1.1E+06	1.7E+06	1.7E+06		1.5E+06	2.3E+06	1.5E+06	
96	Hydroxyfluorene	C ₁₃ H ₁₀ O	[M+Na] ⁺	205.06239	205.06246	-0.36				7.6E+05				2.6E+06
97	Sorbitol	C ₆ H ₁₄ O ₆	[M+Na] ⁺	205.06826	205.06832	-0.30	1.5E+06	4.6E+06	2.8E+06	2.3E+06	1.8E+06	1.4E+06	3.4E+06	
98	Tryptophan	C ₁₁ H ₁₂ N ₂ O ₂	[M+H] ⁺	205.09715	205.09721	-0.29	1.5E+07	1.8E+07	1.3E+07	8.4E+05	1.1E+07	2.3E+06	9.8E+06	
99	Caryophyllene	C ₁₅ H ₂₄	[M+H] ⁺	205.19508	205.19513	-0.26	1.2E+06	2.4E+06	1.4E+06	6.5E+05		2.9E+06	1.2E+06	1.1E+06
100	Oxo-decenoic acid	C ₁₀ H ₁₆ O ₃	[M+Na] ⁺	207.09917	207.09922	-0.27						1.2E+06		
101	Actinamine	C ₈ H ₁₈ N ₂ O ₄	[M+H] ⁺	207.13393	207.13399	-0.27			1.2E+06		1.2E+06			
102	Hydroxybiphenyl	C ₁₂ H ₁₀ O	[M+K] ⁺	209.03632	209.03638	-0.27					1.3E+06			
103	Carboxycyclohexyl-acetic acid	C ₉ H ₁₄ O ₄	[M+Na] ⁺	209.07843	209.07850	-0.35				5.0E+05	1.0E+06	1.3E+06	1.0E+06	1.1E+06
104	Oxodecanoate	C ₁₀ H ₁₈ O ₃	[M+Na] ⁺	209.11482	209.11487	-0.26				8.0E+05		1.0E+06		
105	(Acetamidomethylene)succinate	C ₇ H ₉ NO ₅	[M+Na] ⁺	210.03729	210.03736	-0.29	1.4E+06				1.3E+06			
106	Butenyl-methyl-threonine	C ₉ H ₁₇ NO ₃	[M+Na] ⁺	210.11006	210.11014	-0.36				7.9E+05	3.2E+06	1.8E+06	1.6E+06	1.3E+06
107	Azelaic acid	C ₉ H ₁₆ O ₄	[M+Na] ⁺	211.09408	211.09414	-0.31	1.5E+06		1.4E+06	6.2E+05	1.9E+06	2.4E+06	1.6E+06	1.2E+06
108	Glycyl-L-leucine	C ₈ H ₁₆ N ₂ O ₃	[M+Na] ⁺	211.10531	211.10537	-0.27						1.8E+06		
109	Tridecynoic acid	C ₁₃ H ₂₂ O ₂	[M+H] ⁺	211.16926	211.16934	-0.40		3.7E+06						
110	Propylglutaric acid	C ₈ H ₁₄ O ₄	[M+K] ⁺	213.05237	213.05242	-0.24			1.1E+06		1.2E+06			
111	Citrulline	C ₆ H ₁₃ N ₃ O ₃	[M+K] ⁺	214.05885	214.05891	-0.28	5.9E+06		1.1E+07	7.9E+05	5.5E+06	2.4E+06	4.4E+06	
112	Quinic acid	C ₇ H ₁₂ O ₆	[M+Na] ⁺	215.05261	215.05266	-0.22	1.1E+06				1.4E+06		1.2E+06	
113	Methyl lauric acid	C ₁₃ H ₂₆ O ₂	[M+H] ⁺	215.20056	215.20063	-0.32		2.0E+06				1.1E+06		

ESI(+) FT-ICR MS														
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114	Dihydroxydibenzothiophene	C ₁₂ H ₈ O ₂ S	[M+H] ⁺	217.03178	217.03195	-0.80	1.2E+06				1.4E+06			
115	Methyl-myo-inositol	C ₇ H ₁₄ O ₆	[M+Na] ⁺	217.06826	217.06833	-0.30	1.3E+07		5.5E+07		2.9E+07		1.7E+07	
116	Oxidized Latia luciferin	C ₁₃ H ₂₂ O	[M+Na] ⁺	217.15629	217.15636	-0.32				1.2E+06		2.3E+06		
117	Vulgraon B	C ₁₆ H ₂₄	[M+H] ⁺	217.19508	217.19514	-0.30	1.1E+06	2.9E+06	1.4E+06	4.8E+05		2.9E+06	1.3E+06	1.2E+06
118	Salicyluric acid	C ₉ H ₉ NO ₄	[M+Na] ⁺	218.04238	218.04259	-0.97			1.3E+06					
119	Aldohexose	C ₆ H ₁₂ O ₆	[M+K] ⁺	219.02655	219.02661	-0.28	5.1E+08	1.0E+07	7.4E+08		5.9E+08		6.3E+08	2.4E+06
120	N-Acetylserotonin	C ₁₂ H ₁₄ N ₂ O ₂	[M+H] ⁺	219.11280	219.11281	-0.03					1.0E+06			
121	Amino-dinitrotoluene	C ₇ H ₇ N ₃ O ₄	[M+Na] ⁺	220.03288	220.03287	0.01	1.1E+06		1.6E+06		1.4E+06			
122	Dihydroxy-dihydro-p-cumate	C ₁₀ H ₁₄ O ₄	[M+Na] ⁺	221.07843	221.07852	-0.41		1.7E+06						
123	Prilocaine	C ₁₃ H ₂₀ N ₂ O	[M+H] ⁺	221.16484	221.16488	-0.18						1.0E+06		
124	Dodecanamide	C ₁₂ H ₂₅ NO	[M+Na] ⁺	222.18284	222.18289	-0.26	2.3E+06			3.6E+06	2.4E+06	3.4E+06	2.1E+06	2.5E+06
125	cis-5-Decenedioic acid	C ₁₀ H ₁₆ O ₄	[M+Na] ⁺	223.09408	223.09414	-0.28	1.0E+06			5.3E+05	1.3E+06	2.0E+06	1.0E+06	1.3E+06
126	Amylmercaptapurine	C ₁₀ H ₁₄ N ₄ S	[M+H] ⁺	223.10119	223.10119	0.02	1.6E+06							
127	Oxo-undecanoic acid	C ₁₁ H ₂₀ O ₃	[M+Na] ⁺	223.13047	223.13052	-0.26				8.5E+05		1.4E+06		1.6E+06
128	Carboxycyclohexyl-acetic acid	C ₉ H ₁₄ O ₄	[M+K] ⁺	225.05237	225.05243	-0.25	1.3E+06		1.2E+06					
129	Sebacic acid	C ₁₀ H ₁₈ O ₄	[M+Na] ⁺	225.10973	225.10979	-0.28	1.1E+06			7.0E+05	1.5E+06	2.3E+06		1.4E+06
130	Tetradecadienoic acid	C ₁₄ H ₂₄ O ₂	[M+H] ⁺	225.18491	225.18499	-0.37		1.8E+06						
131	N-Heptanoylglycine	C ₉ H ₁₇ NO ₃	[M+K] ⁺	226.08400	226.08407	-0.27	1.4E+06				1.7E+06			
132	Oxosuberate	C ₈ H ₁₂ O ₅	[M+K] ⁺	227.03163	227.03169	-0.25					1.2E+06			
133	D-Tryptophan	C ₁₁ H ₁₂ N ₂ O ₂	[M+Na] ⁺	227.07910	227.07921	-0.51			1.9E+06		1.6E+06		1.4E+06	
134	Acetyl-hydroxy-lysine	C ₈ H ₁₆ N ₂ O ₄	[M+Na] ⁺	227.10023	227.10028	-0.24	1.3E+06			1.5E+06		1.0E+06		
135	Diazacyclotetradecanedione	C ₁₂ H ₂₂ N ₂ O ₂	[M+H] ⁺	227.17540	227.17549	-0.35				1.6E+06		2.5E+06		
136	Myristoleic acid	C ₁₄ H ₂₆ O ₂	[M+H] ⁺	227.20056	227.20062	-0.30	2.3E+06	3.9E+06	1.4E+06		1.5E+06		1.5E+06	
137	Methylcitric acid	C ₇ H ₁₀ O ₇	[M+Na] ⁺	229.03187	229.03194	-0.29	3.1E+06		5.8E+06		3.3E+06		5.1E+06	
138	Serine-phosphoethanolamine	C ₅ H ₁₃ N ₂ O ₆ P	[M+H] ⁺	229.05840	229.05859	-0.83	1.1E+06							
139	Acetyleugenol	C ₁₂ H ₁₄ O ₃	[M+Na] ⁺	229.08352	229.08374	-0.96		3.0E+06	1.1E+06					
140	Myristic acid	C ₁₄ H ₂₈ O ₂	[M+H] ⁺	229.21621	229.21627	-0.29	1.4E+06	5.8E+06	1.4E+06	9.6E+05		2.4E+06	1.3E+06	1.1E+06
141	Xestoaminol C	C ₁₄ H ₃₁ NO	[M+H] ⁺	230.24784	230.24792	-0.33	2.4E+06	7.2E+06	1.4E+06			2.1E+06		
142	Citric acid	C ₆ H ₈ O ₇	[M+K] ⁺	230.99016	230.99023	-0.27	4.1E+07		5.2E+07		1.4E+07		7.6E+07	

ESI(+) FT-ICR MS														
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143	Heptyloxyphenol	C ₁₃ H ₂₀ O ₂	[M+Na] ⁺	231.13555	231.13563	-0.33				5.1E+05		2.2E+06		2.0E+06
144	L-Arabinitol phosphate	C ₅ H ₁₃ O ₈ P	[M+H] ⁺	233.04208	233.04226	-0.76	4.2E+06		1.4E+07		7.2E+06		4.3E+06	
145	Sinapyl alcohol	C ₁₁ H ₁₄ O ₄	[M+Na] ⁺	233.07843	233.07864	-0.90	1.2E+06							
146	Aplotaxene	C ₁₇ H ₂₈	[M+H] ⁺	233.22638	233.22644	-0.28		2.3E+06		5.1E+05		2.5E+06		
147	Perseitol	C ₇ H ₁₆ O ₇	[M+Na] ⁺	235.07882	235.07889	-0.28	5.3E+06		7.7E+06		7.6E+06		6.6E+06	
148	Hexadecatrienal	C ₁₆ H ₂₆ O	[M+H] ⁺	235.20564	235.20570	-0.25		3.1E+06						
149	Carboxin	C ₁₂ H ₁₃ NO ₂ S	[M+H] ⁺	236.07398	236.07403	-0.23						3.4E+06		
150	Methyl lauric acid	C ₁₃ H ₂₆ O ₂	[M+Na] ⁺	237.18250	237.18258	-0.31				5.0E+05				1.4E+06
151	Hexadecadienal	C ₁₆ H ₂₈ O	[M+H] ⁺	237.22129	237.22136	-0.29		5.5E+06						
152	Acetyl-arginine	C ₈ H ₁₆ N ₄ O ₃	[M+Na] ⁺	239.11146	239.11151	-0.20				1.4E+06				
153	Undecanedioic acid	C ₁₁ H ₂₀ O ₄	[M+Na] ⁺	239.12538	239.12546	-0.35	1.2E+06			1.1E+06	1.6E+06	1.5E+06		1.1E+06
154	Campherene-diol	C ₁₅ H ₂₆ O ₂	[M+H] ⁺	239.20056	239.20064	-0.35		1.6E+06						
155	Hexadecenal	C ₁₆ H ₃₀ O	[M+H] ⁺	239.23694	239.23702	-0.31		2.0E+06				1.8E+06		1.1E+06
156	Anatalline	C ₁₅ H ₁₇ N ₃	[M+H] ⁺	240.14952	240.14960	-0.32		5.0E+06	2.0E+06	1.2E+06		2.2E+06	1.1E+06	
157	Dihydroxy-dihydrodibenzothiophene	C ₁₂ H ₁₀ O ₂ S	[M+Na] ⁺	241.02937	241.02944	-0.29				6.8E+06		3.6E+07		1.0E+07
158	Tridecenyl acetate	C ₁₅ H ₂₈ O ₂	[M+H] ⁺	241.21621	241.21628	-0.28		4.0E+06	1.1E+06					
159	(4E,6E,d14:2) sphingosine	C ₁₄ H ₂₇ NO ₂	[M+H] ⁺	242.21146	242.21153	-0.31			1.2E+06		1.6E+06			
160	Canthin-one	C ₁₄ H ₈ N ₂ O	[M+Na] ⁺	243.05288	243.05309	-0.86	2.6E+06		2.5E+06		2.2E+06			
161	Hydroxy-tryptophan	C ₁₁ H ₁₂ N ₂ O ₃	[M+Na] ⁺	243.07401	243.07423	-0.88	2.3E+06	2.1E+06	1.7E+06	1.6E+06			1.3E+06	
162	Methyl myristic acid	C ₁₅ H ₃₀ O ₂	[M+H] ⁺	243.23186	243.23191	-0.22	1.7E+06	8.7E+06	1.7E+06			2.8E+06	1.4E+06	9.6E+05
163	Acetyl-glucosamine	C ₈ H ₁₅ NO ₆	[M+Na] ⁺	244.07916	244.07923	-0.27	1.7E+06				2.0E+06			
164	Cytidine	C ₉ H ₁₃ N ₃ O ₅	[M+H] ⁺	244.09280	244.09287	-0.28	1.5E+07		5.5E+06		8.5E+06		7.4E+06	
165	Undecanoylglycine	C ₁₃ H ₂₅ NO ₃	[M+H] ⁺	244.19072	244.19079	-0.28	1.8E+07	7.4E+07	9.3E+06	9.0E+06	5.8E+06	8.7E+06	1.9E+07	3.8E+06
166	Amino-tetradecanoic acid	C ₁₄ H ₂₉ NO ₂	[M+H] ⁺	244.22711	244.22719	-0.35		1.9E+07						
167	Apiole	C ₁₂ H ₁₄ O ₄	[M+Na] ⁺	245.07843	245.07850	-0.30				5.0E+05		1.5E+06		1.1E+06
168	Hydroxy-oxo-ionone	C ₁₃ H ₁₈ O ₃	[M+Na] ⁺	245.11482	245.11488	-0.26				1.7E+06	1.3E+06	4.0E+06	1.0E+06	2.7E+06
169	Glutamyl-valine	C ₁₀ H ₁₈ N ₂ O ₅	[M+H] ⁺	247.12885	247.12892	-0.29	1.1E+06							
170	Propylideneisolongifolane	C ₁₈ H ₃₀	[M+H] ⁺	247.24203	247.24210	-0.29		2.5E+06				1.5E+06		
171	Linamarin	C ₁₀ H ₁₇ NO ₆	[M+H] ⁺	248.11286	248.11294	-0.31				1.2E+06				

ESI(+) FT-ICR MS														
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172	Chorismic acid	C ₁₀ H ₁₀ O ₆	[M+Na] ⁺	249.03696	249.03718	-0.88	1.4E+07		3.0E+06		1.4E+07		3.3E+06	
173	Furyl-nitro-furylacrylamide	C ₁₁ H ₈ N ₂ O ₅	[M+H] ⁺	249.05060	249.05073	-0.53		2.7E+06						
174	Diazacyclotetradecanedione	C ₁₂ H ₂₂ N ₂ O ₂	[M+Na] ⁺	249.15735	249.15742	-0.30			1.1E+06		1.8E+06			4.4E+06
175	Myristoleic acid	C ₁₄ H ₂₆ O ₂	[M+Na] ⁺	249.18250	249.18258	-0.32				8.8E+05				1.8E+06
176	Dubamine	C ₁₆ H ₁₁ NO ₂	[M+H] ⁺	250.08626	250.08633	-0.30		4.5E+06		7.2E+05		3.7E+06		
177	Hydroxy-carboxy-oxo-methylocta-dienoate	C ₁₀ H ₁₂ O ₆	[M+Na] ⁺	251.05261	251.05282	-0.84	2.2E+06		3.0E+06		2.1E+06		2.0E+06	
178	Deoxyindenestrol	C ₁₈ H ₁₈ O	[M+H] ⁺	251.14304	251.14317	-0.51	1.3E+06		1.3E+06					
179	Oxo-tridecanoic acid	C ₁₃ H ₂₄ O ₃	[M+Na] ⁺	251.16177	251.16181	-0.18						1.5E+06		
180	Muramic acid	C ₉ H ₁₇ NO ₇	[M+H] ⁺	252.10778	252.10784	-0.24	2.6E+06		2.0E+06		1.6E+06		1.8E+06	
181	N-Decanoylglycine	C ₁₂ H ₂₃ NO ₃	[M+Na] ⁺	252.15701	252.15711	-0.38				1.4E+06				
182	Dodecanedioic acid	C ₁₂ H ₂₂ O ₄	[M+Na] ⁺	253.14103	253.14109	-0.25	1.2E+06			1.0E+06	1.7E+06	2.2E+06		1.5E+06
183	Tetramethyl-undecandiol	C ₁₄ H ₃₀ O ₂	[M+Na] ⁺	253.21380	253.21386	-0.21						2.6E+06		2.0E+06
184	Palmitolinoleic acid	C ₁₆ H ₂₈ O ₂	[M+H] ⁺	253.21621	253.21627	-0.23		6.5E+06				1.5E+06		
185	Goniothalenol	C ₁₃ H ₁₂ O ₄	[M+Na] ⁺	255.06278	255.06299	-0.81	1.4E+06		1.5E+06		1.2E+06			
186	Hexadecenoic acid	C ₁₆ H ₃₀ O ₂	[M+H] ⁺	255.23186	255.23192	-0.24	2.0E+06	2.2E+07	2.3E+06	7.6E+05		3.7E+06	2.4E+06	1.4E+06
187	Palmitic acid	C ₁₆ H ₃₂ O ₂	[M+H] ⁺	257.24751	257.24758	-0.28	2.2E+06	4.7E+07	1.9E+06	1.0E+06		3.7E+06	2.0E+06	1.3E+06
188	Lophophorine	C ₁₃ H ₁₇ NO ₃	[M+Na] ⁺	258.11006	258.11015	-0.33			1.3E+06					
189	Galactosamine phosphate	C ₆ H ₁₄ NO ₈ P	[M+H] ⁺	260.05298	260.05316	-0.69	4.0E+06		2.6E+06		3.3E+06		2.3E+06	
190	Acetyl-glucosaminat	C ₈ H ₁₅ NO ₇	[M+Na] ⁺	260.07407	260.07414	-0.26			1.3E+06					
191	Ketose-phosphate	C ₆ H ₁₃ O ₉ P	[M+H] ⁺	261.03700	261.03711	-0.43	1.4E+06		1.1E+06				1.9E+06	
192	Deoxy-manno-octulosonate	C ₈ H ₁₄ O ₈	[M+Na] ⁺	261.05809	261.05815	-0.25	1.7E+06				2.1E+06		3.1E+06	
193	Methoxychalcone	C ₁₆ H ₁₄ O ₂	[M+Na] ⁺	261.08860	261.08882	-0.83	1.5E+06	1.5E+06	1.2E+06	1.4E+06	2.0E+06			1.0E+06
194	Androstane	C ₁₉ H ₃₂	[M+H] ⁺	261.25768	261.25775	-0.27		3.2E+06	1.8E+06	5.9E+05		3.5E+06	1.3E+06	1.3E+06
195	Tridecenyl acetate	C ₁₅ H ₂₈ O ₂	[M+Na] ⁺	263.19815	263.19822	-0.26				1.7E+06				2.7E+06
196	Dodecylphenol	C ₁₈ H ₃₀ O	[M+H] ⁺	263.23694	263.23700	-0.22		7.3E+06				1.2E+06		
197	Selagine	C ₁₅ H ₁₈ N ₂ O	[M+Na] ⁺	265.13113	265.13133	-0.73				3.0E+06		5.3E+06		1.1E+06
198	Keto myristic acid	C ₁₄ H ₂₆ O ₃	[M+Na] ⁺	265.17742	265.17749	-0.28				6.1E+05				1.7E+06
199	Norlinolenic acid	C ₁₇ H ₂₈ O ₂	[M+H] ⁺	265.21621	265.21627	-0.24		2.3E+06						
200	Octadecadienal	C ₁₈ H ₃₂ O	[M+H] ⁺	265.25259	265.25267	-0.29		9.8E+06						

ESI(+) FT-ICR MS														
No.	Plausible Compound ^a	Molecular formula (M)	Ion	Theor m/z ^b	Exp m/z ^c	Δ ppm ^d	SM _R H ^e	SM _R O ^e	SM _P H ^e	SM _P O ^e	TF _R H ^e	TF _R O ^e	TF _P H ^e	TF _P O ^e
201	Isobutylphendienamide	C ₁₆ H ₂₁ NO	[M+Na] ⁺	266.15153	266.15175	-0.82	9.4E+06	6.6E+06		6.8E+06	4.8E+06	6.1E+06	9.3E+06	3.3E+06
202	Amino-tetradecanoic acid	C ₁₄ H ₂₉ NO ₂	[M+Na] ⁺	266.20905	266.20912	-0.26	1.5E+06		1.2E+06					
203	Methyl-dodecanedioic acid	C ₁₃ H ₂₄ O ₄	[M+Na] ⁺	267.15668	267.15673	-0.17			1.2E+06			1.4E+06		1.3E+06
204	Epoxy-trimethyltrideca-dienoicacid	C ₁₆ H ₂₆ O ₃	[M+H] ⁺	267.19547	267.19553	-0.22		2.1E+06						
205	Pentadecadienyl acetate	C ₁₇ H ₃₀ O ₂	[M+H] ⁺	267.23186	267.23194	-0.31		2.2E+06						
206	Octadecenal	C ₁₈ H ₃₄ O	[M+H] ⁺	267.26824	267.26830	-0.22								1.4E+06
207	Neuraminic acid	C ₉ H ₁₇ NO ₈	[M+H] ⁺	268.10269	268.10279	-0.36	1.8E+06							
208	Adenosine	C ₁₀ H ₁₃ N ₅ O ₄	[M+H] ⁺	268.10403	268.10410	-0.26	2.3E+07		1.3E+07		1.5E+07		6.8E+06	
209	Oxo-pentyl-cyclopentanehexanoic acid	C ₁₆ H ₂₈ O ₃	[M+H] ⁺	269.21112	269.21121	-0.33		5.0E+06						
210	Methyl-hexadecenoic acid	C ₁₇ H ₃₂ O ₂	[M+H] ⁺	269.24751	269.24759	-0.30		1.1E+07	1.2E+06			1.8E+06		
211	Meperidine	C ₁₅ H ₂₁ NO ₂	[M+Na] ⁺	270.14645	270.14667	-0.82	2.5E+06						2.0E+06	
212	Keto palmitic acid	C ₁₆ H ₃₀ O ₃	[M+H] ⁺	271.22677	271.22683	-0.22		7.6E+06				2.6E+06		
213	Erogorgiaene	C ₂₀ H ₃₀	[M+H] ⁺	271.24203	271.24211	-0.31		4.6E+06	1.3E+06			5.2E+06	1.8E+06	2.1E+06
214	Methyl palmitic acid	C ₁₇ H ₃₄ O ₂	[M+H] ⁺	271.26316	271.26324	-0.29		2.3E+07				1.6E+06		
215	Amino-hexadecanoic acid	C ₁₆ H ₃₃ NO ₂	[M+H] ⁺	272.25841	272.25849	-0.29		9.2E+07				1.7E+06		
216	Citrinin	C ₁₃ H ₁₄ O ₅	[M+Na] ⁺	273.07334	273.07335	-0.02	1.1E+06							
217	Glycinol	C ₁₅ H ₁₂ O ₅	[M+H] ⁺	273.07575	273.07582	-0.26							3.1E+06	
218	Methylripariochromene A ([M+Na] ⁺)	C ₁₄ H ₁₈ O ₄	[M+Na] ⁺	273.10973	273.10981	-0.29	2.5E+06	1.8E+06		9.2E+05	2.4E+06	3.3E+06	2.6E+06	2.3E+06
219	Hydroxy palmitic acid	C ₁₆ H ₃₂ O ₃	[M+H] ⁺	273.24242	273.24250	-0.29		2.1E+06						
220	Pimaradiene	C ₂₀ H ₃₂	[M+H] ⁺	273.25768	273.25774	-0.21	1.9E+06	6.3E+06	2.2E+06	9.2E+05		5.0E+06	2.2E+06	1.5E+06
221	Glutamyl-glutamine	C ₁₀ H ₁₇ N ₃ O ₆	[M+H] ⁺	276.11901	276.11907	-0.21	1.4E+06							
222	Phosphogluconic acid	C ₆ H ₁₃ O ₁₀ P	[M+H] ⁺	277.03191	277.03209	-0.65	1.5E+06				1.4E+06		1.6E+06	
223	Gamma Glutamylglutamic acid	C ₁₀ H ₁₆ N ₂ O ₇	[M+H] ⁺	277.10303	277.10309	-0.21	1.4E+06				1.6E+06			
224	methyl-[(formyl-vinyl)-hydroxy-oxo-cyclopentyl]-butanoate	C ₁₃ H ₁₈ O ₅	[M+Na] ⁺	277.10464	277.10487	-0.83	2.2E+06	1.0E+07					1.9E+06	
225	Chrysanthetriol	C ₁₅ H ₂₆ O ₃	[M+H] ⁺	277.17742	277.17748	-0.23						1.3E+06		
226	Hydroxybutanyl-isolongifol-ene	C ₁₉ H ₃₂ O	[M+H] ⁺	277.25259	277.25266	-0.24		3.5E+06						
227	Dihydroxyflavanone	C ₁₅ H ₁₂ O ₄	[M+Na] ⁺	279.06278	279.06302	-0.86					1.3E+06			
228	alhpa-tocopheronolactone	C ₁₆ H ₂₂ O ₄	[M+H] ⁺	279.15909	279.15915	-0.24	8.8E+06	2.5E+07		4.2E+06	4.1E+06	1.5E+07	9.9E+06	4.5E+06

ESI(+) FT-ICR MS														
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229	keto pentadecanoic acid	C ₁₅ H ₂₈ O ₃	[M+Na] ⁺	279.19307	279.19312	-0.20						1.6E+06	1.1E+06	
230	Linolenic acid	C ₁₈ H ₃₀ O ₂	[M+H] ⁺	279.23186	279.23193	-0.26		4.9E+06						
231	Serratine	C ₁₆ H ₂₅ NO ₃	[M+H] ⁺	280.19072	280.19083	-0.39		1.6E+06						
232	Linoleamide	C ₁₈ H ₃₃ NO	[M+H] ⁺	280.26349	280.26358	-0.32		6.9E+06						
233	Apigeniflavan	C ₁₅ H ₁₄ O ₄	[M+Na] ⁺	281.07843	281.07867	-0.86		4.5E+06						
234	Glycero-Phosphocholine	C ₈ H ₂₁ NO ₆ P	[M+Na] ⁺	281.09987	281.09966	0.75		2.7E+06						
235	Methylbatatasin III	C ₁₆ H ₁₈ O ₃	[M+Na] ⁺	281.11482	281.11504	-0.80		4.3E+06						
236	Keto myristic acid	C ₁₄ H ₂₆ O ₃	[M+K] ⁺	281.15135	281.15144	-0.31		6.7E+06						
237	Tetradecanedioic acid	C ₁₄ H ₂₆ O ₄	[M+Na] ⁺	281.17233	281.17238	-0.19	1.6E+06		1.5E+06	9.1E+05	1.7E+06		1.5E+06	
238	Hydroxy-pentadecanoic acid	C ₁₅ H ₃₀ O ₃	[M+Na] ⁺	281.20872	281.20881	-0.32		4.4E+06				2.8E+06		1.7E+06
239	Hydroxy-heptadecatrienoic acid	C ₁₇ H ₂₈ O ₃	[M+H] ⁺	281.21112	281.21120	-0.28		2.1E+06						
240	Linoleic acid	C ₁₈ H ₃₂ O ₂	[M+H] ⁺	281.24751	281.24760	-0.33		1.9E+07				2.1E+06		
241	Heptyl-hydroxy-quinolone	C ₁₆ H ₂₁ NO ₂	[M+Na] ⁺	282.14645	282.14667	-0.80	5.1E+06	1.7E+07	4.5E+06	3.1E+06	3.0E+06	1.9E+06	3.7E+06	
242	Oleamide	C ₁₈ H ₃₅ NO	[M+H] ⁺	282.27914	282.27924	-0.35		2.2E+07						
243	Hemigossypol	C ₁₅ H ₁₆ O ₄	[M+Na] ⁺	283.09408	283.09431	-0.81		4.3E+06						
244	Falcarindiol	C ₁₇ H ₂₄ O ₂	[M+Na] ⁺	283.16685	283.16706	-0.74		1.7E+06						
245	Oleic acid	C ₁₈ H ₃₄ O ₂	[M+H] ⁺	283.26316	283.26322	-0.21	1.6E+06	4.2E+07	1.6E+06	7.4E+05		2.8E+06	1.5E+06	
246	Nonadecanal	C ₁₉ H ₃₈ O	[M+H] ⁺	283.29954	283.29961	-0.24		1.6E+06						
247	Guanosine	C ₁₀ H ₁₃ N ₅ O ₅	[M+H] ⁺	284.09895	284.09901	-0.22	1.0E+07				7.3E+06		3.9E+06	
248	Acrifoline	C ₁₆ H ₂₃ NO ₂	[M+Na] ⁺	284.16210	284.16237	-0.95		1.5E+06						
249	Stearamide	C ₁₈ H ₃₇ NO	[M+H] ⁺	284.29479	284.29487	-0.28		4.8E+06			1.6E+06			
250	Coformycin	C ₁₁ H ₁₆ N ₄ O ₅	[M+H] ⁺	285.11935	285.11943	-0.28		8.8E+06				1.4E+06		
251	Dihexyl maleic acid	C ₁₆ H ₂₈ O ₄	[M+H] ⁺	285.20604	285.20613	-0.33		2.6E+06						
252	Methoxy-hexadecenoic acid	C ₁₇ H ₃₂ O ₃	[M+H] ⁺	285.24242	285.24249	-0.23	2.6E+06	4.7E+06				5.3E+06	1.9E+06	1.3E+06
253	Stearic acid	C ₁₈ H ₃₆ O ₂	[M+H] ⁺	285.27881	285.27889	-0.27		4.4E+07				1.7E+06		
254	Buchananine	C ₁₂ H ₁₅ NO ₇	[M+H] ⁺	286.09213	286.09220	-0.26	1.7E+06		1.2E+06		1.5E+06			
255	Octenoylcarnitine	C ₁₅ H ₂₇ NO ₄	[M+H] ⁺	286.20128	286.20137	-0.30		1.3E+07						
256	Myristoylglycine	C ₁₆ H ₃₁ NO ₃	[M+H] ⁺	286.23767	286.23776	-0.31		2.9E+06						
257	C17 Sphingosine	C ₁₇ H ₃₅ NO ₂	[M+H] ⁺	286.27406	286.27414	-0.29		3.0E+07						

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258	Spisulosine	C ₁₈ H ₃₉ NO	[M+H] ⁺	286.31044	286.31051	-0.24		2.0E+06						
259	Dihydroxy-methoxyisoflavanone	C ₁₆ H ₁₄ O ₅	[M+H] ⁺	287.09140	287.09147	-0.24		2.0E+06						
260	Abscisic acid	C ₁₅ H ₂₀ O ₄	[M+Na] ⁺	287.12538	287.12556	-0.63		1.8E+06						
261	Hydroxy-oxo-hexadecanoic acid	C ₁₆ H ₃₀ O ₄	[M+H] ⁺	287.22169	287.22176	-0.26		2.2E+06						
262	Retinol	C ₂₀ H ₃₀ O	[M+H] ⁺	287.23694	287.23701	-0.24		1.3E+06						
263	Methoxyhexadecanoic acid	C ₁₇ H ₃₄ O ₃	[M+H] ⁺	287.25807	287.25817	-0.34		2.4E+06						
264	Prosopinine	C ₁₆ H ₃₃ NO ₃	[M+H] ⁺	288.25332	288.25338	-0.22	1.8E+06	1.8E+07				2.9E+06	1.3E+06	
265	C17 Sphinganine	C ₁₇ H ₃₇ NO ₂	[M+H] ⁺	288.28971	288.28979	-0.29		1.4E+07						
266	Methoxy-methylisoflavone	C ₁₇ H ₁₄ O ₃	[M+Na] ⁺	289.08352	289.08373	-0.75	2.2E+06	3.6E+06			2.3E+06		2.0E+06	
267	Tributyl phosphate	C ₁₂ H ₂₇ O ₄ P	[M+Na] ⁺	289.15392	289.15409	-0.60						3.8E+06		
268	Heptadecynoic acid	C ₁₇ H ₃₀ O ₂	[M+Na] ⁺	289.21380	289.21387	-0.24						1.4E+06		
269	Androstanedione	C ₁₉ H ₂₈ O ₂	[M+H] ⁺	289.21621	289.21627	-0.22						1.1E+06		
270	Flabellidine	C ₁₈ H ₂₈ N ₂ O	[M+H] ⁺	289.22744	289.22751	-0.24		1.3E+06						
271	Dihydroretinol	C ₂₀ H ₃₂ O	[M+H] ⁺	289.25259	289.25268	-0.30		2.7E+06						
272	Mannosylglycerate	C ₉ H ₁₆ O ₉	[M+Na] ⁺	291.06865	291.06873	-0.27	1.6E+06		2.0E+06		2.3E+06		1.4E+06	
273	Saphenic acid	C ₁₅ H ₁₂ N ₂ O ₃	[M+Na] ⁺	291.07401	291.07391	0.35							1.7E+06	
274	Hydroxybenzopyrene	C ₂₀ H ₁₂ O	[M+Na] ⁺	291.07804	291.07801	0.08	4.7E+06				4.5E+06		7.7E+06	
275	N-Succinyl-diaminopimelate	C ₁₁ H ₁₈ N ₂ O ₇	[M+H] ⁺	291.11868	291.11872	-0.15	1.4E+06							
276	Argininosuccinic acid	C ₁₀ H ₁₈ N ₄ O ₆	[M+H] ⁺	291.12991	291.12999	-0.27		1.4E+06						
277	Palmitolinoleic acid	C ₁₆ H ₂₈ O ₂	[M+K] ⁺	291.17209	291.17217	-0.28		1.3E+07						
278	Oxo-octadecadiynoic acid	C ₁₈ H ₂₆ O ₃	[M+H] ⁺	291.19547	291.19557	-0.34		4.1E+06						
279	Methyl-hexadecenoic acid	C ₁₇ H ₃₂ O ₂	[M+Na] ⁺	291.22945	291.22950	-0.18	1.5E+06			3.4E+06			6.4E+06	4.0E+06
280	Hydroxy-androstanone	C ₁₉ H ₃₀ O ₂	[M+H] ⁺	291.23186	291.23195	-0.32		1.3E+06						
281	Anhydro-N-acetylneuraminic acid	C ₁₁ H ₁₇ NO ₈	[M+H] ⁺	292.10269	292.10274	-0.17	3.7E+06				2.0E+06		1.4E+06	
282	Glucosyl-sn-glycerol	C ₉ H ₁₈ O ₈	[M+K] ⁺	293.06333	293.06339	-0.20	1.3E+06				1.2E+06			
283	Thiamylal	C ₁₂ H ₁₈ N ₂ O ₂ S	[M+K] ⁺	293.07206	293.07183	0.78			1.1E+06					
284	Hydroxy-methoxy-methylflavan	C ₁₇ H ₁₈ O ₃	[M+Na] ⁺	293.11482	293.11504	-0.77	2.5E+06	5.6E+06	2.0E+06		1.6E+06		2.4E+06	
285	Estrone	C ₁₈ H ₂₂ O ₂	[M+Na] ⁺	293.15120	293.15142	-0.75		3.4E+06						
286	Methyl-norandrosta-dienone	C ₁₉ H ₂₆ O	[M+Na] ⁺	293.18759	293.18782	-0.79				1.5E+06		3.5E+06		1.4E+06

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287	Keto palmitic acid	C ₁₆ H ₃₀ O ₃	[M+Na] ⁺	293.20872	293.20878	-0.23	2.7E+06			3.8E+06	1.4E+06	2.3E+06		3.7E+06	2.1E+06
288	Methyl palmitic acid	C ₁₇ H ₃₄ O ₂	[M+Na] ⁺	293.24510	293.24517	-0.22	3.1E+06			2.5E+06	4.8E+06	1.8E+06		3.4E+06	9.0E+06
289	Stearyl alcohol	C ₁₈ H ₃₈ O	[M+Na] ⁺	293.28149	293.28158	-0.32		2.4E+06							
290	N-Acetylmuramic acid	C ₁₁ H ₁₉ NO ₈	[M+H] ⁺	294.11834	294.11836	-0.06		1.5E+06							
291	2-(Carboxy-(methylammonio)propyl)-histidine	C ₁₁ H ₁₉ N ₄ O ₄	[M+Na] ⁺	294.12985	294.12963	0.74	2.0E+07				1.3E+07		1.6E+06		
292	Melosatin B	C ₁₉ H ₁₉ NO ₂	[M+H] ⁺	294.14886	294.14898	-0.42	3.5E+06		3.3E+06		2.3E+06				
293	Dihydrobunolol	C ₁₇ H ₂₇ NO ₃	[M+H] ⁺	294.20637	294.20645	-0.27		3.7E+06							
294	Ribose diphosphate	C ₅ H ₁₂ O ₁₀ P ₂	[M+H] ⁺	294.99785	294.99783	0.06						2.4E+06			
295	Dihydroxy-methoxyflavan	C ₁₆ H ₁₆ O ₄	[M+Na] ⁺	295.09408	295.09432	-0.81		3.0E+06							
296	Tuliposide B	C ₁₁ H ₁₈ O ₉	[M+H] ⁺	295.10236	295.10241	-0.17			3.0E+06				2.8E+06		
297	Aspartame	C ₁₄ H ₁₈ N ₂ O ₅	[M+H] ⁺	295.12885	295.12895	-0.35		2.4E+06							
298	Methallenestrilphenol	C ₁₇ H ₂₀ O ₃	[M+Na] ⁺	295.13047	295.13070	-0.80		3.6E+06							
299	(Butylbenzofuranyl)(hydroxyphenyl)ketone	C ₁₉ H ₁₈ O ₃	[M+H] ⁺	295.13287	295.13298	-0.37	2.6E+06		1.2E+06		2.0E+06				
300	Methyl-tetradecanedioic acid	C ₁₅ H ₂₈ O ₄	[M+Na] ⁺	295.18798	295.18806	-0.27						1.6E+06			
301	Palmitic acid	C ₁₆ H ₃₂ O ₂	[M+K] ⁺	295.20339	295.20346	-0.23				2.0E+06		3.2E+06			3.0E+06
302	Hydroxy palmitic acid	C ₁₆ H ₃₂ O ₃	[M+Na] ⁺	295.22437	295.22444	-0.24				8.8E+05		2.9E+06			
303	Hydroxylinolenic acid	C ₁₈ H ₃₀ O ₃	[M+H] ⁺	295.22677	295.22686	-0.30		4.2E+06				1.2E+06			
304	Methyl-octadecadienoic acid	C ₁₉ H ₃₄ O ₂	[M+H] ⁺	295.26316	295.26325	-0.32		1.8E+06							
305	Eicosenal	C ₂₀ H ₃₈ O	[M+H] ⁺	295.29954	295.29963	-0.30		1.7E+06							
306	Hydroxytetrahydrobiopterin	C ₉ H ₁₅ N ₅ O ₄	[M+K] ⁺	296.07556	296.07584	-0.93	1.4E+06				1.3E+06				
307	(d18:3)sphingosine	C ₁₈ H ₃₃ NO ₂	[M+H] ⁺	296.25841	296.25847	-0.22		4.8E+06							
308	Tetrahydroxyflavan	C ₁₅ H ₁₄ O ₅	[M+Na] ⁺	297.07334	297.07359	-0.83		2.4E+06							
309	Dihydroxy-dimethoxydihydrostilbene	C ₁₆ H ₁₈ O ₄	[M+Na] ⁺	297.10973	297.10997	-0.81		4.0E+06							
310	Hydroxytetradecanedioic acid	C ₁₄ H ₂₆ O ₅	[M+Na] ⁺	297.16724	297.16732	-0.25		5.1E+06				1.5E+06			
311	Dodecanoyl-sn-glycerol	C ₁₅ H ₃₀ O ₄	[M+Na] ⁺	297.20363	297.20373	-0.34		3.1E+06							
312	Hydroxy-octadecadienoic acid	C ₁₈ H ₃₂ O ₃	[M+H] ⁺	297.24242	297.24250	-0.26		7.4E+06				1.9E+06			
313	Methyl-octadecenoic acid	C ₁₉ H ₃₆ O ₂	[M+H] ⁺	297.27881	297.27887	-0.21		4.5E+06				1.2E+06			
314	Phytol	C ₂₀ H ₄₀ O	[M+H] ⁺	297.31519	297.31527	-0.26		2.9E+06							
315	Methylthioadenosine	C ₁₁ H ₁₅ N ₅ O ₃ S	[M+H] ⁺	298.09684	298.09690	-0.20	4.0E+06		4.9E+06		2.4E+06		2.8E+06		

ESI(+) FT-ICR MS														
No.	Plausible Compound ^a	Molecular formula (M)	Ion	Theor m/z ^b	Exp. m/z ^c	Δ ppm _d	SM _R H ^e	SM _R O ^e	SM _P H ^e	SM _P O ^e	TF _R H ^e	TF _R O ^e	TF _P H ^e	TF _P O ^e
316	Lycoflexine	C ₁₇ H ₂₅ NO ₂	[M+Na] ⁺	298.17775	298.17795	-0.68		1.4E+07	1.5E+06	1.7E+06			1.5E+06	
317	N-(oxododecanoyl) homoserine lactone	C ₁₆ H ₂₇ NO ₄	[M+H] ⁺	298.20128	298.20138	-0.32		3.9E+06						
318	Palmitoleoyl Ethanolamide	C ₁₈ H ₃₅ NO ₂	[M+H] ⁺	298.27406	298.27414	-0.28		3.7E+07						
319	Ranunculin	C ₁₁ H ₁₆ O ₈	[M+Na] ⁺	299.07374	299.07378	-0.14					1.6E+06			
320	Dihydroxy myristoic acid	C ₁₄ H ₂₈ O ₄	[M+K] ⁺	299.16192	299.16186	0.20						1.2E+06		1.3E+06
321	Heptadecenedioic acid	C ₁₇ H ₃₀ O ₄	[M+H] ⁺	299.22169	299.22180	-0.38		1.7E+06						
322	Oxooctadecanoic acid	C ₁₈ H ₃₄ O ₃	[M+H] ⁺	299.25807	299.25813	-0.19	2.8E+06	9.3E+06	2.4E+06	8.6E+05		5.4E+06	2.2E+06	1.4E+06
323	Methyl stearic acid	C ₁₉ H ₃₈ O ₂	[M+H] ⁺	299.29446	299.29452	-0.21		9.0E+06				1.3E+06		
324	Lycopsamine	C ₁₅ H ₂₅ NO ₅	[M+H] ⁺	300.18055	300.18064	-0.30		4.5E+06						
325	Coriamyrtin	C ₁₅ H ₁₈ O ₅	[M+Na] ⁺	301.10464	301.10486	-0.72		3.9E+06						
326	Panaxytriol	C ₁₇ H ₂₆ O ₃	[M+Na] ⁺	301.17742	301.17748	-0.21		4.6E+06		5.7E+05		2.9E+06		1.7E+06
327	Tetranor-trihydroxy-prostenoic acid	C ₁₆ H ₂₈ O ₅	[M+H] ⁺	301.20095	301.20098	-0.10		3.5E+06						
328	Methyl-hexadecanedioic acid	C ₁₇ H ₃₂ O ₄	[M+H] ⁺	301.23734	301.23742	-0.28		1.5E+06						
329	Hydroxystearic acid	C ₁₈ H ₃₆ O ₃	[M+H] ⁺	301.27372	301.27379	-0.23		2.0E+06						
330	Nocodazole	C ₁₄ H ₁₁ N ₃ O ₃ S	[M+H] ⁺	302.05939	302.05920	0.62					1.4E+06			
331	N-Acetyl-Glucosamine Phosphate	C ₈ H ₁₆ NO ₉ P	[M+H] ⁺	302.06354	302.06372	-0.57			1.6E+06		1.2E+06		1.2E+06	
332	Sphinganine	C ₁₈ H ₃₉ NO ₂	[M+H] ⁺	302.30536	302.30544	-0.28		2.6E+07						
333	Glyceryl tributyrat	C ₁₅ H ₂₆ O ₆	[M+H] ⁺	303.18022	303.18035	-0.45		2.0E+06						
334	Hydroxy-heptadecatrienoic acid	C ₁₇ H ₂₈ O ₃	[M+Na] ⁺	303.19307	303.19312	-0.18				7.7E+05		2.4E+06		1.5E+06
335	Linoleic acid	C ₁₈ H ₃₂ O ₂	[M+Na] ⁺	303.22945	303.22953	-0.25	1.8E+06		2.6E+06	2.6E+06			4.1E+06	2.9E+06
336	Retinyl ester	C ₂₀ H ₃₀ O ₂	[M+H] ⁺	303.23186	303.23192	-0.21		2.1E+06						
337	Hydroxyphenylacetylglutamic acid	C ₁₃ H ₁₅ NO ₆	[M+Na] ⁺	304.07916	304.07937	-0.71	6.7E+06		1.3E+07		5.9E+06		2.5E+06	
338	Vasconine	C ₁₇ H ₁₆ NO ₂	[M+K] ⁺	305.08126	305.08118	0.27					3.4E+06			
339	Randainol	C ₁₈ H ₁₈ O ₃	[M+Na] ⁺	305.11482	305.11500	-0.61		1.3E+06						
340	Dihydrophaseic acid	C ₁₅ H ₂₂ O ₅	[M+Na] ⁺	305.13594	305.13608	-0.44		3.0E+06						
341	Nopaline	C ₁₁ H ₂₀ N ₄ O ₆	[M+H] ⁺	305.14556	305.14566	-0.32		2.4E+06						
342	Epoxy-trimethyltrideca-dienoic acid	C ₁₆ H ₂₆ O ₃	[M+K] ⁺	305.15135	305.15144	-0.28		2.6E+06						
343	Dehydroretinal	C ₂₀ H ₂₆ O	[M+Na] ⁺	305.18759	305.18784	-0.83		4.1E+06						
344	Arachidonic acid	C ₂₀ H ₃₂ O ₂	[M+H] ⁺	305.24751	305.24758	-0.24		3.4E+06						

ESI(+) FT-ICR MS														
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345	Assoanine	C ₁₇ H ₁₇ NO ₂	[M+K] ⁺	306.08909	306.08900	0.29								1.7E+06
346	Dimethoxyflavanone	C ₁₇ H ₁₆ O ₄	[M+Na] ⁺	307.09408	307.09429	-0.68		2.3E+06						
347	Allogibberic acid	C ₁₈ H ₂₀ O ₃	[M+Na] ⁺	307.13047	307.13070	-0.76		2.7E+06						
348	Methylestra-tetraenediol	C ₁₉ H ₂₄ O ₂	[M+Na] ⁺	307.16685	307.16710	-0.81		1.2E+07						
349	Retinal	C ₂₀ H ₂₈ O	[M+Na] ⁺	307.20324	307.20341	-0.57						1.7E+06		
350	Stearic acid	C ₁₈ H ₃₆ O ₂	[M+Na] ⁺	307.26075	307.26082	-0.21	8.6E+06		5.7E+06		9.0E+06		8.9E+06	
351	Glutathione	C ₁₀ H ₁₇ N ₃ O ₆ S	[M+H] ⁺	308.09108	308.09114	-0.19	2.1E+06		1.8E+06		1.8E+06		1.7E+06	
352	Hydroxy-dimethoxyflavan	C ₁₇ H ₁₈ O ₄	[M+Na] ⁺	309.10973	309.10997	-0.78		6.8E+06						
353	Hydroxyestrone	C ₁₈ H ₂₂ O ₃	[M+Na] ⁺	309.14612	309.14636	-0.79		4.4E+06						
354	Fructoselysine	C ₁₂ H ₂₄ N ₂ O ₇	[M+H] ⁺	309.16563	309.16569	-0.19	2.8E+06		3.2E+06		2.4E+06		2.0E+06	
355	Boldenone	C ₁₉ H ₂₆ O ₂	[M+Na] ⁺	309.18250	309.18272	-0.72	2.1E+06	2.8E+07	2.9E+06		1.9E+06		2.3E+06	
356	Trifluoro-tetradecenyl acetate	C ₁₆ H ₂₇ F ₃ O ₂	[M+H] ⁺	309.20359	309.20370	-0.35		1.3E+07		1.1E+06	1.3E+06	2.4E+06	1.5E+06	1.5E+06
357	Methylembelin	C ₁₈ H ₂₈ O ₄	[M+H] ⁺	309.20604	309.20611	-0.24		2.8E+06						
358	Hydroxy-palmitic acid methyl ester	C ₁₇ H ₃₄ O ₃	[M+Na] ⁺	309.24002	309.24007	-0.18						2.4E+06		1.6E+06
359	Eicosadienoic acid	C ₂₀ H ₃₆ O ₂	[M+H] ⁺	309.27881	309.27891	-0.33		3.9E+06						
360	N-Acetyl-neuraminic acid	C ₁₁ H ₁₉ NO ₉	[M+H] ⁺	310.11326	310.11332	-0.20	2.7E+07	3.0E+06	9.1E+06		1.6E+07		5.1E+06	
361	Galanthamine	C ₁₇ H ₂₁ NO ₃	[M+Na] ⁺	310.14136	310.14160	-0.77	1.8E+06		1.4E+06	2.2E+06				
362	Procyclidine	C ₁₉ H ₂₉ NO	[M+Na] ⁺	310.21414	310.21438	-0.79		6.6E+06						
363	Prosopinine	C ₁₆ H ₃₃ NO ₃	[M+Na] ⁺	310.23526	310.23531	-0.15								1.7E+06
364	Dihydroxy-methoxy-isoflavanol	C ₁₆ H ₁₆ O ₅	[M+Na] ⁺	311.08899	311.08923	-0.76		4.2E+06						
365	Glutamyltyrosine	C ₁₄ H ₁₈ N ₂ O ₆	[M+H] ⁺	311.12376	311.12384	-0.25		3.2E+06						
366	Karwinaphthol B	C ₁₇ H ₂₀ O ₄	[M+Na] ⁺	311.12538	311.12565	-0.87		3.1E+06						
367	Ovalitenin B	C ₁₉ H ₁₈ O ₄	[M+H] ⁺	311.12779	311.12788	-0.30				9.4E+05				
368	Hydroxyestradiol	C ₁₈ H ₂₄ O ₃	[M+Na] ⁺	311.16177	311.16200	-0.75		2.7E+06						
369	Dimethyl-(methoxyphenyl)-ethyl-benzopyranol	C ₂₀ H ₂₂ O ₃	[M+H] ⁺	311.16417	311.16428	-0.35		4.9E+06						
370	Botrydial	C ₁₇ H ₂₆ O ₅	[M+H] ⁺	311.18530	311.18536	-0.19	2.1E+06				1.9E+06		1.6E+06	
371	Dihydroxy-palmitic acid	C ₁₆ H ₃₂ O ₄	[M+Na] ⁺	311.21928	311.21937	-0.29		5.4E+06						
372	Methoprene	C ₁₉ H ₃₄ O ₃	[M+H] ⁺	311.25807	311.25813	-0.20	1.7E+06	3.8E+06	1.6E+06			4.1E+06	1.9E+06	1.3E+06
373	Eicosenoic acid	C ₂₀ H ₃₈ O ₂	[M+H] ⁺	311.29446	311.29452	-0.20		5.5E+06				1.6E+06		

ESI(+) FT-ICR MS														
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374	Dyclonine	C ₁₈ H ₂₇ NO ₂	[M+Na] ⁺	312.19340	312.19362	-0.71				1.5E+06				
375	Methylvisamminol	C ₁₆ H ₁₈ O ₅	[M+Na] ⁺	313.10464	313.10487	-0.72		4.6E+06						
376	epi-Tulipinolide	C ₁₇ H ₂₂ O ₄	[M+Na] ⁺	313.14103	313.14126	-0.73		4.5E+06						
377	Sterculynic acid	C ₁₉ H ₃₀ O ₂	[M+Na] ⁺	313.21380	313.21397	-0.53	1.7E+06		1.8E+06			2.9E+06	1.8E+06	1.2E+06
378	Oxo-nonadecanoic acid	C ₁₉ H ₃₆ O ₃	[M+H] ⁺	313.27372	313.27379	-0.22	4.2E+06	8.0E+06	3.6E+06	1.5E+06	1.4E+06	1.2E+07	3.6E+06	1.8E+06
379	Arachidic acid	C ₂₀ H ₄₀ O ₂	[M+H] ⁺	313.31011	313.31018	-0.22		4.1E+06		7.4E+05		2.1E+06		
380	Heliotrine	C ₁₆ H ₂₇ NO ₅	[M+H] ⁺	314.19620	314.19629	-0.29		4.1E+06						
381	N-palmitoyl glycine	C ₁₈ H ₃₅ NO ₃	[M+H] ⁺	314.26897	314.26906	-0.28		3.3E+06						
382	Margaroyl-ethanolamine	C ₁₉ H ₃₉ NO ₂	[M+H] ⁺	314.30536	314.30544	-0.27		7.3E+06						
383	Amino-dimethyloctadecanol	C ₂₀ H ₄₃ NO	[M+H] ⁺	314.34174	314.34186	-0.38		2.5E+06						
384	Picrotoxinin	C ₁₅ H ₁₆ O ₆	[M+Na] ⁺	315.08391	315.08414	-0.73		2.2E+06						
385	Sugeonyl acetate	C ₁₇ H ₂₄ O ₃	[M+K] ⁺	315.13570	315.13580	-0.30	1.5E+06							
386	Gingerdione	C ₁₇ H ₂₄ O ₄	[M+Na] ⁺	315.15668	315.15678	-0.32		2.3E+06						1.5E+06
387	Hydroxysteroid	C ₁₉ H ₃₂ O ₂	[M+Na] ⁺	315.22945	315.22954	-0.28		2.5E+06						
388	Octadecanedioic acid	C ₁₈ H ₃₄ O ₄	[M+H] ⁺	315.25299	315.25307	-0.25		4.3E+06				2.2E+06		
389	Hydroxy-nonadecanoic acid	C ₁₉ H ₃₈ O ₃	[M+H] ⁺	315.28937	315.28944	-0.22		2.9E+06						
390	Eicosanediol	C ₂₀ H ₄₂ O ₂	[M+H] ⁺	315.32576	315.32584	-0.25		3.4E+06				1.8E+06		
391	Butoctamide hydrogen succinate	C ₁₆ H ₂₉ NO ₅	[M+H] ⁺	316.21185	316.21194	-0.29		1.8E+08						
392	Decanoylcarnitine	C ₁₇ H ₃₃ NO ₄	[M+H] ⁺	316.24824	316.24833	-0.30		1.7E+06						
393	Dehydrophytosphingosine	C ₁₈ H ₃₇ NO ₃	[M+H] ⁺	316.28462	316.28471	-0.30	1.2E+06	2.3E+07	2.5E+06			2.1E+06	1.6E+06	
394	(Butylbenzofuranyl)(hydroxyphenyl)ketone	C ₁₉ H ₁₈ O ₃	[M+Na] ⁺	317.11482	317.11503	-0.68		2.0E+07		2.0E+06		3.5E+06	4.1E+06	1.6E+06
395	[Ethyl-(methoxyphenyl)-pyrazolyl]phenol	C ₁₈ H ₁₈ N ₂ O ₂	[M+Na] ⁺	317.12605	317.12582	0.72						1.4E+06		
396	Docosahexaynoic acid	C ₂₂ H ₂₀ O ₂	[M+H] ⁺	317.15361	317.15370	-0.30						3.1E+06		
397	Methylptelefolonium	C ₁₈ H ₂₂ NO ₄	[M+H] ⁺	317.16216	317.16219	-0.08		4.4E+06				5.0E+06		
398	Phytuberin	C ₁₇ H ₂₆ O ₄	[M+Na] ⁺	317.17233	317.17241	-0.25		3.9E+06						
399	Methyl-octadecadienoic acid	C ₁₉ H ₃₄ O ₂	[M+Na] ⁺	317.24510	317.24513	-0.09						2.0E+06		
400	Propyl-androstenol	C ₂₂ H ₃₆ O	[M+H] ⁺	317.28389	317.28397	-0.25		9.4E+06				1.6E+06		
401	Nilutamide	C ₁₂ H ₁₀ F ₃ N ₃ O ₄	[M+H] ⁺	318.06962	318.06987	-0.80	3.5E+06				3.4E+06			
402	(R)-Prunasin	C ₁₄ H ₁₇ NO ₆	[M+Na] ⁺	318.09481	318.09499	-0.57			1.4E+06					

ESI(+) FT-ICR MS														
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403	Phytosphingosine	C ₁₈ H ₃₉ NO ₃	[M+H] ⁺	318.30027	318.30038	-0.34		3.3E+06						
404	Dimethoxy-methylflavone	C ₁₈ H ₁₆ O ₄	[M+Na] ⁺	319.09408	319.09432	-0.75		2.0E+06						
405	Deoxynivalenol	C ₁₅ H ₂₀ O ₆	[M+Na] ⁺	319.11521	319.11539	-0.57		2.9E+06						
406	Tocopheronic acid	C ₁₆ H ₂₄ O ₅	[M+Na] ⁺	319.15159	319.15181	-0.68		2.5E+06				1.5E+06		
407	Diethylstilbestrol dimethyl ether	C ₂₀ H ₂₄ O ₂	[M+Na] ⁺	319.16685	319.16709	-0.75		6.1E+06						
408	Methano-retinal	C ₂₁ H ₂₈ O	[M+Na] ⁺	319.20324	319.20350	-0.81		7.9E+07				2.4E+06		
409	Keto-octadecenoic acid	C ₁₈ H ₃₂ O ₃	[M+Na] ⁺	319.22437	319.22443	-0.21	1.6E+06		2.2E+06	1.9E+06	1.4E+06		4.0E+06	1.7E+06
410	Phenthoate	C ₁₂ H ₁₇ O ₄ PS ₂	[M+H] ⁺	321.03786	321.03803	-0.52					1.4E+06			
411	Doisynoesol	C ₁₉ H ₂₂ O ₃	[M+Na] ⁺	321.14612	321.14636	-0.76		1.9E+06						
412	Tetranor-oxo-dihydroxy-prostenoic acid	C ₁₆ H ₂₆ O ₅	[M+Na] ⁺	321.16724	321.16735	-0.33		4.1E+06						
413	Methyl-nor-pregnatrienol	C ₂₁ H ₃₀ O	[M+Na] ⁺	321.21889	321.21912	-0.72		1.2E+08				3.5E+06		1.3E+06
414	Keto stearic acid	C ₁₈ H ₃₄ O ₃	[M+Na] ⁺	321.24002	321.24008	-0.20					3.3E+06			
415	Methyl stearic acid	C ₁₉ H ₃₈ O ₂	[M+Na] ⁺	321.27640	321.27640	0.00			1.2E+06	1.6E+06				2.7E+06
416	Phytanol	C ₂₀ H ₄₂ O	[M+Na] ⁺	321.31279	321.31291	-0.38		1.6E+06						
417	Dihydroxy-methoxy-methylflavanone	C ₁₇ H ₁₆ O ₅	[M+Na] ⁺	323.08899	323.08922	-0.70		2.3E+06						
418	Trimethoxyflavan	C ₁₈ H ₂₀ O ₄	[M+Na] ⁺	323.12538	323.12564	-0.81		4.0E+06						
419	Methoxyestrone	C ₁₉ H ₂₄ O ₃	[M+Na] ⁺	323.16177	323.16202	-0.79		5.3E+06						
420	Retinoic acid	C ₂₀ H ₂₈ O ₂	[M+Na] ⁺	323.19815	323.19838	-0.71		8.9E+06						
421	MG(0:0/14:1/0:0)	C ₁₇ H ₃₂ O ₄	[M+Na] ⁺	323.21928	323.21935	-0.23	2.4E+06		2.7E+06	1.5E+06	2.8E+06	3.4E+06	3.3E+06	1.8E+06
422	Allylestrenol	C ₂₁ H ₃₂ O	[M+Na] ⁺	323.23454	323.23476	-0.68		4.4E+07		2.7E+06				3.6E+06
423	Hydroxystearic acid	C ₁₈ H ₃₆ O ₃	[M+Na] ⁺	323.25567	323.25575	-0.26				6.2E+05		2.1E+06		
424	Linoleoyl ethanolamide	C ₂₀ H ₃₇ NO ₂	[M+H] ⁺	324.28971	324.28978	-0.23		5.3E+06						
425	N-Glucosylnicotinate	C ₁₂ H ₁₆ NO ₇	[M+K] ⁺	325.05584	325.05554	0.91							4.5E+06	
426	Dihydroxy-dimethoxyflavan	C ₁₇ H ₁₈ O ₅	[M+Na] ⁺	325.10464	325.10488	-0.72		7.8E+06						
427	Fructofuranose dianhydride	C ₁₂ H ₂₀ O ₁₀	[M+H] ⁺	325.11292	325.11299	-0.22	2.4E+06	4.6E+06	4.1E+06		2.0E+06	1.4E+06	6.6E+06	
428	Ketoestriol	C ₁₈ H ₂₂ O ₄	[M+Na] ⁺	325.14103	325.14127	-0.74		3.6E+06						
429	Allethrin	C ₁₉ H ₂₆ O ₃	[M+Na] ⁺	325.17742	325.17765	-0.72		1.2E+07						
430	Hydroxy-hexadecandioic acid	C ₁₆ H ₃₀ O ₅	[M+Na] ⁺	325.19854	325.19860	-0.18		1.7E+07	1.4E+06	1.9E+06		3.7E+06		1.3E+06
431	3-Hydroxy-palmitic acid methyl ester	C ₁₇ H ₃₄ O ₃	[M+K] ⁺	325.21395	325.21390	0.17						1.9E+06		

ESI(+) FT-ICR MS														
No.	Plausible Compound ^a	Molecular formula (M)	Ion	Theor m/z ^b	Exp m/z ^c	Δppm ^d	SM _R H ^e	SM _R O ^e	SM _P H ^e	SM _P O ^e	TF _R H ^e	TF _R O ^e	TF _P H ^e	TF _P O ^e
432	MG(14:0/0:0/0:0)	C ₁₇ H ₃₄ O ₄	[M+Na] ⁺	325.23493	325.23499	-0.19	2.0E+06			1.3E+06	2.0E+06	4.3E+06		2.8E+06
433	Methyl-eicosenoic acid	C ₂₁ H ₄₀ O ₂	[M+H] ⁺	325.31011	325.31017	-0.19		1.6E+06						
434	Nitrolinoleic acid	C ₁₈ H ₃₁ NO ₄	[M+H] ⁺	326.23258	326.23266	-0.23		3.1E+06						
435	N-oleoyl ethanolamine	C ₂₀ H ₃₉ NO ₂	[M+H] ⁺	326.30536	326.30545	-0.29		1.1E+07						
436	Dihydroxy-prenyloxydihydrochalcone	C ₂₀ H ₂₂ O ₄	[M+H] ⁺	327.15909	327.15913	-0.14		1.3E+06						
437	Hydroxytestosterone	C ₁₉ H ₂₈ O ₃	[M+Na] ⁺	327.19307	327.19329	-0.69		4.8E+06						
438	Isoacitretin	C ₂₁ H ₂₆ O ₃	[M+H] ⁺	327.19547	327.19559	-0.35		2.9E+06				1.7E+06		
439	Arachidonic acid	C ₂₀ H ₃₂ O ₂	[M+Na] ⁺	327.22945	327.22954	-0.27						2.1E+06		
440	Methoxy-hydroxy-octadecadienoic acid	C ₁₉ H ₃₄ O ₄	[M+H] ⁺	327.25299	327.25312	-0.41		1.6E+06						
441	Oxo-eicosanoic acid	C ₂₀ H ₃₈ O ₃	[M+H] ⁺	327.28937	327.28945	-0.25	1.6E+06	3.4E+06	1.5E+06			3.2E+06	1.4E+06	
442	Methyl-eicosanoic acid	C ₂₁ H ₄₂ O ₂	[M+H] ⁺	327.32576	327.32585	-0.28		1.8E+06						
443	Carboxy-chromano	C ₁₈ H ₂₅ O ₄	[M+Na] ⁺	328.16450	328.16430	0.63	3.3E+06		2.6E+06		2.3E+06		3.3E+06	
444	Nitro-octadecenoic acid	C ₁₈ H ₃₃ NO ₄	[M+H] ⁺	328.24824	328.24834	-0.32		2.4E+06						
445	N-palmitoyl alanine	C ₁₉ H ₃₇ NO ₃	[M+H] ⁺	328.28462	328.28475	-0.39		1.8E+06						
446	Dimethylsphingosine	C ₂₀ H ₄₁ NO ₂	[M+H] ⁺	328.32101	328.32109	-0.26		1.4E+07						
447	Confertiflorin	C ₁₇ H ₂₂ O ₅	[M+Na] ⁺	329.13594	329.13618	-0.72		2.8E+06						
448	Dehydroreticuline	C ₁₉ H ₂₂ NO ₄	[M+H] ⁺	329.16216	329.16223	-0.21						1.7E+06		
449	Hydroxyandrosterone	C ₁₉ H ₃₀ O ₃	[M+Na] ⁺	329.20872	329.20885	-0.41		4.0E+06						
450	Icosatrienoic acid	C ₂₀ H ₃₄ O ₂	[M+Na] ⁺	329.24510	329.24518	-0.24		1.3E+07				2.0E+06		
451	MG(16:1/0:0/0:0)	C ₁₉ H ₃₆ O ₄	[M+H] ⁺	329.26864	329.26871	-0.23		8.4E+06		9.1E+05		4.9E+06		
452	Narciclasine	C ₁₄ H ₁₃ NO ₇	[M+Na] ⁺	330.05842	330.05864	-0.67	1.2E+07		7.9E+06		6.1E+06		3.4E+06	
453	Europine	C ₁₆ H ₂₇ NO ₆	[M+H] ⁺	330.19111	330.19124	-0.38		2.7E+06						
454	Keto-decanoylcarnitine	C ₁₇ H ₃₁ NO ₅	[M+H] ⁺	330.22750	330.22755	-0.15		6.8E+06						
455	Dimethylnonanoyl carnitine	C ₁₈ H ₃₅ NO ₄	[M+H] ⁺	330.26389	330.26398	-0.27		6.2E+06				2.3E+06		
456	Palmitoyl Serinol	C ₁₉ H ₃₉ NO ₃	[M+H] ⁺	330.30027	330.30036	-0.27		3.8E+06				1.7E+06		
457	N,N-dimethyl-Safingol	C ₂₀ H ₄₃ NO ₂	[M+H] ⁺	330.33666	330.33674	-0.25		1.3E+07		7.1E+05		4.0E+06		
458	Dihydroxy-(dimethyl-propenyl)chalcone	C ₂₀ H ₂₀ O ₃	[M+Na] ⁺	331.13047	331.13069	-0.68		2.0E+06				3.2E+06		
459	Gambirtannine	C ₂₁ H ₁₈ N ₂ O ₂	[M+H] ⁺	331.14410	331.14379	0.95			1.5E+06					
460	Gestrinone	C ₂₁ H ₂₄ O ₂	[M+Na] ⁺	331.16685	331.16706	-0.62		4.1E+06				1.7E+06		

ESI(+) FT-ICR MS														
No.	Plausible Compound ^a	Molecular formula (M)	Ion	Theor m/z ^b	Exp m/z ^c	Δ ppm ^d	SM _R H ^e	SM _R O ^e	SM _P H ^e	SM _P O ^e	TF _R H ^e	TF _R O ^e	TF _P H ^e	TF _P O ^e
461	Tetraphyllicine	C ₂₀ H ₂₄ N ₂ O	[M+Na] ⁺	331.17808	331.17783	0.77		5.0E+06				7.2E+06		
462	Methylembelin	C ₁₈ H ₂₈ O ₄	[M+Na] ⁺	331.18798	331.18803	-0.14						2.4E+06		1.7E+06
463	Methyl-epoxy-octadecadienoate	C ₁₉ H ₃₂ O ₃	[M+Na] ⁺	331.22437	331.22448	-0.33		2.7E+06				2.0E+06		
464	Eicosadienoic acid	C ₂₀ H ₃₆ O ₂	[M+Na] ⁺	331.26075	331.26082	-0.22				2.6E+06		2.5E+07		1.5E+06
465	Hydroxy-pentanorvitamin D3	C ₂₂ H ₃₄ O ₂	[M+H] ⁺	331.26316	331.26324	-0.24		5.4E+06				3.5E+06		
466	MG(16:0/0:0/0:0)	C ₁₉ H ₃₈ O ₄	[M+H] ⁺	331.28429	331.28437	-0.25		7.8E+06		9.6E+05		8.1E+06	1.5E+06	
467	Geranylgeranylacetone	C ₂₃ H ₃₈ O	[M+H] ⁺	331.29954	331.29959	-0.14						2.0E+06		
468	Melochinone	C ₂₂ H ₂₁ NO ₂	[M+H] ⁺	332.16451	332.16449	0.05						1.4E+06		
469	Pentahydroxy-methoxyflavone	C ₁₆ H ₁₂ O ₈	[M+H] ⁺	333.06049	333.06062	-0.38	2.3E+06				2.7E+06			
470	Cinnamoyl glucoside	C ₁₅ H ₁₈ O ₇	[M+Na] ⁺	333.09447	333.09470	-0.68						1.5E+06		
471	Sanguinarine	C ₂₀ H ₁₄ NO ₄	[M+H] ⁺	333.09956	333.09964	-0.24			1.9E+06					
472	Dihydrocordoin	C ₂₀ H ₂₂ O ₃	[M+Na] ⁺	333.14612	333.14624	-0.37				6.2E+05		2.8E+06	1.2E+06	
473	Dihydro-oxo-phytoenoic acid	C ₁₈ H ₃₀ O ₃	[M+K] ⁺	333.18265	333.18272	-0.20		6.3E+06				2.6E+06		
474	apo-Carotenal	C ₂₂ H ₃₀ O	[M+Na] ⁺	333.21889	333.21912	-0.70		5.7E+06				7.5E+06		
475	Eicosenoic acid	C ₂₀ H ₃₈ O ₂	[M+Na] ⁺	333.27640	333.27650	-0.28				2.7E+06			2.8E+06	
476	Docosatetraenoic acid	C ₂₂ H ₃₆ O ₂	[M+H] ⁺	333.27881	333.27887	-0.20		4.9E+06		9.3E+05		4.1E+06		
477	Xylopine	C ₁₈ H ₁₇ NO ₃	[M+K] ⁺	334.08400	334.08372	0.85					1.4E+06			
478	Hydroxy-methoxyestratriene-carbonitrile	C ₂₀ H ₂₅ NO ₂	[M+Na] ⁺	334.17775	334.17803	-0.84		2.0E+07						
479	Hydroxycinnamyl alcohol glucoside	C ₁₅ H ₂₀ O ₇	[M+Na] ⁺	335.11012	335.11032	-0.59		3.0E+06				2.2E+06		
480	Prenyloxyresveratrol	C ₁₉ H ₂₀ O ₄	[M+Na] ⁺	335.12538	335.12550	-0.34		2.8E+06				1.9E+06		
481	Phenylalanylphenylalanine	C ₁₈ H ₂₀ N ₂ O ₃	[M+Na] ⁺	335.13661	335.13636	0.76						1.6E+06		
482	Triphenyl-hexene	C ₂₄ H ₂₄	[M+Na] ⁺	335.17702	335.17710	-0.22				1.4E+06		1.8E+06		
483	Pregna-dienedione	C ₂₁ H ₂₈ O ₂	[M+Na] ⁺	335.19815	335.19838	-0.68		1.7E+07	1.7E+06	8.5E+05		9.9E+06	1.9E+06	
484	Dihydroxyoctadecadienoic acid	C ₁₈ H ₃₂ O ₄	[M+Na] ⁺	335.21928	335.21935	-0.21				1.2E+06		7.2E+06	1.5E+06	
485	Phytol	C ₂₀ H ₄₀ O	[M+K] ⁺	335.27108	335.27113	-0.16						1.5E+06		
486	Arachidic acid	C ₂₀ H ₄₀ O ₂	[M+Na] ⁺	335.29205	335.29211	-0.18								2.6E+06
487	Dimethyl-eicosatrienoic acid	C ₂₂ H ₃₈ O ₂	[M+H] ⁺	335.29446	335.29452	-0.19						1.9E+06		
488	N-palmitoyl glycine	C ₁₈ H ₃₅ NO ₃	[M+Na] ⁺	336.25091	336.25097	-0.16						1.8E+06		
489	Trimethoxyflavanone	C ₁₈ H ₁₈ O ₅	[M+Na] ⁺	337.10464	337.10483	-0.55		3.2E+06				1.6E+06		

ESI(+) FT-ICR MS														
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490	Dehydro-gibberellin A9	C ₁₉ H ₂₂ O ₄	[M+Na] ⁺	337.14103	337.14126	-0.68		2.4E+06				1.5E+06		
491	oxo-Retinoic acid	C ₂₀ H ₂₆ O ₃	[M+Na] ⁺	337.17742	337.17763	-0.62		3.0E+06				1.7E+06		
492	Methyl-retro-retinoic acid	C ₂₁ H ₃₀ O ₂	[M+Na] ⁺	337.21380	337.21402	-0.65	2.8E+06	2.9E+07	3.2E+06	1.5E+06	2.4E+06	1.5E+07	2.2E+06	
493	Dihydroxyoctadecenoic acid	C ₁₈ H ₃₄ O ₄	[M+Na] ⁺	337.23493	337.23500	-0.21	1.7E+06		2.0E+06	2.0E+06	1.5E+06		2.8E+06	1.8E+06
494	Hydroxy-nonadecanoic acid	C ₁₉ H ₃₈ O ₃	[M+Na] ⁺	337.27132	337.27141	-0.28				6.0E+05		2.9E+06		
495	Eicosanediol	C ₂₀ H ₄₂ O ₂	[M+Na] ⁺	337.30770	337.30773	-0.09								1.7E+06
496	Eicosadienyl acetate	C ₂₂ H ₄₀ O ₂	[M+H] ⁺	337.31011	337.31016	-0.16						1.8E+06		
497	Rosinidin	C ₁₇ H ₁₅ O ₆	[M+Na] ⁺	338.07608	338.07592	0.48			1.5E+06					
498	Ficine	C ₂₀ H ₁₉ NO ₄	[M+H] ⁺	338.13868	338.13865	0.10						1.8E+06		
499	Pentadecanoylglycine	C ₁₇ H ₃₃ NO ₃	[M+K] ⁺	338.20920	338.20922	-0.05						1.6E+06		
500	Dehydrophytosphingosine	C ₁₈ H ₃₇ NO ₃	[M+Na] ⁺	338.26656	338.26666	-0.28				8.5E+05				
501	Hydroxy-trimethoxyflavan	C ₁₈ H ₂₀ O ₅	[M+Na] ⁺	339.12029	339.12051	-0.64						2.1E+06		
502	Gibberellin A9	C ₁₉ H ₂₄ O ₄	[M+Na] ⁺	339.15668	339.15692	-0.69		5.8E+06				3.4E+06		
503	Dihydroxy-methylandrostadienone	C ₂₀ H ₂₈ O ₃	[M+Na] ⁺	339.19307	339.19328	-0.63		8.1E+06	1.5E+06	8.7E+05	1.6E+06	8.3E+06		
504	Hydroxypregnenone	C ₂₁ H ₃₂ O ₂	[M+Na] ⁺	339.22945	339.22966	-0.62		5.5E+06				2.9E+06		
505	Dihydroxy stearic acid	C ₁₈ H ₃₆ O ₄	[M+Na] ⁺	339.25058	339.25064	-0.19	1.8E+06		2.8E+06	2.5E+06	1.6E+06		5.4E+06	1.8E+06
506	Propylandrostenol	C ₂₂ H ₃₆ O	[M+Na] ⁺	339.26584	339.26591	-0.23		1.1E+07		3.8E+06		9.4E+06		
507	Hexadecyl-sn-glycerol	C ₁₉ H ₄₀ O ₃	[M+Na] ⁺	339.28697	339.28705	-0.25		2.7E+06				3.0E+06		
508	Docosenoic acid	C ₂₂ H ₄₂ O ₂	[M+H] ⁺	339.32576	339.32581	-0.16		2.2E+06				2.9E+06		
509	S-Sulfanylgutathione	C ₁₀ H ₁₇ N ₃ O ₆ S ₂	[M+H] ⁺	340.06315	340.06328	-0.36	1.6E+06		1.9E+06		2.0E+06		1.6E+06	
510	N-oleoyl glycine	C ₂₀ H ₃₇ NO ₃	[M+H] ⁺	340.28462	340.28467	-0.15		3.6E+06				1.6E+06		
511	Docosanamide	C ₂₂ H ₄₅ NO	[M+H] ⁺	340.35739	340.35746	-0.19		9.9E+06		3.4E+06		6.5E+06		
512	Trihydroxy-dimethoxyisoflavan	C ₁₇ H ₁₈ O ₆	[M+Na] ⁺	341.09956	341.09981	-0.72		2.5E+06				1.6E+06		
513	Zearalenone	C ₁₈ H ₂₂ O ₅	[M+Na] ⁺	341.13594	341.13618	-0.69		6.5E+06				3.1E+06		
514	Ubiquinone Q2	C ₁₉ H ₂₆ O ₄	[M+Na] ⁺	341.17233	341.17242	-0.28	2.3E+06	2.3E+07	1.8E+06			1.4E+07	2.1E+06	
515	Menthyl O-beta-D-glucoside	C ₁₆ H ₃₀ O ₆	[M+Na] ⁺	341.19346	341.19354	-0.24		4.2E+06						
516	Methantheline	C ₂₁ H ₂₆ NO ₃	[M+H] ⁺	341.19855	341.19858	-0.11	1.9E+06				2.1E+06		1.5E+06	4.4E+06
517	Hydroxy-sacculatadienedial	C ₂₀ H ₃₀ O ₃	[M+Na] ⁺	341.20872	341.20892	-0.60		1.3E+07		1.3E+06		9.0E+06		
518	Canrenone	C ₂₂ H ₂₈ O ₃	[M+H] ⁺	341.21112	341.21120	-0.23		3.8E+06				2.3E+06		

ESI(+) FT-ICR MS														
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519	Pregnanolone	C ₂₁ H ₃₄ O ₂	[M+Na] ⁺	341.24510	341.24527	-0.48				1.3E+06		5.1E+06		
520	Oxo-heneicosanoic acid	C ₂₁ H ₄₀ O ₃	[M+H] ⁺	341.30502	341.30509	-0.20		2.8E+06				3.7E+06		
521	Methyl-heneicosanoic acid	C ₂₂ H ₄₄ O ₂	[M+H] ⁺	341.34141	341.34147	-0.17		3.8E+06		1.3E+06		6.0E+06		
522	Lactosamine	C ₁₂ H ₂₃ NO ₁₀	[M+H] ⁺	342.13947	342.13954	-0.20		1.8E+06						
523	Carboxy-chromanol	C ₁₉ H ₂₇ O ₄	[M+Na] ⁺	342.18016	342.17996	0.57	3.8E+06		2.4E+06		3.8E+06		4.0E+06	
524	Acetyllycopsamine	C ₁₇ H ₂₇ NO ₆	[M+H] ⁺	342.19111	342.19116	-0.13		3.0E+06						
525	Dodecenoylcarnitine	C ₁₉ H ₃₅ NO ₄	[M+H] ⁺	342.26389	342.26395	-0.18		2.4E+06				1.9E+06		
526	N-stearoyl glycine	C ₂₀ H ₃₉ NO ₃	[M+H] ⁺	342.30027	342.30033	-0.17		2.0E+06				1.7E+06		
527	Arctolide	C ₁₇ H ₂₀ O ₆	[M+Na] ⁺	343.11521	343.11542	-0.60		4.1E+06				2.4E+06		
528	Lactose	C ₁₂ H ₂₂ O ₁₁	[M+H] ⁺	343.12349	343.12355	-0.17	2.2E+06	3.8E+06	2.3E+06			1.7E+06	4.6E+06	
529	alpha-Zearalenol	C ₁₈ H ₂₄ O ₅	[M+Na] ⁺	343.15159	343.15183	-0.69		2.4E+06						
530	Phaseollidin hydrate	C ₂₀ H ₂₂ O ₅	[M+H] ⁺	343.15400	343.15406	-0.17		1.6E+06						
531	Hydroxyarachidonic acid	C ₂₀ H ₃₂ O ₃	[M+Na] ⁺	343.22437	343.22447	-0.30		3.0E+06				2.1E+06		
532	Dimethyl-androstanediol	C ₂₁ H ₃₆ O ₂	[M+Na] ⁺	343.26075	343.26084	-0.26		3.4E+06				2.5E+06		
533	Tetrahydroxy-prostaene	C ₂₀ H ₃₈ O ₄	[M+H] ⁺	343.28429	343.28432	-0.10		2.5E+06				4.5E+06		
534	MG(P-18:0e/0:0/0:0)	C ₂₁ H ₄₂ O ₃	[M+H] ⁺	343.32067	343.32071	-0.11						2.2E+06		
535	N-palmitoyl serine	C ₁₉ H ₃₇ NO ₄	[M+H] ⁺	344.27954	344.27959	-0.16		3.9E+06				2.8E+06		
536	epi-Tulipinolide diepoxide	C ₁₇ H ₂₂ O ₆	[M+Na] ⁺	345.13086	345.13106	-0.57		3.4E+06				2.1E+06		
537	Quinidinone	C ₂₀ H ₂₂ N ₂ O ₂	[M+Na] ⁺	345.15735	345.15711	0.69	1.3E+06	4.7E+06	1.7E+06	7.2E+05		7.2E+06	1.7E+06	1.5E+06
538	Tetracosahexaynoic acid	C ₂₄ H ₂₄ O ₂	[M+H] ⁺	345.18491	345.18499	-0.24						2.2E+06		
539	Gingerol	C ₁₉ H ₃₀ O ₄	[M+Na] ⁺	345.20363	345.20369	-0.17						1.4E+06		
540	Lamtidine	C ₁₈ H ₂₈ N ₆ O	[M+H] ⁺	345.23974	345.24005	-0.89		5.7E+06				3.1E+06		
541	Heneicosadienoic acid	C ₂₁ H ₃₈ O ₂	[M+Na] ⁺	345.27640	345.27647	-0.18		2.5E+06				2.2E+06		
542	Dihydroxy arachidic acid	C ₂₀ H ₄₀ O ₄	[M+H] ⁺	345.29994	345.29994	-0.01		3.5E+06				2.6E+06		
543	Portulacaxanthin I	C ₁₄ H ₁₆ N ₂ O ₇	[M+Na] ⁺	347.08497	347.08519	-0.62	1.2E+07		2.1E+07		1.1E+07		2.9E+06	
544	Oxo-dihydroxy-octadecatrienoic acid	C ₁₈ H ₂₈ O ₅	[M+Na] ⁺	347.18289	347.18309	-0.55		3.3E+06				2.5E+06		
545	Docosatetraynoic acid	C ₂₂ H ₂₈ O ₂	[M+Na] ⁺	347.19815	347.19839	-0.69		2.5E+06						
546	Methyl hydroperoxy-octadecatrienoate	C ₁₉ H ₃₂ O ₄	[M+Na] ⁺	347.21928	347.21933	-0.14						1.7E+06		
547	Propano-retinal	C ₂₃ H ₃₂ O	[M+Na] ⁺	347.23454	347.23475	-0.62		2.1E+07		6.3E+05		1.2E+07		

ESI(+) FT-ICR MS														
No.	Plausible Compound ^a	Molecular formula (M)	Ion	Theor m/z ^b	Exp. m/z ^c	Δ ppm _d	SM _R H ^e	SM _R O ^e	SM _P H ^e	SM _P O ^e	TF _R H ^e	TF _R O ^e	TF _P H ^e	TF _P O ^e
548	Heneicosenoic acid	C ₂₁ H ₄₀ O ₂	[M+Na] ⁺	347.29205	347.29212	-0.20				7.6E+05				
549	Pancratistatin	C ₁₄ H ₁₅ NO ₈	[M+Na] ⁺	348.06899	348.06918	-0.56	1.1E+07		6.1E+06		7.9E+06		1.7E+06	
550	Deoxyguanosine monophosphate	C ₁₀ H ₁₄ N ₅ O ₇ P	[M+H] ⁺	348.07036	348.07041	-0.14	8.5E+06		4.2E+06		5.7E+06	1.6E+06	3.6E+06	
551	O-beta-D-Glucosyl-hydroxycinnamate	C ₁₅ H ₁₈ O ₈	[M+Na] ⁺	349.08939	349.08946	-0.21			1.6E+06		1.7E+06			
552	Trihydroxy-prenyldihydrochalcone	C ₂₀ H ₂₂ O ₄	[M+Na] ⁺	349.14103	349.14123	-0.57	4.0E+06		3.1E+06	1.7E+06	3.3E+06	1.6E+07	2.7E+06	
553	Caribine	C ₁₉ H ₂₂ N ₂ O ₃	[M+Na] ⁺	349.15226	349.15200	0.75						2.2E+06		
554	Dinor-iso prostaglandin F2	C ₁₈ H ₃₀ O ₅	[M+Na] ⁺	349.19854	349.19864	-0.26		3.7E+06				2.0E+06		
555	Methyl-eicosanoic acid	C ₂₁ H ₄₂ O ₂	[M+Na] ⁺	349.30770	349.30776	-0.15				1.7E+06		8.7E+06		
556	Biperiden	C ₂₁ H ₂₉ NO	[M+K] ⁺	350.18807	350.18775	0.93								1.6E+06
557	Dihomo-gamma-Linolenoyl ethanolamide Succinyl-enolpyruvyl-hydroxy-cyclohexene-carboxylate	C ₂₂ H ₃₉ NO ₂	[M+H] ⁺	350.30536	350.30539	-0.10		3.9E+06				2.8E+06		
558		C ₁₄ H ₁₆ O ₉	[M+Na] ⁺	351.06865	351.06886	-0.59			1.5E+06		1.6E+06		2.3E+06	
559	Hydroxy-dioxotetranorprostanedioic acid	C ₁₆ H ₂₄ O ₇	[M+Na] ⁺	351.14142	351.14163	-0.59		2.1E+06						
560	Triphenyl-hexene	C ₂₄ H ₂₄	[M+K] ⁺	351.15096	351.15084	0.34								1.8E+06
561	Crocetin	C ₂₀ H ₂₄ O ₄	[M+Na] ⁺	351.15668	351.15688	-0.57		3.1E+06				2.1E+06		
562	Dihydroxypregnatrienone	C ₂₁ H ₂₈ O ₃	[M+Na] ⁺	351.19307	351.19328	-0.60		9.7E+06				4.1E+06		
563	Hydroperoxy-epoxy-octadecenoic acid	C ₁₈ H ₃₂ O ₅	[M+Na] ⁺	351.21419	351.21427	-0.21		7.5E+06		1.3E+06				
564	Retinol Acetate	C ₂₂ H ₃₂ O ₂	[M+Na] ⁺	351.22945	351.22963	-0.50		4.1E+06				3.1E+06		
565	MG(16:1/0:0/0:0)	C ₁₉ H ₃₆ O ₄	[M+Na] ⁺	351.25058	351.25065	-0.19	7.1E+06		8.1E+06		5.8E+06		1.2E+07	4.0E+06
566	Hydroxy-eicosanoic acid	C ₂₀ H ₄₀ O ₃	[M+Na] ⁺	351.28697	351.28700	-0.10						2.7E+06		
567	Ochotensine	C ₂₁ H ₂₁ NO ₄	[M+H] ⁺	352.15433	352.15431	0.07				1.1E+06		3.0E+06		
568	Anandamide (20:2, n-6)	C ₂₂ H ₄₁ NO ₂	[M+H] ⁺	352.32101	352.32106	-0.16		8.8E+06		9.8E+05		3.9E+06		
569	Gibberellin A5	C ₁₉ H ₂₂ O ₅	[M+Na] ⁺	353.13594	353.13615	-0.57		2.7E+06				1.5E+06		
570	Epiiridodial glucoside	C ₁₆ H ₂₆ O ₇	[M+Na] ⁺	353.15707	353.15717	-0.27						1.9E+06		
571	Dicyclohexyl phthalate	C ₂₀ H ₂₆ O ₄	[M+Na] ⁺	353.17233	353.17256	-0.64		3.1E+06				2.3E+06		
572	Octadecanedioic acid	C ₁₈ H ₃₄ O ₄	[M+K] ⁺	353.20887	353.20893	-0.17		1.4E+07		6.9E+05		7.4E+06		
573	Trihydroxy-octadecenoic acid	C ₁₈ H ₃₄ O ₅	[M+Na] ⁺	353.22984	353.22990	-0.17	2.0E+06	1.7E+07		3.4E+06		1.7E+07	2.2E+06	
574	MG(16:0/0:0/0:0)	C ₁₉ H ₃₈ O ₄	[M+Na] ⁺	353.26623	353.26629	-0.17	1.3E+07		1.7E+07		1.5E+07			5.4E+06
575	Eicosanediol	C ₂₀ H ₄₂ O ₂	[M+K] ⁺	353.28164	353.28170	-0.17				1.0E+06				

ESI(+) FT-ICR MS														
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576	Tetracosanal	C ₂₄ H ₄₈ O	[M+H] ⁺	353.37779	353.37779	0.01						1.8E+06		
577	C16 Sphinganine-phosphate	C ₁₆ H ₃₆ NO ₅ P	[M+H] ⁺	354.24039	354.24055	-0.46		4.8E+06				5.9E+06		
578	N-oleoyl alanine	C ₂₁ H ₃₉ NO ₃	[M+H] ⁺	354.30027	354.30035	-0.21		7.8E+06				1.9E+06		
579	Anandamide (20:l, n-9)	C ₂₂ H ₄₃ NO ₂	[M+H] ⁺	354.33666	354.33670	-0.12		1.0E+07				3.3E+06		
580	Dihydroxy-trimethoxydihydrochalcone	C ₁₈ H ₂₀ O ₆	[M+Na] ⁺	355.11521	355.11542	-0.59		2.5E+06				1.6E+06		
581	Dehydro-fluoro-oxotestololactone	C ₁₉ H ₂₁ FO ₄	[M+Na] ⁺	355.13161	355.13165	-0.13		3.5E+06		8.9E+05		3.3E+06		
582	Gibberellin A20	C ₁₉ H ₂₄ O ₅	[M+Na] ⁺	355.15159	355.15182	-0.62		9.9E+06				7.1E+06		
583	Hydroxytridecane-tricarboxylate	C ₁₆ H ₂₈ O ₇	[M+Na] ⁺	355.17272	355.17277	-0.13						1.8E+06		
584	Hydroxyprogesterone	C ₂₀ H ₂₈ O ₄	[M+Na] ⁺	355.18798	355.18818	-0.57		8.7E+06		8.2E+05		5.7E+06		
585	Dihydroxy stearic acid	C ₁₈ H ₃₆ O ₄	[M+K] ⁺	355.22452	355.22455	-0.09	1.5E+06	1.0E+07		1.0E+06		9.9E+06	2.2E+06	
586	Etretinate	C ₂₃ H ₃₀ O ₃	[M+H] ⁺	355.22677	355.22686	-0.25		8.2E+06		3.5E+06		5.5E+06	2.5E+06	4.1E+06
587	Hydroxy-dihydroxy-stearic acid	C ₁₈ H ₃₆ O ₅	[M+Na] ⁺	355.24549	355.24556	-0.19		2.8E+06		7.4E+05		2.2E+06		
588	MG(18:2/0:0/0:0)	C ₂₁ H ₃₈ O ₄	[M+H] ⁺	355.28429	355.28435	-0.17		2.1E+06				2.2E+06		
589	Oxo-docosanoic acid	C ₂₂ H ₄₂ O ₃	[M+H] ⁺	355.32067	355.32074	-0.20		2.4E+06		8.9E+05		2.7E+06		
590	Methyl-docosanoic acid	C ₂₃ H ₄₆ O ₂	[M+H] ⁺	355.35706	355.35713	-0.19				7.3E+05		3.8E+06		
591	N-palmitoyl valine	C ₂₁ H ₄₁ NO ₃	[M+H] ⁺	356.31592	356.31599	-0.19						2.0E+06		
592	Eicosanoyl-ethanolamine	C ₂₂ H ₄₅ NO ₂	[M+H] ⁺	356.35231	356.35238	-0.19		6.1E+06				2.9E+06		
593	Melanin	C ₁₈ H ₁₀ N ₂ O ₄	[M+K] ⁺	357.02722	357.02713	0.24					1.9E+06			
594	Glutathione episulfonium ion	C ₁₂ H ₂₀ N ₃ O ₆ S	[M+Na] ⁺	357.09650	357.09633	0.50	3.8E+06		2.4E+06		3.9E+06		3.9E+06	
595	Vinorine	C ₂₁ H ₂₂ N ₂ O ₂	[M+Na] ⁺	357.15735	357.15707	0.78						1.0E+07		
596	Fluoro-dihydroxy-methylandrosta-dienone	C ₂₀ H ₂₇ FO ₃	[M+Na] ⁺	357.18364	357.18357	0.21		2.5E+06						
597	Asterogenol	C ₂₁ H ₃₄ O ₃	[M+Na] ⁺	357.24002	357.24024	-0.62	1.7E+06	1.8E+07		1.4E+06		1.4E+07	1.7E+06	
598	Docosatrienoic acid	C ₂₂ H ₃₈ O ₂	[M+Na] ⁺	357.27640	357.27648	-0.22				7.4E+05				
599	MG(0:0/18:1/0:0)	C ₂₁ H ₄₀ O ₄	[M+H] ⁺	357.29994	357.30001	-0.19		3.8E+06				4.5E+06		
600	N-palmitoyl threonine	C ₂₀ H ₃₉ NO ₄	[M+H] ⁺	358.29519	358.29526	-0.21		8.0E+06				3.5E+06	1.5E+06	
601	S-Nitrosoglutathione	C ₁₀ H ₁₆ N ₄ O ₇ S	[M+Na] ⁺	359.06319	359.06299	0.57	3.2E+06				2.9E+06			
602	Catharanthine	C ₂₁ H ₂₄ N ₂ O ₂	[M+Na] ⁺	359.17300	359.17273	0.75	6.2E+06	1.4E+07	6.5E+06	2.8E+06	4.8E+06	2.1E+07	6.5E+06	1.1E+07
603	Dihydroxy-eicosatetraenoic acid	C ₂₀ H ₃₂ O ₄	[M+Na] ⁺	359.21928	359.21932	-0.11						1.7E+06		
604	Docosadienoic acid	C ₂₂ H ₄₀ O ₂	[M+Na] ⁺	359.29205	359.29212	-0.19		6.7E+06						

ESI(+) FT-ICR MS														
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605	MG(0:0/18:0/0:0)	C ₂₁ H ₄₂ O ₄	[M+H] ⁺	359.31559	359.31564	-0.15		2.2E+06				4.0E+06		
606	Benzyl viologen	C ₂₄ H ₂₂ N ₂	[M+Na] ⁺	361.16752	361.16723	0.80		1.0E+07				1.1E+07		
607	Dimethoxy-prenylflavan	C ₂₂ H ₂₆ O ₃	[M+Na] ⁺	361.17742	361.17763	-0.59		2.5E+06						
608	Tetrahydroxyandrostanone	C ₁₉ H ₃₀ O ₅	[M+Na] ⁺	361.19854	361.19864	-0.26						2.1E+06		
609	Dihydroxy-eicosatrienoic acid	C ₂₀ H ₃₄ O ₄	[M+Na] ⁺	361.23493	361.23498	-0.12		3.0E+06				2.9E+06		
610	Cyclopentadienylidene-androstanol	C ₂₄ H ₃₄ O	[M+Na] ⁺	361.25019	361.25036	-0.48		2.4E+06				1.7E+06		
611	Clofilium	C ₂₁ H ₃₇ ClN	[M+Na] ⁺	361.25067	361.25041	0.73		2.4E+06						
612	Docosenoic acid	C ₂₂ H ₄₂ O ₂	[M+Na] ⁺	361.30770	361.30775	-0.13				1.1E+06				
613	Docosanamide	C ₂₂ H ₄₅ NO	[M+Na] ⁺	362.33934	362.33937	-0.09								1.4E+06
614	Uridine monophosphate	C ₉ H ₁₃ N ₂ O ₉ P	[M+K] ⁺	362.99903	362.99908	-0.15	1.8E+06							
615	Neobanol	C ₁₈ H ₁₂ O ₆	[M+Na] ⁺	363.02655	363.02645	0.28	4.9E+06		2.1E+06		2.9E+06		2.1E+06	
616	Chelirubine	C ₂₁ H ₁₆ NO ₅	[M+H] ⁺	363.11012	363.11045	-0.90	1.2E+07		1.7E+07		1.4E+07		8.1E+06	
617	Dihydroxy-methoxy-prenyldihydrochalcone	C ₂₁ H ₂₄ O ₄	[M+Na] ⁺	363.15668	363.15688	-0.55		1.7E+06						
618	Hydroxyquinine	C ₂₀ H ₂₄ N ₂ O ₃	[M+Na] ⁺	363.16791	363.16765	0.74		4.5E+06				5.1E+06	1.5E+06	1.8E+06
619	Epoxy-fluoro-hydroxypregnenedione	C ₂₁ H ₂₇ FO ₄	[M+H] ⁺	363.19661	363.19649	0.34				2.4E+06		3.2E+06		2.4E+06
620	Hydroxy-eicosadienoic acid	C ₂₀ H ₃₆ O ₃	[M+K] ⁺	363.22960	363.22964	-0.08		1.8E+06				1.5E+06		
621	Dihydroxy-prostaenoic acid	C ₂₀ H ₃₆ O ₄	[M+Na] ⁺	363.25058	363.25061	-0.08				9.0E+05				
622	Hexadecenoylcholine	C ₂₁ H ₄₂ NO ₂	[M+Na] ⁺	363.31078	363.31057	0.57		5.3E+06	1.4E+06			6.7E+06	2.0E+06	
623	Methyl-heneicosanoic acid	C ₂₂ H ₄₄ O ₂	[M+Na] ⁺	363.32335	363.32337	-0.05								2.1E+06
624	Dioncophylline C	C ₂₃ H ₂₅ NO ₃	[M+H] ⁺	364.19072	364.19074	-0.04		2.8E+06				2.6E+06		
625	Hydroxy-dimethoxy-methylenedioxyflavone	C ₁₈ H ₁₄ O ₇	[M+Na] ⁺	365.06317	365.06338	-0.57	3.3E+06		3.7E+06		3.0E+06		1.9E+06	
626	Lactose	C ₁₂ H ₂₂ O ₁₁	[M+Na] ⁺	365.10543	365.10549	-0.14				2.2E+07				5.8E+06
627	Brosimacutin C	C ₂₀ H ₂₂ O ₅	[M+Na] ⁺	365.13594	365.13602	-0.21						2.8E+06		
628	Dinor-iso prostaglandin F2alpha	C ₁₈ H ₃₀ O ₅	[M+K] ⁺	365.17248	365.17253	-0.13		3.0E+06						
629	Dinor-keto-prostaglandin F1 a	C ₁₈ H ₃₀ O ₆	[M+Na] ⁺	365.19346	365.19355	-0.25		2.2E+06				2.4E+06		
630	Epoxy-docosahexaenoic acid	C ₂₂ H ₃₀ O ₃	[M+Na] ⁺	365.20872	365.20893	-0.57		3.8E+06				2.6E+06		
631	Methyl dihydroxy-oxo-octadecenoate	C ₁₉ H ₃₄ O ₅	[M+Na] ⁺	365.22984	365.22990	-0.16		3.4E+06		6.7E+05		3.5E+06		
632	Tricosahexaenoic acid	C ₂₃ H ₃₄ O ₂	[M+Na] ⁺	365.24510	365.24530	-0.54		5.0E+06				3.1E+06		
633	Eicosanedioic acid	C ₂₀ H ₃₈ O ₄	[M+Na] ⁺	365.26623	365.26629	-0.16	2.1E+06		2.2E+06	2.4E+06	1.8E+06		3.5E+06	2.1E+06

ESI(+) FT-ICR MS														
No.	Plausible Compound ^a	Molecular formula (M)	Ion	Theor m/z ^b	Exp m/z ^c	Δ ppm ^d	SM _R H ^e	SM _R O ^e	SM _P H ^e	SM _P O ^e	TF _R H ^e	TF _R O ^e	TF _P H ^e	TF _P O ^e
634	Hydroxy-heneicosanoic acid	C ₂₁ H ₄₂ O ₃	[M+Na] ⁺	365.30262	365.30272	-0.28				6.6E+05				
635	Methyl-heneicosanediol	C ₂₂ H ₄₆ O ₂	[M+Na] ⁺	365.33900	365.33904	-0.11		1.9E+06		7.2E+05				
636	Dihydroxybenzoxazinone glucoside	C ₁₄ H ₁₇ NO ₉	[M+Na] ⁺	366.07955	366.07976	-0.57	5.0E+06		2.2E+06		5.0E+06			
637	Oxo-dihydroxy-leukotriene B4	C ₂₀ H ₂₉ O ₆	[M+H] ⁺	366.20369	366.20334	0.96						2.4E+06		
638	Sanaganone	C ₂₂ H ₁₆ O ₄	[M+Na] ⁺	367.09408	367.09383	0.69			1.8E+06		2.0E+06			
639	Epiiridotrial glucoside	C ₁₆ H ₂₄ O ₈	[M+Na] ⁺	367.13634	367.13635	-0.03						1.5E+06		
640	Trifluoro-methoxy-norpregna-tetraenol	C ₂₁ H ₂₅ F ₃ O ₂	[M+H] ⁺	367.18794	367.18820	-0.69		6.6E+06				4.2E+06		
641	Hydroxydocosahexaenoic acid	C ₂₂ H ₃₂ O ₃	[M+Na] ⁺	367.22437	367.22457	-0.57	4.7E+06	2.4E+07	4.4E+06	2.9E+06	3.2E+06	2.7E+07	5.4E+06	
642	Dihydroxy-methoxy-octadecenoic acid	C ₁₉ H ₃₆ O ₅	[M+Na] ⁺	367.24549	367.24553	-0.10		8.1E+06		1.3E+06		6.4E+06		
643	Hydroxy-tetranorvitamin D3	C ₂₃ H ₃₆ O ₂	[M+Na] ⁺	367.26075	367.26089	-0.38						1.8E+06		
644	Dihydroxy arachidic acid	C ₂₀ H ₄₀ O ₄	[M+Na] ⁺	367.28188	367.28193	-0.15	1.6E+06		2.1E+06	2.7E+06			2.9E+06	1.8E+06
645	Docosenyl acetate	C ₂₄ H ₄₆ O ₂	[M+H] ⁺	367.35706	367.35714	-0.23		3.1E+06				3.7E+06		
646	N-oleoyl GABA	C ₂₂ H ₄₁ NO ₃	[M+H] ⁺	368.31592	368.31597	-0.13		7.8E+06				4.2E+06		
647	Gibberellin A24	C ₂₀ H ₂₆ O ₅	[M+Na] ⁺	369.16724	369.16747	-0.60		4.3E+06				2.6E+06		
648	Fluoro-hydroxypregnadienedione	C ₂₁ H ₂₇ FO ₃	[M+Na] ⁺	369.18364	369.18359	0.15		3.8E+06						
649	Hydroxytetradecane-tricarboxylate	C ₁₇ H ₃₀ O ₇	[M+Na] ⁺	369.18837	369.18844	-0.18		2.2E+06				2.7E+06		
650	3-Oxo-hydroxysteroid	C ₂₁ H ₃₀ O ₄	[M+Na] ⁺	369.20363	369.20385	-0.60	1.9E+06	2.3E+07		1.9E+06		1.3E+07		
651	(Methylcrotonoyl)oxylupanine	C ₂₀ H ₃₀ N ₂ O ₃	[M+Na] ⁺	369.21486	369.21455	0.85						2.2E+06		
652	MG(0:0/16:0/0:0)	C ₁₉ H ₃₈ O ₄	[M+K] ⁺	369.24017	369.24022	-0.12	7.5E+06		8.1E+06	3.4E+06	4.8E+06		8.2E+06	2.4E+06
653	Oxocholatrienoic Acid	C ₂₄ H ₃₂ O ₃	[M+H] ⁺	369.24242	369.24252	-0.27		2.0E+06						
654	Norcholenediol	C ₂₃ H ₃₈ O ₂	[M+K] ⁺	369.27640	369.27652	-0.31		2.6E+06				3.0E+06		
655	Oxo-tricosanoic acid	C ₂₃ H ₄₄ O ₃	[M+H] ⁺	369.33632	369.33638	-0.14		2.1E+06				2.7E+06		
656	Deoxyvitamin D3	C ₂₇ H ₄₄	[M+H] ⁺	369.35158	369.35162	-0.10	5.0E+06	4.3E+07	6.2E+06	8.4E+06	1.9E+06	1.2E+08	6.7E+06	7.9E+06
657	Dimethyl-docosanoic acid	C ₂₄ H ₄₈ O ₂	[M+H] ⁺	369.37271	369.37273	-0.07	2.2E+06	5.9E+06	2.2E+06	1.9E+06		1.4E+07	1.9E+06	1.9E+06
658	Prostaglandin G1	C ₂₀ H ₃₃ O ₆	[M+H] ⁺	370.23499	370.23464	0.95		7.0E+06	2.6E+06	1.7E+07	5.8E+06	1.4E+07		7.3E+07
659	Tetradecenoylcarnitine	C ₂₁ H ₃₉ NO ₄	[M+H] ⁺	370.29519	370.29525	-0.17		4.6E+06				1.7E+06		
660	N-palmitoyl leucine	C ₂₂ H ₄₃ NO ₃	[M+H] ⁺	370.33157	370.33164	-0.17		6.3E+06				1.1E+07		
661	Dehydro-fluoro-oxotestololactone	C ₁₉ H ₂₁ FO ₄	[M+K] ⁺	371.10555	371.10554	0.02	1.6E+06							
662	Leonuridine	C ₁₅ H ₂₄ O ₉	[M+Na] ⁺	371.13125	371.13134	-0.23		4.9E+06				1.7E+06		

ESI(+) FT-ICR MS														
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663	Bis(dimethoxyphenyl)propanediol	C ₁₉ H ₂₄ O ₆	[M+Na] ⁺	371.14651	371.14673	-0.59		1.6E+06						
664	Fluoro-hydroxypregnenedione	C ₂₁ H ₂₉ FO ₃	[M+Na] ⁺	371.19929	371.19922	0.20		6.6E+06						
665	Deoxy-methylene-keto-PGD2	C ₂₁ H ₃₂ O ₄	[M+Na] ⁺	371.21928	371.21945	-0.46		1.7E+06						
666	Trimethy eicosatrienoic acid	C ₂₃ H ₄₀ O ₂	[M+Na] ⁺	371.29205	371.29212	-0.18		3.6E+07		6.6E+06		3.8E+07		
667	Docosanedioic acid	C ₂₂ H ₄₂ O ₄	[M+H] ⁺	371.31559	371.31564	-0.16	1.8E+06	3.3E+07	3.4E+06	2.4E+06		1.8E+07	2.8E+06	2.1E+06
668	Cholestene	C ₂₇ H ₄₆	[M+H] ⁺	371.36723	371.36719	0.10						1.4E+06		
669	N-(fluro-ethyl) arachidonoyl amine	C ₂₂ H ₃₆ FNO	[M+Na] ⁺	372.26731	372.26761	-0.80								1.7E+06
670	N-stearoyl serine	C ₂₁ H ₄₁ NO ₄	[M+H] ⁺	372.31084	372.31091	-0.19		4.7E+06				2.5E+06		
671	Fluoro-hydroxyandrostenetrione	C ₁₉ H ₂₃ FO ₄	[M+K] ⁺	373.12120	373.12107	0.34					1.6E+06			
672	Deoxyoleandolide	C ₂₀ H ₃₆ O ₆	[M+H] ⁺	373.25847	373.25853	-0.17						3.0E+06		
673	Hydroxy-N-desmethyltamoxifen	C ₂₅ H ₂₇ NO ₂	[M+H] ⁺	374.21146	374.21145	0.02	2.8E+06	9.2E+06	2.6E+06	3.4E+06	2.0E+06	7.3E+06	2.9E+06	8.3E+06
674	MG(18:3/0:0/0:0)	C ₂₁ H ₃₆ O ₄	[M+Na] ⁺	375.25058	375.25066	-0.22		5.7E+06		7.0E+05		3.1E+06		
675	Methyl-(cyclopentadienylidene)-androstanol	C ₂₅ H ₃₆ O	[M+Na] ⁺	375.26584	375.26604	-0.53		4.7E+06				2.5E+06		
676	Prostaglandin H1	C ₂₀ H ₃₃ O ₅	[M+Na] ⁺	376.22202	376.22237	-0.93				3.1E+06		4.5E+06		3.6E+06
677	C16 Sphinganine-phosphate	C ₁₆ H ₃₆ NO ₅ P	[M+Na] ⁺	376.22233	376.22239	-0.15				3.1E+06		4.5E+06	1.7E+06	3.6E+06
678	Anandamide (20:l, n-9)	C ₂₂ H ₄₃ NO ₂	[M+Na] ⁺	376.31860	376.31872	-0.32								1.5E+06
679	Chlorogenic acid	C ₁₆ H ₁₈ O ₉	[M+Na] ⁺	377.08430	377.08421	0.24	1.5E+06		3.5E+06		2.2E+06			
680	Dimethoxyestra-pentaenecarboxylic acid methyl ester	C ₂₂ H ₂₆ O ₄	[M+Na] ⁺	377.17233	377.17254	-0.56		3.2E+06						
681	Yohimbine	C ₂₁ H ₂₆ N ₂ O ₃	[M+Na] ⁺	377.18356	377.18329	0.73	2.2E+06	5.6E+06	2.1E+06	6.7E+05	1.9E+06	7.0E+06	2.5E+06	2.9E+06
682	Hydroperoxy-[epidioxy-(octenyl)-cyclopentyl]-heptenoic acid	C ₁₉ H ₃₀ O ₆	[M+Na] ⁺	377.19346	377.19354	-0.20		2.6E+06				1.6E+06		
683	Hydroxy-mercaptoandrostenone propionate	C ₂₂ H ₃₂ O ₃ S	[M+H] ⁺	377.21449	377.21467	-0.47						2.0E+06		
684	Aspidospermine	C ₂₂ H ₃₀ N ₂ O ₂	[M+Na] ⁺	377.21995	377.21987	0.21		3.2E+06				3.1E+06		1.5E+06
685	trihydroxy-prostadienoic acid	C ₂₀ H ₃₄ O ₅	[M+Na] ⁺	377.22984	377.22995	-0.28		3.4E+06				2.1E+06		
686	MG(18:2/0:0/0:0)	C ₂₁ H ₃₈ O ₄	[M+Na] ⁺	377.26623	377.26628	-0.12				1.9E+06			1.9E+06	1.3E+06
687	Dinor-cholestenynol	C ₂₅ H ₃₈ O	[M+Na] ⁺	377.28149	377.28171	-0.58		3.8E+06				3.0E+06		
688	Lignoceryl alcohol	C ₂₄ H ₅₀ O	[M+Na] ⁺	377.37539	377.37551	-0.31		1.9E+06				2.1E+06		
689	Dioncophylline A	C ₂₄ H ₂₇ NO ₃	[M+H] ⁺	378.20637	378.20639	-0.04		3.7E+06				2.8E+06		
690	Evocarpine	C ₂₃ H ₃₃ NO	[M+K] ⁺	378.21937	378.21904	0.90						2.9E+06		2.8E+06

ESI(+) FT-ICR MS														
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691	O-Feruloyl-D-glucose	C ₁₆ H ₂₀ O ₉	[M+Na] ⁺	379.09995	379.10004	-0.22	2.0E+06		2.2E+06		2.4E+06		1.8E+06	
692	Dihydroxy-methoxy-(hydroxybenzyl) dihydrochalcone	C ₂₃ H ₂₂ O ₅	[M+H] ⁺	379.15400	379.15428	-0.74		2.2E+06						
693	Dioxopregna-dienoic acid methyl ester	C ₂₂ H ₂₈ O ₄	[M+Na] ⁺	379.18798	379.18818	-0.51	1.9E+06	2.2E+06						
694	methyl-dihydroperoxy-octadecatrienoate	C ₁₉ H ₃₂ O ₆	[M+Na] ⁺	379.20911	379.20925	-0.37						1.9E+06		
695	Dehydropregnenolone acetate	C ₂₃ H ₃₂ O ₃	[M+Na] ⁺	379.22437	379.22457	-0.53	1.8E+06	3.2E+06	2.0E+06			2.5E+06	1.9E+06	
696	Hydroxystrenone benzoate	C ₂₅ H ₃₀ O ₃	[M+H] ⁺	379.22677	379.22685	-0.21		2.0E+06						
697	Dihydro PGE1	C ₂₀ H ₃₆ O ₅	[M+Na] ⁺	379.24549	379.24558	-0.21		2.2E+06				2.9E+06		
698	Docosahexaenoic acid ethyl ester	C ₂₄ H ₃₆ O ₂	[M+Na] ⁺	379.26075	379.26095	-0.52		2.8E+06	2.1E+06			2.2E+06		
699	MG(0:0/18:1/0:0)	C ₂₁ H ₄₀ O ₄	[M+Na] ⁺	379.28188	379.28195	-0.17	4.3E+06		5.5E+06	4.6E+06	2.5E+06		7.9E+06	5.8E+06
700	Bisnor-dehydro-cholesterol	C ₂₅ H ₄₀ O	[M+Na] ⁺	379.29714	379.29734	-0.55	2.9E+06	7.8E+06	4.4E+06	2.1E+06	1.8E+06	6.9E+06	4.0E+06	
701	Hydroxydocosanoic acid	C ₂₂ H ₄₄ O ₃	[M+Na] ⁺	379.31827	379.31835	-0.21		3.3E+06		1.2E+06		3.2E+06		1.8E+06
702	cyclo-Dopa glucoside	C ₁₅ H ₁₉ NO ₉	[M+Na] ⁺	380.09520	380.09539	-0.49			3.7E+06					
703	Hydroxydihydrochelirubine	C ₂₁ H ₁₇ NO ₆	[M+H] ⁺	380.11286	380.11291	-0.12			1.5E+06					
704	Propafenone	C ₂₁ H ₂₇ NO ₃	[M+K] ⁺	380.16225	380.16192	0.88						1.9E+06		
705	N-palmitoyl threonine	C ₂₀ H ₃₉ NO ₄	[M+Na] ⁺	380.27713	380.27718	-0.14			2.8E+06		4.3E+06			3.7E+06
706	Tetrahydroxy-methoxyflavone acetate	C ₁₈ H ₁₄ O ₈	[M+Na] ⁺	381.05809	381.05821	-0.31	6.4E+06		5.7E+06		7.2E+06		4.3E+06	
707	Phaseollidin hydrate	C ₂₀ H ₂₂ O ₅	[M+K] ⁺	381.10988	381.10979	0.24	3.6E+06				3.4E+06			
708	Prednisone	C ₂₁ H ₂₆ O ₅	[M+Na] ⁺	381.16724	381.16740	-0.42	1.7E+06	2.3E+06				2.1E+06		
709	PA(14:1/0:0)	C ₁₇ H ₃₃ O ₇ P	[M+H] ⁺	381.20367	381.20384	-0.45	2.1E+06	2.8E+06	2.5E+06		2.3E+06	2.2E+06	2.1E+06	
710	Hydroxy-oxo-tetranorcalciol	C ₂₃ H ₃₄ O ₃	[M+Na] ⁺	381.24002	381.24023	-0.55	1.0E+07	1.2E+07	1.1E+07	3.1E+06	5.5E+06	9.4E+06	1.1E+07	2.1E+06
711	Oxopregnene carboxaldehyde dioxime	C ₂₂ H ₃₄ N ₂ O ₂	[M+Na] ⁺	381.25125	381.25146	-0.56	1.6E+07	2.4E+07	1.6E+07	1.2E+07	4.7E+06	5.7E+06	1.6E+07	2.1E+06
712	Dimethoxy-hydroxy-octadecenoic acid	C ₂₀ H ₃₈ O ₅	[M+Na] ⁺	381.26115	381.26121	-0.17		3.7E+06		1.5E+06				2.6E+06
713	Tetracosapentaenoic acid	C ₂₄ H ₃₈ O ₂	[M+Na] ⁺	381.27640	381.27650	-0.27		3.2E+06		1.0E+06		3.2E+06		
714	MG(0:0/18:0/0:0)	C ₂₁ H ₄₂ O ₄	[M+Na] ⁺	381.29753	381.29760	-0.17	2.2E+07		2.5E+07	5.3E+06	1.9E+07			1.9E+07
715	Pentamethyleicosa-pentaenol	C ₂₅ H ₄₂ O	[M+Na] ⁺	381.31279	381.31299	-0.53		1.7E+06						
716	Oxo-tetracosenoic acid	C ₂₄ H ₄₄ O ₃	[M+H] ⁺	381.33632	381.33632	0.00		1.9E+06				1.8E+06		
717	Trimethyl-docosenoic acid	C ₂₅ H ₄₈ O ₂	[M+H] ⁺	381.37271	381.37271	-0.01						2.4E+06		
718	Symlandine	C ₂₀ H ₃₁ NO ₆	[M+H] ⁺	382.22241	382.22248	-0.18	2.7E+06		4.6E+06		3.4E+06			

ESI(+) FT-ICR MS														
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719	Sphinganine 1-phosphate	C ₁₈ H ₄₀ NO ₅ P	[M+H] ⁺	382.27169	382.27189	-0.52		2.3E+06				3.1E+06		
720	N-dihydroxy-eicosatrienoyl)-ethanolamine	C ₂₂ H ₃₉ NO ₄	[M+H] ⁺	382.29519	382.29524	-0.13		2.0E+06	1.9E+06					
721	N-stearoyl proline	C ₂₃ H ₄₃ NO ₃	[M+H] ⁺	382.33157	382.33166	-0.23	2.1E+06					2.0E+06		
722	Trihydroxy-trimethoxyflavone	C ₁₈ H ₁₆ O ₈	[M+Na] ⁺	383.07374	383.07397	-0.61	9.2E+06							
723	Fisetinidolol-pentamethyl ether	C ₂₀ H ₂₄ O ₆	[M+Na] ⁺	383.14651	383.14671	-0.53	1.7E+07	2.9E+06	2.4E+07		2.3E+07		1.9E+07	
724	Aldosterone	C ₂₁ H ₂₈ O ₅	[M+Na] ⁺	383.18289	383.18312	-0.60	6.0E+06	6.4E+06	5.8E+06		4.4E+06	4.6E+06	5.2E+06	1.8E+06
725	PA(14:0/0:0)	C ₁₇ H ₃₅ O ₇ P	[M+H] ⁺	383.21932	383.21948	-0.44	2.5E+06	4.8E+06	3.6E+06	2.5E+06		3.5E+06	2.8E+06	
726	Dihydroxy-didehydro-dihydro-apo-carotenal	C ₂₅ H ₃₄ O ₃	[M+H] ⁺	383.25807	383.25817	-0.26		2.8E+06		4.2E+06		2.8E+06		6.3E+06
727	MG(18:0/0:0/0:0)	C ₂₁ H ₄₄ O ₃	[M+K] ⁺	383.29220	383.29219	0.05		1.9E+06				2.2E+06		
728	Didehydrovitamin D3	C ₂₇ H ₄₂ O	[M+H] ⁺	383.33084	383.33089	-0.13	3.3E+06	4.6E+06	4.8E+06	1.4E+06	4.2E+06	5.5E+06	4.0E+06	1.9E+06
729	Hydroxy-tetracosenoic acid	C ₂₄ H ₄₆ O ₃	[M+H] ⁺	383.35197	383.35203	-0.15		3.3E+06		1.4E+06		3.6E+06		1.4E+06
730	Mycocerosic acid	C ₂₅ H ₅₀ O ₂	[M+H] ⁺	383.38836	383.38841	-0.13	4.7E+06	4.6E+06	4.9E+06	2.4E+06	3.6E+06	9.9E+06	4.4E+06	3.2E+06
731	Hydroxybenzylsulphoglucosinolate	C ₁₄ H ₁₉ NO ₇ S	[M+K] ⁺	384.05138	384.05139	-0.02			3.0E+06					
732	Mannose-acetylglucosamine	C ₁₄ H ₂₅ NO ₁₁	[M+H] ⁺	384.15004	384.15014	-0.27	2.6E+06		2.8E+06		4.5E+06			
733	Trihydroxy-leukotriene-B4	C ₂₀ H ₃₁ O ₇	[M+H] ⁺	384.21425	384.21391	0.89				3.4E+06		6.6E+06		2.2E+06
734	Hydroxy-tetradecadiencarnitine	C ₂₁ H ₃₇ NO ₅	[M+H] ⁺	384.27445	384.27453	-0.21		2.2E+06						
735	N-oleoyl threonine	C ₂₂ H ₄₁ NO ₄	[M+H] ⁺	384.31084	384.31090	-0.18		3.6E+06	1.7E+06			1.7E+06		
736	N-(Docosanoyl)-ethanolamine	C ₂₄ H ₄₉ NO ₂	[M+H] ⁺	384.38361	384.38368	-0.20		3.7E+06	2.0E+06			3.1E+06		
737	Chelirubine	C ₂₁ H ₁₆ NO ₅	[M+Na] ⁺	385.09207	385.09215	-0.21					1.8E+06			
738	Dihydroxy-tetramethoxyisoflavan	C ₁₉ H ₂₂ O ₇	[M+Na] ⁺	385.12577	385.12596	-0.47	3.8E+06	3.7E+06	2.8E+06		2.4E+06		3.4E+06	
739	Acetyl-maltose	C ₁₄ H ₂₄ O ₁₂	[M+H] ⁺	385.13405	385.13419	-0.36		1.9E+06						
740	Oxo-carboxy-leukotriene B4	C ₂₀ H ₂₆ O ₆	[M+Na] ⁺	385.16216	385.16236	-0.52	6.7E+06	2.4E+06	5.1E+06		5.0E+06		3.7E+06	
741	Epoxy-fluoro-hydroxypregnendione	C ₂₁ H ₂₇ FO ₄	[M+Na] ⁺	385.17856	385.17845	0.28		2.7E+06						
742	Cortisol	C ₂₁ H ₃₀ O ₅	[M+H] ⁺	385.19854	385.19875	-0.52	1.7E+06		2.1E+06					
743	Di-n-heptyl phthalate	C ₂₂ H ₃₄ O ₄	[M+Na] ⁺	385.23493	385.23511	-0.47	5.0E+06		4.3E+06		5.0E+06	3.5E+06	4.0E+06	1.5E+06
744	Norcholenetriol	C ₂₃ H ₃₈ O ₃	[M+Na] ⁺	385.27132	385.27152	-0.52	4.9E+06	9.7E+06	5.4E+06		2.6E+06	6.9E+06	5.7E+06	1.5E+06
745	Tetracosatrienoic acid	C ₂₄ H ₄₂ O ₂	[M+Na] ⁺	385.30770	385.30779	-0.22		5.3E+06	5.9E+06	7.2E+05		1.6E+07	2.8E+06	7.5E+06
746	MG(20:1/0:0/0:0)	C ₂₃ H ₄₄ O ₄	[M+H] ⁺	385.33124	385.33131	-0.19		3.6E+06		8.0E+05		5.3E+06	1.7E+06	
747	Cholecalciferol	C ₂₇ H ₄₄ O	[M+H] ⁺	385.34649	385.34655	-0.15	4.0E+06	8.8E+06	6.8E+06	3.7E+06	2.9E+06	1.2E+07	6.4E+06	3.9E+06

ESI(+) FT-ICR MS														
No.	Plausible Compound ^a	Molecular formula (M)	Ion	Theor m/z ^b	Exp m/z ^c	Δppm ^d	SM _R H ^e	SM _R O ^e	SM _P H ^e	SM _P O ^e	TF _R H ^e	TF _R O ^e	TF _P H ^e	TF _P O ^e
748	Dihydro-trihydroxy-leukotriene B4	C ₂₀ H ₃₃ O ₇	[M+H] ⁺	386.22990	386.22956	0.89		8.4E+06		5.9E+06		9.4E+06	3.6E+06	8.8E+06
749	N-palmitoyl glutamic acid	C ₂₁ H ₃₉ NO ₅	[M+H] ⁺	386.29010	386.29014	-0.10		3.2E+06	1.7E+06					
750	Leonuridine	C ₁₅ H ₂₄ O ₉	[M+K] ⁺	387.10519	387.10525	-0.16	2.3E+06		2.7E+06		2.1E+06		2.1E+06	
751	Gibberellin A8	C ₁₉ H ₂₄ O ₇	[M+Na] ⁺	387.14142	387.14164	-0.55	2.2E+06				2.3E+06			
752	Pinoresinol dimethyl ether	C ₂₂ H ₂₆ O ₆	[M+H] ⁺	387.18022	387.18028	-0.18	2.2E+06		2.0E+06	1.5E+06	2.0E+06		2.2E+06	
753	Dihydrocortisol	C ₂₁ H ₃₂ O ₅	[M+Na] ⁺	387.21419	387.21441	-0.56	2.5E+06	1.8E+06	2.2E+06		1.7E+06			
754	Robustadial A	C ₂₃ H ₃₀ O ₅	[M+H] ⁺	387.21660	387.21667	-0.18		2.4E+06						
755	Anacardic acid	C ₂₂ H ₃₆ O ₃	[M+K] ⁺	387.22960	387.22967	-0.17	2.8E+06	4.7E+06	3.3E+06			3.5E+06	3.4E+06	
756	Oxo-hydroxy-dimethyl-prostadienoic acid	C ₂₂ H ₃₆ O ₄	[M+Na] ⁺	387.25058	387.25072	-0.37	4.2E+06	4.0E+06			3.2E+06	2.3E+06		2.1E+06
757	(Ladderane-octanyl)-sn-glycerol	C ₂₃ H ₄₀ O ₃	[M+Na] ⁺	387.28697	387.28702	-0.15	1.7E+06	1.0E+07	3.3E+06	3.2E+06		1.1E+07	4.6E+06	5.4E+06
758	Tetracosadienoic acid	C ₂₄ H ₄₄ O ₂	[M+Na] ⁺	387.32335	387.32345	-0.25		1.9E+06						
759	Ulifloxacin	C ₁₆ H ₁₆ FN ₃ O ₃ S	[M+K] ⁺	388.05280	388.05277	0.08					5.1E+06			
760	Hydroxymyristoylcarnitine	C ₂₁ H ₄₁ NO ₅	[M+H] ⁺	388.30575	388.30580	-0.13	1.7E+06	3.0E+06	2.4E+06			1.9E+06	1.6E+06	
761	Diacetoxyscirpenol	C ₁₉ H ₂₆ O ₇	[M+Na] ⁺	389.15707	389.15728	-0.52	1.5E+07		1.4E+07		8.9E+06		1.2E+07	
762	Cortolone	C ₂₁ H ₃₄ O ₅	[M+Na] ⁺	389.22984	389.23017	-0.84								1.3E+06
763	Tetracosenoic acid	C ₂₄ H ₄₆ O ₂	[M+Na] ⁺	389.33900	389.33907	-0.18	1.8E+06		2.8E+06				4.6E+06	3.8E+06
764	Amino-tetrahydroxyeicosenoic acid	C ₂₀ H ₃₉ NO ₆	[M+H] ⁺	390.28501	390.28505	-0.08	2.2E+06	2.9E+06	2.8E+06		2.0E+06	2.3E+06	1.9E+06	
765	N-oleoyl GABA	C ₂₂ H ₄₁ NO ₃	[M+Na] ⁺	390.29786	390.29798	-0.29								1.6E+06
766	Phosphatidyl-D-myo-inositol	C ₁₁ H ₁₉ O ₁₃ P	[M+H] ⁺	391.06360	391.06378	-0.44	2.3E+06				2.1E+06			
767	N-[(Methylenedioxyphenyl)-(mercaptomethyl)-oxopropyl]-alanine	C ₁₆ H ₂₀ N ₂ O ₆ S	[M+Na] ⁺	391.09343	391.09319	0.61	2.1E+06		1.9E+06		2.2E+06			
768	O-Feruloylquininate	C ₁₇ H ₂₀ O ₉	[M+Na] ⁺	391.09995	391.10017	-0.55	2.7E+06		2.2E+06		2.5E+06		1.9E+06	
769	Dihydroxy-methoxy-prenyloxyflavone	C ₂₁ H ₂₀ O ₆	[M+Na] ⁺	391.11521	391.11542	-0.54	1.6E+06							
770	O-Acetylajmaline	C ₂₂ H ₂₈ N ₂ O ₃	[M+Na] ⁺	391.19921	391.19894	0.71	4.3E+06	1.1E+07	4.4E+06	2.0E+06	3.7E+06	1.4E+07	4.5E+06	8.2E+06
771	Trifluoro-LTB4	C ₂₀ H ₂₉ F ₃ O ₄	[M+H] ⁺	391.20907	391.20918	-0.27		2.9E+06				1.9E+06		1.5E+06
772	MG(18:3/0:0/0:0)	C ₂₁ H ₃₆ O ₄	[M+K] ⁺	391.22452	391.22457	-0.14	2.0E+06		1.9E+06			2.5E+06	1.9E+06	
773	Cortol	C ₂₁ H ₃₆ O ₅	[M+Na] ⁺	391.24549	391.24556	-0.15		2.6E+06				2.1E+06		
774	Didesmethyl tocotrienol	C ₂₅ H ₃₆ O ₂	[M+Na] ⁺	391.26075	391.26093	-0.46			1.8E+06					
775	Diisooctyl phthalate	C ₂₄ H ₃₈ O ₄	[M+H] ⁺	391.28429	391.28434	-0.13	3.6E+07	4.0E+07	1.2E+07	5.0E+06	2.4E+07	2.5E+07	1.4E+07	7.1E+06

ESI(+) FT-ICR MS														
No.	Plausible Compound ^a	Molecular formula (M)	Ion	Theor m/z ^b	Exp m/z ^c	Δppm ^d	SM _R H ^e	SM _R O ^e	SM _P H ^e	SM _P O ^e	TF _R H ^e	TF _R O ^e	TF _P H ^e	TF _P O ^e
776	Tricosenoic acid	C ₂₃ H ₄₄ O ₂	[M+K] ⁺	391.29729	391.29730	-0.03				1.8E+06				
777	Oxo-tricosanoic acid	C ₂₃ H ₄₄ O ₃	[M+Na] ⁺	391.31827	391.31833	-0.16								3.4E+06
778	Flavoxate	C ₂₄ H ₂₅ NO ₄	[M+H] ⁺	392.18563	392.18555	0.22						3.2E+06		
779	N-oleoyl alanine	C ₂₁ H ₃₉ NO ₃	[M+K] ⁺	392.25615	392.25626	-0.27	2.0E+06							
780	N-palmitoyl isoleucine	C ₂₂ H ₄₃ NO ₃	[M+Na] ⁺	392.31351	392.31358	-0.16	1.6E+06			2.7E+06			2.5E+06	4.8E+06
781	Stemonone	C ₁₉ H ₁₄ O ₈	[M+Na] ⁺	393.05809	393.05829	-0.51	3.9E+06			1.1E+07	3.6E+06		2.3E+07	
782	Pentahydroxy-trimethoxyflavone	C ₁₈ H ₁₆ O ₁₀	[M+H] ⁺	393.08162	393.08169	-0.17				1.7E+06				
783	C-p-Hydroxybenzylkaempferol	C ₂₂ H ₁₆ O ₇	[M+H] ⁺	393.09688	393.09721	-0.84				1.7E+06				
784	Unaniso flavan [Isoflavans [PK1208]] ([M+Na] ⁺)	C ₂₂ H ₂₆ O ₅	[M+Na] ⁺	393.16724	393.16744	-0.50		2.6E+06			2.6E+06			
785	Oxo-pentanorvitamin D3 6,19-sulfur dioxide adduct	C ₂₂ H ₃₂ O ₄ S	[M+H] ⁺	393.20941	393.20956	-0.40	1.4E+08	9.9E+06	1.3E+08	1.1E+07	1.5E+08	1.9E+07	1.0E+08	1.3E+07
786	Hydroxy-PGE1	C ₂₀ H ₃₄ O ₆	[M+Na] ⁺	393.22476	393.22493	-0.42		2.7E+06		1.3E+06		2.4E+06		2.2E+06
787	Hydroxychole-trienoic Acid	C ₂₄ H ₃₄ O ₃	[M+Na] ⁺	393.24002	393.24022	-0.52	7.5E+06	9.7E+06	1.1E+07	4.5E+06	3.7E+06	6.6E+06	1.1E+07	2.0E+06
788	Oxo-docosanoic acid	C ₂₂ H ₄₂ O ₃	[M+K] ⁺	393.27655	393.27660	-0.12	2.1E+06			3.3E+06	1.8E+06		3.0E+06	
789	Docosanedioic acid	C ₂₂ H ₄₂ O ₄	[M+Na] ⁺	393.29753	393.29761	-0.20					5.6E+06			
790	Norcholestenone	C ₂₆ H ₄₂ O	[M+Na] ⁺	393.31279	393.31299	-0.51	4.2E+06	6.4E+06	4.6E+06	3.9E+06	1.8E+06	6.7E+06	3.7E+06	
791	Hydroxy-tricosanoic acid	C ₂₃ H ₄₆ O ₃	[M+Na] ⁺	393.33392	393.33399	-0.18		3.3E+06		1.5E+06		3.7E+06		1.8E+06
792	(Triaza-indenoanthracenyl)-acetic acid ethylester	C ₂₂ H ₁₇ N ₃ O ₂	[M+K] ⁺	394.09524	394.09560	-0.91				2.1E+06			1.9E+06	
793	Tylophorine	C ₂₄ H ₂₇ NO ₄	[M+H] ⁺	394.20128	394.20117	0.30						3.2E+06		4.6E+06
794	N-palmitoyl histidine	C ₂₂ H ₃₉ N ₃ O ₃	[M+H] ⁺	394.30642	394.30648	-0.15	3.0E+06			5.1E+06			1.9E+06	
795	Hydroxy-trimethoxy-methylenedioxyflavone	C ₁₉ H ₁₆ O ₈	[M+Na] ⁺	395.07374	395.07394	-0.51	5.2E+06			7.6E+06	4.4E+06		3.4E+06	
796	Veraguensin	C ₂₂ H ₂₈ O ₅	[M+Na] ⁺	395.18289	395.18284	0.15	2.6E+06				2.6E+06			
797	Hydroxy-pregnenedione acetate	C ₂₃ H ₃₂ O ₄	[M+Na] ⁺	395.21928	395.21947	-0.48	2.4E+06	3.2E+06	2.6E+06		1.8E+06	2.4E+06	2.8E+06	
798	Deoxyoleandolide	C ₂₀ H ₃₆ O ₆	[M+Na] ⁺	395.24041	395.24046	-0.13	2.8E+06			2.8E+06	2.5E+06	3.9E+06	3.0E+06	5.6E+06
799	Hydroxycholadienoic Acid	C ₂₄ H ₃₆ O ₃	[M+Na] ⁺	395.25567	395.25587	-0.52	1.5E+07	1.7E+07	1.7E+07	5.0E+06	5.1E+06	1.2E+07	1.9E+07	2.7E+06
800	Dysideapalaunic acid	C ₂₅ H ₄₀ O ₂	[M+Na] ⁺	395.29205	395.29223	-0.46	2.1E+06	2.8E+06	2.4E+06			2.3E+06	2.4E+06	
801	Dihydroxy-docosanoic acid	C ₂₂ H ₄₄ O ₄	[M+Na] ⁺	395.31318	395.31323	-0.12		3.7E+06	2.0E+06	1.6E+06		4.6E+06		2.6E+06
802	Hexacosenoic acid	C ₂₆ H ₅₀ O ₂	[M+H] ⁺	395.38836	395.38839	-0.08	1.8E+06	2.5E+06	2.0E+06			3.4E+06	1.8E+06	
803	Deacetylcolchicine	C ₂₀ H ₂₃ NO ₅	[M+K] ⁺	396.12078	396.12061	0.43								2.6E+06
804	PC(O-10:1/0:0)	C ₁₈ H ₃₈ NO ₆ P	[M+H] ⁺	396.25095	396.25110	-0.37	1.7E+07	2.0E+07	8.6E+06	1.3E+07	1.0E+07	4.9E+06	1.6E+07	3.0E+06

ESI(+) FT-ICR MS														
No.	Plausible Compound ^a	Molecular formula (M)	Ion	Theor m/z ^b	Exp m/z ^c	Δ ppm ^d	SM _R H ^e	SM _R O ^e	SM _P H ^e	SM _P O ^e	TF _R H ^e	TF _R O ^e	TF _P H ^e	TF _P O ^e
805	Prostaglandin E2 ethanolamide	C ₂₂ H ₃₇ NO ₅	[M+H] ⁺	396.27445	396.27450	-0.11	1.9E+06		2.1E+06					
806	Dihydroxy-tetramethoxyflavone	C ₁₉ H ₁₈ O ₈	[M+Na] ⁺	397.08939	397.08955	-0.41	2.3E+06				2.4E+06			
807	Hydroxy-dioxopregn-enoic acid	C ₂₂ H ₃₀ O ₅	[M+Na] ⁺	397.19854	397.19876	-0.54	2.8E+06	1.2E+07	2.6E+06	3.0E+06	2.5E+06	4.5E+06	2.6E+06	1.8E+06
808	Hydroxy-tetranorvitamin D3 carboxylic acid	C ₂₃ H ₃₄ O ₄	[M+Na] ⁺	397.23493	397.23512	-0.48	4.1E+06	3.5E+06	4.3E+06		2.9E+06	3.6E+06	3.7E+06	
809	Hydroxycholenoic Acid	C ₂₄ H ₃₈ O ₃	[M+Na] ⁺	397.27132	397.27150	-0.46	1.0E+08	1.3E+07	9.9E+07	6.9E+06	5.3E+07	1.2E+07	9.4E+07	9.6E+06
810	Pentacosadiynoic acid	C ₂₅ H ₄₂ O ₂	[M+Na] ⁺	397.30770	397.30788	-0.46	2.2E+06	1.8E+06					1.9E+06	
811	Hydroxynervonic acid	C ₂₅ H ₄₈ O ₃	[M+H] ⁺	397.36762	397.36769	-0.18		2.7E+06	1.9E+06	2.1E+06		3.5E+06	2.1E+06	1.9E+06
812	Trimethyl-tricosanoic acid	C ₂₆ H ₅₂ O ₂	[M+H] ⁺	397.40401	397.40405	-0.10	5.0E+06	5.7E+06	4.6E+06	2.4E+06	2.5E+06	1.0E+07	4.2E+06	3.3E+06
813	PC(4:0/4:0)	C ₁₆ H ₃₂ NO ₈ P	[M+H] ⁺	398.19383	398.19400	-0.43							2.0E+06	
814	N-(trihydroxy-prostadienoyl)-ethanolamine	C ₂₂ H ₃₉ NO ₅	[M+H] ⁺	398.29010	398.29017	-0.18			2.0E+06					
815	Hexadecenoyl carnitine	C ₂₃ H ₄₃ NO ₄	[M+H] ⁺	398.32649	398.32659	-0.26		2.9E+06				2.1E+06		
816	Dihydroxy-tetramethoxypterocarpan	C ₁₉ H ₂₀ O ₈	[M+Na] ⁺	399.10504	399.10524	-0.51	2.8E+06		2.1E+06		2.7E+06			
817	Hydroxy-pentamethoxyisoflavan	C ₂₀ H ₂₄ O ₇	[M+Na] ⁺	399.14142	399.14163	-0.52	6.8E+06	5.4E+06	4.7E+06		4.5E+06		4.4E+06	
818	S-Adenosyl-L-methionine	C ₁₅ H ₂₂ N ₆ O ₅ S	[M+H] ⁺	399.14452	399.14455	-0.09	2.8E+06		5.2E+06		3.6E+06		3.2E+06	
819	Oxocortisol	C ₂₁ H ₂₈ O ₆	[M+Na] ⁺	399.17781	399.17799	-0.44	2.0E+06		2.7E+06		2.5E+06			
820	di-O-hexanoyl-glucopyranose	C ₁₈ H ₃₂ O ₈	[M+Na] ⁺	399.19894	399.19898	-0.10				1.3E+06	2.6E+06	2.9E+06		
821	MG(0:0/20:5/0:0)	C ₂₃ H ₃₆ O ₄	[M+Na] ⁺	399.25058	399.25069	-0.26	7.5E+06	5.3E+06	5.9E+06	1.7E+06	4.8E+06	4.5E+06	4.2E+06	2.1E+06
822	Oxoprevitamin D3	C ₂₇ H ₄₂ O ₂	[M+H] ⁺	399.32576	399.32578	-0.05	1.7E+06	2.4E+06	1.8E+06		1.8E+06	3.3E+06		
823	Axillarenic acid	C ₂₄ H ₄₆ O ₄	[M+H] ⁺	399.34689	399.34693	-0.10	2.2E+06	4.3E+06	1.8E+06			7.1E+06		2.1E+06
824	Methylvitamin D3	C ₂₈ H ₄₆ O	[M+H] ⁺	399.36214	399.36221	-0.16		1.7E+06	1.9E+06			3.4E+06		
825	L-Palmitoylcarnitine	C ₂₃ H ₄₅ NO ₄	[M+H] ⁺	400.34214	400.34219	-0.14	4.9E+06	7.3E+06	5.9E+06	1.7E+06	3.0E+06	4.9E+06	6.3E+06	2.3E+06
826	Hydroxyvernolide	C ₁₉ H ₂₂ O ₈	[M+Na] ⁺	401.12069	401.12089	-0.50	3.0E+06		2.4E+06		2.1E+06		2.1E+06	
827	Dihydroxy-methoxy-(hydroxybenzyl)dihydrochalcone	C ₂₃ H ₂₂ O ₅	[M+H] ⁺	401.13594	401.13614	-0.49	2.5E+06							
828	Epoxy-fluoro-hydroxypregnendione	C ₂₁ H ₂₇ FO ₄	[M+K] ⁺	401.15250	401.15238	0.30	2.6E+06		2.9E+06		3.7E+06			
829	Gibberellin A17	C ₂₀ H ₂₆ O ₇	[M+Na] ⁺	401.15707	401.15726	-0.45	2.0E+06				2.1E+06			
830	Trioxo-cholenoic Acid	C ₂₄ H ₃₂ O ₅	[M+H] ⁺	401.23225	401.23233	-0.20		6.1E+06		2.4E+06		3.5E+06		2.9E+06
831	MG(20:4/0:0/0:0)	C ₂₃ H ₃₈ O ₄	[M+Na] ⁺	401.26623	401.26642	-0.48	1.7E+07	3.0E+07	1.7E+07	4.4E+06	6.7E+06	1.9E+07	2.0E+07	2.4E+06
832	Cholesta-tetraenone	C ₂₇ H ₃₈ O	[M+Na] ⁺	401.28149	401.28169	-0.49						8.4E+06	4.0E+06	

ESI(+) FT-ICR MS														
No.	Plausible Compound ^a	Molecular formula (M)	Ion	Theor m/z ^b	Exp m/z ^c	Δ ppm ^d	SM _R H ^e	SM _R O ^e	SM _P H ^e	SM _P O ^e	TF _R H ^e	TF _R O ^e	TF _P H ^e	TF _P O ^e
833	Cholantriol	C ₂₄ H ₄₂ O ₃	[M+Na] ⁺	401.30262	401.30267	-0.14		2.0E+06				2.9E+06		1.8E+06
834	Hydroxyvitamin D3	C ₂₇ H ₄₄ O ₂	[M+H] ⁺	401.34141	401.34146	-0.13	2.5E+06	5.0E+06	2.4E+06	1.8E+06	1.8E+06	7.4E+06	2.7E+06	2.4E+06
835	Leukotriene B4 ethanolamide	C ₂₂ H ₃₇ NO ₄	[M+Na] ⁺	402.26148	402.26168	-0.50								1.7E+06
836	Sphingofungin F	C ₂₁ H ₃₉ NO ₆	[M+H] ⁺	402.28501	402.28504	-0.06		2.2E+06	4.5E+06			3.5E+06	2.6E+06	
837	N-propyl-dimethyl-docosatetraenoyl amine	C ₂₇ H ₄₇ NO	[M+H] ⁺	402.37304	402.37310	-0.13		3.2E+06	2.5E+06			4.1E+06	2.2E+06	
838	Tetracenomycin D3	C ₂₀ H ₁₂ O ₈	[M+Na] ⁺	403.04244	403.04266	-0.54	2.5E+06		3.2E+06		3.3E+06			
839	Chaparrin	C ₂₀ H ₂₈ O ₇	[M+Na] ⁺	403.17272	403.17288	-0.39	3.1E+06		2.8E+06		2.4E+06		2.6E+06	
840	Oxo-hydroxy-dimethyl-prostadienoic acid	C ₂₂ H ₃₆ O ₄	[M+K] ⁺	403.22452	403.22454	-0.05			2.2E+06					
841	Dihydroxy-diperoxy-eicosadienoic acid	C ₂₀ H ₃₄ O ₈	[M+H] ⁺	403.23264	403.23268	-0.08		4.5E+06	2.6E+06			3.0E+06		
842	Dihydroxy-oxo-dimethyl-prostadienoic acid	C ₂₂ H ₃₆ O ₅	[M+Na] ⁺	403.24549	403.24566	-0.42		2.7E+06		1.9E+06		2.1E+06		
843	Arachidonyl Glycerol ether	C ₂₃ H ₄₀ O ₃	[M+K] ⁺	403.26090	403.26091	-0.01					1.9E+06			
844	MG(0:0/20:3/0:0)	C ₂₃ H ₄₀ O ₄	[M+Na] ⁺	403.28188	403.28192	-0.10		4.5E+06		2.3E+06		4.5E+06	3.3E+06	2.8E+06
845	Oxo-tetracosenoic acid	C ₂₄ H ₄₄ O ₃	[M+Na] ⁺	403.31827	403.31830	-0.08								2.0E+06
846	Pentacosenoic acid	C ₂₅ H ₄₈ O ₂	[M+Na] ⁺	403.35465	403.35473	-0.19				1.3E+06				2.3E+06
847	N-palmitoyl phenylalanine	C ₂₅ H ₄₁ NO ₃	[M+H] ⁺	404.31592	404.31594	-0.05	2.0E+06						2.1E+06	
848	Dihydroxy-dimethoxy-prenylisoflavone (Methyl-(methylpropyl)benzeneacetate)-	C ₂₂ H ₂₂ O ₆	[M+Na] ⁺	405.13086	405.13105	-0.46	3.9E+06		3.3E+06					
849	Glucopyranuronic acid	C ₁₉ H ₂₆ O ₈	[M+Na] ⁺	405.15199	405.15217	-0.44	1.0E+07		7.8E+06		8.9E+06		6.2E+06	
850	Dioxocholatrienoic Acid	C ₂₄ H ₃₀ O ₄	[M+Na] ⁺	405.20363	405.20370	-0.17						2.1E+06		
851	Hydroxy-mercapto-pregnendione acetate	C ₂₃ H ₃₂ O ₄ S	[M+H] ⁺	405.20941	405.20959	-0.45			2.7E+06					
852	Sarcostin	C ₂₁ H ₃₄ O ₆	[M+Na] ⁺	405.22476	405.22499	-0.56	1.7E+06	3.3E+06		2.3E+06		2.2E+06		2.2E+06
853	Dihydroxy-didehydro-dihydro-apo-beta-carotenal	C ₂₅ H ₃₄ O ₃	[M+Na] ⁺	405.24002	405.23993	0.20	2.1E+06		3.2E+06				2.8E+06	
854	Methyl trihydroxy-methyl-prostadienoate	C ₂₂ H ₃₈ O ₅	[M+Na] ⁺	405.26115	405.26121	-0.16		1.9E+06						
855	MG(0:0/20:2/0:0)	C ₂₃ H ₄₂ O ₄	[M+Na] ⁺	405.29753	405.29756	-0.06		3.0E+06						2.1E+06
856	Dehydroprevitamin D3	C ₂₇ H ₄₂ O	[M+Na] ⁺	405.31279	405.31294	-0.38					1.6E+06			
857	O-fucopyranosyl-acetamido-deoxyglucopyranose	C ₁₄ H ₂₅ NO ₁₀	[M+Na] ⁺	406.11101	406.11106	-0.13	2.0E+06							
858	Hydroxy-tetradecadiencarnitine	C ₂₁ H ₃₇ NO ₅	[M+Na] ⁺	406.25639	406.25643	-0.09						2.7E+06		
859	N-oleoyl threonine	C ₂₂ H ₄₁ NO ₄	[M+Na] ⁺	406.29278	406.29284	-0.14				4.1E+06				3.2E+06
860	Indolylmethyl-desulfoglucosinolate	C ₁₆ H ₂₀ N ₂ O ₆ S	[M+K] ⁺	407.06737	407.06719	0.43							1.7E+07	

ESI(+) FT-ICR MS														
No.	Plausible Compound ^a	Molecular formula (M)	Ion	Theor m/z ^b	Experimental m/z ^c	Δ ppm ^d	SM _R H ^e	SM _R O ^e	SM _P H ^e	SM _P O ^e	TF _R H ^e	TF _R O ^e	TF _P H ^e	TF _P O ^e
861	Dihydroxy-dimethoxy-prenylflavanone	C ₂₂ H ₂₄ O ₆	[M+Na] ⁺	407.14651	407.14668	-0.42	1.1E+07	2.8E+06	9.6E+06		5.5E+06		6.7E+06	
862	Argentine	C ₂₃ H ₂₆ N ₄ O ₃	[M+H] ⁺	407.20777	407.20812	-0.87				1.2E+06				3.1E+06
863	Dihydroxy-(p-menthenyl)-methoxychalcone	C ₂₆ H ₃₀ O ₄	[M+H] ⁺	407.22169	407.22179	-0.26								1.8E+06
864	Hexacosahexaenoic acid	C ₂₆ H ₄₀ O ₂	[M+Na] ⁺	407.29205	407.29225	-0.50	2.2E+06	2.8E+06	2.9E+06		1.6E+06	3.7E+06	2.9E+06	1.7E+06
865	Diapophytofluene	C ₃₀ H ₄₆	[M+H] ⁺	407.36723	407.36727	-0.09		3.4E+06				2.6E+06		
866	Hydroxy-(morpholinylmethyl)estratrienone	C ₂₃ H ₃₁ NO ₃	[M+K] ⁺	408.19355	408.19317	0.94						4.6E+06		
867	N-palmitoyl glutamic acid	C ₂₁ H ₃₉ NO ₅	[M+Na] ⁺	408.27204	408.27220	-0.38								2.9E+06
868	N-palmitoyl leucine	C ₂₂ H ₄₃ NO ₃	[M+K] ⁺	408.28745	408.28748	-0.06	2.8E+06		2.6E+06			3.7E+06		
869	Hydroxychalcone-glucoside	C ₂₁ H ₂₂ O ₇	[M+Na] ⁺	409.12577	409.12583	-0.14		1.0E+07						
870	Di-O-methyl-prenylafzelechinol	C ₂₂ H ₂₆ O ₆	[M+Na] ⁺	409.16216	409.16228	-0.30		3.2E+06						2.9E+06
871	Epoxy-dioxopregnenyl acetate	C ₂₃ H ₃₀ O ₅	[M+Na] ⁺	409.19854	409.19869	-0.35							3.4E+06	
872	Oleandolide	C ₂₀ H ₃₄ O ₇	[M+Na] ⁺	409.21967	409.21979	-0.28		3.0E+06			4.5E+06	2.1E+06		
873	Dioxocholenoic Acid	C ₂₄ H ₃₄ O ₄	[M+Na] ⁺	409.23493	409.23511	-0.44	2.2E+06	2.7E+06	2.6E+06			2.6E+06	3.3E+06	
874	Deoxyerythronolide B	C ₂₁ H ₃₈ O ₆	[M+Na] ⁺	409.25606	409.25612	-0.14		6.2E+06		1.3E+06		3.7E+06		3.2E+06
875	Testosterone isocaproate	C ₂₅ H ₃₈ O ₃	[M+Na] ⁺	409.27132	409.27152	-0.49	2.1E+07	6.4E+07	3.1E+07	1.1E+07	9.9E+06	2.9E+07	2.2E+07	5.6E+06
876	DG(18:0/2:0/0:0)	C ₂₃ H ₄₆ O ₄	[M+Na] ⁺	409.32883	409.32888	-0.12		4.1E+06	2.6E+06	9.8E+05		4.5E+06	2.6E+06	3.3E+06
877	Epoxycholestane	C ₂₇ H ₄₆ O	[M+Na] ⁺	409.34409	409.34413	-0.11	4.5E+06	1.3E+07	6.9E+06	7.9E+06	2.5E+06	2.8E+07	6.2E+06	1.0E+07
878	Oxohexacosenoic acid	C ₂₆ H ₄₈ O ₃	[M+H] ⁺	409.36762	409.36768	-0.14						2.4E+06		
879	Diapophytoene	C ₃₀ H ₄₈	[M+H] ⁺	409.38288	409.38292	-0.11	6.5E+06	2.0E+07	9.0E+06	2.7E+06	2.7E+06	1.8E+07	8.6E+06	5.8E+06
880	Phthienoic acid	C ₂₇ H ₅₂ O ₂	[M+H] ⁺	409.40401	409.40408	-0.18		2.8E+06				2.6E+06		
881	Linustatin	C ₁₆ H ₂₇ NO ₁₁	[M+H] ⁺	410.16569	410.16559	0.24				1.7E+06		1.9E+06		
882	Hexamethoxychalcone	C ₂₁ H ₂₄ O ₇	[M+Na] ⁺	411.14142	411.14158	-0.38		2.0E+06						
883	Methyl bisepidioxo-hydroperoxy-octadecenoate	C ₁₉ H ₃₂ O ₈	[M+Na] ⁺	411.19894	411.19906	-0.30		2.3E+06						
884	Dihydroxyandrostenone diacetate	C ₂₃ H ₃₂ O ₅	[M+Na] ⁺	411.21419	411.21441	-0.52	8.2E+06	5.1E+06	6.6E+06		6.3E+06	4.5E+06	6.4E+06	
885	Hydroxy-oxo-cholenoic Acid	C ₂₄ H ₃₆ O ₄	[M+Na] ⁺	411.25058	411.25077	-0.47	3.9E+06	4.0E+06	4.0E+06	2.3E+06	2.3E+06	3.4E+06	4.2E+06	2.1E+06
886	Desoxyscalarin	C ₂₅ H ₄₀ O ₃	[M+Na] ⁺	411.28697	411.28714	-0.43	2.5E+06	3.4E+06	3.7E+06	1.4E+06	1.9E+06	2.8E+06	2.8E+06	
887	Gama-Tocotrienol	C ₂₈ H ₄₂ O ₂	[M+H] ⁺	411.32576	411.32579	-0.08		3.5E+06						
888	Serratene	C ₃₀ H ₅₀	[M+H] ⁺	411.39853	411.39857	-0.09	5.3E+07	5.7E+07	5.1E+07	1.4E+07	1.4E+07	9.2E+07	3.8E+07	3.4E+07
889	Methyl-hexacosanoic acid	C ₂₇ H ₅₄ O ₂	[M+H] ⁺	411.41966	411.41972	-0.14	2.5E+06	3.0E+06	2.6E+06			4.9E+06	2.1E+06	2.1E+06

ESI(+) FT-ICR MS														
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890	N-oleoyl glutamic acid	C ₂₃ H ₄₁ N O ₅	[M+H] ⁺	412.30575	412.30583	-0.19		1.2E+07						
891	Lignoceroyl-ethanolamine	C ₂₆ H ₅₃ N O ₂	[M+H] ⁺	412.41491	412.41495	-0.09		4.4E+06	2.9E+06			3.4E+06	1.9E+06	
892	Erioflorin acetate	C ₂₁ H ₂₆ O ₇	[M+Na] ⁺	413.15707	413.15727	-0.48	3.0E+06		2.7E+06		2.5E+06		2.6E+06	
893	Hydroxy-dihydrojasmonic acid glucoside	C ₁₈ H ₃₀ O ₉	[M+Na] ⁺	413.17820	413.17831	-0.26					2.4E+06			
894	Rehmaionoside B	C ₁₉ H ₃₄ O ₈	[M+Na] ⁺	413.21459	413.21465	-0.16	6.8E+06		6.3E+06		8.0E+06	1.9E+06	6.4E+06	
895	Dihydroxy-dinor-secovitamin D3	C ₂₅ H ₄₂ O ₃	[M+Na] ⁺	413.30262	413.30280	-0.43	1.8E+06	2.6E+06	2.0E+06			2.8E+06		
896	MG(0:0/22:1/0:0)	C ₂₅ H ₄₈ O ₄	[M+H] ⁺	413.36254	413.36259	-0.12	2.1E+06	2.8E+06				4.7E+06		
897	Iceaine	C ₂₂ H ₃₃ N O ₄	[M+K] ⁺	414.20412	414.20434	-0.54					2.4E+06			
898	Tetrahydroxy-trimethoxyflavone	C ₁₈ H ₁₆ O ₉	[M+K] ⁺	415.04259	415.04264	-0.12				8.7E+07				1.8E+08
899	Epi-Eupatoroxin	C ₂₀ H ₂₄ O ₈	[M+Na] ⁺	415.13634	415.13653	-0.45	2.6E+06				2.0E+06			
900	Picrasin G	C ₂₁ H ₂₈ O ₇	[M+Na] ⁺	415.17272	415.17294	-0.51	2.4E+06		2.7E+06		2.6E+06			
901	Isodomedin	C ₂₂ H ₃₂ O ₆	[M+Na] ⁺	415.20911	415.20932	-0.51	2.4E+06							
902	EstraTriene-3,6α,17β-triol triacetate	C ₂₄ H ₃₀ O ₆	[M+H] ⁺	415.21152	415.21157	-0.14		9.6E+07		4.1E+06		6.6E+06		
903	Dihydroxycholanoic acid	C ₂₄ H ₄₀ O ₄	[M+Na] ⁺	415.28188	415.28210	-0.54	9.7E+06	8.1E+06	1.0E+07		4.6E+06	3.9E+06	1.2E+07	
904	Alpinine	C ₂₃ H ₂₉ N O ₆	[M+H] ⁺	416.20676	416.20684	-0.18	1.8E+06							
905	Hydroxyhexadecanoylcarnitine	C ₂₃ H ₄₅ N O ₅	[M+H] ⁺	416.33705	416.33711	-0.14	2.2E+06		2.9E+06					
906	Tomatidine	C ₂₇ H ₄₅ N O ₂	[M+H] ⁺	416.35231	416.35237	-0.14			2.5E+06				2.4E+06	
907	Gibberellin A28	C ₂₀ H ₂₆ O ₈	[M+Na] ⁺	417.15199	417.15217	-0.44	3.3E+06							
908	Briantheine W	C ₂₄ H ₃₂ O ₆	[M+H] ⁺	417.22717	417.22724	-0.18		3.5E+06						
909	Hydroxyeicosatetraenoate glyceryl ester	C ₂₃ H ₃₈ O ₅	[M+H] ⁺	417.26115	417.26135	-0.48	3.6E+07	3.4E+06	2.6E+07		1.5E+07	3.4E+06	2.0E+07	
910	Dihydroxyvitamin D3	C ₂₇ H ₄₄ O ₃	[M+H] ⁺	417.33632	417.33639	-0.16		2.6E+06				3.0E+06		
911	Tetramethyl-docosenoic acid	C ₂₆ H ₅₀ O ₂	[M+Na] ⁺	417.37030	417.37034	-0.09				1.9E+06				
912	Cyclovirobuxine C	C ₂₇ H ₄₈ N ₂ O	[M+H] ⁺	417.38394	417.38400	-0.13	3.0E+06				2.8E+06		2.4E+06	
913	Sphingofungin E	C ₂₁ H ₃₉ N O ₇	[M+H] ⁺	418.27993	418.27999	-0.15	2.2E+06							

914	N-Oleoyl Dopamine	C ₂₆ H ₄₃ N O ₃	[M+H] ⁺	418.33157	418.33164	-0.16	7.2E+06	2.1E+06	4.1E+06	2.4E+06	1.3E+07	5.3E+06
915	N-(hydroxy-methyl-ethyl)-dimethyl- docosatetraenoyl amine	C ₂₇ H ₄₇ N O ₂	[M+H] ⁺	418.36796	418.36802	-0.15					2.4E+06	
916	Melengestrol acetate	C ₂₅ H ₃₂ O ₄	[M+Na] ⁺	419.21928	419.21953	-0.60		2.5E+06				
917	methyl-[epidioxy-(hydroperoxy-pentenyl)- cyclopentyl]-octanoate	C ₂₂ H ₃₆ O ₆	[M+Na] ⁺	419.24041	419.24049	-0.18		2.5E+06			2.0E+06	

ESI(+) FT-ICR MS														
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918	Estradiol cyclopentylpropionate	C ₂₆ H ₃₆ O ₃	[M+Na] ⁺	419.25567	419.25589	-0.54	2.9E+06	3.5E+06	3.4E+06			2.7E+06	3.5E+06	
919	Norcholanpentol	C ₂₃ H ₄₀ O ₅	[M+Na] ⁺	419.27680	419.27688	-0.20				2.6E+06	2.6E+06	4.7E+06		2.6E+06
920	N-oleoyl asparagine	C ₂₂ H ₄₀ N ₂ O ₄	[M+Na] ⁺	419.28803	419.28809	-0.15		2.0E+06		1.4E+06		3.0E+06		
921	Palmitoyl glucuronide	C ₂₂ H ₄₂ O ₇	[M+H] ⁺	419.30033	419.30038	-0.12	3.4E+06				2.7E+06		3.8E+06	
922	Trihydroxy-norvitamin D3	C ₂₆ H ₄₂ O ₄	[M+H] ⁺	419.31559	419.31566	-0.17	9.7E+06	1.1E+07	4.3E+06	1.2E+06	2.4E+06	5.9E+06	5.3E+06	2.4E+06
923	Isovitamin D2	C ₂₈ H ₄₄ O	[M+Na] ⁺	419.32844	419.32862	-0.44		2.9E+06				2.7E+06		
924	Ethamoxytriphetol	C ₂₇ H ₃₃ NO ₃	[M+H] ⁺	420.25332	420.25331	0.02				1.6E+06		2.4E+06		5.5E+06
925	Trihydroxy-dimethoxy-prenylflavone	C ₂₂ H ₂₂ O ₇	[M+Na] ⁺	421.12577	421.12599	-0.51	3.8E+06							
926	C17 Sphingosine-1-phosphate	C ₁₇ H ₃₉ N ₂ O ₅ P	[M+K] ⁺	421.22282	421.22314	-0.76		8.5E+06		1.4E+06		7.7E+06		
927	Pregna-triene-diol diacetate	C ₂₅ H ₃₄ O ₄	[M+Na] ⁺	421.23493	421.23508	-0.36		2.3E+06						
928	Dihydroxy-tetradehydro-norvitamin D3	C ₂₆ H ₃₈ O ₃	[M+Na] ⁺	421.27132	421.27151	-0.46	2.2E+06	2.7E+06	2.9E+06			2.8E+06	3.3E+06	
929	Hydroxy-didehydrovitamin D3	C ₂₇ H ₄₂ O ₂	[M+Na] ⁺	421.30770	421.30791	-0.50					2.1E+06			
930	Tetracosanedioic acid	C ₂₄ H ₄₆ O ₄	[M+Na] ⁺	421.32883	421.32891	-0.19					2.5E+06		6.8E+06	
931	Methylvitamin D3	C ₂₈ H ₄₆ O	[M+Na] ⁺	421.34409	421.34428	-0.45	1.1E+07			6.0E+06	3.9E+06			3.5E+06
932	Fenpyroximate	C ₂₄ H ₂₇ N ₃ O ₄	[M+H] ⁺	422.20743	422.20783	-0.94							3.2E+06	
933	N-acetylsphingosine phosphate	C ₂₀ H ₄₀ NO ₆ P	[M+H] ⁺	422.26660	422.26681	-0.50	3.7E+06		3.0E+06	3.9E+06	3.6E+06	2.0E+06	4.7E+06	
934	Ticarcillin	C ₁₅ H ₁₆ N ₂ O ₆ S ₂	[M+K] ⁺	423.00814	423.00829	-0.37	5.2E+06		6.2E+06		4.8E+06		6.7E+06	
935	Tetracenomycin F2	C ₂₀ H ₁₆ O ₈	[M+K] ⁺	423.04768	423.04758	0.23	4.3E+07		1.7E+07				1.4E+07	
936	Lophirone J	C ₂₅ H ₂₀ O ₅	[M+Na] ⁺	423.12029	423.12051	-0.51			1.1E+07					
937	Isopropylidenedioxy-methylprogesterone	C ₂₅ H ₃₆ O ₄	[M+Na] ⁺	423.25058	423.25077	-0.45			3.6E+06			2.5E+06	3.3E+06	
938	Dihydroxy-didehydro-norvitamin D3	C ₂₆ H ₄₀ O ₃	[M+Na] ⁺	423.28697	423.28717	-0.48	1.1E+07	9.1E+06	8.0E+06	2.4E+06	4.8E+06	8.0E+06	8.2E+06	2.2E+06
939	Diapolycopene	C ₃₀ H ₄₀	[M+K] ⁺	423.30222	423.30244	-0.52	5.5E+06	9.8E+06	1.8E+07	4.5E+06	2.7E+06	1.2E+07	1.5E+07	3.7E+06
940	Didecanoylglycerol	C ₂₃ H ₄₄ O ₅	[M+Na] ⁺	423.30810	423.30816	-0.16		3.4E+06				2.6E+06		2.4E+06
941	Hydroxyvitamin D3	C ₂₇ H ₄₄ O ₂	[M+Na] ⁺	423.32335	423.32349	-0.34	3.7E+06		4.8E+06		2.2E+06			
942	Theonellasterol B	C ₃₀ H ₄₆ O	[M+H] ⁺	423.36214	423.36217	-0.06						2.1E+06		
943	Octacosenoic acid	C ₂₈ H ₅₄ O ₂	[M+H] ⁺	423.41966	423.41970	-0.09	6.0E+06	8.0E+06	6.9E+06	2.1E+06	2.5E+06	1.2E+07	6.8E+06	2.9E+06
944	O-Methylandrocymbine	C ₂₂ H ₂₇ NO ₅	[M+K] ⁺	424.15208	424.15192	0.38		2.6E+06		2.4E+06		4.0E+06		8.5E+06
945	Myxalamid B	C ₂₅ H ₃₉ NO ₃	[M+Na] ⁺	424.28221	424.28241	-0.46	5.1E+08	5.1E+08	3.1E+08	3.4E+08	3.0E+08	1.2E+08	4.8E+08	9.5E+07
946	Deoxythymidine 5'-diphosphate	C ₁₀ H ₁₆ N ₂ O ₁₁ P	[M+Na] ⁺	425.01215	425.01222	-0.16							2.0E+06	

ESI(+) FT-ICR MS														
No.	Plausible Compound ^a	Molecular formula (M)	Ion	Theo r m/z ^b	Exp m/z ^c	Δppm ^d	SM _R H ^e	SM _R O ^e	SM _P H ^e	SM _P O ^e	TF _R H ^e	TF _R O ^e	TF _P H ^e	TF _P O ^e
947	Hydroxy-(glucosyloxy)-anthraquinone	C ₂₀ H ₁₈ O ₉	[M+Na] ⁺	425.08430	425.08447	-0.40	2.2E+06		2.1E+06		2.6E+06		3.3E+06	
948	p-Coumaroyl-dihydro-dihydroxy-phenylcoumarin	C ₂₄ H ₁₈ O ₆	[M+Na] ⁺	425.09956	425.09976	-0.47		1.2E+07						
949	Tomentolide A	C ₂₅ H ₂₂ O ₅	[M+Na] ⁺	425.13594	425.13615	-0.48	2.9E+07	3.4E+06	2.3E+07	1.5E+07	2.1E+07	1.5E+07	2.1E+07	3.2E+06
950	Sphenostylin D	C ₂₂ H ₂₆ O ₇	[M+Na] ⁺	425.15707	425.15725	-0.41	3.3E+06		2.8E+06		3.4E+06		2.3E+06	
951	Dihydroxy-diperoxy-eicosadienoic acid	C ₂₀ H ₃₄ O ₈	[M+Na] ⁺	425.21459	425.21466	-0.16					1.9E+06			6.1E+06
952	Trioxo-cholan-oic Acid	C ₂₄ H ₃₄ O ₅	[M+Na] ⁺	425.22984	425.23006	-0.49	3.9E+06	6.7E+06	3.5E+06		3.9E+06	3.1E+06	3.9E+06	
953	Erythronolide B	C ₂₁ H ₃₈ O ₇	[M+Na] ⁺	425.25097	425.25107	-0.23						2.1E+06		
954	MG(0:0/22:6/0:0)	C ₂₅ H ₃₈ O ₄	[M+Na] ⁺	425.26623	425.26643	-0.47	4.0E+06	9.9E+06	5.3E+07	2.2E+06	5.1E+06	6.3E+06	2.3E+07	2.7E+06
955	Dihydroxy-norprevitamin D3	C ₂₆ H ₄₂ O ₃	[M+Na] ⁺	425.30262	425.30281	-0.46	3.7E+06	3.5E+06	4.7E+06		2.8E+06	3.8E+06	4.1E+06	
956	Diaponeurosporene	C ₃₀ H ₄₂	[M+Na] ⁺	425.31787	425.31804	-0.40	3.0E+06		2.2E+06			3.3E+06	3.0E+06	
957	Hydroxycholesterol	C ₂₇ H ₄₆ O ₂	[M+Na] ⁺	425.33900	425.33906	-0.13		2.9E+06				5.0E+06		3.6E+06
958	Glutinine	C ₃₀ H ₄₈ O	[M+H] ⁺	425.37779	425.37784	-0.11	3.2E+06	8.9E+06	4.3E+06			7.4E+06	4.2E+06	3.4E+06
959	Octacosanoic acid	C ₂₈ H ₅₆ O ₂	[M+H] ⁺	425.43531	425.43535	-0.09	3.4E+06	4.3E+06	4.1E+06	1.9E+06		6.6E+06	3.5E+06	2.1E+06
960	Oleoylcarnitine	C ₂₅ H ₄₇ NO ₄	[M+H] ⁺	426.35779	426.35783	-0.11	3.6E+06	3.8E+06	4.8E+06		4.3E+06	2.9E+06	5.8E+06	
961	S-Glutathionyl-L-cysteine	C ₁₃ H ₂₂ N ₄ O ₈ S ₂	[M+H] ⁺	427.09518	427.09522	-0.10	3.2E+06		2.7E+06		3.2E+06			
962	Hexamethoxyflavanone	C ₂₁ H ₂₄ O ₈	[M+Na] ⁺	427.13634	427.13653	-0.44	2.9E+06		3.4E+06		3.6E+06		4.8E+06	
963	Chromolaenide	C ₂₂ H ₂₈ O ₇	[M+Na] ⁺	427.17272	427.17294	-0.51	3.0E+06		2.6E+06		2.7E+06			
964	Hydroxy-dioxo-cholanoic Acid	C ₂₄ H ₃₆ O ₅	[M+Na] ⁺	427.24549	427.24563	-0.30		2.4E+06				2.2E+06		
965	Hydroxy-didehydrovitamin D3 lactone	C ₂₇ H ₃₈ O ₄	[M+H] ⁺	427.28429	427.28395	0.79	9.4E+06	9.8E+06	5.7E+06	1.2E+07	9.1E+06	3.5E+06	1.3E+07	3.1E+06
966	Leupeptin	C ₂₀ H ₃₈ N ₆ O ₄	[M+H] ⁺	427.30273	427.30307	-0.80	2.7E+06	3.4E+06	3.3E+06		3.0E+06	3.6E+06	4.3E+06	
967	Dihydroxy-norsecovitamin D3	C ₂₆ H ₄₄ O ₃	[M+Na] ⁺	427.31827	427.31842	-0.35		3.0E+06				2.9E+06		
968	Hexacosanedioic acid	C ₂₆ H ₅₀ O ₄	[M+H] ⁺	427.37819	427.37821	-0.05	2.6E+06	3.2E+06				5.8E+06		1.8E+06
969	Neophenol	C ₃₀ H ₅₀ O	[M+H] ⁺	427.39344	427.39348	-0.09	7.0E+06	1.6E+07	9.4E+06	2.8E+06	3.4E+06	2.0E+07	7.7E+06	5.4E+06
970	Stearoylcarnitine	C ₂₅ H ₄₉ NO ₄	[M+H] ⁺	428.37344	428.37348	-0.10	2.9E+07	2.5E+07	3.7E+07	5.7E+06	1.9E+07	1.8E+07	4.4E+07	9.6E+06
971	Dopaxanthin	C ₁₈ H ₁₈ N ₂ O ₈	[M+K] ⁺	429.06947	429.06928	0.45	2.8E+06		3.5E+06		4.3E+06			
972	Hydroxy-dihydrojasmonic acid glucoside	C ₁₈ H ₃₀ O ₉	[M+K] ⁺	429.15214	429.15218	-0.09	2.5E+06							
973	Isomontanolide	C ₂₂ H ₃₀ O ₇	[M+Na] ⁺	429.18837	429.18857	-0.46	1.2E+07		8.3E+06		6.1E+06		5.5E+06	
974	Ketodeoxycholic acid	C ₂₄ H ₃₈ O ₄	[M+K] ⁺	429.24017	429.24021	-0.10	1.4E+08	5.6E+07	4.6E+07	1.4E+07	9.9E+07	3.7E+07	4.3E+07	1.0E+07
975	Trihydroxy-choenoic Acid	C ₂₄ H ₃₈ O ₅	[M+Na] ⁺	429.26115	429.26132	-0.41	1.0E+07	3.9E+06	8.0E+06		6.4E+06	3.9E+06	6.4E+06	2.6E+06

ESI(+) FT-ICR MS														
No.	Plausible Compound ^a	Molecular formula (M)	Ion	Theor m/z ^b	Exp. m/z ^c	Δ ppm _d	SM _R H ^e	SM _R O ^e	SM _P H ^e	SM _P O ^e	TF _R H ^e	TF _R O ^e	TF _P H ^e	TF _P O ^e
976	Dihydroxynoroxavitamin D3	C ₂₅ H ₄₂ O ₄	[M+Na] ⁺	429.29753	429.29772	-0.44	7.7E+06	1.2E+07	8.3E+06	4.0E+06	3.6E+06	8.6E+06	7.5E+06	
977	Diapophytofluene	C ₃₀ H ₄₆	[M+Na] ⁺	429.34917	429.34895	0.52								2.6E+06
978	Fucosterol epoxide	C ₂₉ H ₄₈ O ₂	[M+H] ⁺	429.37271	429.37276	-0.13	2.2E+06	3.3E+06	2.6E+06	1.3E+06		4.6E+06		1.9E+06
979	CMP-aminoethylphosphonate	C ₁₁ H ₂₀ N ₄ O ₁₀ P ₂	[M+H] ⁺	431.07274	431.07235	0.91					2.7E+06			
980	Ginkgolide A	C ₂₀ H ₂₄ O ₉	[M+Na] ⁺	431.13125	431.13144	-0.43	2.5E+06			1.0E+06				
981	Bleekerine	C ₂₃ H ₂₄ N ₂ O ₅	[M+Na] ⁺	431.15774	431.15765	0.21								2.1E+06
982	Vernoflexuoside	C ₂₁ H ₂₈ O ₈	[M+Na] ⁺	431.16764	431.16778	-0.33	2.7E+06							
983	PGE2 methyl ester acetate	C ₂₃ H ₃₆ O ₆	[M+Na] ⁺	431.24041	431.24064	-0.53	4.9E+06		3.6E+06					
984	Hydroxypregnenedione hydrogen succinate	C ₂₅ H ₃₄ O ₆	[M+H] ⁺	431.24282	431.24292	-0.24		4.2E+06						
985	Trihydroxy-cholanoic Acid	C ₂₄ H ₄₀ O ₅	[M+Na] ⁺	431.27680	431.27697	-0.41	5.7E+06	2.7E+06			3.9E+06	2.4E+06		
986	Oxo-hexacosenoic acid	C ₂₆ H ₄₈ O ₃	[M+Na] ⁺	431.34957	431.34963	-0.14		2.7E+06		2.6E+06				2.9E+06
987	C27-Phthienoic acid	C ₂₇ H ₅₂ O ₂	[M+Na] ⁺	431.38595	431.38596	-0.01				1.4E+06				2.8E+06
988	Sphingofungin D	C ₂₂ H ₄₁ NO ₇	[M+H] ⁺	432.29558	432.29563	-0.11	3.5E+06		2.3E+06		2.1E+06		2.5E+06	
989	Specionin	C ₂₀ H ₂₆ O ₉	[M+Na] ⁺	433.14690	433.14707	-0.39	3.5E+06				2.9E+06			
990	Gama-Tocotrienol	C ₂₈ H ₄₂ O ₂	[M+Na] ⁺	433.30770	433.30786	-0.37			2.2E+06					
991	MG(0:0/22:2/0:0)	C ₂₅ H ₄₆ O ₄	[M+Na] ⁺	433.32883	433.32891	-0.19		2.6E+06	2.2E+06	1.1E+06		4.7E+06		3.4E+06
992	Hexacosenoic acid	C ₂₆ H ₅₀ O ₂	[M+K] ⁺	433.34424	433.34427	-0.06	2.9E+06	3.9E+06	3.7E+06			5.0E+06	3.4E+06	
993	Acetophenazine	C ₂₃ H ₂₉ N ₃ O ₂ S	[M+Na] ⁺	434.18727	434.18688	0.90	4.6E+06							
994	Grayanotoxin I	C ₂₂ H ₃₆ O ₇	[M+Na] ⁺	435.23532	435.23543	-0.23		3.6E+06				2.4E+06		
995	Oleoylglycerone phosphate	C ₂₁ H ₃₉ O ₇ P	[M+H] ⁺	435.25062	435.25077	-0.34	3.5E+06	6.5E+06			2.8E+06			
996	Dihydroxy-cyclo-didehydroepivitamin D3	C ₂₇ H ₄₀ O ₃	[M+Na] ⁺	435.28697	435.28713	-0.38	3.1E+06	3.6E+06	3.8E+06			3.8E+06	3.8E+06	
997	Ficisterol	C ₂₉ H ₄₈ O	[M+Na] ⁺	435.35974	435.35992	-0.41	1.1E+07	1.4E+07	1.2E+07	5.2E+06	3.8E+06	1.6E+07	1.1E+07	3.9E+06
998	Hydroxyhexacosanoic acid	C ₂₆ H ₅₂ O ₃	[M+Na] ⁺	435.38087	435.38092	-0.11		2.4E+06				3.8E+06		
999	N-stearoyl glutamic acid	C ₂₃ H ₄₃ NO ₅	[M+Na] ⁺	436.30334	436.30335	-0.01				1.1E+06				
1000	Estra-triene-triol triacetate	C ₂₄ H ₃₀ O ₆	[M+Na] ⁺	437.19346	437.19351	-0.12							2.3E+06	
1001	Methyl hydroperoxy-bisepidioxy-eicosadienoate	C ₂₁ H ₃₄ O ₈	[M+Na] ⁺	437.21459	437.21463	-0.09						2.1E+06		
1002	Lupulone	C ₂₆ H ₃₈ O ₄	[M+Na] ⁺	437.26623	437.26641	-0.40		2.1E+06	2.1E+06				3.0E+06	
1003	Dihydroxy-methano-norvitamin D3	C ₂₇ H ₄₂ O ₃	[M+Na] ⁺	437.30262	437.30280	-0.42	1.4E+07		9.9E+06	3.6E+06	5.1E+06		9.5E+06	
1004	Hydroxy-campestenone	C ₂₈ H ₄₆ O ₂	[M+Na] ⁺	437.33900	437.33914	-0.32		2.6E+06	2.3E+06			4.3E+06	3.0E+06	

ESI(+) FT-ICR MS														
No.	Plausible Compound ^a	Molecular formula (M)	Ion	Theor m/z ^b	Exp. m/z ^c	Δ ppm _d	SM _R H ^e	SM _R O ^e	SM _P H ^e	SM _P O ^e	TF _R H ^e	TF _R O ^e	TF _P H ^e	TF _P O ^e
1005	MG(22:0/0:0/0:0)	C ₂₅ H ₅₀ O ₄	[M+Na] ⁺	437.36013	437.36017	-0.09	2.0E+06	4.5E+06		1.9E+06		6.4E+06		3.0E+06
1006	Tridecyl oleate	C ₂₉ H ₅₆ O ₂	[M+H] ⁺	437.43531	437.43533	-0.06	4.8E+06	6.9E+06	5.9E+06	1.8E+06	2.4E+06	1.1E+07	6.0E+06	3.0E+06
1007	Fluphenazine	C ₂₂ H ₂₆ F ₃ N ₃ OS	[M+H] ⁺	438.18214	438.18176	0.88			6.8E+06		5.7E+06		4.7E+06	
1008	Lunarine	C ₂₅ H ₃₁ N ₃ O ₄	[M+H] ⁺	438.23873	438.23912	-0.89	2.4E+07		2.2E+07	3.8E+06	2.5E+07	5.2E+06	1.8E+07	3.9E+06
1009	Erioflorin methacrylate	C ₂₃ H ₂₈ O ₇	[M+Na] ⁺	439.17272	439.17294	-0.49	3.0E+06	6.6E+06	5.8E+06				5.4E+06	
1010	Alfentanil	C ₂₁ H ₃₂ N ₆ O ₃	[M+Na] ⁺	439.24281	439.24246	0.81	3.1E+06				4.2E+06			
1011	Dihydroxyandrosthenone dipropionate	C ₂₅ H ₃₆ O ₅	[M+Na] ⁺	439.24549	439.24570	-0.46	2.7E+06	3.6E+06	2.8E+06			2.6E+06	2.3E+06	
1012	Epoxy-dihydroxy-norvitamin D3	C ₂₆ H ₄₀ O ₄	[M+Na] ⁺	439.28188	439.28199	-0.25	3.5E+06	2.2E+06	3.1E+06				3.4E+06	
1013	Calcitriol	C ₂₇ H ₄₄ O ₃	[M+Na] ⁺	439.31827	439.31839	-0.27	3.2E+06		4.5E+06	3.0E+06	2.3E+06		4.9E+06	5.2E+06
1014	Beta-tocopherol	C ₂₈ H ₄₈ O ₂	[M+Na] ⁺	439.35465	439.35469	-0.09	5.0E+06	3.6E+07	1.6E+07	1.2E+07	2.4E+06	5.0E+07	2.2E+07	1.8E+07
1015	Pentacosanoylglycine	C ₂₇ H ₅₃ NO ₃	[M+H] ⁺	440.40982	440.40987	-0.11		4.4E+07		3.6E+06		5.3E+06		
1016	Hallactone B	C ₂₀ H ₂₄ O ₉ S	[M+H] ⁺	441.12138	441.12154	-0.36					3.1E+06		2.8E+06	
1017	Syringaresinol	C ₂₂ H ₂₆ O ₈	[M+Na] ⁺	441.15199	441.15212	-0.30	2.2E+06							
1018	Trihydroxy-methylpregnendione acetate	C ₂₄ H ₃₄ O ₆	[M+Na] ⁺	441.22476	441.22493	-0.39		2.3E+06						
1019	Dihydroxy-pregnanone diacetate	C ₂₅ H ₃₈ O ₅	[M+Na] ⁺	441.26115	441.26132	-0.40		2.2E+06						
1020	Trifluoro-hydroxy-norvitamin D3	C ₂₆ H ₃₉ F ₃ O ₂	[M+H] ⁺	441.29749	441.29757	-0.18	8.6E+06	1.2E+07	4.3E+06	4.0E+06	2.7E+06	9.8E+06	8.4E+06	6.5E+06
1021	apo-Carotenol	C ₃₀ H ₄₂ O	[M+Na] ⁺	441.31279	441.31299	-0.45		2.5E+06				3.5E+06		2.5E+06
1022	Dihomo-hydroxy epivitamin D2	C ₃₀ H ₄₈ O ₂	[M+H] ⁺	441.37271	441.37279	-0.19		4.2E+06						
1023	MG(0:0/24:1/0:0)	C ₂₇ H ₅₂ O ₄	[M+H] ⁺	441.39384	441.39392	-0.18		2.2E+06				4.7E+06		
1024	Glycyphyllin	C ₂₁ H ₂₄ O ₉	[M+Na] ⁺	443.13125	443.13144	-0.42							2.5E+06	
1025	Eupacunolin	C ₂₂ H ₂₈ O ₈	[M+Na] ⁺	443.16764	443.16784	-0.45	4.4E+06		3.4E+06		2.7E+06			
1026	Fluoro-trihydroxypregnadiendione acetate	C ₂₃ H ₂₉ FO ₆	[M+Na] ⁺	443.18404	443.18411	-0.15		2.6E+06				2.4E+06		
1027	PG(13:0/0:0)	C ₁₉ H ₃₉ O ₉ P	[M+H] ⁺	443.24045	443.24062	-0.39	2.7E+06				2.6E+06			
1028	Scillirosidin	C ₂₆ H ₃₄ O ₆	[M+H] ⁺	443.24282	443.24293	-0.26		5.1E+06						
1029	Testosterone phenylpropionate	C ₂₈ H ₃₆ O ₃	[M+Na] ⁺	443.25567	443.25582	-0.35	2.9E+06							
1030	Hydroperoxy-squalene	C ₃₀ H ₅₀ O ₂	[M+H] ⁺	443.38836	443.38842	-0.14		4.5E+06				3.9E+06		
1031	Bis[(phenyl-propyl)phenyl]amine	C ₃₀ H ₃₁ N	[M+K] ⁺	444.20881	444.20843	0.85		2.4E+06				3.3E+06		
1032	Hydroxy-octadecanoylcarnitine	C ₂₅ H ₄₉ NO ₅	[M+H] ⁺	444.36835	444.36841	-0.13	2.4E+06		3.5E+06			3.2E+06	3.0E+06	
1033	Enantiomultijugin	C ₂₄ H ₂₂ O ₇	[M+Na] ⁺	445.12577	445.12605	-0.62	5.1E+06							

ESI(+) FT-ICR MS														
No.	Plausible Compound ^a	Molecular formula (M)	Ion	Theor m/z ^b	Exp m/z ^c	Δ ppm ^d	SM _R H ^e	SM _R O ^e	SM _P H ^e	SM _P O ^e	TF _R H ^e	TF _R O ^e	TF _P H ^e	TF _P O ^e
1034	Octenol-3-o-D-xylopyranosyl-glucopyranoside	C ₁₉ H ₃₄ O ₁₀	[M+Na] ⁺	445.20442	445.20449	-0.16					3.9E+06			
1035	Trihydroxy-oxo-cholanoic Acid	C ₂₄ H ₃₈ O ₆	[M+Na] ⁺	445.25606	445.25632	-0.58					3.0E+06			
1036	Methyl-butanoyloxy-villanovanediol	C ₂₅ H ₄₂ O ₅	[M+Na] ⁺	445.29245	445.29266	-0.48	1.7E+07	3.3E+07	1.7E+07	6.6E+06	6.9E+06	1.7E+07	2.1E+07	2.8E+06
1037	Grandidentatin	C ₂₁ H ₂₈ O ₉	[M+Na] ⁺	447.16255	447.16273	-0.39	4.8E+06				3.6E+06		3.7E+06	
1038	Didrovaltratum	C ₂₂ H ₃₂ O ₈	[M+Na] ⁺	447.19894	447.19912	-0.41	4.5E+06				3.1E+06			
1039	Difenoxin	C ₂₈ H ₂₈ N ₂ O ₂	[M+Na] ⁺	447.20430	447.20408	0.49		3.8E+06						
1040	Pravastatin	C ₂₃ H ₃₆ O ₇	[M+Na] ⁺	447.23532	447.23554	-0.49	5.9E+06		5.0E+06		4.2E+06		4.6E+06	
1041	Alpha-Tocotrienol	C ₂₉ H ₄₄ O ₂	[M+Na] ⁺	447.32335	447.32359	-0.53		2.6E+06	3.3E+06			3.6E+06	3.9E+06	
1042	Trihydroxy-homovitamin D3	C ₂₈ H ₄₆ O ₄	[M+H] ⁺	447.34689	447.34698	-0.20		5.5E+06			4.0E+06			
1043	Glutinine	C ₃₀ H ₄₈ O	[M+Na] ⁺	447.35974	447.35997	-0.52	2.4E+06							
1044	Tephrosin A	C ₂₄ H ₂₆ O ₇	[M+Na] ⁺	449.15707	449.15725	-0.40	5.0E+06	3.0E+06	5.1E+06		3.1E+06			
1045	Abcisic acid glucose ester	C ₂₁ H ₃₀ O ₉	[M+Na] ⁺	449.17820	449.17842	-0.47	1.1E+07		9.0E+06		9.5E+06		6.7E+06	
1046	Dihydroxy-oxo-prostadienoic acid glyceryl ester	C ₂₃ H ₃₈ O ₇	[M+Na] ⁺	449.25097	449.25113	-0.35		2.8E+06						
1047	Glutathionylaminopropylcadaverine	C ₁₈ H ₃₆ N ₆ O ₅ S	[M+H] ⁺	449.25407	449.25438	-0.70						2.6E+06		
1048	Hydroxy-gama-tocotrienol	C ₂₈ H ₄₂ O ₃	[M+Na] ⁺	449.30262	449.30286	-0.53		4.7E+06	3.1E+06			5.6E+06	3.4E+06	2.3E+06
1049	Hydroxy-methylvitamin D2	C ₂₉ H ₄₆ O ₂	[M+Na] ⁺	449.33900	449.33922	-0.49			3.3E+06					
1050	Hexacosanedioic acid	C ₂₆ H ₅₀ O ₄	[M+Na] ⁺	449.36013	449.36020	-0.15				3.2E+06				
1051	Methylene-stigmastanol	C ₃₀ H ₅₀ O	[M+Na] ⁺	449.37539	449.37548	-0.21					4.6E+06			
1052	tetramethyl-hexacosadienoic acid	C ₃₀ H ₅₆ O ₂	[M+H] ⁺	449.43531	449.43528	0.06						3.0E+06		
1053	Tetrahydroxyflavanone 6-C-glucoside	C ₂₁ H ₂₂ O ₁₁	[M+H] ⁺	451.12349	451.12359	-0.23			2.8E+06					
1054	Furcadin	C ₂₀ H ₂₈ O ₁₀	[M+Na] ⁺	451.15747	451.15770	-0.51	1.3E+07		1.1E+07		1.1E+07		7.5E+06	
1055	Heteroflavanone B	C ₂₄ H ₂₈ O ₇	[M+Na] ⁺	451.17272	451.17290	-0.39	1.7E+07	3.0E+06	1.2E+07		9.8E+06		7.8E+06	
1056	Hydroxyvitamin D3 lactone	C ₂₇ H ₄₀ O ₄	[M+Na] ⁺	451.28188	451.28213	-0.55		3.0E+06						
1057	Chaksine	C ₂₂ H ₃₈ N ₆ O ₄	[M+H] ⁺	451.30273	451.30311	-0.83		4.7E+06				4.2E+06		2.8E+06
1058	Dihydroxy-methyl-didehydrovitamin D3	C ₂₈ H ₄₄ O ₃	[M+Na] ⁺	451.31827	451.31846	-0.43	8.3E+06	8.9E+06	6.7E+06	4.0E+06	3.8E+06	7.4E+06	6.6E+06	
1059	Myristyl oleate	C ₃₀ H ₅₈ O ₂	[M+H] ⁺	451.45096	451.45101	-0.12	1.2E+07	1.8E+07	1.5E+07	3.8E+06	3.8E+06	3.0E+07	1.5E+07	6.7E+06
1060	Tomatidinol	C ₂₇ H ₄₃ NO ₂	[M+K] ⁺	452.29254	452.29284	-0.67				3.8E+06				
1061	N-oleoyl phenylalanine	C ₂₇ H ₄₃ NO ₃	[M+Na] ⁺	452.31351	452.31374	-0.49	7.5E+06		4.4E+06	8.9E+06	7.9E+06	2.6E+06	9.9E+06	2.6E+06
1062	Dimethyl-bis(methoxyphenyl)benzopyranol acetate	C ₂₇ H ₂₆ O ₅	[M+Na] ⁺	453.16724	453.16746	-0.48	6.3E+06	4.6E+08	9.6E+06	3.4E+07	5.0E+06	4.8E+07	6.6E+06	1.4E+07

ESI(+) FT-ICR MS														
No.	Plausible Compound ^a	Molecular formula (M)	Ion	Theor m/z ^b	Exp m/z ^c	Δ ppm ^d	SM _R H ^e	SM _R O ^e	SM _P H ^e	SM _P O ^e	TF _R H ^e	TF _R O ^e	TF _P H ^e	TF _P O ^e
1063	PA(18:4/0:0)	C ₂₁ H ₃₅ O ₇ P	[M+Na] ⁺	453.20126	453.20146	-0.44	3.8E+06							
1064	Phenyl-trinor-PGF2alpha isopropyl ester	C ₂₆ H ₃₈ O ₅	[M+Na] ⁺	453.26115	453.26133	-0.41	7.1E+06	4.5E+06	3.8E+06		4.5E+06	2.9E+06	5.2E+06	
1065	Solagenin	C ₂₇ H ₄₂ O ₄	[M+Na] ⁺	453.29753	453.29764	-0.23	2.7E+06	3.6E+06	2.4E+06			2.9E+06	3.8E+06	
1066	Difluoro-dihydroxyvitamin D3	C ₂₇ H ₄₂ F ₂ O ₃	[M+H] ⁺	453.31748	453.31714	0.75					3.9E+06			
1067	Methyl-epi-dihydroxyvitamin D3	C ₂₈ H ₄₆ O ₃	[M+Na] ⁺	453.33392	453.33410	-0.41	4.0E+06	4.7E+06	5.1E+06				4.4E+06	2.4E+06
1068	Alpha-Tocopherol	C ₂₉ H ₅₀ O ₂	[M+Na] ⁺	453.37030	453.37035	-0.10		5.7E+06	7.7E+06			1.8E+07		
1069	Tetradecyl-hexadecanoate	C ₃₀ H ₆₀ O ₂	[M+H] ⁺	453.46661	453.46664	-0.08	4.9E+06	5.9E+06	5.4E+06	1.6E+06		9.4E+06	4.8E+06	3.4E+06
1070	Sphingofungin D	C ₂₂ H ₄₁ NO ₇	[M+Na] ⁺	454.27752	454.27756	-0.08								2.4E+06
1071	Spironolactone	C ₂₄ H ₃₂ O ₄ S	[M+K] ⁺	455.16529	455.16558	-0.64		3.4E+07						
1072	Alfentanil	C ₂₁ H ₃₂ N ₆ O ₃	[M+H] ⁺	455.21675	455.21648	0.59					4.0E+06			
1073	Diaponeurosporenic acid	C ₃₀ H ₄₀ O ₂	[M+Na] ⁺	455.29205	455.29226	-0.46	4.5E+06	5.6E+06	4.5E+06			3.8E+06	5.4E+06	
1074	Trifluoro-hydroxyvitamin D3	C ₂₇ H ₄₁ F ₃ O ₂	[M+Na] ⁺	455.31314	455.31323	-0.20		4.4E+06				3.9E+06		2.9E+06
1075	Hydroxy-gama-tocopherol	C ₂₈ H ₄₈ O ₃	[M+Na] ⁺	455.34957	455.34962	-0.13		9.2E+06	3.8E+06	3.0E+06		1.0E+07	7.0E+06	5.4E+06
1076	Pelargonidin 3-O-glucoside	C ₂₁ H ₂₁ O ₁₀	[M+Na] ⁺	456.10269	456.10253	0.36	4.8E+06		3.9E+06		6.4E+06			
1077	Arachidyl carnitine	C ₂₇ H ₅₃ NO ₄	[M+H] ⁺	456.40474	456.40480	-0.13			2.6E+06				2.6E+06	
1078	Heptamethoxyflavanone (Diphenylethenylidene)bis[N,N-dimethylbenzenamine]	C ₂₂ H ₂₆ O ₉	[M+Na] ⁺	457.14690	457.14715	-0.54	2.6E+06						2.4E+06	
1079		C ₃₀ H ₃₀ N ₂	[M+K] ⁺	457.20406	457.20448	-0.91	2.8E+06				3.5E+06			
1080	Trihydroxy-oxavitamin D3	C ₂₆ H ₄₂ O ₅	[M+Na] ⁺	457.29245	457.29264	-0.43	2.5E+06							
1081	Trihydroxy-dihydrovitamin D3	C ₂₇ H ₄₆ O ₄	[M+Na] ⁺	457.32883	457.32892	-0.20		4.1E+06				4.4E+06		
1082	Salvisyriacolide	C ₂₅ H ₄₀ O ₆	[M+Na] ⁺	459.27171	459.27192	-0.45	2.4E+07		1.4E+07		1.2E+07		1.1E+07	
1083	Varanic acid	C ₂₆ H ₄₄ O ₅	[M+Na] ⁺	459.30810	459.30830	-0.43	1.4E+07	1.2E+07	1.4E+07	4.7E+06	6.3E+06	5.7E+06	1.6E+07	3.1E+06
1084	Cholestane-tetrol	C ₂₇ H ₄₈ O ₄	[M+Na] ⁺	459.34448	459.34449	-0.02						3.4E+06		
1085	Tetramethy-tetracosadienoic acid	C ₂₈ H ₅₂ O ₂	[M+K] ⁺	459.35989	459.35987	0.04							2.4E+06	
1086	Oxo-octacosenoic acid	C ₂₈ H ₅₂ O ₃	[M+Na] ⁺	459.38087	459.38091	-0.10		2.3E+06						
1087	Militarinone A	C ₂₆ H ₃₇ NO ₆	[M+H] ⁺	460.26936	460.26943	-0.14		5.4E+06						
1088	(Methyl-butanoyloxy)-villanovanediol	C ₂₅ H ₄₂ O ₆	[M+Na] ⁺	461.28736	461.28755	-0.42	5.3E+07	4.5E+06	3.5E+07		2.3E+07		2.6E+07	
1089	Nor-cholestanpentol	C ₂₆ H ₄₆ O ₅	[M+Na] ⁺	461.32375	461.32387	-0.27		2.7E+06						
1090	Ophirasterol	C ₃₁ H ₅₀ O	[M+Na] ⁺	461.37539	461.37556	-0.38	6.9E+06	1.7E+07	1.3E+07	3.7E+06		1.6E+07	1.3E+07	4.1E+06

ESI(+) FT-ICR MS														
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1091	Carboxy-gama-tocotrienol	C ₂₈ H ₃₉ O ₄	[M+Na] ⁺	462.27406	462.27381	0.53								3.0E+06
1092	D-Glucosylsphingosine	C ₂₄ H ₄₇ NO ₇	[M+H] ⁺	462.34253	462.34258	-0.12		3.7E+06	2.7E+06			3.1E+06	2.5E+06	
1093	Amurensisin	C ₂₂ H ₁₆ O ₁₀	[M+Na] ⁺	463.06357	463.06366	-0.19	1.2E+07		1.1E+07		1.1E+07		4.2E+06	
1094	Deacetyl-debenzoylbaccatin III	C ₂₂ H ₃₂ O ₉	[M+Na] ⁺	463.19385	463.19397	-0.24	4.4E+06				4.8E+06			
1095	Cyclopropyl-dihydroxy-didehydro-norvitamin D3	C ₂₉ H ₄₄ O ₃	[M+Na] ⁺	463.31827	463.31845	-0.41	8.6E+06	9.2E+06	8.1E+06	4.3E+06	2.6E+06	6.5E+06	8.1E+06	2.6E+06
1096	Dihomo-hydroxy-epivitamin D2	C ₃₀ H ₄₈ O ₂	[M+Na] ⁺	463.35465	463.35481	-0.34			3.7E+06					
1097	MG(24:1/0:0/0:0)	C ₂₇ H ₅₂ O ₄	[M+Na] ⁺	463.37578	463.37582	-0.08			3.8E+06	4.1E+06			5.0E+06	
1098	Methylcycloartaenol	C ₃₁ H ₅₂ O	[M+Na] ⁺	463.39104	463.39122	-0.39	6.1E+06	1.1E+07	8.7E+06	3.3E+06	2.8E+06	1.1E+07	7.3E+06	3.3E+06
1099	Adenylsuccinic acid	C ₁₄ H ₁₈ N ₅ O ₁₁ P	[M+H] ⁺	464.08132	464.08093	0.84					3.2E+06			
1100	D-Glucosyldihydrosphingosine	C ₂₄ H ₄₉ NO ₇	[M+H] ⁺	464.35818	464.35820	-0.03		3.1E+06	3.0E+06			2.8E+06	2.9E+06	
1101	Hydroxy-tetramethoxy-prenyloxyflavone	C ₂₄ H ₂₆ O ₈	[M+Na] ⁺	465.15199	465.15219	-0.42	5.2E+06		4.9E+06		4.2E+06		3.3E+06	
1102	Lusitanicoside	C ₂₁ H ₃₀ O ₁₀	[M+Na] ⁺	465.17312	465.17332	-0.43	8.3E+06		6.4E+06		5.9E+06		5.5E+06	
1103	Psychotrine	C ₂₈ H ₃₆ N ₂ O ₄	[M+H] ⁺	465.27478	465.27483	-0.10	4.8E+06		6.1E+06					
1104	Dihydroxy-dimethyl-didehydrovitamin D3	C ₂₉ H ₄₆ O ₃	[M+Na] ⁺	465.33392	465.33411	-0.41	1.3E+07	1.1E+07	9.3E+06	4.7E+06	5.0E+06	9.6E+06	8.7E+06	3.0E+06
1105	Sphingosine-1-phosphocholine	C ₂₃ H ₄₉ N ₂ O ₅ P	[M+H] ⁺	465.34519	465.34535	-0.35	4.3E+06			4.2E+06				
1106	Hopendiol	C ₃₀ H ₅₀ O ₂	[M+Na] ⁺	465.37030	465.37034	-0.09	6.3E+06	3.9E+07	9.4E+06	7.6E+06	3.5E+06		1.6E+07	1.5E+07
1107	MG(24:0/0:0/0:0)	C ₂₇ H ₅₄ O ₄	[M+Na] ⁺	465.39143	465.39147	-0.08		4.9E+06		2.2E+06		7.0E+06	3.5E+06	3.8E+06
1108	Pentadecyl oleate	C ₃₁ H ₆₀ O ₂	[M+H] ⁺	465.46661	465.46663	-0.04	1.1E+07	1.6E+07	1.4E+07	3.6E+06	4.6E+06	2.7E+07	1.3E+07	6.2E+06
1109	Codonocarpine	C ₂₆ H ₃₁ N ₃ O ₅	[M+H] ⁺	466.23365	466.23404	-0.84					3.7E+06			
1110	Sphingosyl-phosphocholine	C ₂₃ H ₅₀ N ₂ O ₅ P	[M+H] ⁺	466.35301	466.35271	0.65	1.4E+07	2.9E+07	2.3E+07	6.8E+06	4.2E+06	2.0E+07	2.7E+07	6.3E+06
1111	Dihydrophaseic acid O-beta-D-glucoside	C ₂₁ H ₃₂ O ₁₀	[M+Na] ⁺	467.18877	467.18896	-0.41	6.5E+07		5.0E+07		3.9E+07		3.2E+07	
1112	Dehydro-clavulone	C ₂₅ H ₃₂ O ₇	[M+Na] ⁺	467.20402	467.20421	-0.40		2.8E+06						
1113	Bufotalin	C ₂₆ H ₃₆ O ₆	[M+Na] ⁺	467.24041	467.24055	-0.30		2.5E+06						
1114	Dihydroxyvitamin D3 lactone	C ₂₇ H ₄₀ O ₅	[M+Na] ⁺	467.27680	467.27697	-0.37	4.4E+06	3.6E+06	4.6E+06			3.6E+06	3.9E+06	
1115	Trihydroxyvitamin D2	C ₂₈ H ₄₄ O ₄	[M+Na] ⁺	467.31318	467.31332	-0.30	3.0E+06							
1116	Ethyl-dihydroxyvitamin D3	C ₂₉ H ₄₈ O ₃	[M+Na] ⁺	467.34957	467.34972	-0.33	3.5E+06	3.3E+06	4.2E+06			5.3E+06	3.9E+06	
1117	Triacotatetraenoic acid	C ₃₀ H ₅₂ O ₂	[M+Na] ⁺	467.38595	467.38599	-0.09		6.6E+06	2.6E+06			5.6E+06	3.3E+06	
1118	Dynorphin A	C ₁₈ H ₃₉ N ₉ O ₄	[M+Na] ⁺	468.30172	468.30139	0.71		2.8E+06						
1119	Catechinol O-beta-D-galactopyranoside	C ₂₁ H ₂₄ O ₁₂	[M+H] ⁺	469.13405	469.13411	-0.12	5.0E+06		4.3E+06		6.9E+06			

ESI(+) FT-ICR MS														
No.	Plausible Compound ^a	Molecular formula (M)	Ion	Theor m/z ^b	Exp. m/z ^c	Δ ppm _d	SM _{RH} ^e	SM _{RO} ^e	SM _{PH} ^e	SM _{PO} ^e	TF _{RH} ^e	TF _{RO} ^e	TF _{PH} ^e	TF _{PO} ^e
1120	Ptilosteroid A	C ₂₁ H ₃₄ O ₈ S	[M+Na] ⁺	469.18666	469.18706	-0.85	6.2E+06		5.1E+06		5.1E+06			
1121	PG(15:1(9Z)/0:0)	C ₂₁ H ₄₁ O ₉ P	[M+H] ⁺	469.25610	469.25624	-0.30	3.2E+06	3.8E+06				2.9E+06		
1122	Trifluoro-dihydroxy-didehydrovitamin D3	C ₂₇ H ₃₉ F ₃ O ₃	[M+H] ⁺	469.29241	469.29263	-0.48		2.8E+06						
1123	Trihydroxy-homovitamin D3	C ₂₈ H ₄₆ O ₄	[M+Na] ⁺	469.32883	469.32891	-0.17				2.3E+06				
1124	Hydroxy-tocopherol [primary alcohol] ([M+Na] ⁺)	C ₂₉ H ₅₀ O ₃	[M+Na] ⁺	469.36522	469.36526	-0.10		3.2E+06		2.2E+06		7.0E+06		3.4E+06
1125	Kalbreclasine	C ₂₀ H ₂₃ NO ₁₂	[M+H] ⁺	470.12930	470.12932	-0.05	3.5E+06		5.3E+06		3.2E+06			
1126	PS(14:0/0:0)	C ₂₀ H ₄₀ NO ₉ P	[M+H] ⁺	470.25134	470.25150	-0.32			3.9E+06	7.6E+06	5.3E+06		7.1E+06	
1127	Diiodo-hydroxyphenylpyruvate	C ₉ H ₆ I ₂ O ₄	[M+K] ⁺	470.79871	470.79880	-0.18	2.9E+06				4.7E+06			4.4E+06
1128	Temocaprilat	C ₂₁ H ₂₄ N ₂ O ₅ S ₂	[M+Na] ⁺	471.10188	471.10218	-0.62		4.4E+06		5.3E+06				
1129	Artonin P D-Galactosyl-3-(N-acetyl-beta-D-galactosaminy)-L-serine	C ₂₅ H ₂₀ O ₈	[M+Na] ⁺	471.10504	471.10522	-0.38				3.6E+07				5.0E+07
1130		C ₁₇ H ₃₀ N ₂ O ₁₃	[M+H] ⁺	471.18207	471.18207	-0.02	4.0E+06		5.3E+06		2.7E+06			
1131	Usambarensine	C ₂₉ H ₂₈ N ₄	[M+K] ⁺	471.19456	471.19425	0.66				1.3E+06				6.4E+06
1132	Estradiol glucuronide	C ₂₄ H ₃₂ O ₈	[M+Na] ⁺	471.19894	471.19913	-0.40	5.4E+06	5.0E+06	4.2E+06		3.9E+06		5.8E+06	
1133	Stigmatellin X	C ₂₈ H ₃₈ O ₆	[M+H] ⁺	471.27412	471.27421	-0.20		3.7E+06						
1134	Trihydroxyvitamin D3	C ₂₇ H ₄₄ O ₄	[M+K] ⁺	471.28712	471.28708	0.08			4.2E+06					
1135	Trifluoro-dihydroxyvitamin D3	C ₂₇ H ₄₁ F ₃ O ₃	[M+H] ⁺	471.30806	471.30814	-0.17		4.2E+06	2.6E+06			3.2E+06		2.9E+06
1136	Hydroxy-gama-tocopherol	C ₂₈ H ₄₈ O ₃	[M+K] ⁺	471.32350	471.32349	0.03	3.3E+06							
1137	Chlorogenin	C ₂₈ H ₄₈ O ₄	[M+Na] ⁺	471.34448	471.34453	-0.10		3.8E+06				4.8E+06		
1138	Tetramethyl-hexacosadienoic acid	C ₃₀ H ₅₆ O ₂	[M+Na] ⁺	471.41725	471.41734	-0.18		5.6E+06		1.2E+06				2.8E+06
1139	Glucosquerellin	C ₁₄ H ₂₇ NO ₉ S ₃	[M+Na] ⁺	472.07402	472.07360	0.88			3.7E+06					
1140	Nigakilactone E	C ₂₄ H ₃₄ O ₈	[M+Na] ⁺	473.21459	473.21476	-0.37	1.5E+07		1.1E+07		1.0E+07		7.2E+06	
1141	Laserpitin	C ₂₅ H ₃₈ O ₇	[M+Na] ⁺	473.25097	473.25118	-0.43	3.0E+06							
1142	Trihydroxy-cholestanoic acid	C ₂₇ H ₄₆ O ₅	[M+Na] ⁺	473.32375	473.32395	-0.44	8.9E+06	1.5E+07	9.7E+06	4.1E+06	4.2E+06	9.2E+06	9.5E+06	
1143	Dihydroxy-dimethylhexadehydro-homovitamin D3	C ₃₀ H ₄₄ O ₃	[M+Na] ⁺	475.31827	475.31853	-0.55	1.1E+07	1.2E+07	4.5E+06			5.7E+07	7.6E+06	1.1E+07
1144	Phylloquinol	C ₃₁ H ₄₈ O ₂	[M+Na] ⁺	475.35465	475.35488	-0.48			3.0E+06					
1145	Tetrahydrogeranylgeranyl diphosphate	C ₂₀ H ₄₀ O ₇ P ₂	[M+Na] ⁺	477.21415	477.21454	-0.81			2.8E+06				7.0E+06	
1146	Dihydroxy-dimethyl-tetradehydro-	C ₃₀ H ₄₆ O ₃	[M+Na] ⁺	477.33392	477.33409	-0.37	2.7E+06	3.6E+06				2.9E+06		

homovitamin D3						
1147	Vitamin D3 butyrate	$C_{31}H_{50}O_2$	[M+Na] ⁺	477.37030	477.37050	-0.42
						3.3E+06

ESI(+) FT-ICR MS														
No.	Plausible Compound ^a	Molecular formula (M)	Ion	Theo r m/z ^b	Exp . m/z ^c	Δ ppm ^d	SM _R H ^e	SM _R O ^e	SM _P H ^e	SM _P O ^e	TF _R H ^e	TF _R O ^e	TF _P H ^e	TF _P O ^e
1148	Ethyl-trimethyl-hydroxycholestadiene	C ₃₂ H ₅₄ O	[M+Na] ⁺	477.40669	477.40688	-0.41	4.3E+06	1.0E+07	7.3E+06	3.1E+06		9.4E+06	6.9E+06	3.0E+06
1149	PS(13:0/0:0)	C ₁₉ H ₃₈ NO ₉ P	[M+Na] ⁺	478.21764	478.21766	-0.03	2.8E+06						2.5E+06	
1150	Abyssinoflavanone V	C ₂₅ H ₂₈ O ₇	[M+K] ⁺	479.14666	479.14709	-0.89								9.4E+06
1151	Minabeolide-7	C ₂₈ H ₄₀ O ₅	[M+Na] ⁺	479.27680	479.27698	-0.39	2.7E+06	1.2E+07	2.8E+06	2.9E+06				
1152	Trihydroxy-tetradehydrodihomoepivitamin D3	C ₂₉ H ₄₄ O ₄	[M+Na] ⁺	479.31318	479.31337	-0.40		3.2E+06						
1153	Butyl-dihydroxy-didehydro-norvitamin D3	C ₃₀ H ₄₈ O ₃	[M+Na] ⁺	479.34957	479.34975	-0.38	9.0E+06		8.6E+06	4.8E+06	3.5E+06	9.2E+06	8.9E+06	2.8E+06
1154	Palmityl oleate	C ₃₂ H ₆₂ O ₂	[M+H] ⁺	479.48226	479.48230	-0.09	1.6E+07	2.5E+07	2.0E+07	5.0E+06	5.3E+06	4.4E+07	1.9E+07	9.0E+06
1155	Hexahydroxyflavone 3-glucoside	C ₂₁ H ₂₀ O ₁₃	[M+H] ⁺	481.09767	481.09775	-0.17	3.8E+06				3.8E+06			
1156	3-Sulfodeoxycholic acid	C ₂₃ H ₃₈ O ₇ S	[M+Na] ⁺	481.22305	481.22325	-0.43		1.1E+07	2.9E+06			6.9E+06		
1157	PA(10:0/10:0)	C ₂₃ H ₄₅ O ₈ P	[M+H] ⁺	481.29248	481.29267	-0.40	4.1E+06	4.7E+06	3.6E+06	2.8E+06		4.7E+06	3.2E+06	
1158	Dihydroxy-trihomovitamin D3	C ₃₀ H ₅₀ O ₃	[M+Na] ⁺	481.36522	481.36535	-0.27	4.9E+06		7.4E+06	5.4E+06	3.1E+06	1.4E+07	1.0E+07	9.0E+06
1159	Hexadecyl hexadecanoate	C ₃₂ H ₆₄ O ₂	[M+H] ⁺	481.49791	481.49794	-0.07	5.2E+06	6.5E+06	5.9E+06	2.0E+06	2.9E+06	1.2E+07	5.7E+06	3.6E+06
1160	Cer(d18:1/12:0)	C ₃₀ H ₅₉ NO ₃	[M+H] ⁺	482.45677	482.45680	-0.06		3.9E+06				2.6E+06		
1161	6-Acetylpicropolin	C ₂₄ H ₂₈ O ₉	[M+Na] ⁺	483.16255	483.16277	-0.45	4.6E+06		3.4E+06		4.0E+06			
1162	Dihydroxypregnrtrione(hydrogensuccinate)	C ₂₅ H ₃₂ O ₈	[M+Na] ⁺	483.19894	483.19924	-0.62		3.4E+06						
1163	Hydrocortisone caproate	C ₂₇ H ₄₀ O ₆	[M+Na] ⁺	483.27171	483.27190	-0.39	4.1E+06	6.8E+06	3.8E+06		2.8E+06	4.5E+06	3.3E+06	
1164	Thiaclycobenzylnordihomosecocholestatrienetriol	C ₃₀ H ₄₂ O ₃ S	[M+H] ⁺	483.29274	483.29287	-0.26			3.0E+06					
1165	Dihydroxyvitamin D3	C ₂₉ H ₄₈ O ₃	[M+K] ⁺	483.32350	483.32339	0.24								1.6E+07
1166	Ethylthornasterol	C ₂₉ H ₄₈ O ₄	[M+Na] ⁺	483.34448	483.34443	0.10						3.0E+06		
1167	Myrrhanol A	C ₃₀ H ₅₂ O ₃	[M+Na] ⁺	483.38087	483.38090	-0.08		8.2E+06		1.7E+06		4.6E+06		3.2E+06
1168	Triacontanedioic acid	C ₃₀ H ₅₈ O ₄	[M+H] ⁺	483.44079	483.44086	-0.15						3.5E+06		
1169	Tetrahydrofolic acid	C ₁₉ H ₂₃ N ₇ O ₆	[M+K] ⁺	484.13414	484.13383	0.64	4.6E+06		8.6E+06		6.0E+06		3.4E+06	
1170	Dynorphin A (6-8)	C ₁₈ H ₃₉ N ₉ O ₄	[M+K] ⁺	484.27566	484.27532	0.70	2.7E+06							
1171	Uridine triphosphate	C ₉ H ₁₅ N ₂ O ₁₅ P ₃	[M+H] ⁺	484.97580	484.97557	0.48							3.4E+06	
1172	Digalloyl-beta-D-glucose	C ₂₀ H ₂₀ O ₁₄	[M+H] ⁺	485.09258	485.09266	-0.15			3.4E+06		3.7E+06			
1173	Diospyrin	C ₂₁ H ₂₄ O ₁₃	[M+H] ⁺	485.12897	485.12896	0.02	3.1E+06				4.3E+06			
1174	Dihydroxy-dimethoxychalcone glucoside	C ₂₃ H ₂₆ O ₁₀	[M+Na] ⁺	485.14182	485.14201	-0.39	3.4E+06				3.5E+06			
1175	Dehydrotestosterone glucuronide	C ₂₅ H ₃₄ O ₈	[M+Na] ⁺	485.21459	485.21474	-0.30	4.1E+06	7.5E+06	4.4E+06				5.5E+06	
1176	Dehydroecdysone	C ₂₇ H ₄₂ O ₆	[M+Na] ⁺	485.28736	485.28749	-0.28	3.1E+06	4.0E+06				3.4E+06		

		ESI(+) FT-ICR MS												
No.	Plausible Compound ^a	Molecular formula (M)	Ion	Theor m/z ^b	Exp. m/z ^c	Δ ppm _d	SM _R H ^e	SM _R O ^e	SM _P H ^e	SM _P O ^e	TF _R H ^e	TF _R O ^e	TF _P H ^e	TF _P O ^e
1177	Hydroxy-alpha-tocopherol	C ₂₉ H ₅₀ O ₃	[M+K] ⁺	485.33915	485.33925	-0.20			3.6E+06					3.4E+06
1178	N-tert-Butyloxycarbonyl-deacetyl-leupeptin	C ₂₃ H ₄₄ N ₆ O ₅	[M+H] ⁺	485.34460	485.34493	-0.68					2.8E+06	4.1E+06		
1179	(Hydroxypropyl)-dihydroxy-norvitamin D3	C ₂₉ H ₅₀ O ₄	[M+Na] ⁺	485.36013	485.36024	-0.23	4.2E+06		4.2E+06		4.3E+06			3.6E+06
1180	Methylthioheptyl glucosinolate	C ₁₅ H ₂₉ NO ₉ S ₃	[M+Na] ⁺	486.08967	486.08932	0.71								4.4E+06
1181	D-Glucosyldihydrosphingosine	C ₂₄ H ₄₉ NO ₇	[M+Na] ⁺	486.34012	486.34032	-0.40					3.9E+06			
1182	hydroxynorandrostene-dione glucuronide	C ₂₄ H ₃₂ O ₉	[M+Na] ⁺	487.19385	487.19405	-0.41	5.4E+06		5.1E+06		3.7E+06			
1183	N-Acetyl-leu-leu-tyr-amide	C ₂₃ H ₃₆ N ₄ O ₅	[M+K] ⁺	487.23173	487.23127	-0.94		1.4E+07		4.7E+06				8.8E+06
1184	Tetrahydroxy-cholestenoic acid	C ₂₇ H ₄₄ O ₆	[M+Na] ⁺	487.30301	487.30317	-0.32	5.4E+06	5.0E+06	4.3E+06			3.3E+06	5.2E+06	
1185	Hydroxy-[(hydroxy-methylethyl)phenyl]-pentanorvitamin D3	C ₃₁ H ₄₄ O ₃	[M+Na] ⁺	487.31827	487.31845	-0.37		3.1E+06				3.0E+06		
1186	Trihydroxycoprostanoic acid	C ₂₈ H ₄₈ O ₅	[M+Na] ⁺	487.33940	487.33957	-0.36	6.6E+06	7.6E+06	7.5E+06		3.7E+06	4.8E+06	5.8E+06	
1187	Tetramethyl-hexacosadienoic acid	C ₃₀ H ₅₆ O ₂	[M+K] ⁺	487.39119	487.39124	-0.10			4.0E+06					
1188	Hydroxycyanidin glucoside	C ₂₁ H ₂₁ O ₁₂	[M+Na] ⁺	488.09252	488.09240	0.25					3.3E+06			
1189	Eriotriochin	C ₂₇ H ₃₀ O ₇	[M+Na] ⁺	489.18837	489.18858	-0.42	4.7E+06							
1190	Hydroxy-androstane glucuronide	C ₂₅ H ₃₈ O ₈	[M+Na] ⁺	489.24589	489.24599	-0.21	3.3E+06							
1191	Difluoro-dihydroxy-homovitamin D3	C ₂₈ H ₄₄ F ₂ O ₃	[M+Na] ⁺	489.31507	489.31524	-0.34						4.3E+06		
1192	Tetrahydroxy-cholestanoic acid	C ₂₇ H ₄₆ O ₆	[M+Na] ⁺	489.31866	489.31886	-0.41	2.7E+07	4.8E+07	2.6E+07	1.1E+07	1.3E+07	2.5E+07	3.1E+07	4.4E+06
1193	Hydroxy-castasterone	C ₂₈ H ₅₀ O ₅	[M+Na] ⁺	489.35505	489.35496	0.17						3.5E+06		
1194	Paucin	C ₂₃ H ₃₂ O ₁₀	[M+Na] ⁺	491.18877	491.18896	-0.40	5.1E+06		6.0E+06		5.0E+06			4.7E+06
1195	Diphenoxylate	C ₃₀ H ₃₂ N ₂ O ₂	[M+K] ⁺	491.20954	491.20995	-0.84					3.4E+06			
1196	Repaglinide	C ₂₇ H ₃₆ N ₂ O ₄	[M+K] ⁺	491.23067	491.23020	0.95	1.3E+07		9.3E+06		8.4E+06			2.1E+07
1197	Hydroxyandrostane-3-glucuronide	C ₂₅ H ₄₀ O ₈	[M+Na] ⁺	491.26154	491.26173	-0.38	1.4E+07		9.9E+06		8.0E+06			7.3E+06
1198	(Hydroxy-propynyl)-didehydrovitamin D3	C ₃₀ H ₄₄ O ₄	[M+Na] ⁺	491.31318	491.31336	-0.37						3.2E+06		
	Dihydroxy-dimethyl-tetradehydro-dihomovitamin													
1199	D3	C ₃₁ H ₄₈ O ₃	[M+Na] ⁺	491.34957	491.34969	-0.25		3.4E+06	3.9E+06			3.8E+06	3.6E+06	
1200	Limonin	C ₂₆ H ₃₀ O ₈	[M+Na] ⁺	493.18329	493.18345	-0.33	8.7E+06		8.9E+06		5.6E+06			5.7E+06
1201	Mucronine B	C ₂₈ H ₃₆ N ₄ O ₄	[M+H] ⁺	493.28093	493.28056	0.75		4.6E+06				4.2E+06		
	Trihydroxy-dimethyl-tetradehydro-homo-epivitamin													
1202	D3	C ₃₀ H ₄₆ O ₄	[M+Na] ⁺	493.32883	493.32902	-0.38		3.1E+06						
1203	N-stearoyl tryptophan	C ₂₉ H ₄₆ N ₂ O ₃	[M+Na] ⁺	493.34006	493.33976	0.62								3.5E+06

ESI(+) FT-ICR MS														
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1204	Trioctanoylglycerol	C ₂₇ H ₅₀ O ₆	[M+Na] ⁺	493.34996	493.35000	-0.08		4.9E+06				4.3E+06		3.5E+06
1205	(Carboxylpropyl)vitamin D3	C ₃₁ H ₅₀ O ₃	[M+Na] ⁺	493.36522	493.36537	-0.31	8.2E+06	8.2E+06	8.3E+06		3.3E+06	8.5E+06	7.2E+06	2.9E+06
1206	Heptadecyl oleate	C ₃₃ H ₆₄ O ₂	[M+H] ⁺	493.49791	493.49792	-0.03	1.9E+07	2.4E+07	2.3E+07	5.3E+06	7.5E+06	5.0E+07	2.2E+07	1.1E+07
1207	Pentahydroxy-dimethoxyflavone L-arabinopyranoside	C ₂₂ H ₂₂ O ₁₃	[M+H] ⁺	495.11332	495.11337	-0.11	9.6E+06		3.6E+06		1.0E+07			
1208	Deoxylimonate	C ₂₆ H ₃₂ O ₈	[M+Na] ⁺	495.19894	495.19914	-0.41	3.0E+07		2.1E+07		1.4E+07		1.4E+07	
1209	Oxolycoclavanol	C ₃₀ H ₄₈ O ₄	[M+Na] ⁺	495.34448	495.34459	-0.23		4.5E+06	2.9E+06			4.6E+06	4.4E+06	
1210	Dihydroxy-dimethyl-dihomovitamin D3	C ₃₁ H ₅₂ O ₃	[M+Na] ⁺	495.38087	495.38098	-0.24	4.1E+06	8.7E+06	6.1E+06	3.4E+06		9.5E+06	6.4E+06	6.2E+06
1211	Heptadecyl-palmitate	C ₃₃ H ₆₆ O ₂	[M+H] ⁺	495.51356	495.51359	-0.06	5.9E+06	6.8E+06	6.4E+06	2.3E+06		1.4E+07	6.5E+06	4.1E+06
1212	PG(17:1/0:0)	C ₂₃ H ₄₅ O ₉ P	[M+H] ⁺	497.28740	497.28753	-0.26	1.1E+07	8.2E+06	7.3E+06	4.3E+06	6.1E+06	5.7E+06	6.3E+06	
1213	Dihydroxy-methoxy-dimethylvitamin D3	C ₃₀ H ₅₀ O ₄	[M+Na] ⁺	497.36013	497.36014	-0.01			4.3E+06			1.2E+07	8.9E+06	8.8E+06
1214	Deoxytubulosine	C ₂₉ H ₃₇ N ₃ O ₂	[M+K] ⁺	498.25174	498.25206	-0.65			2.7E+06					
1215	Calofloride	C ₃₀ H ₃₆ O ₅	[M+Na] ⁺	499.24549	499.24571	-0.43			3.5E+06					
1216	PG(17:0/0:0)	C ₂₃ H ₄₇ O ₉ P	[M+H] ⁺	499.30305	499.30320	-0.31			3.1E+06					
1217	Cucurbitacin S	C ₃₀ H ₄₂ O ₆	[M+H] ⁺	499.30542	499.30552	-0.20		5.1E+06		5.2E+06				
1218	Dammarenetriol	C ₃₀ H ₅₂ O ₃	[M+K] ⁺	499.35480	499.35485	-0.09			3.9E+06					
1219	D-glucopyranosyl-eicosandiol	C ₂₆ H ₅₂ O ₇	[M+Na] ⁺	499.36052	499.36056	-0.07						3.2E+06		
1220	Methoxy-estradiol glucuronide	C ₂₅ H ₃₄ O ₉	[M+Na] ⁺	501.20950	501.20967	-0.33	5.0E+06				4.5E+06			
1221	O-alpha- glucopyranosyl nonadecandiol	C ₂₅ H ₅₀ O ₇	[M+K] ⁺	501.31881	501.31880	0.03		3.6E+06						
1222	Dihydroxy-(hydroxypropoxy)-norvitamin D3	C ₂₉ H ₅₀ O ₅	[M+Na] ⁺	501.35505	501.35517	-0.25		3.4E+06			3.3E+06			
1223	Hydroxyglucobrassicin	C ₁₆ H ₁₉ N ₂ O ₁₀ S ₂	[M+K] ⁺	502.01127	502.01121	0.12				1.2E+07				1.8E+07
1224	Acevaltrate	C ₂₄ H ₃₂ O ₁₀	[M+K] ⁺	503.18877	503.18891	-0.28	2.9E+06							
1225	Hydroxyecdysone	C ₂₇ H ₄₄ O ₇	[M+Na] ⁺	503.29792	503.29810	-0.35	3.6E+07	4.1E+06	2.3E+07		1.6E+07	3.5E+06	1.7E+07	
1226	epi-Brassinolide	C ₂₈ H ₄₈ O ₆	[M+Na] ⁺	503.33431	503.33450	-0.38	1.7E+07	1.4E+07	1.8E+07	4.3E+06	9.2E+06	7.1E+06	1.8E+07	4.4E+06
1227	Dihydroxy-dimethyl-hexadehydro-trihomovitamin D3	C ₃₂ H ₄₈ O ₃	[M+Na] ⁺	503.34957	503.34973	-0.32			3.8E+06			4.2E+06	3.7E+06	
1228	Pederin	C ₂₅ H ₄₅ NO ₉	[M+H] ⁺	504.31671	504.31652	0.37				4.7E+06	2.8E+06			3.4E+06
1229	Thymidine 5'-triphosphate	C ₁₀ H ₁₇ N ₂ O ₁₄ P ₃	[M+Na] ⁺	504.97848	504.97825	0.46					3.9E+06			
1230	Hydroxycholesterol sulfate	C ₂₇ H ₄₆ O ₅ S	[M+Na] ⁺	505.29582	505.29616	-0.68	3.5E+06							
1231	Dihydroxy-diethyl-tetradehydro-homovitamin	C ₃₂ H ₅₀ O ₃	[M+Na] ⁺	505.36522	505.36540	-0.36		3.2E+06	3.3E+06				3.6E+06	

ESI(+) FT-ICR MS														
No.	Plausible Compound ^a	Molecular formula (M)	Ion	Theo r m/z ^b	Exp . m/z ^c	Δppm ^d	SM _R H ^e	SM _R O ^e	SM _P H ^e	SM _P O ^e	TF _R H ^e	TF _R O ^e	TF _P H ^e	TF _P O ^e
1232	Triacontanedioic acid	C ₃₀ H ₅₈ O ₄	[M+Na] ⁺	505.42273	505.42280	-0.13				2.3E+06				4.5E+06
1233	Hydroxyandrostane-glucuronide	C ₂₅ H ₄₀ O ₉	[M+Na] ⁺	507.25645	507.25648	-0.05	3.9E+06				3.6E+06			
1234	Cholestan heptol	C ₂₇ H ₄₈ O ₇	[M+Na] ⁺	507.32922	507.32919	0.07		6.4E+06						
1235	Stearyl oleate	C ₃₄ H ₆₆ O ₂	[M+H] ⁺	507.51356	507.51358	-0.05	2.0E+07	2.7E+07	2.4E+07	5.1E+06	6.1E+06	5.3E+07	2.3E+07	1.1E+07
1236	Trihydroxy-prenylchalcone O-glucoside	C ₂₆ H ₃₀ O ₉	[M+Na] ⁺	509.17820	509.17838	-0.35	7.0E+06		5.7E+06		5.0E+06			
1237	Hydrocortisone cypionate	C ₂₉ H ₄₂ O ₆	[M+Na] ⁺	509.28736	509.28767	-0.61		3.4E+06						
1238	Alisol C	C ₃₀ H ₄₆ O ₅	[M+Na] ⁺	509.32375	509.32393	-0.37	4.1E+06	4.4E+06	4.6E+06			3.9E+06	4.8E+06	
1239	Diethyl-dihydroxy-methano-oxavitamin D3	C ₃₁ H ₅₀ O ₄	[M+Na] ⁺	509.36013	509.36031	-0.36		3.7E+06	3.3E+06			4.5E+06		
1240	Epoxy-ethoxyhopan-ol	C ₃₂ H ₅₄ O ₃	[M+Na] ⁺	509.39652	509.39670	-0.37		3.8E+06	3.9E+06			5.1E+06		
1241	Mycocerosic acid (C34)	C ₃₄ H ₆₈ O ₂	[M+H] ⁺	509.52921	509.52923	-0.05	5.6E+06	6.7E+06	5.9E+06	2.1E+06		1.2E+07	5.6E+06	3.7E+06
1242	Formyldihydrofolate	C ₂₀ H ₂₁ N ₇ O ₇	[M+K] ⁺	510.11341	510.11311	0.59	3.9E+06				3.5E+06			
1243	PG(18:1(9Z)/0:0)	C ₂₄ H ₄₇ O ₉ P	[M+H] ⁺	511.30305	511.30325	-0.41	6.3E+06	7.4E+06	4.8E+06		4.6E+06	6.1E+06	4.3E+06	
1244	Acetoxy-dihydroxy-methyl-secocholestadienone	C ₃₀ H ₄₈ O ₅	[M+Na] ⁺	511.33940	511.33954	-0.28		5.9E+06						
1245	Cholestadienol benzoate	C ₃₄ H ₄₈ O ₂	[M+Na] ⁺	511.35465	511.35484	-0.37	3.1E+06	5.4E+06	4.8E+06			5.1E+06	7.2E+06	
1246	Trihydroxy-diethylvitamin D3	C ₃₁ H ₅₂ O ₄	[M+Na] ⁺	511.37578	511.37586	-0.15		3.3E+06				3.9E+06		
1247	Raucaffricine	C ₂₇ H ₃₂ N ₂ O ₈	[M+H] ⁺	513.22314	513.22269	0.88	7.5E+06		8.1E+06				6.6E+06	
1248	Epoxy-acetoxy-cholestentriol	C ₂₉ H ₄₆ O ₆	[M+Na] ⁺	513.31866	513.31881	-0.29	3.2E+06	3.7E+06					3.5E+06	
1249	Dihydroxy-(hydroxypropoxy)vitamin D3	C ₃₀ H ₅₀ O ₅	[M+Na] ⁺	513.35505	513.35508	-0.07		1.6E+07		3.5E+06		7.9E+06	7.1E+06	6.6E+06
1250	Aragusteroketal	C ₃₁ H ₅₄ O ₄	[M+Na] ⁺	513.39143	513.39151	-0.15						6.2E+06		
1251	Cyanidin acetylglucoside	C ₂₃ H ₂₃ O ₁₂	[M+Na] ⁺	514.10817	514.10796	0.41	6.9E+06		1.1E+07		6.5E+06		5.1E+06	
1252	Caryoptin	C ₂₆ H ₃₆ O ₉	[M+Na] ⁺	515.22515	515.22526	-0.21	4.7E+06							
1253	Dihydroxy-phenylvitamin D3	C ₃₃ H ₄₈ O ₃	[M+Na] ⁺	515.34957	515.34974	-0.34		4.3E+06						
1254	Xenisterol-a	C ₃₀ H ₅₂ O ₅	[M+Na] ⁺	515.37070	515.37085	-0.30		6.0E+06						
1255	PI(12:0/0:0)	C ₂₁ H ₄₁ O ₁₂ P	[M+H] ⁺	517.24084	517.24099	-0.28	2.6E+07		2.0E+07		1.8E+07		1.4E+07	</

ESI(+) FT-ICR MS														
No.	Plausible Compound ^a	Molecular formula (M)	Ion	Theor m/z ^b	Exp. m/z ^c	Δ ppm _d	SM _R H ^e	SM _R O ^e	SM _P H ^e	SM _P O ^e	TF _R H ^e	TF _R O ^e	TF _P H ^e	TF _P O ^e
1261	Glauucarubin	C ₂₅ H ₃₆ O ₁₀	[M+Na] ⁺	519.22007	519.22028	-0.41	4.7E+06							
1262	Emetine	C ₂₉ H ₄₀ N ₂ O ₄	[M+K] ⁺	519.26197	519.26147	0.96	7.2E+06				7.1E+06		1.1E+07	
1263	20,26-Dihydroxyecdysone	C ₂₇ H ₄₄ O ₈	[M+Na] ⁺	519.29284	519.29307	-0.44	1.4E+07		1.3E+07		7.9E+06		6.9E+06	
1264	Hydroxy-epi-brassinolide	C ₂₈ H ₄₈ O ₇	[M+Na] ⁺	519.32922	519.32945	-0.42	6.5E+06				5.6E+06			
1265	Tetratriacontahexaenoic acid	C ₃₄ H ₅₆ O ₂	[M+Na] ⁺	519.41725	519.41736	-0.20			3.2E+06				3.7E+06	
1266	Ceforanide	C ₂₀ H ₂₁ N ₇ O ₆ S ₂	[M+H] ⁺	520.10675	520.10628	0.90					6.4E+06			
1267	PS(16:0/0:0)	C ₂₂ H ₄₄ NO ₉ P	[M+Na] ⁺	520.26459	520.26487	-0.53					3.0E+06		3.4E+06	
1268	Epiiridodial glucoside tetraacetate	C ₂₄ H ₃₄ O ₁₁	[M+Na] ⁺	521.19933	521.19951	-0.34	4.1E+06							
1269	Triacantanedioic acid	C ₃₀ H ₅₈ O ₄	[M+K] ⁺	521.39667	521.39672	-0.09	6.9E+06				3.7E+06			
1270	Tetratriacontapentaenoic acid	C ₃₄ H ₅₈ O ₂	[M+Na] ⁺	521.43290	521.43299	-0.16		9.4E+06	4.6E+06	1.6E+06		1.1E+07	7.6E+06	5.5E+06
1271	Nonadecyl oleate	C ₃₅ H ₆₈ O ₂	[M+H] ⁺	521.52921	521.52921	0.00	1.4E+07	1.9E+07	1.7E+07	3.6E+06	5.7E+06	4.0E+07	1.6E+07	8.5E+06
1272	Hexafluoro-dihydroxy-didehydrovitamin D3	C ₂₇ H ₃₆ F ₆ O ₃	[M+H] ⁺	523.26414	523.26442	-0.52			5.5E+06				4.4E+06	
1273	Deoxocucurbitacin I	C ₃₀ H ₄₄ O ₆	[M+Na] ⁺	523.30301	523.30326	-0.48	3.4E+06	9.7E+06						
1274	Cholestan-octol	C ₂₇ H ₄₈ O ₈	[M+Na] ⁺	523.32414	523.32409	0.09					3.1E+06			
1275	Hydroxylanostane-dione acetate	C ₃₂ H ₅₂ O ₄	[M+Na] ⁺	523.37578	523.37592	-0.27		4.6E+06	4.0E+06			4.2E+06		
1276	Dihydroxy-hexamethylvitamin D3	C ₃₃ H ₅₆ O ₃	[M+Na] ⁺	523.41217	523.41235	-0.35		4.1E+06	4.8E+06			4.6E+06	4.4E+06	
1277	Tetratriacontatetraenoic acid	C ₃₄ H ₆₀ O ₂	[M+Na] ⁺	523.44855	523.44857	-0.03		5.6E+06	3.8E+06			6.2E+06	4.9E+06	3.8E+06
1278	Octadecyl-heptadecanoate	C ₃₅ H ₇₀ O ₂	[M+H] ⁺	523.54486	523.54486	0.00	5.1E+06	5.4E+06	4.8E+06		3.0E+06	9.8E+06	4.9E+06	3.5E+06
1279	Geranioloxalatatum flavone	C ₂₇ H ₃₄ O ₉	[M+Na] ⁺	525.20950	525.20968	-0.34	5.6E+06							
1280	Hexafluoro-Dihydroxyvitamin D3	C ₂₇ H ₃₈ F ₆ O ₃	[M+H] ⁺	525.27979	525.27999	-0.38	7.3E+06		7.2E+06		9.3E+06		7.8E+06	
1281	PG(19:1/0:0)	C ₂₅ H ₄₉ O ₉ P	[M+H] ⁺	525.31870	525.31885	-0.30	4.4E+06	5.3E+06	3.4E+06			3.9E+06		
1282	Kestose	C ₁₈ H ₃₂ O ₁₆	[M+Na] ⁺	527.15826	527.15825	0.02		4.4E+06	4.7E+06	5.1E+06			9.2E+06	
1283	Eudesobovatol A	C ₃₃ H ₄₄ O ₄	[M+Na] ⁺	527.31318	527.31336	-0.34		3.3E+06						
1284	PG(19:0/0:0)	C ₂₅ H ₅₁ O ₉ P	[M+H] ⁺	527.33435	527.33439	-0.07		5.7E+06				4.3E+06		
1285	PG(O-20:0/0:0)	C ₂₆ H ₅₅ O ₈ P	[M+H] ⁺	527.37073	527.37071	0.04						4.3E+06		
1286	Peonidin 3-(6''-acetylglucoside)	C ₂₄ H ₂₅ O ₁₂	[M+Na] ⁺	528.12382	528.12359	0.45	4.2E+07		3.8E+07		3.9E+07		2.2E+07	
1287	(Hydroxypropoxy)vitamin D3	C ₃₀ H ₅₀ O ₅	[M+K] ⁺	529.32898	529.32902	-0.07					3.3E+06			
1288	Aragusteroketal	C ₃₁ H ₅₄ O ₄	[M+K] ⁺	529.36537	529.36538	-0.01			4.7E+06				4.5E+06	
1289	Hydroxy-norgeminivitamin D3	C ₃₁ H ₅₄ O ₅	[M+Na] ⁺	529.38635	529.38643	-0.16	3.6E+06	3.5E+06	3.0E+06			5.0E+06	3.8E+06	

ESI(+) FT-ICR MS														
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1290	Delphinidin (acetylglucoside)	C ₂₃ H ₂₃ O ₁₃	[M+Na] ⁺	530.10309	530.10283	0.48	3.6E+06			4.9E+06				
1291	Mucronine B	C ₂₈ H ₃₆ N ₄ O ₄	[M+K] ⁺	531.23682	531.23646	0.67		9.2E+06				7.4E+06		
1292	Hexafluoro-hydroxyvitamin D3	C ₂₇ H ₃₈ F ₆ O ₂	[M+Na] ⁺	531.26682	531.26729	-0.88	5.4E+06			4.1E+06				
1293	Trihydroxy-carboxymethylcholestanoic acid	C ₂₉ H ₄₈ O ₇	[M+Na] ⁺	531.32922	531.32941	-0.34	7.7E+06			6.6E+06	4.6E+06		5.6E+06	
1294	Acetoxy-methylcholestantetrol	C ₃₀ H ₅₂ O ₆	[M+Na] ⁺	531.36561	531.36575	-0.26	6.5E+06	1.0E+07	8.3E+06		4.4E+06	5.1E+06	6.4E+06	
1295	DG(14:1/14:0/0:0)	C ₃₁ H ₅₈ O ₅	[M+Na] ⁺	533.41765	533.41771	-0.12		6.7E+06				6.5E+06		4.0E+06
1296	Gibberellin A2 O-beta-D-glucoside	C ₂₅ H ₃₆ O ₁₁	[M+Na] ⁺	535.21498	535.21516	-0.32	5.1E+06				4.5E+06			
1297	Trihydroxyecdysone	C ₂₇ H ₄₄ O ₉	[M+Na] ⁺	535.28775	535.28796	-0.39	1.4E+07		1.0E+07		8.9E+06		9.4E+06	
1298	Dimyristyl-sn-glycerol	C ₃₁ H ₆₀ O ₅	[M+Na] ⁺	535.43330	535.43334	-0.08		7.8E+06		2.0E+06		7.8E+06	5.7E+06	6.0E+06
1299	Eicosanyl oleate	C ₃₆ H ₇₀ O ₂	[M+H] ⁺	535.54486	535.54488	-0.04	1.5E+07	2.0E+07	1.7E+07	3.9E+06	4.6E+06	3.6E+07	1.6E+07	7.9E+06
1300	PC(P-20:0/0:0)	C ₂₈ H ₅₈ NO ₆ P	[M+H] ⁺	536.40745	536.40700	0.84						3.6E+06		
1301	Nomilin	C ₂₈ H ₃₄ O ₉	[M+Na] ⁺	537.20950	537.20985	-0.64	9.9E+06		1.1E+07		9.3E+06		7.3E+06	
1302	Phthioceranic acid (C36)	C ₃₆ H ₇₂ O ₂	[M+H] ⁺	537.56051	537.56057	-0.11	3.5E+06	4.1E+06	3.8E+06			8.7E+06	4.1E+06	3.1E+06
1303	N-Palmitoylsphingosine	C ₃₄ H ₆₇ NO ₃	[M+H] ⁺	538.51937	538.51943	-0.11		4.7E+06						
1304	L-Olivosyl-oleandolide	C ₂₆ H ₄₄ O ₁₀	[M+Na] ⁺	539.28267	539.28272	-0.10	4.9E+06				6.1E+06			
1305	Fusidic acid	C ₃₁ H ₄₈ O ₆	[M+Na] ⁺	539.33431	539.33454	-0.42	5.5E+06	6.3E+06						
1306	Tetratriacontatetraenoic acid	C ₃₄ H ₆₀ O ₂	[M+K] ⁺	539.42249	539.42256	-0.13	3.6E+06							
1307	Carboxypyranocyanidin 3-O-beta-glucopyranoside	C ₂₄ H ₂₁ O ₁₃	[M+Na] ⁺	540.08744	540.08718	0.48	6.1E+06		4.9E+06		4.8E+06		4.6E+06	
1308	Hexacosanoyl carnitine	C ₃₃ H ₆₅ NO ₄	[M+H] ⁺	540.49864	540.49865	-0.03		6.1E+06						
1309	Hexafluoro-hydroxyvitamin D2	C ₂₈ H ₃₈ F ₆ O ₂	[M+Na] ⁺	543.26682	543.26641	0.76	6.1E+06							
1310	Dihydroxy-(hydroxymethylphenyl)-didehydrovitamin D3	C ₃₄ H ₄₈ O ₄	[M+Na] ⁺	543.34448	543.34471	-0.42				4.9E+06				
1311	Ophrysananin	C ₂₃ H ₂₁ O ₁₄	[M+Na] ⁺	544.08235	544.08217	0.33	1.1E+07		1.0E+07		1.0E+07		8.9E+06	
1312	Trilobolide	C ₂₇ H ₃₈ O ₁₀	[M+Na] ⁺	545.23572	545.23591	-0.35	6.1E+06			6.2E+06				
1313	Oleoylglycerophosphocholine	C ₂₆ H ₅₃ NO ₇ P	[M+Na] ⁺	545.34519	545.34496	0.42	3.2E+06	9.7E+06		4.4E+06		4.9E+06		4.4E+06
1314	Westiellamide	C ₂₇ H ₄₂ N ₆ O ₆	[M+H] ⁺	547.32386	547.32433	-0.85	8.3E+07		4.1E+07		2.7E+07		3.6E+07	
1315	DG(14:1/15:0/0:0)	C ₃₂ H ₆₀ O ₅	[M+Na] ⁺	547.43330	547.43329	0.01		1.1E+07	4.6E+06	3.8E+06		9.8E+06	8.4E+06	5.4E+06
1316	Retinyl palmitate	C ₃₆ H ₆₀ O ₂	[M+Na] ⁺	547.44855	547.44865	-0.18		5.2E+06				3.9E+06		
1317	bacteriohopane-tetrol	C ₃₅ H ₆₂ O ₄	[M+H] ⁺	547.47209	547.47208	0.01						7.5E+06		

ESI(+) FT-ICR MS														
No.	Plausible Compound ^a	Molecular formula (M)	Ion	Theor m/z ^b	Exp m/z ^c	Δ ppm ^d	SM _R H ^e	SM _R O ^e	SM _P H ^e	SM _P O ^e	TF _R H ^e	TF _R O ^e	TF _P H ^e	TF _P O ^e
1318	DG(14:0/14:1/0:0)	C ₃₁ H ₅₈ O ₅	[M+K] ⁺	549.39158	549.39163	-0.08	6.6E+06							
1319	Anhydrobacteriohopantetrol	C ₃₅ H ₅₈ O ₃	[M+Na] ⁺	549.42782	549.42799	-0.31	5.3E+06	5.9E+06	5.6E+06				4.8E+06	
1320	DG(14:0/15:0/0:0)	C ₃₂ H ₆₂ O ₅	[M+Na] ⁺	549.44895	549.44897	-0.03		1.4E+07	5.8E+06	3.7E+06		1.5E+07	9.0E+06	7.3E+06
1321	Hydroxypthioceranic acid (C33)	C ₃₃ H ₆₆ O ₃	[M+K] ⁺	549.46436	549.46425	0.19	6.7E+06	3.8E+07	1.5E+07	6.7E+06		3.7E+07	2.1E+07	1.3E+07
1322	Heneicosanyl oleate	C ₃₇ H ₇₂ O ₂	[M+H] ⁺	549.56051	549.56053	-0.04	1.0E+07	1.3E+07	1.2E+07	3.0E+06		2.7E+07	1.1E+07	6.0E+06
1323	Pachymic acid	C ₃₃ H ₅₂ O ₅	[M+Na] ⁺	551.37070	551.37096	-0.48		6.1E+06	2.2E+07			6.3E+06	8.5E+06	
1324	Dimyristyl-sn-glycerol	C ₃₁ H ₆₀ O ₅	[M+K] ⁺	551.40723	551.40712	0.21	1.2E+07				4.4E+06			
1325	Anhydrobacteriohopaneterol	C ₃₅ H ₆₀ O ₃	[M+Na] ⁺	551.44347	551.44360	-0.25	4.0E+06	5.3E+06	5.0E+06			5.3E+06	5.7E+06	
1326	Hexatriacontatetraenoic acid	C ₃₆ H ₆₄ O ₂	[M+Na] ⁺	551.47985	551.47989	-0.07		8.3E+06	5.0E+06	1.7E+06		9.5E+06	6.8E+06	5.7E+06
1327	(Tetradecenyl)-(octadecenoyl)-sn-glycerol	C ₃₅ H ₆₆ O ₄	[M+H] ⁺	551.50339	551.50339	-0.01	1.0E+07	9.2E+06	7.2E+06	2.5E+06	3.5E+06	2.0E+07	7.3E+06	5.5E+06
1328	Phthioceranic acid (C37)	C ₃₇ H ₇₄ O ₂	[M+H] ⁺	551.57616	551.57616	0.00						6.6E+06		
1329	((O-hydroxy-ethane)-hydroxy-propane)-hopane	C ₃₅ H ₆₂ O ₃	[M+Na] ⁺	553.45912	553.45906	0.10						9.4E+06		
1330	Calactin	C ₂₉ H ₄₀ O ₉	[M+Na] ⁺	555.25645	555.25664	-0.34	7.5E+06							
1331	Mayolene-16	C ₃₄ H ₆₀ O ₄	[M+Na] ⁺	555.43838	555.43843	-0.08		5.0E+06				5.4E+06		
1332	Cer(t18:0/16:0)	C ₃₄ H ₆₉ NO ₄	[M+H] ⁺	556.52994	556.52990	0.06		4.7E+06				4.0E+06		
1333	PG(20:3/0:0)	C ₂₆ H ₄₇ O ₉ P	[M+Na] ⁺	557.28499	557.28449	0.90	4.9E+06							
1334	Cyanidin (malonylglucoside)	C ₂₄ H ₂₃ O ₁₄	[M+Na] ⁺	558.09800	558.09776	0.43	5.2E+07		3.1E+07		4.9E+07		1.6E+07	
1335	DG(14:1/16:1/0:0)	C ₃₃ H ₆₀ O ₅	[M+Na] ⁺	559.43330	559.43330	0.00		8.1E+06	4.9E+06			7.7E+06	6.9E+06	5.3E+06
1336	Hexatriacontylic acid	C ₃₆ H ₇₂ O ₂	[M+Na] ⁺	559.54245	559.54242	0.06				4.9E+06				
1337	PG(22:4/0:0)	C ₂₈ H ₄₉ O ₉ P	[M+H] ⁺	561.31870	561.31889	-0.35		1.1E+07				4.4E+06		
1338	Deferoxamine	C ₂₅ H ₄₈ N ₆ O ₈	[M+H] ⁺	561.36064	561.36092	-0.49	1.2E+07		1.3E+07		1.1E+07		1.5E+07	
1339	DG(14:0/16:1/0:0)	C ₃₃ H ₆₂ O ₅	[M+Na] ⁺	561.44895	561.44896	-0.02	5.6E+06	2.4E+07	9.4E+06	5.0E+06			1.5E+07	1.2E+07
1340	Methyl-hexatriacontahexaenoic acid	C ₃₇ H ₆₂ O ₂	[M+Na] ⁺	561.46420	561.46438	-0.31	4.4E+06		4.6E+06			3.7E+06	4.6E+06	
1341	Aminobacteriohopanetetrol	C ₃₅ H ₆₃ NO ₄	[M+H] ⁺	562.48299	562.48300	-0.02			9.9E+06					
1342	Tetrahydroaldosterone glucuronide	C ₂₇ H ₄₀ O ₁₁	[M+Na] ⁺	563.24628	563.24630	-0.03	4.7E+06							
1343	DG(14:1/15:0/0:0)	C ₃₂ H ₆₀ O ₅	[M+K] ⁺	563.40723	563.40706	0.31					3.8E+06			
1344	DG(14:0/16:0/0:0)	C ₃₃ H ₆₄ O ₅	[M+Na] ⁺	563.46460	563.46463	-0.06	6.0E+06	2.1E+07	7.5E+06	6.1E+06		2.4E+07	1.2E+07	1.1E+07
1345	CE(10:0)	C ₃₇ H ₆₄ O ₂	[M+Na] ⁺	563.47985	563.47988	-0.05		1.1E+07	5.2E+06	2.2E+06		1.2E+07		6.7E+06
1346	Docosanyl oleate	C ₃₈ H ₇₄ O ₂	[M+H] ⁺	563.57616	563.57615	0.01	8.2E+06	1.0E+07	8.7E+06	3.3E+06	4.4E+06	2.0E+07	9.0E+06	5.0E+06

ESI(+) FT-ICR MS														
No.	Plausible Compound ^a	Molecular formula (M)	Ion	Theor m/z ^b	Exp. m/z ^c	Δ ppm _d	SM _R H ^e	SM _R O ^e	SM _P H ^e	SM _P O ^e	TF _R H ^e	TF _R O ^e	TF _P H ^e	TF _P O ^e
1347	Cortolone-3-glucuronide	C ₂₇ H ₄₂ O ₁₁	[M+Na] ⁺	565.26193	565.26209	-0.28	2.2E+07		2.0E+07		1.6E+07		1.8E+07	
1348	(D-ribonyl)hopane	C ₃₅ H ₅₈ O ₄	[M+Na] ⁺	565.42273	565.42293	-0.36	1.7E+07	1.6E+07	2.0E+07	9.4E+06	5.0E+06	1.4E+07	2.0E+07	4.7E+06
1349	Methyl-anhydrobacteriohopanetetrol	C ₃₆ H ₆₂ O ₃	[M+Na] ⁺	565.45912	565.45923	-0.19		5.9E+06	3.9E+06			6.7E+06		
1350	Tetramethyl-tetratriacontanoic acid	C ₃₈ H ₇₆ O ₂	[M+H] ⁺	565.59181	565.59182	-0.02						5.5E+06		
1351	Hemiglutaryloxy-dihydroxyvitamin D3	C ₃₃ H ₅₂ O ₆	[M+Na] ⁺	567.36561	567.36591	-0.53							3.7E+06	
1352	DG(14:0/18:1/0:0)	C ₃₅ H ₆₆ O ₅	[M+H] ⁺	567.49830	567.49829	0.02						3.5E+06		
1353	Adouetine Y	C ₃₄ H ₄₀ N ₄ O ₄	[M+H] ⁺	569.31223	569.31191	0.57			8.4E+06					
1354	Cholest-dienol O-beta-D-glucopyranoside	C ₃₃ H ₅₄ O ₆	[M+Na] ⁺	569.38126	569.38130	-0.07		4.1E+06				3.5E+06		
1355	Retinyl linolate	C ₃₈ H ₅₈ O ₂	[M+Na] ⁺	569.43290	569.43309	-0.34					8.3E+07	1.1E+07	6.1E+06	
1356	Hexaprenyl-methoxy-benzoquinol	C ₃₇ H ₅₆ O ₃	[M+Na] ⁺	571.41217	571.41206	0.18		4.6E+06	4.2E+06			4.1E+06	5.1E+06	
1357	Dihydrochlorobactene	C ₄₀ H ₅₄	[M+K] ⁺	573.38571	573.38557	0.25						6.3E+06		
1358	Canthiumine	C ₃₃ H ₃₆ N ₄ O ₄	[M+Na] ⁺	575.26288	575.26259	0.50						6.7E+06		
1359	Lithocholate O-glucuronide	C ₃₀ H ₄₈ O ₉	[M+Na] ⁺	575.31905	575.31924	-0.32	7.1E+06				5.0E+06			
1360	DG(15:0/16:1/0:0)	C ₃₄ H ₆₄ O ₅	[M+Na] ⁺	575.46460	575.46459	0.01	7.2E+06	2.9E+07	1.2E+07	6.4E+06	3.5E+06	2.9E+07	1.7E+07	1.3E+07
1361	Octatriacontahexaenoic acid	C ₃₈ H ₆₄ O ₂	[M+Na] ⁺	575.47985	575.47999	-0.24	4.1E+06	6.2E+06	4.2E+06			6.0E+06	5.0E+06	
1362	Toonacilin	C ₃₁ H ₃₈ O ₉	[M+Na] ⁺	577.24080	577.24100	-0.33	8.3E+06		6.7E+06		6.0E+06			
1363	6,8a-Seco-6,8a-deoxy-5-oxoavermectin "1b" aglycone	C ₃₃ H ₄₆ O ₇	[M+Na] ⁺	577.31357	577.31370	-0.22		7.7E+06	3.7E+06					
1364	PA(P-16:0/12:0)	C ₃₁ H ₆₁ O ₇ P	[M+H] ⁺	577.42277	577.42289	-0.21	2.8E+07	3.2E+07	4.1E+07	7.2E+06	7.0E+06	2.5E+07	4.4E+07	7.7E+06
1365	DG(15:0/16:0/0:0)	C ₃₄ H ₆₆ O ₅	[M+Na] ⁺	577.48025	577.48028	-0.05	6.7E+06	2.9E+07	1.0E+07	7.6E+06		3.2E+07	1.5E+07	1.4E+07
1366	Octatriacontapentaenoic acid	C ₃₈ H ₆₆ O ₂	[M+Na] ⁺	577.49550	577.49549	0.02		7.6E+06	5.2E+06	2.1E+06		7.6E+06	5.5E+06	4.4E+06
1367	Tricosanyl oleate	C ₃₉ H ₇₆ O ₂	[M+H] ⁺	577.59181	577.59182	-0.02	6.0E+06	7.0E+06	6.1E+06			1.5E+07	5.9E+06	4.2E+06
1368	PA(O-16:0/12:0)	C ₃₁ H ₆₃ O ₇ P	[M+H] ⁺	579.43842	579.43855	-0.23	3.1E+07	3.0E+07	4.0E+07	8.6E+06	7.7E+06	2.6E+07	4.1E+07	7.5E+06
1369	Chloroxanthin	C ₄₀ H ₆₀ O	[M+Na] ⁺	579.45364	579.45381	-0.30	6.7E+06	1.1E+07	1.5E+07		3.6E+06	1.1E+07	1.4E+07	
1370	Octatriacontatetraenoic acid	C ₃₈ H ₆₈ O ₂	[M+Na] ⁺	579.51115	579.51118	-0.05		6.9E+06	4.1E+06			7.9E+06		
1371	Hexadecyl-tricosanoate	C ₃₉ H ₇₈ O ₂	[M+H] ⁺	579.60746	579.60749	-0.05						4.1E+06		
1372	Dihydroergotamine (Acetoxymethylphenyl)-dihydroxy-didehydrovitamin	C ₃₃ H ₃₇ N ₅ O ₅	[M+H] ⁺	584.28675	584.28661	0.23			4.9E+06					
1373	D3	C ₃₆ H ₅₀ O ₅	[M+Na] ⁺	585.35505	585.35536	-0.54		3.4E+06						
1374	Cholesterol glucuronide	C ₃₃ H ₅₄ O ₇	[M+Na] ⁺	585.37617	585.37634	-0.28	5.9E+06							

ESI(+) FT-ICR MS														
No.	Plausible Compound ^a	Molecular formula (M)	Ion	Theo r m/z ^b	Exp m/z ^c	Δppm ^d	SM _R H ^e	SM _R O ^e	SM _P H ^e	SM _P O ^e	TF _R H ^e	TF _R O ^e	TF _P H ^e	TF _P O ^e
1375	DG(14:0/18:3/0:0)	C ₃₅ H ₆₂ O ₅	[M+Na] ⁺	585.44895	585.44895	0.00		5.0E+06				4.9E+06		
1376	Phycocyanobilin	C ₃₃ H ₃₈ N ₄ O ₆	[M+H] ⁺	587.28641	587.28643	-0.03	1.0E+07		8.0E+06		7.3E+06		7.3E+06	
1377	DG(14:0/18:2/0:0)	C ₃₅ H ₆₄ O ₅	[M+Na] ⁺	587.46460	587.46462	-0.03	7.0E+06	2.6E+07	1.2E+07	5.4E+06	3.7E+06	2.6E+07	1.8E+07	1.1E+07
1378	Antiarigenin O-antiaroside	C ₂₉ H ₄₂ O ₁₁	[M+Na] ⁺	589.26193	589.26206	-0.22	8.5E+06		6.3E+06		6.6E+06			
1379	Sarmentoloside	C ₂₉ H ₄₄ O ₁₁	[M+Na] ⁺	591.27758	591.27761	-0.05	3.9E+06							
1380	PA(P-16:0/13:0)	C ₃₂ H ₆₃ O ₇ P	[M+H] ⁺	591.43842	591.43854	-0.20	3.8E+07	3.6E+07	5.7E+07	9.6E+06	7.5E+06	3.1E+07	5.8E+07	7.9E+06
1381	Dihydroanhydrorhodovibrin	C ₄₁ H ₆₀ O	[M+Na] ⁺	591.45364	591.45383	-0.33			5.0E+06					
1382	DG(14:0/18:0/0:0)	C ₃₅ H ₆₈ O ₅	[M+Na] ⁺	591.49590	591.49591	-0.02	8.6E+06	2.9E+07	1.1E+07	8.3E+06	4.4E+06	3.5E+07	1.6E+07	1.7E+07
1383	Coixenolide	C ₃₈ H ₇₀ O ₄	[M+H] ⁺	591.53469	591.53475	-0.11						4.0E+06		
1384	Tetracosanyl oleate	C ₄₀ H ₇₈ O ₂	[M+H] ⁺	591.60746	591.60742	0.06	5.3E+06	6.2E+06	5.2E+06	1.7E+06		1.4E+07	5.4E+06	4.5E+06
1385	Avermectin B1b aglycone	C ₃₃ H ₄₆ O ₈	[M+Na] ⁺	593.30849	593.30869	-0.34		7.3E+06						
1386	PA(12:0/16:0)	C ₃₁ H ₆₁ O ₈ P	[M+H] ⁺	593.41768	593.41795	-0.45		4.0E+06						
1387	PA(O-16:0/13:0)	C ₃₂ H ₆₅ O ₇ P	[M+H] ⁺	593.45407	593.45418	-0.18	3.6E+07	3.2E+07	4.7E+07	1.1E+07	9.1E+06	3.0E+07	4.8E+07	7.6E+06
1388	Dihydrospheroidene	C ₄₁ H ₆₂ O	[M+Na] ⁺	593.46929	593.46945	-0.28	5.0E+06	6.5E+06	1.0E+07			6.7E+06	9.7E+06	
1389	Cer(d18:0/20:0)	C ₃₈ H ₇₇ NO ₃	[M+H] ⁺	596.59762	596.59773	-0.18						3.6E+06		
1390	DG(15:0/18:3/0:0)	C ₃₆ H ₆₄ O ₅	[M+Na] ⁺	599.46460	599.46466	-0.11		4.7E+06				3.9E+06		
1391	Albanol A	C ₃₄ H ₂₆ O ₈	[M+K] ⁺	601.12593	601.12642	-0.82							4.2E+06	
1392	Hexaprenyl-methyl-hydroxy-methoxy-benzoquinol	C ₃₈ H ₅₈ O ₄	[M+Na] ⁺	601.42273	601.42293	-0.34		3.9E+06	5.4E+06				4.9E+06	
1393	DG(15:0/18:2/0:0)	C ₃₆ H ₆₆ O ₅	[M+Na] ⁺	601.48025	601.48028	-0.05	4.4E+06	1.3E+07	6.0E+06	3.4E+06		1.3E+07	1.1E+07	5.6E+06
1394	PA(P-16:0/14:1)	C ₃₃ H ₆₃ O ₇ P	[M+H] ⁺	603.43842	603.43853	-0.19	2.7E+07	3.1E+07	4.5E+07	7.0E+06	5.4E+06	2.4E+07	4.5E+07	7.6E+06
1395	DG(15:0/18:1/0:0)	C ₃₆ H ₆₈ O ₅	[M+Na] ⁺	603.49590	603.49588	0.03	6.3E+06	2.3E+07	9.1E+06	5.7E+06	3.7E+06		1.5E+07	1.1E+07
1396	Polidocanol	C ₃₀ H ₆₂ O ₁₀	[M+Na] ⁺	605.42352	605.42356	-0.06		8.6E+06	4.1E+06	4.6E+06	4.2E+06	1.2E+07	8.7E+06	7.4E+06
1397	PA(O-16:0/14:1)	C ₃₃ H ₆₅ O ₇ P	[M+H] ⁺	605.45407	605.45420	-0.21	5.6E+07	5.5E+07	8.3E+07	1.3E+07	1.1E+07	4.6E+07	8.4E+07	1.1E+07
1398	DG(15:0/18:0/0:0)	C ₃₆ H ₇₀ O ₅	[M+Na] ⁺	605.51155	605.51157	-0.04	4.6E+06	1.7E+07	6.0E+06	5.4E+06		2.1E+07	1.2E+07	8.6E+06
1399	Hydroxypthioceranic acid (C37)	C ₃₇ H ₇₄ O ₃	[M+K] ⁺	605.52696	605.52690	0.09						4.5E+06		
1400	Pentacosanyl oleate	C ₄₁ H ₈₀ O ₂	[M+H] ⁺	605.62311	605.62304	0.11	3.9E+06					6.6E+06	4.0E+06	
1401	Pubescenol	C ₃₂ H ₄₀ O ₁₀	[M+Na] ⁺	607.25137	607.25151	-0.23	6.1E+06							
1402	Ouabain	C ₂₉ H ₄₄ O ₁₂	[M+Na] ⁺	607.27250	607.27257	-0.12	5.4E+06							
1403	PA(O-16:0/14:0)	C ₃₃ H ₆₇ O ₇ P	[M+H] ⁺	607.46972	607.46985	-0.22	4.5E+07	3.5E+07	4.9E+07	1.1E+07	1.0E+07	3.2E+07	5.0E+07	8.3E+06

ESI(+) FT-ICR MS														
No.	Plausible Compound ^a	Molecular formula (M)	Ion	Theo r m/z ^b	Exp m/z ^c	Δppm ^d	SM _R H ^e	SM _R O ^e	SM _P H ^e	SM _P O ^e	TF _R H ^e	TF _R O ^e	TF _P H ^e	TF _P O ^e
1404	5-Oxoavermectin "2b" aglycone	C ₃₃ H ₄₆ O ₉	[M+Na] ⁺	609.30340	609.30356	-0.26		5.6E+06						
1405	Niguldipine	C ₃₆ H ₃₉ N ₃ O ₆	[M+H] ⁺	610.29116	610.29160	-0.72	5.4E+06		7.5E+06		5.6E+06			
1406	Glucosylkaempferol 3-O-glucoside	C ₂₇ H ₃₀ O ₁₆	[M+H] ⁺	611.16066	611.16073	-0.11							6.3E+06	
1407	Cyclo[D-trp-D-asp-L-pro-D-val-L-leu]	C ₃₁ H ₄₂ N ₆ O ₇	[M+H] ⁺	611.31877	611.31922	-0.73		6.9E+06				3.7E+06		
1408	Hydroxyvitamin D2 (beta-glucuronide)	C ₃₄ H ₅₂ O ₈	[M+Na] ⁺	611.35544	611.35557	-0.21		1.1E+07						
1409	DG(14:0/20:4/0:0)	C ₃₇ H ₆₄ O ₅	[M+Na] ⁺	611.46460	611.46461	-0.01		5.2E+06				4.4E+06		
1410	Glutathione disulfide	C ₂₀ H ₃₂ N ₆ O ₁₂ S ₂	[M+H] ⁺	613.15924	613.15938	-0.22			3.8E+06				4.9E+06	
1411	(O-D-glucopyranosyl)-keto-hexacosanediol	C ₃₂ H ₆₂ O ₈	[M+K] ⁺	613.40763	613.40779	-0.26	3.7E+06							
1412	DG(14:0/20:3/0:0)	C ₃₇ H ₆₆ O ₅	[M+Na] ⁺	613.48025	613.48028	-0.05		9.5E+06	4.8E+06	1.9E+06		1.0E+07	8.0E+06	5.3E+06
1413	Myricetin (triacetylxyloside)	C ₂₆ H ₂₄ O ₁₅	[M+K] ⁺	615.07468	615.07457	0.17	1.3E+07		4.7E+06		4.9E+06		8.9E+06	
1414	Ubiquinol-6	C ₃₉ H ₆₀ O ₄	[M+Na] ⁺	615.43838	615.43861	-0.37		4.9E+06	5.2E+06				5.9E+06	
1415	DG(14:0/20:2/0:0)	C ₃₇ H ₆₈ O ₅	[M+Na] ⁺	615.49590	615.49591	-0.02	9.2E+06	2.8E+07	1.3E+07	5.9E+06		2.9E+07	1.7E+07	1.2E+07
1416	Tetracosyl-palmitate	C ₄₀ H ₈₀ O ₂	[M+Na] ⁺	615.60505	615.60500	0.09						6.2E+06		
1417	PA(P-16:0/15:1)	C ₃₄ H ₆₅ O ₇ P	[M+H] ⁺	617.45407	617.45418	-0.19	1.7E+07	1.7E+07	2.8E+07	7.7E+06	4.6E+06	1.4E+07	2.6E+07	5.5E+06
1418	Hexadecanoyl-(octadecenoyl)-sn-glycerol	C ₃₇ H ₇₀ O ₅	[M+Na] ⁺	617.51155	617.51153	0.02	1.3E+07	2.9E+07	1.1E+07	6.7E+06		3.2E+07	1.5E+07	1.2E+07
1419	Cholesteryl ester	C ₄₁ H ₇₀ O ₂	[M+Na] ⁺	617.52680	617.52687	-0.10		4.7E+06	4.2E+06			6.1E+06	4.5E+06	3.3E+06
1420	CerP(d18:1/16:0)	C ₃₄ H ₆₈ NO ₆ P	[M+H] ⁺	618.48570	618.48519	0.83						3.8E+06		
1421	O-[beta-D-glucopyranosyl]-furostantriol	C ₃₃ H ₅₆ O ₉	[M+Na] ⁺	619.38165	619.38184	-0.30	2.1E+07	3.7E+06	1.4E+07		1.1E+07		1.0E+07	
1422	PA(12:0/18:1)	C ₃₃ H ₆₃ O ₈ P	[M+H] ⁺	619.43333	619.43357	-0.38		4.2E+06				4.0E+06		
1423	PA(O-16:0/15:1)	C ₃₄ H ₆₇ O ₇ P	[M+H] ⁺	619.46972	619.46979	-0.11	3.5E+07	3.1E+07	4.9E+07	9.2E+06	6.8E+06	2.8E+07	4.9E+07	7.0E+06
1424	DG(14:0/20:0/0:0)	C ₃₇ H ₇₂ O ₅	[M+Na] ⁺	619.52720	619.52717	0.04	4.3E+06	9.8E+06	4.6E+06	3.6E+06		1.3E+07	7.2E+06	1.0E+07
1425	Hexacosanyl oleate	C ₄₂ H ₈₂ O ₂	[M+H] ⁺	619.63876	619.63883	-0.12						4.6E+06		
1426	Kurilensoside G	C ₃₂ H ₅₄ O ₁₀	[M+Na] ⁺	621.36092	621.36101	-0.15	7.9E+06				4.0E+06		5.9E+06	
1427	PA(12:0/18:0)	C ₃₃ H ₆₅ O ₈ P	[M+H] ⁺	621.44898	621.44914	-0.25	5.2E+06	5.4E+06	4.1E+06			5.1E+06	4.9E+06	
1428	PA(O-16:0/15:0)	C ₃₄ H ₆₉ O ₇ P	[M+H] ⁺	621.48537	621.48547	-0.16	2.3E+07	1.9E+07	2.8E+07	8.2E+06	6.6E+06	1.9E+07	2.7E+07	6.1E+06
1429	Cer(d18:0/22:1)	C ₄₀ H ₇₉ NO ₃	[M+H] ⁺	622.61327	622.61326	0.02		3.5E+06						
1430	Hydroxy-oxobaccatin III	C ₃₁ H ₃₆ O ₁₂	[M+Na] ⁺	623.20990	623.21001	-0.18	4.0E+06				3.5E+06		3.8E+06	
1431	Avermectin A2b aglycone	C ₃₄ H ₅₀ O ₉	[M+Na] ⁺	625.33470	625.33486	-0.26	4.8E+06	6.8E+06	4.0E+06		4.2E+06	4.5E+06		
1432	(O-glucopyranosyl)-keto-octacosanediol	C ₃₄ H ₆₆ O ₈	[M+Na] ⁺	625.46499	625.46511	-0.18	4.4E+06		4.9E+06		4.3E+06		5.0E+06	

ESI(+) FT-ICR MS														
No.	Plausible Compound ^a	Molecular formula (M)	Ion	Theor m/z ^b	Exp m/z ^c	Δ ppm ^d	SM _R H ^e	SM _R O ^e	SM _P H ^e	SM _P O ^e	TF _R H ^e	TF _R O ^e	TF _P H ^e	TF _P O ^e
1433	DG(15:0/20:4/0:0)	C ₃₈ H ₆₆ O ₅	[M+Na] ⁺	625.48025	625.48038	-0.21		5.0E+06	4.3E+06			5.2E+06		
1434	N-((methyl-hexadecanoyloxy)-methyl-tetradecanoyl)-L-serine	C ₃₇ H ₇₁ NO ₆	[M+H] ⁺	626.53542	626.53539	0.04	5.7E+06	6.3E+06	8.2E+06			7.5E+06	7.9E+06	
1435	Cerbertin	C ₃₂ H ₄₄ O ₁₁	[M+Na] ⁺	627.27758	627.27777	-0.30	3.4E+07		2.5E+07		2.0E+07		1.9E+07	
1436	DG(15:0/20:3/0:0)	C ₃₈ H ₆₈ O ₅	[M+Na] ⁺	627.49590	627.49580	0.16		4.4E+06				3.6E+06		
1437	Pentacosanyl oleate	C ₄₁ H ₈₀ O ₂	[M+Na] ⁺	627.60505	627.60510	-0.07			5.5E+06	3.6E+06				
1438	DG(14:0/20:3/0:0)	C ₃₇ H ₆₆ O ₅	[M+K] ⁺	629.45418	629.45423	-0.07	8.9E+06							
1439	DG(15:0/20:2/0:0)	C ₃₈ H ₇₀ O ₅	[M+Na] ⁺	629.51155	629.51145	0.15		6.4E+06	4.0E+06			8.6E+06	5.5E+06	4.6E+06
1440	Tetracosanyl oleate	C ₄₀ H ₇₈ O ₂	[M+K] ⁺	629.56334	629.56349	-0.24					4.4E+06			
1441	Methyl-tetracosanoic acid	C ₄₁ H ₈₂ O ₂	[M+Na] ⁺	629.62070	629.62085	-0.23						3.7E+06		
1442	PA(P-16:0/16:1)	C ₃₅ H ₆₇ O ₇ P	[M+H] ⁺	631.46972	631.46982	-0.16	3.4E+07	3.0E+07	4.5E+07	1.0E+07	6.0E+06	2.6E+07	4.1E+07	6.8E+06
1443	DG(15:0/20:1/0:0)	C ₃₈ H ₇₂ O ₅	[M+Na] ⁺	631.52720	631.52716	0.05		6.7E+06	3.9E+06			7.3E+06		5.7E+06
1444	15:1 Cholesteryl ester	C ₄₂ H ₇₂ O ₂	[M+Na] ⁺	631.54245	631.54250	-0.08		4.2E+06	4.5E+06			7.1E+06	5.1E+06	
1445	PA(O-16:0/16:1)	C ₃₅ H ₆₉ O ₇ P	[M+H] ⁺	633.48537	633.48548	-0.17	5.2E+07	3.2E+07	4.3E+07	8.9E+06	5.8E+06	2.8E+07	4.1E+07	6.0E+06
1446	DG(15:0/20:0/0:0)	C ₃₈ H ₇₄ O ₅	[M+Na] ⁺	633.54285	633.54287	-0.04		5.0E+06				8.5E+06		4.4E+06
1447	15:0 Cholesteryl ester	C ₄₂ H ₇₄ O ₂	[M+Na] ⁺	633.55810	633.55805	0.08			4.1E+06	2.2E+06		6.5E+06	3.8E+06	4.7E+06
1448	Cholestane-tetrol-glucuronide	C ₃₃ H ₅₆ O ₁₀	[M+Na] ⁺	635.37657	635.37673	-0.25	6.2E+07		4.1E+07		2.7E+07		3.0E+07	
1449	DG(14:0/22:6/0:0)	C ₃₉ H ₆₄ O ₅	[M+Na] ⁺	635.46460	635.46476	-0.26			4.0E+06					
1450	PA(O-16:0/16:0)	C ₃₅ H ₇₁ O ₇ P	[M+H] ⁺	635.50102	635.50112	-0.16	1.5E+07	1.1E+07	1.6E+07	8.4E+06	5.9E+06	1.0E+07	1.5E+07	5.7E+06
1451	(D-xylopyranosyloxy)-epoxycholestan-pentol	C ₃₂ H ₅₄ O ₁₁	[M+Na] ⁺	637.35583	637.35587	-0.06	4.9E+06							
1452	Evasterioside D	C ₃₃ H ₅₈ O ₁₀	[M+Na] ⁺	637.39222	637.39234	-0.20	1.4E+07	7.1E+06	1.1E+07		8.1E+06	4.6E+06	9.1E+06	
1453	DG(14:0/22:5/0:0)	C ₃₉ H ₆₆ O ₅	[M+Na] ⁺	637.48025	637.48037	-0.19	4.7E+06	6.2E+06	5.0E+06			5.8E+06	4.4E+06	
1454	Avermectin A2a aglycone	C ₃₅ H ₅₂ O ₉	[M+Na] ⁺	639.35035	639.35054	-0.29		5.8E+06						
1455	PG(12:0/14:0)	C ₃₂ H ₆₃ O ₁₀ P	[M+H] ⁺	639.42316	639.42325	-0.14	4.2E+06							
1456	DG(14:0/22:4/0:0)	C ₃₉ H ₆₈ O ₅	[M+Na] ⁺	639.49590	639.49590	0.00	5.7E+06	1.3E+07	8.7E+06	2.5E+06		9.0E+06	9.3E+06	5.1E+06
1457	Bryotoxin A	C ₃₂ H ₄₂ O ₁₂	[M+Na] ⁺	641.25685	641.25695	-0.16	6.8E+06							
1458	(O-D-glucopyranosyl)-keto-octacosanetriol	C ₃₄ H ₆₆ O ₉	[M+Na] ⁺	641.45990	641.45995	-0.07	3.6E+06				4.4E+06			
1459	DG(14:1/22:2/0:0)	C ₃₉ H ₇₀ O ₅	[M+Na] ⁺	641.51155	641.51151	0.05	4.9E+06	1.2E+07				9.3E+06	6.9E+06	4.7E+06
1460	Hexacosanyl oleate	C ₄₂ H ₈₂ O ₂	[M+Na] ⁺	641.62070	641.62054	0.25		5.8E+06						5.3E+06

ESI(+) FT-ICR MS														
No.	Plausible Compound ^a	Molecular formula (M)	Ion	Theor m/z ^b	Exp. m/z ^c	Δ ppm _d	SM _{RH} ^e	SM _{RO} ^e	SM _{PH} ^e	SM _{PO} ^e	TF _{RH} ^e	TF _{RO} ^e	TF _{PH} ^e	TF _{PO} ^e
1461	Myricetin 3,3'-digalactoside	C ₂₇ H ₃₀ O ₁₈	[M+H] ⁺	643.15049	643.15061	-0.19					4.2E+06			
1462	(Ladderane-hexanoyl)-ladderane-octanyl)-sn-glycerol	C ₄₁ H ₆₄ O ₄	[M+Na] ⁺	643.46968	643.46975	-0.10		4.8E+06	5.7E+06				6.6E+06	
1463	DG(14:0/22:2/0:0)	C ₃₉ H ₇₂ O ₅	[M+Na] ⁺	643.52720	643.52717	0.05	6.5E+06	1.5E+07	6.3E+06	3.6E+06		1.3E+07	8.6E+06	5.9E+06
1464	Pentacosanyl oleate	C ₄₁ H ₈₀ O ₂	[M+K] ⁺	643.57899	643.57879	0.31					4.0E+06			
1465	Galactosylceramide (d18:1/12:0)	C ₃₆ H ₆₉ NO ₈	[M+H] ⁺	644.50959	644.50939	0.32						3.7E+06		
1466	PA(12:0/20:2)	C ₃₅ H ₆₅ O ₈ P	[M+H] ⁺	645.44898	645.44911	-0.19	4.0E+06					4.3E+06		
1467	PA(O-16:0/17:2)	C ₃₆ H ₆₉ O ₇ P	[M+H] ⁺	645.48537	645.48549	-0.18	8.5E+06	7.2E+06	1.3E+07			6.8E+06	1.1E+07	
1468	DG(14:0/22:1/0:0)	C ₃₉ H ₇₄ O ₅	[M+Na] ⁺	645.54285	645.54285	-0.01		6.9E+06				5.9E+06		3.9E+06
1469	Vitamin D3 palmitate	C ₄₃ H ₇₄ O ₂	[M+Na] ⁺	645.55810	645.55807	0.05	5.1E+06	1.2E+07	6.1E+06	4.2E+06		1.8E+07	7.9E+06	8.5E+06
1470	DG(17:2/20:5/0:0)	C ₄₀ H ₆₄ O ₅	[M+Na] ⁺	647.46460	647.46467	-0.11	4.8E+06	4.0E+06					5.4E+06	
1471	PA(O-16:0/17:1)	C ₃₆ H ₇₁ O ₇ P	[M+H] ⁺	647.50102	647.50113	-0.17	1.1E+07	8.7E+06	1.3E+07			7.9E+06	1.2E+07	
1472	DG(14:0/22:0/0:0)	C ₃₉ H ₇₆ O ₅	[M+Na] ⁺	647.55850	647.55850	-0.01		4.0E+06				5.5E+06		5.0E+06
1473	16:0 Cholesteryl ester	C ₄₃ H ₇₆ O ₂	[M+Na] ⁺	647.57375	647.57371	0.07						7.5E+06		4.1E+06
1474	Cer (d18:1/24:1(15Z))	C ₄₂ H ₈₁ NO ₃	[M+H] ⁺	648.62892	648.62860	0.50						4.1E+06		
1475	Hydroxykaempferol caffeylglucoside	C ₃₀ H ₂₆ O ₁₅	[M+Na] ⁺	649.11639	649.11653	-0.21	4.3E+06						7.0E+06	
1476	O-(Glc)-spirostantriol	C ₃₄ H ₅₈ O ₁₀	[M+Na] ⁺	649.39222	649.39242	-0.31	2.5E+08	4.2E+06	1.6E+08	6.0E+06	1.0E+08	9.8E+06	1.1E+08	
1477	Methoxy-methyloctadecenynoyl anhydride	C ₄₀ H ₆₆ O ₅	[M+Na] ⁺	649.48025	649.48050	-0.38	9.8E+06	5.6E+06	5.1E+06				5.8E+06	
1478	PA(O-16:0/17:0)	C ₃₆ H ₇₃ O ₇ P	[M+H] ⁺	649.51667	649.51673	-0.10	7.2E+06	4.7E+06	7.2E+06			6.2E+06	5.8E+06	
1479	Squalamine	C ₃₄ H ₆₅ N ₃ O ₅ S	[M+Na] ⁺	650.45371	650.45322	0.76						5.5E+06		
1480	Perhydroazepino-N-carbonyl-L-Leu-D-Trp-D-Trp	C ₃₅ H ₄₄ N ₆ O ₅	[M+Na] ⁺	651.32654	651.32632	0.34			3.7E+06		3.5E+06			
1481	PI(P-20:0/0:0)	C ₂₉ H ₅₇ O ₁₁ P	[M+K] ⁺	651.32701	651.32646	0.84					3.5E+06			
1482	PA(13:0/18:3)	C ₃₄ H ₆₁ O ₈ P	[M+Na] ⁺	651.39963	651.39914	0.75	1.6E+07		1.5E+07		8.3E+06			
1483	DG(15:0/22:5/0:0)	C ₄₀ H ₆₈ O ₅	[M+Na] ⁺	651.49590	651.49617	-0.41	3.9E+06	4.4E+06	4.2E+06			4.4E+06	4.6E+06	
1484	PI(22:2/0:0)	C ₃₁ H ₅₇ O ₁₂ P	[M+H] ⁺	653.36604	653.36622	-0.27		5.5E+06						
1485	PG(12:0/15:0)	C ₃₃ H ₆₅ O ₁₀ P	[M+H] ⁺	653.43881	653.43879	0.03	5.4E+06	4.6E+06	3.9E+06					
1486	PA(P-16:0/18:4)	C ₃₇ H ₆₅ O ₇ P	[M+H] ⁺	653.45407	653.45422	-0.23			4.2E+06					
1487	DG(15:0/22:4/0:0)	C ₄₀ H ₇₀ O ₅	[M+Na] ⁺	653.51155	653.51163	-0.12	3.7E+06	5.5E+06				6.1E+06	4.5E+06	
1488	Oleanoic acid 3-O-glucuronide	C ₃₆ H ₅₆ O ₉	[M+Na] ⁺	655.38165	655.38200	-0.53		7.5E+06						

ESI(+) FT-ICR MS														
No.	Plausible Compound ^a	Molecular formula (M)	Ion	Theor m/z ^b	Exp. m/z ^c	Δ ppm _d	SM _R H ^e	SM _R O ^e	SM _P H ^e	SM _P O ^e	TF _R H ^e	TF _R O ^e	TF _P H ^e	TF _P O ^e
1489	PA(O-16:0/18:4)	C ₃₇ H ₆₇ O ₇ P	[M+H] ⁺	655.46972	655.46981	-0.14	9.1E+06	1.0E+07	2.2E+07	5.3E+06		7.1E+06	1.1E+07	
1490	Hexahydroxy-methoxyflavone neohesperidoside	C ₂₈ H ₃₂ O ₁₈	[M+H] ⁺	657.16614	657.16601	0.20					3.8E+06			
1491	Enalkiren	C ₃₅ H ₅₆ N ₆ O ₆	[M+H] ⁺	657.43341	657.43378	-0.56	6.5E+06							
1492	PA(O-16:0/18:3)	C ₃₇ H ₆₉ O ₇ P	[M+H] ⁺	657.48537	657.48548	-0.18	1.6E+07	1.3E+07	2.3E+07	6.0E+06		9.6E+06	1.4E+07	
1493	PA(O-16:0/18:2)	C ₃₇ H ₇₁ O ₇ P	[M+H] ⁺	659.50102	659.50116	-0.21	2.3E+07	1.5E+07	2.2E+07	8.2E+06	4.0E+06	1.2E+07	1.7E+07	4.3E+06
1494	DG(15:0/22:1/0:0)	C ₄₀ H ₇₆ O ₅	[M+Na] ⁺	659.55850	659.55849	0.01						3.9E+06		
1495	17:1 Cholesteryl ester	C ₄₄ H ₇₆ O ₂	[M+Na] ⁺	659.57375	659.57381	-0.09						7.0E+06	4.3E+06	
1496	Purpureacin-1	C ₃₇ H ₆₆ O ₈	[M+Na] ⁺	661.46499	661.46503	-0.07	4.6E+06		4.3E+06			3.8E+06		
1497	PA(O-16:0/18:1)	C ₃₇ H ₇₃ O ₇ P	[M+H] ⁺	661.51667	661.51680	-0.20	1.4E+07	6.3E+06	9.5E+06			5.2E+06	8.4E+06	
1498	2-Octaprenylphenol	C ₄₆ H ₇₀ O	[M+Na] ⁺	661.53189	661.53200	-0.17	8.1E+06	1.3E+07	1.3E+07	5.6E+06		1.8E+07	1.1E+07	6.9E+06
1499	Mosesin 4	C ₃₅ H ₆₀ O ₁₀	[M+Na] ⁺	663.40787	663.40811	-0.36	1.4E+07		1.3E+07		7.4E+06		8.1E+06	
1500	DG(16:0/22:6/0:0)	C ₄₁ H ₆₈ O ₅	[M+Na] ⁺	663.49590	663.49587	0.04	3.5E+06							
1501	PA(16:0e/18:0)	C ₃₇ H ₇₅ O ₇ P	[M+H] ⁺	663.53232	663.53237	-0.08	5.9E+06	3.7E+06	5.8E+06		4.0E+06	4.6E+06	5.7E+06	
1502	16:0 Cholesteryl ester	C ₄₃ H ₇₆ O ₂	[M+K] ⁺	663.54769	663.54766	0.05			3.8E+06					
1503	DG(16:0/22:5/0:0)	C ₄₁ H ₇₀ O ₅	[M+Na] ⁺	665.51155	665.51177	-0.33		4.5E+06	4.4E+06			5.2E+06		
1504	Squalamine	C ₃₄ H ₆₅ N ₃ O ₅ S	[M+K] ⁺	666.42765	666.42713	0.78	6.8E+06				4.3E+06		6.5E+06	
1505	PI(22:6/0:0)	C ₃₁ H ₄₉ O ₁₂ P	[M+Na] ⁺	667.28538	667.28484	0.82			5.5E+06				6.3E+06	
1506	DG(16:0/22:4/0:0)	C ₄₁ H ₇₂ O ₅	[M+Na] ⁺	667.52720	667.52724	-0.07			3.9E+06					
1507	Finaconitine	C ₃₃ H ₄₆ N ₂ O ₁₀	[M+K] ⁺	669.27841	669.27786	0.81							4.8E+06	
1508	(O-galactopyranosyl)-keto-triacontanetriol	C ₃₆ H ₇₀ O ₉	[M+Na] ⁺	669.49120	669.49133	-0.19	5.5E+06							
1509	18:2 Cholesteryl ester	C ₄₅ H ₇₆ O ₂	[M+Na] ⁺	671.57375	671.57358	0.26						5.6E+06		
1510	Galactosylceramide	C ₃₈ H ₇₃ NO ₈	[M+H] ⁺	672.54089	672.54095	-0.08		4.3E+06				4.9E+06		
1511	Thapsigargin	C ₃₄ H ₅₀ O ₁₂	[M+Na] ⁺	673.31945	673.31965	-0.29	1.1E+07		1.1E+07		8.2E+06		9.4E+06	
1512	18:1 Cholesteryl ester	C ₄₅ H ₇₈ O ₂	[M+Na] ⁺	673.58940	673.58936	0.06		5.1E+06		1.7E+06		7.1E+06		4.3E+06
1513	N-Acetyl-leu-leu-leu-leu-tyr-amide	C ₃₅ H ₅₈ N ₆ O ₇	[M+H] ⁺	675.44397	675.44440	-0.63	4.2E+06							
1514	DG(17:1/22:6/0:0)	C ₄₂ H ₆₈ O ₅	[M+Na] ⁺	675.49590	675.49605	-0.23	5.6E+06	4.0E+06						
1515	DG(17:0/22:6/0:0)	C ₄₂ H ₇₀ O ₅	[M+Na] ⁺	677.51155	677.51172	-0.26	7.7E+06							
1516	PA(O-16:0/19:0)	C ₃₈ H ₇₇ O ₇ P	[M+H] ⁺	677.54797	677.54766	0.45			3.7E+06					
1517	PG(12:0/17:1)	C ₃₅ H ₆₇ O ₁₀ P	[M+H] ⁺	679.45446	679.45446	0.01	5.9E+06	3.9E+06			4.4E+06			

ESI(+) FT-ICR MS														
No.	Plausible Compound ^a	Molecular formula (M)	Ion	Theor m/z ^b	Exp. m/z ^c	Δ ppm _d	SM _R H ^e	SM _R O ^e	SM _P H ^e	SM _P O ^e	TF _R H ^e	TF _R O ^e	TF _P H ^e	TF _P O ^e
1518	PI(21:0/0:0)	C ₃₀ H ₅₉ O ₁₂ P	[M+K] ⁺	681.33757	681.33694	0.94				1.2E+07				1.4E+07
1519	PG(12:0/17:0)	C ₃₅ H ₆₉ O ₁₀ P	[M+H] ⁺	681.47011	681.47028	-0.25	4.8E+06							
1520	Mannosyl-1beta-phosphomycoketide C30	C ₃₆ H ₇₃ O ₉ P	[M+H] ⁺	681.50650	681.50650	0.00	4.0E+06	5.1E+06						
1521	PA(O-16:0/20:3)	C ₃₉ H ₇₃ O ₇ P	[M+H] ⁺	685.51667	685.51664	0.04				3.6E+06				
1522	DG(15:0/24:1/0:0)	C ₄₂ H ₈₀ O ₅	[M+Na] ⁺	687.58980	687.58948	0.46						3.6E+06		
1523	PA(O-16:0/20:1)	C ₃₉ H ₇₇ O ₇ P	[M+H] ⁺	689.54797	689.54790	0.10				3.8E+06				4.2E+06
1524	DG(15:0/24:0/0:0)	C ₄₂ H ₈₂ O ₅	[M+Na] ⁺	689.60545	689.60530	0.21						3.6E+06		
1525	Peonidin 3-glucoside-5-(6''-acetylglucoside)	C ₃₀ H ₃₅ O ₁₇	[M+Na] ⁺	690.17665	690.17641	0.34	4.9E+06			4.6E+06	5.4E+06			
1526	PG(P-16:0/15:1)	C ₃₇ H ₇₁ O ₉ P	[M+H] ⁺	691.49085	691.49104	-0.28						3.6E+06		
1527	PA(O-16:0/20:0)	C ₃₉ H ₇₉ O ₇ P	[M+H] ⁺	691.56362	691.56372	-0.15				3.8E+06				4.2E+06
1528	Monensin	C ₃₆ H ₆₂ O ₁₁	[M+Na] ⁺	693.41843	693.41864	-0.30	1.9E+08			1.2E+08	5.4E+06	7.8E+07		8.2E+07
1529	PG(12:0/18:1)	C ₃₆ H ₆₉ O ₁₀ P	[M+H] ⁺	693.47011	693.47027	-0.23		4.5E+06			6.2E+06			
1530	PG(12:0/18:0)	C ₃₆ H ₇₁ O ₁₀ P	[M+H] ⁺	695.48576	695.48586	-0.14	3.7E+06							
1531	Mannosyl-phosphomycoketide C31	C ₃₇ H ₇₅ O ₉ P	[M+H] ⁺	695.52215	695.52197	0.25		4.1E+06						
1532	GalCer(d18:1/16:0)	C ₄₀ H ₇₇ NO ₈	[M+H] ⁺	700.57219	700.57206	0.19						4.3E+06		
1533	PA(14:0/22:1)	C ₃₉ H ₇₅ O ₈ P	[M+H] ⁺	703.52723	703.52741	-0.25	5.8E+06							
1534	DG(16:0/24:0/0:0)	C ₄₃ H ₈₄ O ₅	[M+Na] ⁺	703.62110	703.62106	0.05						4.0E+06		
1535	DG(19:0/22:6/0:0)	C ₄₄ H ₇₄ O ₅	[M+Na] ⁺	705.54285	705.54269	0.23	7.3E+06							4.0E+06
1536	SM(d18:0/16:0)	C ₃₉ H ₈₁ N ₂ O ₆ P	[M+H] ⁺	705.59050	705.59063	-0.18		3.9E+06						
1537	PG(12:0/19:1)	C ₃₇ H ₇₁ O ₁₀ P	[M+H] ⁺	707.48576	707.48588	-0.16	7.6E+06	6.4E+06			9.8E+06	5.9E+06	4.3E+06	
1538	Mannosyl-1beta-phosphomycoketide C32	C ₃₈ H ₇₇ O ₉ P	[M+H] ⁺	709.53780	709.53798	-0.25		5.0E+06				4.0E+06		
1539	O-alpha-D-glucopyranosyl-(tetradecanoyloxy)- eicosanol	C ₄₀ H ₇₈ O ₈	[M+Na] ⁺	709.55889	709.55884	0.07	6.2E+06	4.1E+06	9.5E+06		4.0E+06			1.2E+07
1540	Dihexadecanoyl-sn-glycero-3-O-(N,N,N- trimethyl)- homoserine	C ₄₂ H ₈₁ NO ₇	[M+H] ⁺	712.60858	712.60865	-0.10	4.2E+06			4.7E+06				
1541	(O-D-glucopyranosyl)-keto-dotriacontanetriol	C ₃₈ H ₇₄ O ₉	[M+K] ⁺	713.49644	713.49639	0.07	5.8E+06							
1542	Scillaren A	C ₃₆ H ₅₂ O ₁₃	[M+Na] ⁺	715.33001	715.33019	-0.24	1.6E+07			1.5E+07	8.6E+06			8.7E+06
1543	PA(O-16:0/22:1)	C ₄₁ H ₈₁ O ₇ P	[M+H] ⁺	717.57927	717.57939	-0.17	4.2E+06			4.2E+06				
1544	PA(O-16:0/22:0)	C ₄₁ H ₈₃ O ₇ P	[M+H] ⁺	719.59492	719.59505	-0.18	4.4E+06			4.3E+06				4.4E+06
1545	Cyanidin 3-(6''-malonylglucoside)-5-glucoside	C ₃₀ H ₃₃ O ₁₉	[M+Na] ⁺	720.15082	720.15055	0.38	4.7E+06			4.9E+06	4.3E+06			

ESI(+) FT-ICR MS														
No.	Plausible Compound ^a	Molecular formula (M)	Ion	Theor m/z ^b	Exp. m/z ^c	Δ ppm _d	SM _R H ^e	SM _R O ^e	SM _P H ^e	SM _P O ^e	TF _R H ^e	TF _R O ^e	TF _P H ^e	TF _P O ^e
1546	PG(12:0/20:1)	C ₃₈ H ₇₃ O ₁₀ P	[M+H] ⁺	721.50141	721.50152	-0.15	7.0E+06	7.3E+06	4.2E+06		8.8E+06		6.1E+06	
1547	PG(12:0/20:0)	C ₃₈ H ₇₅ O ₁₀ P	[M+H] ⁺	723.51706	723.51726	-0.27	3.9E+06							
1548	PA(O-20:0/17:2)	C ₄₀ H ₇₇ O ₇ P	[M+Na] ⁺	723.52991	723.53056	-0.90	9.5E+06	4.0E+07	2.3E+07	1.3E+07	8.7E+06	2.1E+07	2.5E+07	1.8E+07
1549	Crasseride 2a	C ₄₁ H ₈₀ O ₈	[M+Na] ⁺	723.57454	723.57455	-0.01	4.2E+06		7.7E+06			4.2E+06	1.1E+07	
1550	PC(12:0/18:2)	C ₃₈ H ₇₂ NO ₈ P	[M+Na] ⁺	724.48878	724.48941	-0.88		1.4E+07						
1551	PG(13:0/18:3)	C ₃₇ H ₆₇ O ₁₀ P	[M+Na] ⁺	725.43641	725.43582	0.81	4.4E+06							
1552	Ecdysone palmitate	C ₄₃ H ₇₄ O ₇	[M+Na] ⁺	725.53268	725.53276	-0.12		4.7E+06	4.2E+06					
1553	DG(18:0/24:1/0:0)	C ₄₅ H ₈₆ O ₅	[M+Na] ⁺	729.63675	729.63677	-0.03						3.7E+06		
1554	PA(O-18:0/20:5)	C ₄₁ H ₇₃ O ₇ P	[M+Na] ⁺	731.49861	731.49813	0.66	6.5E+06							
1555	PA(16:0/22:1)	C ₄₁ H ₇₉ O ₈ P	[M+H] ⁺	731.55853	731.55870	-0.23	5.4E+06							
1556	PA(O-20:0/19:1)	C ₄₂ H ₈₃ O ₇ P	[M+H] ⁺	731.59492	731.59486	0.08			4.6E+06					
1557	PG(13:0/20:2)	C ₃₉ H ₇₃ O ₁₀ P	[M+H] ⁺	733.50141	733.50132	0.12	5.1E+06							
1558	DG(21:0/22:6/0:0)	C ₄₆ H ₇₈ O ₅	[M+Na] ⁺	733.57415	733.57418	-0.04	5.3E+06	4.2E+06	4.1E+06				3.8E+06	
1559	PA(O-18:0/21:0)	C ₄₂ H ₈₅ O ₇ P	[M+H] ⁺	733.61057	733.61058	-0.02			4.6E+06					
1560	Digitalin	C ₃₆ H ₅₆ O ₁₄	[M+Na] ⁺	735.35623	735.35639	-0.22	4.9E+06				4.2E+06			
1561	PG(13:0/20:1)	C ₃₉ H ₇₅ O ₁₀ P	[M+H] ⁺	735.51706	735.51726	-0.26	6.9E+06	7.1E+06	4.1E+06		5.8E+06	5.0E+06	4.5E+06	
1562	PA(O-16:0/22:2)	C ₄₁ H ₇₉ O ₇ P	[M+Na] ⁺	737.54556	737.54622	-0.89				6.6E+06				1.1E+07
1563	O-glucopyranosyl-(hexadecanoyloxy)-eicosanol	C ₄₂ H ₈₂ O ₈	[M+Na] ⁺	737.59019	737.59014	0.07	4.9E+06		8.8E+06			4.5E+06	9.9E+06	
1564	ADP-Ribosyl-L-arginine	C ₂₁ H ₃₅ N ₉ O ₁₅ P ₂	[M+Na] ⁺	738.16201	738.16164	0.50	3.8E+06				4.0E+06			
1565	Chalcomycin	C ₃₅ H ₅₆ O ₁₄	[M+K] ⁺	739.33017	739.33009	0.10	4.3E+06							
1566	PG(12:0/20:3)	C ₃₈ H ₆₉ O ₁₀ P	[M+Na] ⁺	739.45206	739.45156	0.67	1.1E+07		8.9E+06					
1567	PC(P-14:0/18:1)	C ₄₀ H ₇₉ NO ₇ P	[M+Na] ⁺	739.54864	739.54860	0.05							4.1E+06	
1568	Glc-Cer(d18:1/18:0)	C ₄₂ H ₇₉ NO ₉	[M+H] ⁺	742.58276	742.58271	0.07	5.4E+06							
1569	Butanoyloxyfucoxanthin	C ₄₆ H ₆₄ O ₈	[M+H] ⁺	745.46740	745.46792	-0.70		1.9E+07		5.8E+06		1.0E+07		5.1E+06
1570	DG(22:1/22:6/0:0)	C ₄₇ H ₇₈ O ₅	[M+Na] ⁺	745.57415	745.57422	-0.10	3.9E+06		4.3E+06			4.4E+06	6.3E+06	
1571	PA(O-18:0/22:1)	C ₄₃ H ₈₅ O ₇ P	[M+H] ⁺	745.61057	745.61090	-0.44			3.8E+06				3.8E+06	
1572	TG(14:0/14:0/14:0)	C ₄₅ H ₈₆ O ₆	[M+Na] ⁺	745.63166	745.63150	0.22		3.7E+06				5.0E+06		
1573	PI(12:0/14:1)	C ₃₅ H ₆₅ O ₁₃ P	[M+Na] ⁺	747.40550	747.40604	-0.72				2.6E+06		4.7E+06		8.9E+06
1574	PG(12:0/22:2)	C ₄₀ H ₇₅ O ₁₀ P	[M+H] ⁺	747.51706	747.51705	0.02			3.6E+06					

ESI(+) FT-ICR MS														
No.	Plausible Compound ^a	Molecular formula (M)	Ion	Theor m/z ^b	Exp m/z ^c	Δ ppm ^d	SM _R H ^e	SM _R O ^e	SM _P H ^e	SM _P O ^e	TF _R H ^e	TF _R O ^e	TF _P H ^e	TF _P O ^e
1575	DG(20:5/24:1/0:0)	C ₄₇ H ₈₀ O ₅	[M+Na] ⁺	747.58980	747.59001	-0.29	4.4E+06			4.6E+06				5.2E+06
1576	Hexadecanoyl-(octadecenoyl)-sn-glycero-phospho-sn-glycerol	C ₄₀ H ₇₇ O ₁₀ P	[M+H] ⁺	749.53271	749.53286	-0.19	6.8E+06	6.5E+06	4.6E+06			6.0E+06	5.6E+06	
1577	PG(12:0/22:0)	C ₄₀ H ₇₉ O ₁₀ P	[M+H] ⁺	751.54836	751.54865	-0.38	3.7E+06	3.3E+06	3.9E+06					4.0E+06
1578	PA(18:0/22:2)	C ₄₃ H ₈₁ O ₈ P	[M+H] ⁺	757.57418	757.57411	0.10			3.6E+06					
1579	PA(O-20:0/20:5)	C ₄₃ H ₇₇ O ₇ P	[M+Na] ⁺	759.52991	759.52940	0.67	4.9E+06							
1580	PA(18:0/22:1)	C ₄₃ H ₈₃ O ₈ P	[M+H] ⁺	759.58983	759.58995	-0.16	7.6E+06	6.8E+06	9.9E+06			6.8E+06	9.2E+06	
1581	PA(P-20:0/21:0)	C ₄₄ H ₈₇ O ₇ P	[M+H] ⁺	759.62622	759.62604	0.23			3.7E+06					
1582	PA(O-18:0/22:4)	C ₄₃ H ₇₉ O ₇ P	[M+Na] ⁺	761.54556	761.54513	0.57	7.1E+06							
1583	PA(18:0/22:0)	C ₄₃ H ₈₅ O ₈ P	[M+H] ⁺	761.60548	761.60559	-0.14	8.8E+06	6.3E+06	9.2E+06	4.0E+06		6.9E+06	9.3E+06	
1584	PG(13:0/22:1)	C ₄₁ H ₇₉ O ₁₀ P	[M+H] ⁺	763.54836	763.54849	-0.17	6.1E+06	4.5E+06	4.1E+06		3.7E+06	4.5E+06	4.5E+06	
1585	PG(P-18:0/17:2)	C ₄₁ H ₇₇ O ₉ P	[M+Na] ⁺	767.51974	767.52041	-0.87	6.8E+07		8.9E+07		3.3E+07			
1586	GalCer(d16:1/23:0)	C ₄₅ H ₈₇ NO ₈	[M+H] ⁺	770.65045	770.65021	0.31	3.9E+06							
1587	PA(19:0/22:2)	C ₄₄ H ₈₃ O ₈ P	[M+H] ⁺	771.58983	771.58993	-0.12			5.8E+06			6.4E+06	6.0E+06	
1588	DG(22:6/24:1/0:0)	C ₄₉ H ₈₂ O ₅	[M+Na] ⁺	773.60545	773.60556	-0.15	1.1E+07	1.1E+07	1.6E+07	3.0E+06		1.1E+07	1.6E+07	
1589	PA(O-20:0/22:1)	C ₄₅ H ₈₉ O ₇ P	[M+H] ⁺	773.64187	773.64195	-0.11			3.4E+06					
1590	DG(22:5/24:1/0:0)	C ₄₉ H ₈₄ O ₅	[M+Na] ⁺	775.62110	775.62119	-0.12	1.1E+07	1.0E+07	1.4E+07			1.0E+07	1.4E+07	
1591	Chikusetsusaponin Ia	C ₄₁ H ₇₀ O ₁₂	[M+Na] ⁺	777.47595	777.47592	0.04	3.8E+06							
1592	PG(14:0/22:1)	C ₄₂ H ₈₁ O ₁₀ P	[M+H] ⁺	777.56401	777.56419	-0.22	5.1E+06	3.9E+06			3.4E+06		4.5E+06	
1593	PI(12:0/18:1)	C ₃₉ H ₇₃ O ₁₃ P	[M+H] ⁺	781.48616	781.48618	-0.03		5.6E+06						
1594	Hexadecanoyl-(octadecenoyl)-sn-glycero-phosphocholine	C ₄₂ H ₈₃ NO ₈ P	[M+Na] ⁺	783.57485	783.57444	0.52		4.1E+06						
1595	PA(20:1/22:2)	C ₄₅ H ₈₃ O ₈ P	[M+H] ⁺	783.58983	783.58985	-0.02							3.7E+06	
1596	PA(20:0/22:2)	C ₄₅ H ₈₅ O ₈ P	[M+H] ⁺	785.60548	785.60555	-0.08	1.2E+07	1.0E+07	1.6E+07	2.6E+06		1.2E+07	1.7E+07	
1597	PA(20:0/22:1)	C ₄₅ H ₈₇ O ₈ P	[M+H] ⁺	787.62113	787.62116	-0.03	2.7E+07	2.1E+07	3.5E+07	5.7E+06	4.4E+06	2.4E+07	3.5E+07	5.3E+06
1598	PA(20:0/22:0)	C ₄₅ H ₈₉ O ₈ P	[M+H] ⁺	789.63678	789.63685	-0.08	2.1E+07	1.5E+07	2.6E+07	7.9E+06	4.9E+06	1.8E+07	2.4E+07	4.4E+06
1599	PG(P-20:0/17:2)	C ₄₃ H ₈₁ O ₉ P	[M+Na] ⁺	795.55104	795.55142	-0.48			4.8E+06					
1600	GalCer(d18:2/23:0)	C ₄₇ H ₈₉ NO ₈	[M+H] ⁺	796.66610	796.66605	0.06	3.5E+06							
1601	TG(16:1/14:0/16:1)	C ₄₉ H ₉₀ O ₆	[M+Na] ⁺	797.66296	797.66290	0.08	5.3E+06	1.8E+07	8.1E+06	4.3E+06		2.5E+07	1.1E+07	8.0E+06
1602	GalCer(d18:1/23:0)	C ₄₇ H ₉₁ NO ₈	[M+H] ⁺	798.68175	798.68169	0.07	3.3E+06							

ESI(+) FT-ICR MS														
No.	Plausible Compound ^a	Molecular formula (M)	Ion	Theor m/z ^b	Exp m/z ^c	Δ ppm ^d	SM _R H ^e	SM _R O ^e	SM _P H ^e	SM _P O ^e	TF _R H ^e	TF _R O ^e	TF _P H ^e	TF _P O ^e
1603	PA(21:0/22:2)	C ₄₆ H ₈₇ O ₈ P	[M+H] ⁺	799.62113	799.62124	-0.13	1.7E+07	1.4E+07	2.7E+07	4.2E+06	3.7E+06	1.7E+07	2.5E+07	4.5E+06
1604	TG(16:0/14:0/16:1)	C ₄₉ H ₉₂ O ₆	[M+Na] ⁺	799.67861	799.67858	0.04	7.2E+06	2.6E+07	9.7E+06	5.0E+06			1.5E+07	1.3E+07
1605	MGDG(18:2/18:2)	C ₄₅ H ₇₈ O ₁₀	[M+Na] ⁺	801.54872	801.54897	-0.31	1.0E+07		8.7E+06		5.7E+06			
1606	PA(21:0/22:1)	C ₄₆ H ₈₉ O ₈ P	[M+H] ⁺	801.63678	801.63694	-0.19	3.6E+07	2.9E+07	5.0E+07	6.6E+06	6.6E+06	3.4E+07	4.9E+07	7.5E+06
1607	Dodecanoyl-hexadecanoyl-octadecanoyl-sn-glycerol	C ₄₉ H ₉₄ O ₆	[M+Na] ⁺	801.69426	801.69437	-0.14	4.3E+06	1.3E+07	3.7E+06	3.8E+06		1.9E+07	8.4E+06	7.2E+06
1608	PE(16:0/22:6)	C ₄₃ H ₇₄ NO ₉ P	[M+Na] ⁺	802.49934	802.49989	-0.69		4.3E+07	3.6E+06			4.4E+06	4.4E+06	
1609	PA(21:0/22:0)	C ₄₆ H ₉₁ O ₈ P	[M+H] ⁺	803.65243	803.65260	-0.21	2.6E+07	1.9E+07	3.2E+07	5.9E+06	5.3E+06	2.1E+07	3.1E+07	6.5E+06
1610	PE(20:5/22:6)	C ₄₇ H ₇₂ NO ₈ P	[M+H] ⁺	810.50683	810.50692	-0.11	3.1E+07		8.5E+06		1.4E+07		9.9E+06	
1611	PS(14:0/22:2)	C ₄₂ H ₇₈ NO ₁₀ P	[M+Na] ⁺	810.52556	810.52628	-0.89	4.2E+07		2.6E+07		1.4E+07		1.4E+07	
1612	PA(22:1/22:2)	C ₄₇ H ₈₇ O ₈ P	[M+H] ⁺	811.62113	811.62131	-0.22	8.3E+06	7.7E+06	1.2E+07			7.6E+06	1.2E+07	
1613	PE(20:4/22:6)	C ₄₇ H ₇₄ NO ₈ P	[M+H] ⁺	812.52248	812.52240	0.10							3.6E+06	
1614	PA(22:0/22:2)	C ₄₇ H ₈₉ O ₈ P	[M+H] ⁺	813.63678	813.63692	-0.17	3.4E+07	3.0E+07	4.8E+07	6.2E+06	5.6E+06	3.4E+07	4.7E+07	6.6E+06
1615	Leucomycin A4	C ₄₁ H ₆₇ NO ₁₅	[M+H] ⁺	814.45835	814.45855	-0.25							4.4E+06	
1616	PA(22:0/22:0)	C ₄₇ H ₉₃ O ₈ P	[M+H] ⁺	817.66808	817.66821	-0.15	3.5E+07	2.5E+07	4.1E+07	7.8E+06	7.2E+06	2.8E+07	3.9E+07	7.3E+06
1617	Diginatin	C ₄₁ H ₆₄ O ₁₅	[M+Na] ⁺	819.41374	819.41403	-0.35	9.9E+06		7.2E+06		5.0E+06			
1618	PG(O-18:0/22:0)	C ₄₆ H ₉₃ O ₉ P	[M+H] ⁺	821.66300	821.66284	0.19						4.3E+06		
1619	Spongipregnenoloside D	C ₄₀ H ₆₄ O ₁₆	[M+Na] ⁺	823.40866	823.40889	-0.28	3.9E+06							
1620	TG(16:1/14:0/18:2)	C ₅₁ H ₉₂ O ₆	[M+Na] ⁺	823.67861	823.67851	0.13	4.6E+06	1.4E+07	6.5E+06	2.9E+06		1.7E+07	9.0E+06	5.9E+06
1621	TG(16:0/14:0/18:2)	C ₅₁ H ₉₄ O ₆	[M+Na] ⁺	825.69426	825.69422	0.05	9.7E+06	3.2E+07	1.3E+07	5.0E+06		4.4E+07	1.9E+07	1.5E+07
1622	Glucosylceramide (d18:1/25:0)	C ₄₉ H ₉₅ NO ₈	[M+H] ⁺	826.71305	826.71309	-0.05	3.9E+06		4.0E+06					
1623	PI(P-16:0/17:2)	C ₄₂ H ₇₇ O ₁₂ P	[M+Na] ⁺	827.50449	827.50393	0.67	5.3E+06							
1624	TG(16:0/14:0/18:1)	C ₅₁ H ₉₆ O ₆	[M+Na] ⁺	827.70991	827.70987	0.05	8.2E+06	3.2E+07	1.1E+07	6.0E+06		4.6E+07	1.7E+07	1.4E+07
1625	TG(16:0/14:0/18:0)	C ₅₁ H ₉₈ O ₆	[M+Na] ⁺	829.72556	829.72549	0.09		1.2E+07	3.7E+06	3.0E+06		1.6E+07	5.7E+06	6.6E+06
1626	TG(16:0/16:0/18:1)	C ₅₃ H ₁₀₀ O ₆	[M+H] ⁺	833.75927	833.75998	-0.85						3.3E+06		
1627	TG(16:1/16:1/17:2)	C ₅₂ H ₉₂ O ₆	[M+Na] ⁺	835.67861	835.67872	-0.13		3.6E+06				4.9E+06		
1628	TG(16:0/16:1/17:2)	C ₅₂ H ₉₄ O ₆	[M+Na] ⁺	837.69426	837.69436	-0.11	4.8E+06	1.0E+07	5.4E+06	1.9E+06		1.3E+07	9.1E+06	5.9E+06
1629	GalCer(d18:1/26:1)	C ₅₀ H ₉₅ NO ₈	[M+H] ⁺	838.71305	838.71309	-0.05	4.3E+06		5.8E+06					
1630	TG(15:0/18:1/16:1)	C ₅₂ H ₉₆ O ₆	[M+Na] ⁺	839.70991	839.70996	-0.05	6.2E+06	2.2E+07	1.0E+07	4.1E+06		3.1E+07	1.4E+07	1.0E+07
1631	GalCer(d18:0/26:1)	C ₅₀ H ₉₇ NO ₈	[M+H] ⁺	840.72870	840.72879	-0.11	4.1E+06		5.6E+06					

ESI(+) FT-ICR MS														
No.	Plausible Compound ^a	Molecular formula (M)	Ion	Theo r m/z ^b	Exp . m/z ^c	Δppm _d	SM _R H ^e	SM _R O ^e	SM _P H ^e	SM _P O ^e	TF _R H ^e	TF _R O ^e	TF _P H ^e	TF _P O ^e
1632	TG(15:0/18:1/16:0)	C ₅₂ H ₉₈ O ₆	[M+Na] ⁺	841.72556	841.72563	-0.08	5.4E+06	1.9E+07	6.8E+06	3.9E+06		2.7E+07	1.4E+07	9.0E+06
1633	TG(16:0/16:0/17:0)	C ₅₂ H ₁₀₀ O ₆	[M+Na] ⁺	843.74121	843.74131	-0.11		6.1E+06		3.4E-01		9.0E+06		4.5E+06
1634	SM(d18:1/26:0)	C ₄₉ H ₁₀₀ N ₂ O ₆ P	[M+H] ⁺	844.73918	844.73917	0.01						3.7E+06		
1635	Glycyrrhizinate	C ₄₂ H ₆₂ O ₁₆	[M+Na] ⁺	845.39301	845.39337	-0.42	5.7E+06		5.6E+06					
1636	TG(16:0/14:0/18:0)	C ₅₁ H ₉₈ O ₆	[M+K] ⁺	845.69950	845.69959	-0.11					6.1E+06			
1637	TG(16:0/16:1/18:3)	C ₅₃ H ₉₄ O ₆	[M+Na] ⁺	849.69426	849.69415	0.13		5.8E+06	3.6E+06			7.1E+06		
1638	TG(16:1/16:1)/17:2)	C ₅₂ H ₉₂ O ₆	[M+K] ⁺	851.65255	851.65274	-0.22	4.7E+06		6.3E+06					
1639	TG(16:0/16:0/18:3)	C ₅₃ H ₉₆ O ₆	[M+Na] ⁺	851.70991	851.70990	0.01	5.3E+06	1.7E+07	7.3E+06	2.8E+06		1.9E+07	9.6E+06	6.4E+06
1640	TG(16:0/16:1/17:2)	C ₅₂ H ₉₄ O ₆	[M+K] ⁺	853.66820	853.66815	0.06					3.3E+06			
1641	TG(16:0/16:0/18:2)	C ₅₃ H ₉₈ O ₆	[M+Na] ⁺	853.72556	853.72549	0.09	1.1E+07	2.8E+07	9.9E+06	4.1E+06			1.4E+07	9.7E+06
1642	TG(16:0/16:0/18:1)	C ₅₃ H ₁₀₀ O ₆	[M+Na] ⁺	855.74121	855.74112	0.11		2.5E+07	5.6E+06	3.5E+06			1.2E+07	8.3E+06
1643	TG(15:0/18:1/16:0)	C ₅₂ H ₉₈ O ₆	[M+K] ⁺	857.69950	857.69949	0.01					8.0E+06			
1644	TG(16:0/16:0/18:0)	C ₅₃ H ₁₀₂ O ₆	[M+Na] ⁺	857.75686	857.75688	-0.02		4.4E+06				5.7E+06		3.6E+06
1645	TG(16:0/16:0/17:0)	C ₅₂ H ₁₀₀ O ₆	[M+K] ⁺	859.71515	859.71496	0.22	1.7E+07		2.0E+07		4.1E+06			
1646	TG(16:1/16:1/18:3)	C ₅₃ H ₉₂ O ₆	[M+K] ⁺	863.65255	863.65276	-0.24			4.2E+06				3.4E+06	
1647	TG(15:0/16:0/20:4)	C ₅₄ H ₉₆ O ₆	[M+Na] ⁺	863.70991	863.70987	0.05		4.8E+06	4.3E+06			5.9E+06	4.3E+06	3.1E+06
1648	LacCer(d18:0/16:0)	C ₄₆ H ₈₉ NO ₁₃	[M+H] ⁺	864.64067	864.64020	0.54	3.6E+06							
1649	PG(20:4/22:6)	C ₄₈ H ₇₅ O ₁₀ P	[M+Na] ⁺	865.49901	865.49892	0.10	2.1E+07		2.4E+07		2.1E+07		2.8E+07	
1650	TG(15:0/16:0/20:3)	C ₅₄ H ₉₈ O ₆	[M+Na] ⁺	865.72556	865.72540	0.18	3.3E+06	1.0E+07	5.7E+06	1.8E+06		1.3E+07	7.4E+06	5.5E+06
1651	TG(15:0/16:0/20:2)	C ₅₄ H ₁₀₀ O ₆	[M+Na] ⁺	867.74121	867.74110	0.13	4.3E+06	1.3E+07	6.7E+06	2.5E+06		1.7E+07	9.1E+06	5.9E+06
1652	TG(16:0/16:1/19:0)	C ₅₄ H ₁₀₂ O ₆	[M+Na] ⁺	869.75686	869.75678	0.09		7.6E+06	4.0E+06	1.7E+06		1.1E+07	4.4E+06	5.6E+06
1653	Pheophytin a	C ₅₅ H ₇₄ N ₄ O ₅	[M+H] ⁺	871.57320	871.57339	-0.22				1.8E+06				2.8E+06
1654	TG(16:0/16:0/19:0)	C ₅₄ H ₁₀₄ O ₆	[M+Na] ⁺	871.77251	871.77223	0.32						3.5E+06		
1655	PG(O-20:0/22:6)	C ₄₈ H ₈₅ O ₉ P	[M+K] ⁺	875.55628	875.55613	0.17						4.4E+06		
1656	TG(16:0/16:0/20:5)	C ₅₅ H ₉₆ O ₆	[M+Na] ⁺	875.70991	875.71004	-0.15			3.8E+06			5.5E+06		3.0E+06
1657	Ditetradecanoyl-sn-glycero-3-phospho-lyso tetradecanoylglycerol	C ₄₈ H ₉₃ O ₁₁ P	[M+H] ⁺	877.65283	877.65309	-0.30	5.7E+06	3.5E+06						
1658	TG(16:0/17:2/18:3)	C ₅₄ H ₉₄ O ₆	[M+K] ⁺	877.66820	877.66819	0.01			3.8E+06					
1659	TG(16:0/16:0/20:4)	C ₅₅ H ₉₈ O ₆	[M+Na] ⁺	877.72556	877.72559	-0.03	4.6E+06	1.2E+07	7.7E+06	2.4E+06		1.2E+07	7.9E+06	5.5E+06

ESI(+) FT-ICR MS														
No.	Plausible Compound ^a	Molecular formula (M)	Ion	Theor m/z ^b	Exp. m/z ^c	Δ ppm _d	SM _R H ^e	SM _R O ^e	SM _P H ^e	SM _P O ^e	TF _R H ^e	TF _R O ^e	TF _P H ^e	TF _P O ^e
1660	TG(16:0/16:0/20:3)	C ₅₅ H ₁₀₀ O ₆	[M+Na] ⁺	879.74121	879.74115	0.07	8.5E+06	1.8E+07	8.7E+06	3.1E+06		1.9E+07	8.2E+06	6.7E+06
1661	Thevetin B	C ₄₂ H ₆₆ O ₁₈	[M+Na] ⁺	881.41414	881.41436	-0.25	3.6E+06							
1662	TG(15:0/16:0/20:3)	C ₅₄ H ₉₈ O ₆	[M+K] ⁺	881.69950	881.69960	-0.11					3.4E+06			
1663	TG(16:0/16:0/20:2)	C ₅₅ H ₁₀₂ O ₆	[M+Na] ⁺	881.75686	881.75692	-0.07	1.3E+07	2.1E+07	6.6E+06	2.8E+06		2.2E+07	9.5E+06	6.6E+06
1664	TG(15:0/16:0/20:2)	C ₅₄ H ₁₀₀ O ₆	[M+K] ⁺	883.71515	883.71506	0.10					4.4E+06			
1665	TG(16:0/16:0/20:1)	C ₅₅ H ₁₀₄ O ₆	[M+Na] ⁺	883.77251	883.77254	-0.03	1.1E+07	9.5E+06				7.4E+06		3.5E+06
1666	TG(16:0/16:1/19:0)	C ₅₄ H ₁₀₂ O ₆	[M+K] ⁺	885.73080	885.73116	-0.41					4.9E+06			
1667	TG(16:0/16:0/20:0)	C ₅₅ H ₁₀₆ O ₆	[M+Na] ⁺	885.78816	885.78809	0.08						3.3E+06		
1668	TG(16:0/16:0/19:0)	C ₅₄ H ₁₀₄ O ₆	[M+K] ⁺	887.74645	887.74642	0.04	5.1E+06		5.5E+06				5.5E+06	
1669	TG(16:0/17:0/20:5)	C ₅₆ H ₉₈ O ₆	[M+Na] ⁺	889.72556	889.72590	-0.38						3.4E+06		
1670	TG(16:0/16:0/20:5)	C ₅₅ H ₉₆ O ₆	[M+K] ⁺	891.68385	891.68415	-0.34	5.1E+06							
1671	TG(16:0/17:0/20:4)	C ₅₆ H ₁₀₀ O ₆	[M+Na] ⁺	891.74121	891.74122	-0.01		3.7E+06				4.6E+06		
1672	TG(16:0/16:0/20:4)	C ₅₅ H ₉₈ O ₆	[M+K] ⁺	893.69950	893.69981	-0.35					4.8E+06			
1673	TG(16:0/16:0/20:3)	C ₅₅ H ₁₀₀ O ₆	[M+K] ⁺	895.71515	895.71526	-0.12					4.6E+06			
1674	TG(16:0/17:0/20:2)	C ₅₆ H ₁₀₄ O ₆	[M+Na] ⁺	895.77251	895.77245	0.07						4.6E+06		
1675	TG(16:0/16:0/20:2)	C ₅₅ H ₁₀₂ O ₆	[M+K] ⁺	897.73080	897.73087	-0.08					4.7E+06			
1676	TG(16:0/16:1/21:0)	C ₅₆ H ₁₀₆ O ₆	[M+Na] ⁺	897.78816	897.78820	-0.04						3.7E+06		
1677	TG(16:0/16:0/20:1)	C ₅₅ H ₁₀₄ O ₆	[M+K] ⁺	899.74645	899.74642	0.03				3.1E+06				
1678	TG(18:3/18:0/18:3)	C ₅₇ H ₉₈ O ₆	[M+Na] ⁺	901.72556	901.72543	0.15		1.0E+07	5.8E+06			7.0E+06	4.1E+06	3.6E+06
1679	TG(16:0/16:0/20:0)	C ₅₅ H ₁₀₆ O ₆	[M+K] ⁺	901.76210	901.76215	-0.05	5.7E+06		4.3E+06				4.8E+06	
1680	LacCer(d18:0/16:0)	C ₄₆ H ₈₉ NO ₁₃	[M+K] ⁺	902.59655	902.59596	0.66			3.3E+06					
1681	PC(22:0/22:0)	C ₅₂ H ₁₀₄ NO ₈ P	[M+H] ⁺	902.75723	902.75671	0.58	4.6E+06							
1682	TG(18:2/18:1/18:2)	C ₅₇ H ₁₀₀ O ₆	[M+Na] ⁺	903.74121	903.74118	0.03	3.5E+06	1.2E+07	6.5E+06			7.6E+06	5.0E+06	4.2E+06
1683	TG(17:2/18:1/18:2)	C ₅₆ H ₉₈ O ₆	[M+K] ⁺	905.69950	905.69969	-0.21			3.5E+06					
1684	TG(18:2/16:0/20:2)	C ₅₇ H ₁₀₂ O ₆	[M+Na] ⁺	905.75686	905.75680	0.07		1.2E+07	6.3E+06	1.7E+06		8.9E+06	5.4E+06	3.8E+06
1685	TG(17:2/18:1/18:1)	C ₅₆ H ₁₀₀ O ₆	[M+K] ⁺	907.71515	907.71528	-0.14	4.7E+06		7.7E+06					
1686	TG(18:1/18:1/18:1)	C ₅₇ H ₁₀₄ O ₆	[M+Na] ⁺	907.77251	907.77250	0.02	8.0E+06	1.5E+07	6.0E+06	1.8E+06		1.2E+07	5.3E+06	3.9E+06
1687	TG(17:2/18:0/18:1)	C ₅₆ H ₁₀₂ O ₆	[M+K] ⁺	909.73080	909.73080	0.00	6.8E+06		9.6E+06					
1688	TG(18:1/18:0/18:1)	C ₅₇ H ₁₀₆ O ₆	[M+Na] ⁺	909.78816	909.78808	0.09		6.5E+06				6.3E+06		3.2E+06

ESI(+) FT-ICR MS														
No.	Plausible Compound ^a	Molecular formula (M)	Ion	Theor m/z ^b	Exp. m/z ^c	Δ ppm _d	SM _R H ^e	SM _R O ^e	SM _P H ^e	SM _P O ^e	TF _R H ^e	TF _R O ^e	TF _P H ^e	TF _P O ^e
1689	TG(17:2/18:0/18:0)	C ₅₆ H ₁₀₄ O ₆	[M+K] ⁺	911.74645	911.74636	0.10	7.3E+06	6.2E+06	1.0E+07					
1690	TG(18:0/18:0/18:1)	C ₅₇ H ₁₀₈ O ₆	[M+Na] ⁺	911.80381	911.80355	0.29	6.7E+06	5.6E+06				4.4E+06		
1691	TG(17:1/18:0/18:0)	C ₅₆ H ₁₀₆ O ₆	[M+K] ⁺	913.76210	913.76204	0.06	6.5E+06		6.9E+06				6.2E+06	
1692	TG(18:0/18:0/18:0)	C ₅₇ H ₁₁₀ O ₆	[M+Na] ⁺	913.81946	913.81951	-0.05		3.4E+06				3.4E+06		
1693	TG(17:0/18:0/18:0)	C ₅₆ H ₁₀₈ O ₆	[M+K] ⁺	915.77775	915.77753	0.24	4.1E+06		3.8E+06				4.5E+06	
1694	Galabiosylceramide (d18:1/20:0)	C ₅₀ H ₉₅ NO ₁₃	[M+H] ⁺	918.68762	918.68774	-0.13	4.2E+06							
1695	TG(18:2/18:1/18:2)	C ₅₇ H ₁₀₀ O ₆	[M+K] ⁺	919.71515	919.71498	0.19					5.0E+06			
1696	TG(18:2/18:2/19:0)	C ₅₈ H ₁₀₄ O ₆	[M+Na] ⁺	919.77251	919.77250	0.01						3.0E+06		
1697	TG(18:2/16:0/20:2)	C ₅₇ H ₁₀₂ O ₆	[M+K] ⁺	921.73080	921.73074	0.07					4.1E+06			
1698	TG(18:1/16:0/20:2)	C ₅₇ H ₁₀₄ O ₆	[M+K] ⁺	923.74645	923.74630	0.16					4.2E+06			
1699	TG(18:0/18:0/18:2)	C ₅₇ H ₁₀₆ O ₆	[M+K] ⁺	925.76210	925.76225	-0.16			1.0E+07				7.4E+06	
1700	TG(16:1/18:0/21:0)	C ₅₈ H ₁₁₀ O ₆	[M+Na] ⁺	925.81946	925.81954	-0.08		3.3E+06				4.3E+06		
1701	TG(18:0/18:0/18:1)	C ₅₇ H ₁₀₈ O ₆	[M+K] ⁺	927.77775	927.77789	-0.15			8.2E+06					
1702	TG(16:0/17:0/22:0)	C ₅₈ H ₁₁₂ O ₆	[M+Na] ⁺	927.83511	927.83508	0.03						3.3E+06		
1703	TG(18:0/18:0/18:0)	C ₅₇ H ₁₁₀ O ₆	[M+K] ⁺	929.79340	929.79350	-0.11			4.3E+06					
1704	TG(17:0/17:2/21:0)	C ₅₈ H ₁₀₈ O ₆	[M+K] ⁺	939.77775	939.77802	-0.29	3.5E+06		4.1E+06				3.9E+06	
1705	TG(18:0/18:0/20:1)	C ₅₉ H ₁₁₂ O ₆	[M+Na] ⁺	939.83511	939.83521	-0.10						4.2E+06		
1706	TG(18:0/18:1/19:0)	C ₅₈ H ₁₁₀ O ₆	[M+K] ⁺	941.79340	941.79354	-0.14	4.0E+06		5.6E+06					
1707	TG(16:0/18:0/21:0)	C ₅₈ H ₁₁₂ O ₆	[M+K] ⁺	943.80905	943.80902	0.03			4.3E+06				3.9E+06	
1708	TG(18:2/18:2/20:0)	C ₅₉ H ₁₀₆ O ₆	[M+K] ⁺	949.76210	949.76176	0.36			3.4E+06					
1709	TG(18:1/18:1/20:1)	C ₅₉ H ₁₀₈ O ₆	[M+K] ⁺	951.77775	951.77772	0.03							3.8E+06	
1710	TG(18:0/18:2/21:0)	C ₆₀ H ₁₁₂ O ₆	[M+Na] ⁺	951.83511	951.83469	0.44						3.4E+06		
1711	Thyroxine glucuronide	C ₂₁ H ₁₉ I ₄ NO ₁₀	[M+H] ⁺	953.72606	953.72642	-0.37			2.8E+06					
1712	TG(18:2/19:0/19:0)	C ₅₉ H ₁₁₀ O ₆	[M+K] ⁺	953.79340	953.79320	0.21	5.0E+06		6.5E+06				5.2E+06	
1713	TG(18:1/19:0/19:0)	C ₅₉ H ₁₁₂ O ₆	[M+K] ⁺	955.80905	955.80873	0.34			8.4E+06					
1714	TG(19:0/19:0/19:0)	C ₆₀ H ₁₁₆ O ₆	[M+Na] ⁺	955.86641	955.86635	0.07						2.9E+06		
1715	TG(16:0/20:0/20:0)	C ₅₉ H ₁₁₄ O ₆	[M+K] ⁺	957.82470	957.82449	0.22	4.1E+06		5.2E+06				4.7E+06	
1716	PC(22:0/24:1)	C ₅₄ H ₁₀₆ NO ₈ P	[M+K] ⁺	966.72877	966.72945	-0.71							3.9E+06	
1717	TG(18:0/18:2/21:0)	C ₆₀ H ₁₁₂ O ₆	[M+K] ⁺	967.80905	967.80881	0.25			5.2E+06				4.5E+06	

ESI(+) FT-ICR MS													
No.	Plausible Compound ^a	Molecular formula (M)	Ion	Theo r m/z ^b	Exp . m/z ^c	Δ ppm ^d	SM _R H ^e	SM _R O ^e	SM _P H ^e	SM _P O ^e	TF _R H ^e	TF _R O ^e	TF _P H ^e TF _P O ^e
1718	PC(22:0/24:0)	C ₅₄ H ₁₀₈ NO ₈ P	[M+K] ⁺	968.74442	968.74507	-0.68							3.4E+06
1719	TG(18:0/20:1/20:1)	C ₆₁ H ₁₁₄ O ₆	[M+K] ⁺	981.82470	981.82486	-0.16			4.7E+06				4.4E+06
1720	Tomatine	C ₅₀ H ₈₃ NO ₂₁	[M+H] ⁺	1034.55304	1034.55351	-0.46			9.7E+06				3.6E+06
1721	Acetyl-sphingosine-tetraacetyl-GalCer(d18:1/h24:0)	C ₅₈ H ₁₀₃ NO ₁₄	[M+H] ⁺	1038.74513	1038.74449	0.62							3.5E+06

^a Cer: Ceramide; GalCer: Galactosylceramide; GlcCer: Glucosylceramide; LacCer: Lactosylceramide; MG: Monoacylglycerol; DG: Diacylglycerol; TG: Triacylglycerol; MGDG: Monoacyldiacylglycerol; PA: Phosphatidic acid; PC: Phosphatidylcholine; PE: Phosphatidylethanolamine; PG: Glycerophospholipids; PI: Phosphatidylinositol; PS: Phosphatidylserine;; SM: Sphingomyelin

^b Theor. stands for calculated exact mass to charge ratio

^c Exp. stands for experimental m/z value

^d The error expressed in parts per million (ppm)

^e SM_RH and SM_RO stand for hydroalcoholic and organic portions of red San Marzano extracts, respectively; SM_PH and SM_PO stand for hydroalcoholic and organic portions of pink San Marzano extracts, respectively. TF_RH and TF_RO stand for hydroalcoholic and organic portions of red Torpedino di Fondi extracts, respectively; TF_PH and TF_PO stand for hydroalcoholic and organic portions of pink Torpedino di Fondi extracts, respectively.

Table S3: Comprehensive list of metabolites detected in hydroalcoholic and organic fractions of pink and red San Marzano (SM) and Torpedino di Fondi (TF) extracts using ESI(-) FT-ICR MS.

ESI(-) FTICR-MS														
No.	Plausible compound ^a	Molecular formula (M)	Ion	Theor. m/z ^b	Exp. m/z ^c	Δppm ^d	SM _R H ^e	SM _R O ^e	SM _P H ^e	SM _P O ^e	TF _R H ^e	TF _R O ^e	TF _P H ^e	TF _P O ^e
1	L-Serine	C ₃ H ₇ NO ₃	[M-H]-	104.03532	104.03540	0.77	1.0E+06	5.6E+06		1.2E+06	1.4E+06		3.2E+06	2.3E+06
2	2-Furoic acid	C ₅ H ₄ O ₃	[M-H]-	111.00877	111.00886	0.81	1.9E+06		1.5E+06				1.4E+07	
3	Oxopentenoic acid	C ₅ H ₆ O ₃	[M-H]-	113.02442	113.02448	0.53							1.4E+06	
4	Maleic acid	C ₄ H ₄ O ₄	[M-H]-	115.00368	115.00376	0.70							2.4E+06	
5	Glutarate semialdehyde	C ₅ H ₈ O ₃	[M-H]-	115.04007	115.04012	0.43		1.3E+06						
6	L-Valine	C ₅ H ₁₁ NO ₂	[M-H]-	116.07170	116.07177	0.60		1.4E+06						
7	Succinic acid	C ₄ H ₆ O ₄	[M-H]-	117.01933	117.01941	0.68		1.1E+06					4.0E+06	
8	D-Threonine	C ₄ H ₉ NO ₃	[M-H]-	118.05097	118.05105	0.68		2.0E+06					1.6E+06	
9	D-Erythrose	C ₄ H ₈ O ₄	[M-H]-	119.03498	119.03508	0.84	2.8E+06				1.3E+06		5.0E+06	
10	o-Hydroxybenzaldehyde	C ₇ H ₆ O ₂	[M-H]-	121.02950	121.02957	0.58		1.1E+06						
11	2-Oxo-4E-hexenoic acid	C ₆ H ₈ O ₃	[M-H]-	127.04007	127.04017	0.79							1.2E+06	
12	Pyroglutamic acid	C ₅ H ₇ NO ₃	[M-H]-	128.03532	128.03540	0.62	1.4E+07	3.2E+07	1.5E+06	5.5E+06	1.1E+07	1.2E+07	3.9E+07	1.5E+07
13	2-Oxoglutarate semialdehyde	C ₅ H ₆ O ₄	[M-H]-	129.01933	129.01942	0.70							1.5E+06	
14	3-Oxohexanoic acid	C ₆ H ₁₀ O ₃	[M-H]-	129.05572	129.05580	0.62		1.4E+06						1.1E+06
15	Octanol	C ₈ H ₁₈ O	[M-H]-	129.12849	129.12858	0.70							1.0E+06	
16	L-Leucine	C ₆ H ₁₃ NO ₂	[M-H]-	130.08735	130.08743	0.61		3.2E+06					1.1E+06	
17	Glutaric acid	C ₅ H ₈ O ₄	[M-H]-	131.03498	131.03506	0.61		1.2E+06					3.4E+06	
18	L-Asparagine	C ₄ H ₈ N ₂ O ₃	[M-H]-	131.04622	131.04630	0.61							3.3E+06	
19	L-Aspartic acid	C ₄ H ₇ NO ₄	[M-H]-	132.03023	132.03032	0.68	1.0E+07	1.3E+06	3.0E+06		2.1E+06		3.0E+07	

ESI(-) FTICR-MS														
No.	Plausible compound ^a	Molecular formula (M)	Ion	Theor. m/z ^b	Exp. m/z ^c	Δppm ^d	SM _R H ^e	SM _R O ^e	SM _P H ^e	SM _P O ^e	TF _R H ^e	TF _R O ^e	TF _P H ^e	TF _P O ^e
20	Malic acid	C ₄ H ₆ O ₅	[M-H]-	133.01425	133.01434	0.68	3.5E+06			5.9E+06		1.4E+06		3.0E+07
21	Threonic acid	C ₄ H ₈ O ₅	[M-H]-	135.02990	135.03000	0.74								1.8E+06
22	4-Nitroaniline	C ₆ H ₆ N ₂ O ₂	[M-H]-	137.03565	137.03573	0.58		7.2E+06		1.9E+06	2.5E+06	2.7E+06	1.6E+07	4.2E+06
23	Dimethylmaleic acid	C ₆ H ₈ O ₄	[M-H]-	143.03498	143.03507	0.63	2.0E+06	1.5E+06			1.3E+06		3.9E+06	1.3E+06
24	Oxoglutaric acid	C ₅ H ₆ O ₅	[M-H]-	145.01425	145.01435	0.69								1.3E+06
25	Methylglutaric acid	C ₆ H ₁₀ O ₄	[M-H]-	145.05063	145.05072	0.62	2.2E+06	9.9E+06		4.8E+06	2.5E+06	5.5E+06	1.5E+07	1.0E+07
26	L-Glutamine	C ₅ H ₁₀ N ₂ O ₃	[M-H]-	145.06187	145.06197	0.69	2.9E+06		2.0E+06		1.3E+06		1.9E+07	
27	L-Glutamic acid	C ₅ H ₉ NO ₄	[M-H]-	146.04588	146.04597	0.62	2.8E+07	1.6E+06	5.7E+06		3.4E+06		6.8E+07	1.8E+06
28	Hydroxyglutarate	C ₅ H ₈ O ₅	[M-H]-	147.02990	147.02998	0.54								2.8E+06
29	2-Deoxyribonic acid	C ₅ H ₁₀ O ₅	[M-H]-	149.04555	149.04565	0.67	1.4E+06							2.5E+06
30	Diethylphosphoric acid	C ₄ H ₁₁ O ₄ P	[M-H]-	153.03222	153.03230	0.52							1.0E+06	
31	L-Histidine	C ₆ H ₉ N ₃ O ₂	[M-H]-	154.06220	154.06228	0.52							1.6E+06	
32	Isopropylmaleic acid	C ₇ H ₁₀ O ₄	[M-H]-	157.05063	157.05071	0.51		2.4E+06					2.0E+06	1.4E+06
33	Oxooctanoic acid	C ₈ H ₁₄ O ₃	[M-H]-	157.08702	157.08709	0.45		4.0E+06		1.5E+06		1.6E+06		2.3E+06
34	Methyl-octanoic acid	C ₉ H ₁₈ O ₂	[M-H]-	157.12340	157.12348	0.51		1.4E+06			1.1E+06	1.1E+06	1.7E+06	1.3E+06
35	Pimelic acid	C ₇ H ₁₂ O ₄	[M-H]-	159.06628	159.06637	0.57		4.7E+06		2.0E+06	1.9E+06	2.1E+06	4.3E+06	4.4E+06
36	N-Methyl-L-glutamic acid	C ₆ H ₁₁ NO ₄	[M-H]-	160.06153	160.06159	0.37							1.1E+06	
37	Hydroxyadipic acid	C ₆ H ₁₀ O ₅	[M-H]-	161.04555	161.04563	0.50	4.2E+06	1.6E+06	1.5E+06		2.5E+06		1.1E+07	1.8E+06
38	L-Phenylalanine	C ₉ H ₁₁ NO ₂	[M-H]-	164.07170	164.07178	0.49		2.1E+06		1.3E+06	1.2E+06		1.4E+06	1.7E+06
39	Formylsalicylic acid	C ₈ H ₆ O ₄	[M-H]-	165.01933	165.01937	0.24							1.8E+06	
40	D-Ribonic acid	C ₅ H ₁₀ O ₆	[M-H]-	165.04046	165.04054	0.48					1.2E+06		4.8E+06	

ESI(-) FTICR-MS														
No.	Plausible compound ^a	Molecular formula (M)	Ion	Theor. m/z ^b	Exp. m/z ^c	Δppm ^d	SM _R H ^e	SM _R O ^e	SM _P H ^e	SM _P O ^e	TF _R H ^e	TF _R O ^e	TF _P H ^e	TF _P O ^e
41	Uric acid	C ₅ H ₄ N ₄ O ₃	[M-H]-	167.02106	167.02115	0.54								1.2E+06
42	N-Cyclopropylammelide	C ₆ H ₈ N ₄ O ₂	[M-H]-	167.05745	167.05731	-0.84								1.3E+06
43	2-Octenedioic acid	C ₈ H ₁₂ O ₄	[M-H]-	171.06628	171.06637	0.53		1.3E+06					1.4E+06	1.4E+06
44	Oxo-nonanoic acid	C ₉ H ₁₆ O ₃	[M-H]-	171.10267	171.10276	0.53		3.1E+06		1.4E+06		1.3E+06	1.4E+06	1.9E+06
45	Decanoic acid	C ₁₀ H ₂₀ O ₂	[M-H]-	171.13905	171.13914	0.53		1.2E+06					1.1E+06	1.2E+06
46	N-Acetyl-L-leucine	C ₈ H ₁₅ NO ₃	[M-H]-	172.09792	172.09799	0.41		1.0E+06						
47	Dehydroascorbic acid	C ₆ H ₆ O ₆	[M-H]-	173.00916	173.00924	0.46	4.3E+06		1.4E+06		2.4E+06		2.6E+07	
48	Shikimic acid	C ₇ H ₁₀ O ₅	[M-H]-	173.04555	173.04564	0.52					1.6E+06		3.2E+06	1.4E+06
49	2-Propylglutaric acid	C ₈ H ₁₄ O ₄	[M-H]-	173.08193	173.08200	0.40	1.5E+06	5.7E+06		3.0E+06	1.8E+06	3.9E+06	4.8E+06	6.3E+06
50	Hydroxy pelargonic acid	C ₉ H ₁₈ O ₃	[M-H]-	173.11832	173.11840	0.46		1.1E+06					1.3E+06	1.2E+06
51	N-Formyl-L-glutamic acid	C ₆ H ₉ NO ₅	[M-H]-	174.04080	174.04084	0.23		1.0E+06					9.7E+05	
52	Argininic acid	C ₆ H ₁₃ N ₃ O ₃	[M-H]-	174.08841	174.08850	0.52		7.0E+06		3.2E+06	1.6E+06	5.1E+06	2.3E+06	4.6E+06
53	Ascorbic acid	C ₆ H ₈ O ₆	[M-H]-	175.02481	175.02488	0.40	3.0E+06		1.5E+06				1.0E+07	
54	Isopropylmalic acid	C ₇ H ₁₂ O ₅	[M-H]-	175.06120	175.06126	0.34							1.5E+06	
55	Hexose-1,5-lactone	C ₆ H ₁₀ O ₆	[M-H]-	177.04046	177.04053	0.40							1.6E+06	
56	Fluorenone	C ₁₃ H ₈ O	[M-H]-	179.05024	179.05020	-0.22	5.8E+06						7.1E+06	
57	Aldohexose	C ₆ H ₁₂ O ₆	[M-H]-	179.05611	179.05619	0.45	2.8E+08	3.8E+06	7.5E+07	3.9E+06	1.1E+08	3.3E+06	4.4E+08	8.8E+06
58	Amino-piperidinecarboxylic acid	C ₆ H ₁₂ N ₂ O ₂	[M+Cl]-	179.05928	179.05942	0.78	2.9E+06							
59	L-Tyrosine	C ₉ H ₁₁ NO ₃	[M-H]-	180.06662	180.06669	0.39		3.1E+06		2.3E+06		3.8E+06		3.9E+06
60	Mannitol	C ₆ H ₁₄ O ₆	[M-H]-	181.07176	181.07183	0.39		1.4E+06			1.1E+06	1.6E+06	1.1E+06	1.4E+06
61	Tartaric acid	C ₄ H ₆ O ₆	[M+Cl]-	184.98584	184.98574	-0.54							1.0E+06	

ESI(-) FTICR-MS														
No.	Plausible compound ^a	Molecular formula (M)	Ion	Theor. m/z ^b	Exp. m/z ^c	Δppm ^d	SM _R H ^e	SM _R O ^e	SM _P H ^e	SM _P O ^e	TF _R H ^e	TF _R O ^e	TF _P H ^e	TF _P O ^e
62	Oxodecanoic acid	C ₁₀ H ₁₈ O ₃	[M-H]-	185.11832	185.11837	0.27		1.3E+06						1.2E+06
63	2-(Acetamidomethylene)	C ₇ H ₉ NO ₅	[M-H]-	186.04080	186.04087	0.38							9.2E+05	
64	Oxo-amino-nonanoic acid	C ₉ H ₁₇ NO ₃	[M-H]-	186.11357	186.11364	0.38		2.8E+06		1.8E+06	1.6E+06	1.9E+06	1.3E+06	2.1E+06
65	Nonanedioic acid	C ₉ H ₁₆ O ₄	[M-H]-	187.09758	187.09766	0.43		4.9E+06		2.9E+06	2.3E+06	3.5E+06	7.0E+06	4.6E+06
66	Hydroxy-decanoic acid	C ₁₀ H ₂₀ O ₃	[M-H]-	187.13397	187.13402	0.27								1.2E+06
67	N-Acetyl-L-glutamic acid	C ₇ H ₁₁ NO ₅	[M-H]-	188.05645	188.05652	0.37							1.5E+06	
68	Oxalosuccinic acid	C ₆ H ₆ O ₇	[M-H]-	189.00408	189.00415	0.37							1.3E+06	
69	Dehydroquinic acid	C ₇ H ₁₀ O ₆	[M-H]-	189.04046	189.04052	0.32							1.3E+06	
70	Hydroxysuberic acid	C ₈ H ₁₄ O ₅	[M-H]-	189.07685	189.07695	0.53							1.2E+06	9.9E+05
71	Citric acid	C ₆ H ₈ O ₇	[M-H]-	191.01973	191.01980	0.37	1.5E+08		1.2E+08		4.8E+07		4.5E+08	1.6E+06
72	Quinic acid	C ₇ H ₁₂ O ₆	[M-H]-	191.05611	191.05618	0.37					2.7E+06		2.0E+07	
73	D-Glucuronic acid	C ₆ H ₁₀ O ₇	[M-H]-	193.03538	193.03545	0.36	9.7E+06				2.9E+06		3.5E+06	
74	Galactonic acid	C ₆ H ₁₂ O ₇	[M-H]-	195.05103	195.05108	0.26	2.6E+07	2.1E+06	1.1E+06	1.3E+06	2.1E+06	8.4E+07	8.8E+06	
75	Dodecenoic acid	C ₁₂ H ₂₂ O ₂	[M-H]-	197.15470	197.15475	0.25							1.2E+06	
76	L-Threonine O-3-phosphate	C ₄ H ₁₀ NO ₆ P	[M-H]-	198.01730	198.01736	0.30	1.8E+06							
77	Dihydroclavaminic acid	C ₈ H ₁₂ N ₂ O ₄	[M-H]-	199.07243	199.07253	0.50								9.3E+05
78	Decenedioic acid	C ₁₀ H ₁₆ O ₄	[M-H]-	199.09758	199.09762	0.20		1.1E+06						
79	Hydroxy-undecenoic acid	C ₁₁ H ₂₀ O ₃	[M-H]-	199.13397	199.13405	0.40		1.1E+06						1.1E+06
80	Lauric acid	C ₁₂ H ₂₄ O ₂	[M-H]-	199.17035	199.17043	0.40		4.0E+06		2.2E+06	1.4E+06	4.2E+06	1.3E+07	3.9E+06
81	Diethyl oxalpropionic acid	C ₉ H ₁₄ O ₅	[M-H]-	201.07685	201.07692	0.35		1.9E+06		1.2E+06		1.3E+06	1.6E+06	1.8E+06
82	Sebacic acid	C ₁₀ H ₁₈ O ₄	[M-H]-	201.11323	201.11330	0.35		4.4E+06		2.6E+06	2.9E+06	2.5E+06	3.3E+06	6.1E+06

ESI(-) FTICR-MS														
No.	Plausible compound ^a	Molecular formula (M)	Ion	Theor. m/z ^b	Exp. m/z ^c	Δppm ^d	SM _R H ^e	SM _R O ^e	SM _P H ^e	SM _P O ^e	TF _R H ^e	TF _R O ^e	TF _P H ^e	TF _P O ^e
83	L-Tryptophan	C ₁₁ H ₁₂ N ₂ O ₂	[M-H]-	203.08260	203.08266	0.30		2.0E+06		1.3E+06		3.2E+06		2.2E+06
84	Diethyl-methyl-hydroxysuccinate	C ₉ H ₁₆ O ₅	[M-H]-	203.09250	203.09253	0.15							9.9E+05	
85	Acetyl-hydroxy-L-lysine	C ₈ H ₁₆ N ₂ O ₄	[M-H]-	203.10373	203.10379	0.30		1.2E+06						
86	Methylcitric acid	C ₇ H ₁₀ O ₇	[M-H]-	205.03538	205.03543	0.24	1.0E+07		1.5E+06		1.6E+06		1.9E+07	
87	Naphthalenesulfonic acid	C ₁₀ H ₈ O ₃ S	[M-H]-	207.01214	207.01221	0.34		1.6E+06				1.4E+06	4.4E+06	2.8E+06
88	beta-D-Sedoheptulopyranose	C ₇ H ₁₄ O ₇	[M-H]-	209.06668	209.06672	0.19	7.7E+06				1.3E+06		2.9E+06	
89	Oxo-dodecenoic acid	C ₁₂ H ₂₀ O ₃	[M-H]-	211.13397	211.13400	0.14		1.1E+06						
90	Methyl-dodecenoic acid	C ₁₃ H ₂₄ O ₂	[M-H]-	211.17035	211.17041	0.28		1.6E+06					1.5E+06	1.4E+06
91	Oxododecanoic acid	C ₁₂ H ₂₂ O ₃	[M-H]-	213.14962	213.14971	0.42		1.2E+06						1.0E+06
92	Methyl-dodecanoic acid	C ₁₃ H ₂₆ O ₂	[M-H]-	213.18600	213.18607	0.33	1.7E+06	9.6E+06		4.9E+06	3.2E+06	1.1E+07	2.5E+07	1.0E+07
93	N-Nonanoylglycine	C ₁₁ H ₂₁ NO ₃	[M-H]-	214.14487	214.14495	0.37		1.5E+06						1.0E+06
94	Bergapten	C ₁₂ H ₈ O ₄	[M-H]-	215.03498	215.03507	0.42							3.3E+06	
95	Hydroxy-dodecanoic acid	C ₁₂ H ₂₄ O ₃	[M-H]-	215.16527	215.16541	0.65								1.1E+06
96	Hydroxydecanedioic acid	C ₁₀ H ₁₈ O ₅	[M-H]-	217.10815	217.10823	0.37		1.2E+06					1.0E+06	1.2E+06
97	O-Succinylhomoserine	C ₈ H ₁₃ NO ₆	[M-H]-	218.06701	218.06707	0.28							1.0E+06	
98	Dihydroxykynurenate	C ₁₀ H ₇ NO ₅	[M-H]-	220.02515	220.02516	0.05			1.7E+06		1.2E+06			
99	Acetyl-glucose	C ₈ H ₁₄ O ₇	[M-H]-	221.06668	221.06673	0.23	1.9E+06		1.2E+06				1.4E+06	
100	Tetradecadienoic acid	C ₁₄ H ₂₄ O ₂	[M-H]-	223.17035	223.17041	0.27							1.0E+06	
101	Myristoleic acid	C ₁₄ H ₂₆ O ₂	[M-H]-	225.18600	225.18607	0.31	4.1E+06	3.2E+07		1.6E+07	1.1E+07	4.1E+07	4.0E+07	3.8E+07
102	Dihydroxy-diepoxy-undecadienol	C ₁₁ H ₁₆ O ₅	[M-H]-	227.09250	227.09256	0.26		1.2E+06					1.5E+06	1.5E+06
103	Myristic acid	C ₁₄ H ₂₈ O ₂	[M-H]-	227.20165	227.20172	0.31	1.2E+07	9.9E+07	2.0E+06	4.4E+07	3.0E+07	9.3E+07	2.0E+08	9.7E+07

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104	D-Arabinose 5-phosphate	C ₅ H ₁₁ O ₈ P	[M-H]-	229.01188	229.01188	0.00							1.3E+06	
105	Dodecanedioic acid	C ₁₂ H ₂₂ O ₄	[M-H]-	229.14453	229.14461	0.35		1.6E+06					1.4E+06	1.2E+06
106	N-Acetyl-D-glucosamine	C ₈ H ₁₅ NO ₇	[M-H]-	236.07758	236.07760	0.08							1.1E+06	
107	Deoxy-manno-octulosonate	C ₈ H ₁₄ O ₈	[M-H]-	237.06159	237.06164	0.21							3.0E+06	
108	Campherene-diol	C ₁₅ H ₂₆ O ₂	[M-H]-	237.18600	237.18603	0.13		1.3E+06					1.3E+06	
109	Carboxy-methyl-propyl-furanpropanoic acid	C ₁₂ H ₁₆ O ₅	[M-H]-	239.09250	239.09256	0.25							1.2E+06	
110	Tridecenyl acetate	C ₁₅ H ₂₈ O ₂	[M-H]-	239.20165	239.20172	0.29	8.6E+06	6.7E+07	1.3E+06	3.2E+07	2.2E+07	8.3E+07	7.3E+07	7.7E+07
111	Myo-Inositol phosphate	C ₆ H ₁₁ O ₈ P	[M-H]-	241.01188	241.01206	0.75							4.4E+06	
112	Keto myristic acid	C ₁₄ H ₂₆ O ₃	[M-H]-	241.18092	241.18100	0.33		1.9E+06						2.2E+06
113	Methyl myristic acid	C ₁₅ H ₃₀ O ₂	[M-H]-	241.21730	241.21737	0.29	2.4E+07	2.1E+08	4.1E+06	8.3E+07	5.8E+07	1.8E+08	3.1E+08	1.9E+08
114	Uridine	C ₉ H ₁₂ N ₂ O ₆	[M-H]-	243.06226	243.06229	0.12			1.1E+06				2.1E+06	
115	Methyl-dodecanedioic acid	C ₁₃ H ₂₄ O ₄	[M-H]-	243.16018	243.16025	0.29		1.8E+06				1.5E+06	1.7E+06	1.5E+06
116	2-Hydroxymyristic acid	C ₁₄ H ₂₈ O ₃	[M-H]-	243.19657	243.19664	0.29		1.8E+06			1.2E+06		1.3E+06	2.0E+06
117	Glycerophosphoglycerol	C ₆ H ₁₅ O ₈ P	[M-H]-	245.04318	245.04331	0.53	3.0E+06		1.4E+06				2.7E+06	
118	Hydroxyindoleacetyl glycine	C ₁₂ H ₁₂ N ₂ O ₄	[M-H]-	247.07243	247.07231	-0.49		1.2E+06						1.3E+06
119	Hexadecatrienoic acid	C ₁₆ H ₂₆ O ₂	[M-H]-	249.18600	249.18604	0.16		1.2E+06						
120	Muramic acid	C ₉ H ₁₇ NO ₇	[M-H]-	250.09323	250.09329	0.24			6.3E+06				1.3E+06	
121	Hexadecynoic acid	C ₁₆ H ₂₈ O ₂	[M-H]-	251.20165	251.20171	0.24		1.4E+07		6.4E+06	4.1E+06	1.6E+07	1.1E+07	1.6E+07
122	N-(Aminobutyryl)-L-histidine	C ₁₁ H ₁₈ N ₄ O ₃	[M-H]-	253.13061	253.13063	0.08		1.6E+06					1.1E+06	
123	Palmitoleic acid	C ₁₆ H ₃₀ O ₂	[M-H]-	253.21730	253.21736	0.24	8.6E+07	7.1E+08	1.1E+07	3.2E+08	2.1E+08	7.7E+08	5.6E+08	7.6E+08
124	Oxo-pentadecanoic acid	C ₁₅ H ₂₈ O ₃	[M-H]-	255.19657	255.19664	0.27		4.5E+06		2.2E+06		3.7E+06	3.5E+06	4.4E+06

[illegible]

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No.	Plausible compound ^a	Molecular formula (M)	Ion	Theor . m/z ^b	Exp. m/z ^c	Δ ppm ^d	SM _R H ^e	SM _R O ^e	SM _P H ^e	SM _P O ^e	TF _R H ^e	TF _R O ^e	TF _P H ^e	TF _P O ^e
146	(L-Glutamyl)-glutamine	C ₁₀ H ₁₇ N ₃ O ₆	[M-H]-	274.10446	274.10451	0.18	1.5E+06							
147	Gamma Glutamylglutamic acid	C ₁₀ H ₁₆ N ₂ O ₇	[M-H]-	275.08847	275.08855	0.29	1.3E+06							
148	Linolenic acid	C ₁₈ H ₃₀ O ₂	[M-H]-	277.21730	277.21736	0.22	2.3E+06	1.1E+07		4.9E+06	5.2E+06	1.3E+07	1.2E+07	1.1E+07
149	Linoleic acid	C ₁₈ H ₃₂ O ₂	[M-H]-	279.23295	279.23301	0.21	3.2E+07	1.7E+08	4.1E+06	7.9E+07	7.6E+07	2.0E+08	1.7E+08	1.9E+08
150	Xylobiose	C ₁₀ H ₁₈ O ₉	[M-H]-	281.08781	281.08784	0.11							1.5E+06	
151	Dihydrophaseic acid	C ₁₅ H ₂₂ O ₅	[M-H]-	281.13945	281.13951	0.21							1.1E+06	
152	Dehydrolupanine	C ₁₅ H ₂₂ N ₂ O	[M+Cl]-	281.14261	281.14283	0.78							1.4E+06	
153	Hydroxy-heptadecadienoic acid	C ₁₇ H ₃₀ O ₃	[M-H]-	281.21222	281.21228	0.21		2.2E+06					2.7E+06	2.4E+06
154	Oleic acid	C ₁₈ H ₃₄ O ₂	[M-H]-	281.24860	281.24866	0.21	8.1E+07	5.0E+08	1.0E+07	2.2E+08	1.8E+08	5.5E+08	5.4E+08	5.1E+08
155	Guanosine	C ₁₀ H ₁₃ N ₅ O ₅	[M-H]-	282.08439	282.08443	0.14	2.1E+06						1.3E+06	
156	Dihydrosantonin	C ₁₅ H ₂₀ O ₃	[M+Cl]-	283.11065	283.11055	-0.35							2.5E+06	1.7E+06
157	Dihexyl maleic acid	C ₁₆ H ₂₈ O ₄	[M-H]-	283.19148	283.19155	0.25		1.8E+06					1.6E+06	1.4E+06
158	Methoxy-hexadecenoic acid	C ₁₇ H ₃₂ O ₃	[M-H]-	283.22787	283.22793	0.21		4.6E+06		2.0E+06	2.4E+06	4.1E+06	3.9E+06	5.2E+06
159	Stearic acid	C ₁₈ H ₃₆ O ₂	[M-H]-	283.26425	283.26431	0.21	6.1E+07	3.3E+08	2.8E+07	1.6E+08	1.0E+08	2.5E+08	4.3E+08	3.5E+08
160	Abscisic alcohol	C ₁₅ H ₂₂ O ₃	[M+Cl]-	285.12630	285.12618	-0.42		2.5E+06				1.5E+06		1.7E+06
161	Hydroxy-oxo-hexadecanoic acid	C ₁₆ H ₃₀ O ₄	[M-H]-	285.20713	285.20720	0.25		3.4E+06		1.4E+06	1.6E+06	2.3E+06	3.2E+06	3.2E+06
162	Hydroxy-palmitic acid methyl ester	C ₁₇ H ₃₄ O ₃	[M-H]-	285.24352	285.24358	0.21	1.6E+06	4.8E+06		2.1E+06	1.7E+06	5.0E+06	4.3E+06	5.1E+06
163	Dihydrokaempferol	C ₁₅ H ₁₂ O ₆	[M-H]-	287.05611	287.05619	0.28							1.2E+06	
164	Dihydroxy-palmitic acid	C ₁₆ H ₃₂ O ₄	[M-H]-	287.22278	287.22285	0.24		7.7E+06					3.2E+06	1.8E+06
165	Sedoheptulose-phosphate	C ₇ H ₁₅ O ₁₀ P	[M-H]-	289.03301	289.03305	0.14	2.8E+06							
166	Malonyl-D-tryptophan	C ₁₄ H ₁₄ N ₂ O ₅	[M-H]-	289.08300	289.08305	0.17	1.7E+06							

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167	Anhydro-N-acetylneuraminic acid	C ₁₁ H ₁₇ NO ₈	[M-H]-	290.08814	290.08819	0.17	6.1E+07	1.4E+06	1.9E+07		9.2E+06		1.6E+07	
168	Hydroxysteroid	C ₁₉ H ₃₂ O ₂	[M-H]-	291.23295	291.23301	0.21		3.6E+06			9.0E+05		1.3E+06	1.7E+06
169	N-Glycosyl-L-asparagine	C ₁₀ H ₁₈ N ₂ O ₈	[M-H]-	293.09904	293.09908	0.14	1.9E+07		5.6E+06		2.8E+06		3.5E+06	
170	Hydroxylinolenic acid	C ₁₈ H ₃₀ O ₃	[M-H]-	293.21222	293.21228	0.20		6.7E+06			1.5E+06	2.6E+06	2.1E+06	2.9E+06
171	Methyl-octadecadienoic acid	C ₁₉ H ₃₄ O ₂	[M-H]-	293.24860	293.24866	0.20	2.6E+06	2.4E+07		5.3E+06	4.4E+06	1.3E+07	9.1E+06	1.2E+07
172	Tocopheronic acid	C ₁₆ H ₂₄ O ₅	[M-H]-	295.15510	295.15515	0.17		1.8E+06						
173	Ropinirole	C ₁₆ H ₂₄ N ₂ O	[M+Cl]-	295.15826	295.15851	0.85		1.2E+06						
174	Methanoxyethano-isolongifol-ene	C ₁₈ H ₂₈ O	[M-H]-	295.18342	295.18350	0.27		6.2E+06					1.9E+06	
175	Deoxymethynolide	C ₁₇ H ₂₈ O ₄	[M-H]-	295.19148	295.19152	0.14		1.4E+06						
176	Hydroxy-linoleic acid	C ₁₈ H ₃₂ O ₃	[M-H]-	295.22787	295.22793	0.20	2.4E+06	2.3E+07		4.3E+06	2.9E+06	8.9E+06	7.2E+06	1.1E+07
177	Methyl-octadecenoic acid	C ₁₉ H ₃₆ O ₂	[M-H]-	295.26425	295.26431	0.20	4.1E+06	6.3E+07		1.0E+07	8.6E+06	2.7E+07	2.5E+07	2.4E+07
178	N-oxododecanoyl-homoserine lactone	C ₁₆ H ₂₇ NO ₄	[M-H]-	296.18673	296.18685	0.41		1.6E+06						
179	Tetranor-oxo-dihydroxy-prostenoic acid	C ₁₆ H ₂₆ O ₅	[M-H]-	297.17075	297.17077	0.07		7.2E+06					1.6E+06	
180	Heptadecenedioic acid	C ₁₇ H ₃₀ O ₄	[M-H]-	297.20713	297.20718	0.17		1.7E+06						
181	Keto stearic acid	C ₁₈ H ₃₄ O ₃	[M-H]-	297.24352	297.24357	0.17	2.8E+06	4.1E+07		8.4E+06	4.8E+06	1.4E+07	1.2E+07	1.8E+07
182	Methyl stearic acid	C ₁₉ H ₃₈ O ₂	[M-H]-	297.27990	297.27996	0.20	3.8E+06	5.6E+07		7.9E+06	6.5E+06	1.8E+07	2.2E+07	1.9E+07
183	Pentadecanoylglycine	C ₁₇ H ₃₃ NO ₃	[M-H]-	298.23877	298.23882	0.17		4.3E+06		1.1E+06				1.6E+06
184	[(Dihydro-hydroxy-naphthalenyl)thio]- oxopropanoic acid	C ₁₃ H ₁₂ O ₄ S	[M+Cl]-	299.01503	299.01503	0.00	1.7E+06		1.4E+06					
185	Salidroside	C ₁₄ H ₂₀ O ₇	[M-H]-	299.11363	299.11368	0.17		1.3E+06						
186	Tetranor-trihydroxy-prostenoic acid	C ₁₆ H ₂₈ O ₅	[M-H]-	299.18640	299.18647	0.23		7.3E+06		1.7E+06		1.9E+06	2.1E+06	4.3E+06

ESI(-) FTICR-MS														
No.	Plausible compound ^a	Molecular formula (M)	Ion	Theor. m/z ^b	Exp. m/z ^c	Δppm ^d	SM _R H ^e	SM _R O ^e	SM _P H ^e	SM _P O ^e	TF _R H ^e	TF _R O ^e	TF _P H ^e	TF _P O ^e
187	Retinoic acid	C ₂₀ H ₂₈ O ₂	[M-H]-	299.20165	299.20172	0.23		1.9E+06						
188	Tetradecenoyl-glycerol	C ₁₇ H ₃₂ O ₄	[M-H]-	299.22278	299.22283	0.17		1.6E+07		1.4E+06	1.4E+06		4.5E+06	2.5E+06
189	Hydroxystearic acid	C ₁₈ H ₃₆ O ₃	[M-H]-	299.25917	299.25923	0.20	2.4E+06	2.1E+07		3.0E+06	3.1E+06	6.8E+06	6.5E+06	6.7E+06
190	N-Acetyl-D-Glucosamine 6-Phosphate	C ₈ H ₁₆ NO ₉ P	[M-H]-	300.04899	300.04903	0.13	2.4E+06		1.5E+06				1.7E+06	
191	Xanthoxic acid	C ₁₅ H ₂₂ O ₄	[M+Cl]-	301.12121	301.12108	-0.43	1.2E+06	6.2E+06			1.2E+06			
192	Tributyryn	C ₁₅ H ₂₆ O ₆	[M-H]-	301.16566	301.16573	0.23		4.7E+06					1.8E+06	1.2E+06
193	Hydroxy-hexadecan-dioic acid	C ₁₆ H ₃₀ O ₅	[M-H]-	301.20205	301.20208	0.10		4.0E+06					1.7E+06	
194	Eicosapentaenoic acid	C ₂₀ H ₃₀ O ₂	[M-H]-	301.21730	301.21734	0.13		1.8E+06						
195	MG(0:0/14:0/0:0)	C ₁₇ H ₃₄ O ₄	[M-H]-	301.23843	301.23847	0.13		1.9E+07					4.8E+06	
196	Adenosine	C ₁₀ H ₁₃ N ₅ O ₄	[M+Cl]-	302.06616	302.06631	0.50	1.8E+06							
197	Nopaline	C ₁₁ H ₂₀ N ₄ O ₆	[M-H]-	303.13101	303.13104	0.10		2.5E+06						
198	Trihydroxy palmitic acid	C ₁₆ H ₃₂ O ₅	[M-H]-	303.21770	303.21775	0.16		2.4E+06					1.3E+06	
199	Arachidonic acid	C ₂₀ H ₃₂ O ₂	[M-H]-	303.23295	303.23301	0.20		5.6E+06			1.5E+06		2.5E+06	3.0E+06
200	20:3(5Z,13Z,16Z)	C ₂₀ H ₃₄ O ₂	[M-H]-	305.24860	305.24866	0.20	3.7E+06	4.1E+07		9.0E+06	8.5E+06	2.4E+07	1.7E+07	2.1E+07
201	Glutathione	C ₁₀ H ₁₇ N ₃ O ₆ S	[M-H]-	306.07653	306.07655	0.07	2.2E+06						5.9E+06	
202	Amino-hexadecanoic acid	C ₁₆ H ₃₃ NO ₂	[M+Cl]-	306.22053	306.22056	0.10		2.2E+06						
203	Obscurine	C ₁₇ H ₂₄ N ₂ O	[M+Cl]-	307.15826	307.15850	0.78		3.6E+06					2.2E+06	
204	Eicosadienoic acid	C ₂₀ H ₃₆ O ₂	[M-H]-	307.26425	307.26431	0.20	7.9E+06	9.5E+07		1.8E+07	1.8E+07	4.7E+07	4.0E+07	4.1E+07
205	N-Acetyl-a-neuraminic acid	C ₁₁ H ₁₉ NO ₉	[M-H]-	308.09870	308.09875	0.16	9.2E+07	6.0E+06	2.5E+07		1.2E+07		2.3E+08	
206	Sauroxine	C ₁₇ H ₂₆ N ₂ O	[M+Cl]-	309.17392	309.17418	0.84	2.7E+07	9.7E+08	1.3E+07	4.9E+06	6.8E+06	1.2E+07	2.8E+08	2.2E+07
207	Epoxy-oxo-octadecenoic acid	C ₁₈ H ₃₀ O ₄	[M-H]-	309.20713	309.20722	0.29		2.8E+06						1.7E+06

ESI(-) FTICR-MS

No.	Plausible compound ^a	Molecular formula (M)	Ion	Theor . m/z ^b	Exp. m/z ^c	Δ ppm ^d	SM _R H ^e	SM _R O ^e	SM _P H ^e	SM _P O ^e	TF _R H ^e	TF _R O ^e	TF _P H ^e	TF _P O ^e
208	Octadecenyl acetate	C ₂₀ H ₃₈ O ₂	[M-H]-	309.27990	309.27996	0.19	5.9E+06	8.5E+07		1.3E+07	1.3E+07	3.4E+07	3.7E+07	3.0E+07
209	Alanyltryptophan	C ₁₄ H ₁₇ N ₃ O ₃	[M+Cl]-	310.09639	310.09665	0.84	2.1E+06							
210	O-(beta-D-Xylopyranosyl)-D-glucopyranose	C ₁₁ H ₂₀ O ₁₀	[M-H]-	311.09837	311.09841	0.13							2.9E+06	
211	Octadecadiynoic acid	C ₁₈ H ₂₈ O ₂	[M+Cl]-	311.17833	311.17838	0.16		1.3E+07					4.0E+06	
212	Dihydroxy-octadecadienoic acid	C ₁₈ H ₃₂ O ₄	[M-H]-	311.22278	311.22285	0.22		1.0E+07		1.4E+06			3.4E+06	2.9E+06
213	Oxo-nonadecanoic acid	C ₁₉ H ₃₆ O ₃	[M-H]-	311.25917	311.25920	0.10		1.4E+06						
214	Arachidic acid	C ₂₀ H ₄₀ O ₂	[M-H]-	311.29555	311.29561	0.19	6.2E+06	8.6E+07	1.4E+06	1.3E+07	1.2E+07	2.7E+07	3.8E+07	2.7E+07
215	Lycomarasmine B	C ₉ H ₁₅ N ₃ O ₇	[M+Cl]-	312.06040	312.06039	-0.03	1.7E+06		1.1E+06					
216	Oxo-retinoate	C ₂₀ H ₂₅ O ₃	[M-H]-	312.17309	312.17324	0.48							2.4E+06	
217	N-palmitoyl glycine	C ₁₈ H ₃₅ NO ₃	[M-H]-	312.25442	312.25447	0.16		3.8E+06						
218	5'-Phosphoribosyl-N-formylglycinamide	C ₈ H ₁₅ N ₂ O ₉ P	[M-H]-	313.04424	313.04438	0.45	1.8E+06							
219	Dihydroxy-octadecenoic acid	C ₁₈ H ₃₄ O ₄	[M-H]-	313.23843	313.23850	0.22	2.0E+06	1.8E+07		2.3E+06	1.6E+06	4.0E+06	7.0E+06	5.0E+06
220	Hydroxy-nonadecanoic acid	C ₁₉ H ₃₈ O ₃	[M-H]-	313.27482	313.27485	0.10		2.1E+06					1.3E+06	
221	Belladine	C ₁₉ H ₂₅ NO ₃	[M-H]-	314.17617	314.17630	0.41		1.7E+06						
222	Dihydroxy-octadecanoic acid	C ₁₈ H ₃₆ O ₄	[M-H]-	315.25408	315.25416	0.25		6.6E+06					2.6E+06	1.3E+06
223	Methyladenosine	C ₁₁ H ₁₅ N ₅ O ₄	[M+Cl]-	316.08181	316.08198	0.54	1.9E+06							
224	Hexahydroxyflavone	C ₁₅ H ₁₀ O ₈	[M-H]-	317.03029	317.03037	0.25	3.3E+06		1.3E+06					
225	Methylinosine	C ₁₁ H ₁₄ N ₄ O ₅	[M+Cl]-	317.06582	317.06603	0.66	1.8E+06							
226	Menthyl O-beta-D-glucoside	C ₁₆ H ₃₀ O ₆	[M-H]-	317.19696	317.19703	0.22		1.6E+06						
227	Cucumopine	C ₁₁ H ₁₃ N ₃ O ₆	[M+Cl]-	318.04984	318.05004	0.63			1.6E+06					
228	Ethyl-androstane-diol	C ₂₁ H ₃₆ O ₂	[M-H]-	319.26425	319.26432	0.22		2.4E+06					1.5E+06	

ESI(-) FTICR-MS														
No.	Plausible compound ^a	Molecular formula (M)	Ion	Theor. m/z ^b	Exp. m/z ^c	Δppm ^d	SM _R H ^e	SM _R O ^e	SM _P H ^e	SM _P O ^e	TF _R H ^e	TF _R O ^e	TF _P H ^e	TF _P O ^e
229	Gingerol	C ₁₉ H ₃₀ O ₄	[M-H]-	321.20713	321.20717	0.12		1.6E+06						
230	Methyl-androstanetriol	C ₂₀ H ₃₄ O ₃	[M-H]-	321.24352	321.24356	0.12		2.1E+06						
231	Methyl-eicosadienoic acid	C ₂₁ H ₃₈ O ₂	[M-H]-	321.27990	321.27998	0.25		5.0E+06		1.5E+06			2.3E+06	2.2E+06
232	Cytidine 3'-phosphate	C ₉ H ₁₄ N ₃ O ₈ P	[M-H]-	322.04457	322.04462	0.16	7.2E+06		2.0E+06				2.0E+06	
233	Orotidine	C ₁₀ H ₁₂ N ₂ O ₈	[M+Cl]-	323.02877	323.02862	-0.46	5.1E+07		1.4E+07		2.9E+06		1.3E+07	
234	Fructofuranose dianhydride	C ₁₂ H ₂₀ O ₁₀	[M-H]-	323.09837	323.09841	0.12							3.4E+06	
235	Flabellidine	C ₁₈ H ₂₈ N ₂ O	[M+Cl]-	323.18957	323.18980	0.71		3.3E+06					2.3E+06	
236	Hydroxy-eicosadienoic acid	C ₂₀ H ₃₆ O ₃	[M-H]-	323.25917	323.25921	0.12		3.0E+06					1.3E+06	
237	Heneicosenoic acid	C ₂₁ H ₄₀ O ₂	[M-H]-	323.29555	323.29562	0.22		7.6E+06		1.9E+06	2.0E+06	4.4E+06	4.0E+06	3.1E+06
238	N-Glycoloyl-neuramate	C ₁₁ H ₁₉ NO ₁₀	[M-H]-	324.09362	324.09364	0.06	1.2E+06						1.7E+06	
239	O-beta-D-Glucosyl-coumarate	C ₁₅ H ₁₈ O ₈	[M-H]-	325.09289	325.09292	0.09	4.1E+06		1.5E+06				3.5E+06	
240	2-O-Fucopyranosyl-galactose	C ₁₂ H ₂₂ O ₁₀	[M-H]-	325.11402	325.11407	0.15							2.3E+07	
241	Oxo-eicosanoic acid	C ₂₀ H ₃₈ O ₃	[M-H]-	325.27482	325.27488	0.18		5.2E+06					2.2E+06	2.0E+06
242	Heneicosanoic acid	C ₂₁ H ₄₂ O ₂	[M-H]-	325.31120	325.31127	0.22	2.5E+06	2.5E+07		4.0E+06	4.4E+06	8.6E+06	1.3E+07	8.4E+06
243	N-palmitoyl alanine	C ₁₉ H ₃₇ NO ₃	[M-H]-	326.27007	326.27011	0.12		2.2E+06						
244	Steryl sulfate	C ₁₇ H ₂₈ O ₄ S	[M-H]-	327.16355	327.16359	0.12		2.6E+06					2.4E+06	
245	Difluoro-hexadecanoic acid	C ₁₆ H ₃₀ F ₂ O ₂	[M+Cl]-	327.19079	327.19106	0.83	1.8E+06	2.3E+07	2.3E+06				7.3E+06	2.1E+06
246	Trihydroxy-octadecadienoic acid	C ₁₈ H ₃₂ O ₅	[M-H]-	327.21770	327.21777	0.21		4.7E+06		1.4E+06		1.8E+06	1.9E+06	3.1E+06
247	MG(0:0/16:1(9Z)/0:0)	C ₁₉ H ₃₆ O ₄	[M-H]-	327.25408	327.25414	0.18	2.0E+06	2.0E+07		2.2E+06	2.0E+06	4.5E+06	7.1E+06	4.6E+06
248	Hydroxy-eicosanoic acid	C ₂₀ H ₄₀ O ₃	[M-H]-	327.29047	327.29051	0.12		3.0E+06					1.7E+06	
249	MG(0:0/16:0/0:0)	C ₁₉ H ₃₈ O ₄	[M-H]-	329.26973	329.26979	0.18		6.2E+06					2.3E+06	

ESI(-) FTICR-MS														
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250	Pentahydroxy-methoxyflavone	C ₁₆ H ₁₂ O ₈	[M-H]-	331.04594	331.04601	0.21	3.6E+07			4.0E+06		1.5E+06		
251	Hydroxytridecane-tricarboxylic acid	C ₁₆ H ₂₈ O ₇	[M-H]-	331.17623	331.17630	0.21		1.4E+06						
252	Hydroxy-dihydroxy-stearic acid	C ₁₈ H ₃₆ O ₅	[M-H]-	331.24900	331.24905	0.15		1.0E+07					5.2E+06	
253	Adrenic acid	C ₂₂ H ₃₆ O ₂	[M-H]-	331.26425	331.26432	0.21	1.9E+06	1.3E+07		2.7E+06	2.1E+06	5.5E+06	5.5E+06	4.9E+06
254	Albendazole sulfone	C ₁₂ H ₁₅ N ₃ O ₄ S	[M+Cl]-	332.04773	332.04743	-0.90	2.6E+06						1.4E+06	
255	Galactosyl-sn-glycerol-phosphate	C ₉ H ₁₉ O ₁₁ P	[M-H]-	333.05922	333.05927	0.15	1.8E+06		1.4E+06				7.9E+06	
256	Docosatrienoic acid	C ₂₂ H ₃₈ O ₂	[M-H]-	333.27990	333.27996	0.18	2.9E+06	2.4E+07		5.3E+06	5.9E+06	1.5E+07	1.2E+07	1.2E+07
257	Acetyl-beta-D-glucosaminy-l-asparagine	C ₁₂ H ₂₁ N ₃ O ₈	[M-H]-	334.12559	334.12563	0.12	2.6E+06		2.2E+06		1.9E+06		3.7E+06	
258	Palmitoylethanolamide	C ₁₈ H ₃₇ NO ₂	[M+Cl]-	334.25183	334.25188	0.15		1.6E+06						
259	Eicosadienyl acetate	C ₂₂ H ₄₀ O ₂	[M-H]-	335.29555	335.29560	0.15	2.1E+06	1.7E+07		3.4E+06	4.0E+06	8.7E+06	9.0E+06	7.6E+06
260	Deoxy-hydroxymethylcytidine-phosphate	C ₁₀ H ₁₆ N ₃ O ₈ P	[M-H]-	336.06022	336.06040	0.54	1.3E+06							
261	Shiromodiol diacetate	C ₁₉ H ₃₀ O ₅	[M-H]-	337.20205	337.20206	0.03		1.2E+06						
262	Docosenoic acid	C ₂₂ H ₄₂ O ₂	[M-H]-	337.31120	337.31126	0.18	2.4E+06	2.0E+07		3.7E+06	4.1E+06	9.8E+06	1.0E+07	7.6E+06
263	N-oleoyl glycine	C ₂₀ H ₃₇ NO ₃	[M-H]-	338.27007	338.27012	0.15		1.3E+06						
264	Ketolactose	C ₁₂ H ₂₀ O ₁₁	[M-H]-	339.09328	339.09335	0.21							1.6E+06	
265	Methyl-fucopyranosyl-galactoside	C ₁₃ H ₂₄ O ₁₀	[M-H]-	339.12967	339.12972	0.15					1.6E+06		5.9E+06	
266	Hydroperoxy-eicosadienoic acid	C ₂₀ H ₃₆ O ₄	[M-H]-	339.25408	339.25412	0.12		4.8E+06					2.0E+06	
267	Oxo-heneicosanoic acid	C ₂₁ H ₄₀ O ₃	[M-H]-	339.29047	339.29055	0.24		3.4E+06						
268	Methyl-heneicosanoic acid	C ₂₂ H ₄₄ O ₂	[M-H]-	339.32685	339.32691	0.18	5.8E+06	6.3E+07	1.2E+06	9.9E+06	1.7E+07	2.4E+07	3.2E+07	2.1E+07
269	Glucosaminy-l-myo-inositol	C ₁₂ H ₂₃ NO ₁₀	[M-H]-	340.12492	340.12493	0.03							2.0E+06	
270	Stearoylglycine	C ₂₀ H ₃₉ NO ₃	[M-H]-	340.28572	340.28577	0.15		1.9E+06						

ESI(-) FTICR-MS

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271	Caffeic acid 3-glucoside	C ₁₅ H ₁₈ O ₉	[M-H]-	341.08781	341.08784	0.09	1.2E+07		3.7E+06		1.8E+06		4.4E+06	
272	Glucosyl-glucose	C ₁₂ H ₂₂ O ₁₁	[M-H]-	341.10894	341.10899	0.15	3.7E+06	2.3E+07	2.9E+06	3.6E+06	4.4E+06	5.7E+06	1.1E+07	6.6E+06
273	Methyl-dihydroxy-oxo-octadecenoate	C ₁₉ H ₃₄ O ₅	[M-H]-	341.23335	341.23342	0.21		3.1E+06			1.8E+06		1.5E+06	
274	Eicosanedioic acid	C ₂₀ H ₃₈ O ₄	[M-H]-	341.26973	341.26979	0.18	2.1E+06	1.6E+07		2.9E+06	5.4E+06	5.8E+06	7.0E+06	7.5E+06
275	Hydroxy-heneicosanoic acid	C ₂₁ H ₄₂ O ₃	[M-H]-	341.30612	341.30619	0.21		1.5E+06						
276	N-palmitoyl serine	C ₁₉ H ₃₇ NO ₄	[M-H]-	342.26498	342.26502	0.12		2.5E+06						
277	Maltitol	C ₁₂ H ₂₄ O ₁₁	[M-H]-	343.12459	343.12462	0.09							1.7E+06	
278	Affinisine	C ₂₀ H ₂₄ N ₂ O	[M+Cl]-	343.15826	343.15850	0.70					1.9E+06		2.2E+06	
279	Dihydroxy-methoxy-octadecenoic acid	C ₁₉ H ₃₆ O ₅	[M-H]-	343.24900	343.24907	0.20		4.4E+07			1.5E+07		2.2E+07	1.3E+06
280	Sulfadoxine	C ₁₂ H ₁₄ N ₄ O ₄ S	[M+Cl]-	345.04298	345.04266	-0.93	4.1E+06	2.2E+06			1.5E+06			
281	Dihydroxy-Octadecanedioic acid	C ₁₈ H ₃₄ O ₆	[M-H]-	345.22826	345.22829	0.09		2.1E+06						
282	Deoxyguanosine 5'-monophosphate	C ₁₀ H ₁₄ N ₅ O ₇ P	[M-H]-	346.05581	346.05585	0.12	1.3E+08	1.7E+06	3.3E+07		1.5E+07		2.6E+07	
283	Leonuridine	C ₁₅ H ₂₄ O ₉	[M-H]-	347.13476	347.13479	0.09		6.7E+06			3.3E+06		2.1E+06	
284	Hydroxy-(methoxymethyl)-methyl-androstan- one	C ₂₂ H ₃₆ O ₃	[M-H]-	347.25917	347.25922	0.14		2.4E+06						1.5E+06
285	Dihydropteroic acid	C ₁₄ H ₁₄ N ₆ O ₃	[M+Cl]-	349.08214	349.08205	-0.26	3.0E+06							
286	MG(18:3/0:0/0:0)	C ₂₁ H ₃₆ O ₄	[M-H]-	351.25408	351.25408	0.00		1.7E+06						
287	Tricosenoic acid	C ₂₃ H ₄₄ O ₂	[M-H]-	351.32685	351.32692	0.20		5.9E+06			1.8E+06		3.2E+06	2.3E+06
288	N-palmitoyl proline	C ₂₁ H ₃₉ NO ₃	[M-H]-	352.28572	352.28588	0.45							1.4E+06	
289	Chlorogenic acid	C ₁₆ H ₁₈ O ₉	[M-H]-	353.08781	353.08786	0.14	1.1E+07	1.8E+06	1.4E+07		3.9E+06		1.1E+08	
290	MG(0:0/18:2/0:0)	C ₂₁ H ₃₈ O ₄	[M-H]-	353.26973	353.26980	0.20		6.8E+06			1.8E+06		2.3E+06	1.6E+06

ESI(-) FTICR-MS														
No.	Plausible compound ^a	Molecular formula (M)	Ion	Theor. m/z ^b	Exp. m/z ^c	Δppm ^d	SM _R H ^e	SM _R O ^e	SM _P H ^e	SM _P O ^e	TF _R H ^e	TF _R O ^e	TF _P H ^e	TF _P O ^e
291	Oxo-docosanoic acid	C ₂₂ H ₄₂ O ₃	[M-H]-	353.30612	353.30619	0.20		3.6E+06				1.9E+06	1.6E+06	1.7E+06
292	Methyl-docosanoic acid	C ₂₃ H ₄₆ O ₂	[M-H]-	353.34250	353.34256	0.17	6.1E+06	6.4E+07	1.4E+06	9.9E+06	1.8E+07	2.6E+07	3.3E+07	2.2E+07
293	N-palmitoyl valine	C ₂₁ H ₄₁ NO ₃	[M-H]-	354.30137	354.30143	0.17		1.7E+06						
294	Feruloyl-glucose	C ₁₆ H ₂₀ O ₉	[M-H]-	355.10346	355.10350	0.11	2.2E+06		1.4E+06				1.8E+06	
295	Prostaglandin F1alpha	C ₂₀ H ₃₆ O ₅	[M-H]-	355.24900	355.24907	0.20		3.6E+06				1.8E+06		2.5E+06
296	MG(0:0/18:1/0:0)	C ₂₁ H ₄₀ O ₄	[M-H]-	355.28538	355.28545	0.20	1.9E+06	1.1E+07		2.2E+06	3.5E+06	3.9E+06	4.4E+06	5.2E+06
297	Hydroxydocosanoic acid	C ₂₂ H ₄₄ O ₃	[M-H]-	355.32177	355.32183	0.17		9.0E+06			3.0E+06	4.4E+06	3.9E+06	2.9E+06
298	N-palmitoyl threonine	C ₂₀ H ₃₉ NO ₄	[M-H]-	356.28063	356.28070	0.20		1.8E+06						
299	Epideoxyloganic acid	C ₁₆ H ₂₄ O ₉	[M-H]-	359.13476	359.13477	0.03	3.1E+06						1.8E+06	
300	Cholanediol	C ₂₄ H ₄₂ O ₂	[M-H]-	361.31120	361.31123	0.08		1.9E+06					1.5E+06	
301	Methylthiopropyl-desulfoglucosinolate	C ₁₁ H ₂₁ NO ₆ S ₂	[M+Cl]-	362.05043	362.05076	0.91	1.0E+07		2.1E+06		3.5E+06		4.0E+06	
302	Guanosine monophosphate	C ₁₀ H ₁₄ N ₅ O ₈ P	[M-H]-	362.05072	362.05077	0.14	1.0E+07		1.7E+06		3.5E+06		4.0E+06	
303	Docosenyl acetate	C ₂₄ H ₄₆ O ₂	[M-H]-	365.34250	365.34256	0.16	1.1E+07	2.4E+07		4.3E+06	7.3E+06	1.0E+07	1.3E+07	8.6E+06
304	Tetracosanoic acid	C ₂₄ H ₄₈ O ₂	[M-H]-	367.35815	367.35821	0.16	8.9E+07	2.1E+08	3.9E+06	3.5E+07	6.9E+07	8.9E+07	1.3E+08	7.4E+07
305	N-palmitoyl leucine	C ₂₂ H ₄₃ NO ₃	[M-H]-	368.31702	368.31711	0.24		1.7E+06						
306	Heptahydroxyflavone	C ₁₅ H ₁₀ O ₉	[M+Cl]-	369.00188	369.00187	-0.03	1.5E+06							
307	Methoxytaxifolin	C ₁₆ H ₁₄ O ₈	[M+Cl]-	369.03827	369.03814	-0.35			1.6E+06					
308	Fluoro-hydroxyandrostene-trione	C ₁₉ H ₂₃ FO ₄	[M+Cl]-	369.12744	369.12734	-0.27		2.8E+06	1.5E+06					
309	Amylose	C ₁₄ H ₂₆ O ₁₁	[M-H]-	369.14024	369.14029	0.14							1.8E+06	
310	Keto-prostaglandin F1	C ₂₀ H ₃₄ O ₆	[M-H]-	369.22826	369.22828	0.05		1.6E+06						
311	Docosanedioic acid	C ₂₂ H ₄₂ O ₄	[M-H]-	369.30103	369.30109	0.16	1.1E+07	1.9E+07		3.9E+06	5.3E+06	7.5E+06	8.4E+06	1.1E+07

ESI(-) FTICR-MS														
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312	Hydroxy-tricosanoic acid	C ₂₃ H ₄₆ O ₃	[M-H]-	369.33742	369.33746	0.11	5.1E+06	8.8E+06			3.6E+06		4.4E+06	3.0E+06
313	N-stearoyl serine	C ₂₁ H ₄₁ NO ₄	[M-H]-	370.29628	370.29636	0.22		2.7E+06						
314	Deoxyoleandolide	C ₂₀ H ₃₆ O ₆	[M-H]-	371.24391	371.24397	0.16	7.9E+06	9.3E+06			9.5E+06	2.1E+06	4.8E+06	2.9E+06
315	Urate D-ribonucleotide	C ₁₀ H ₁₃ N ₄ O ₁₀ P	[M-H]-	379.02965	379.02937	-0.74							1.6E+06	
316	Diphyllin	C ₂₁ H ₁₆ O ₇	[M-H]-	379.08233	379.08269	0.95		2.1E+07				2.7E+06	5.8E+06	
317	MG(0:0/20:3/0:0)	C ₂₃ H ₄₀ O ₄	[M-H]-	379.28538	379.28545	0.18		1.6E+06						
318	Pentacosenoic acid	C ₂₅ H ₄₈ O ₂	[M-H]-	379.35815	379.35820	0.13	5.1E+06	8.9E+06		2.4E+06	3.4E+06	4.7E+06	6.0E+06	4.1E+06
319	Amino-formylamino-(phosphoribosylamino)pyrimidine	C ₁₀ H ₁₆ N ₅ O ₉ P	[M-H]-	380.06129	380.06130	0.03	3.4E+06							
320	PA(14:0/0:0)	C ₁₇ H ₃₅ O ₇ P	[M-H]-	381.20476	381.20494	0.47		3.1E+06			1.8E+06		2.1E+06	
321	Heptadecenyl-resorcinol	C ₂₃ H ₃₈ O ₂	[M+Cl]-	381.25658	381.25673	0.39							1.5E+06	
322	MG(0:0/20:2/0:0)	C ₂₃ H ₄₂ O ₄	[M-H]-	381.30103	381.30108	0.13		1.7E+06						
323	Hydroxy-tetracosenoic acid	C ₂₄ H ₄₆ O ₃	[M-H]-	381.33742	381.33749	0.18		3.8E+06			2.3E+06		2.4E+06	2.2E+06
324	Isopentacosanoic acid	C ₂₅ H ₅₀ O ₂	[M-H]-	381.37380	381.37386	0.16	6.4E+07	1.4E+08	3.2E+06	3.5E+07	5.9E+07	6.3E+07	1.0E+08	6.4E+07
325	PC(8:0/0:0)	C ₁₆ H ₃₄ NO ₇ P	[M-H]-	382.20001	382.20022	0.55		1.7E+06						1.7E+06
326	Acetyl-maltose	C ₁₄ H ₂₄ O ₁₂	[M-H]-	383.11950	383.11952	0.05							1.7E+06	
327	Sativic acid	C ₁₈ H ₃₆ O ₆	[M+Cl]-	383.22059	383.22064	0.13					1.6E+06		2.2E+06	
328	MG(0:0/20:1/0:0)	C ₂₃ H ₄₄ O ₄	[M-H]-	383.31668	383.31673	0.13	9.2E+06	1.7E+07		4.6E+06	5.8E+06	7.1E+06	8.4E+06	1.3E+07
329	Hydroxy-tetracosanoic acid	C ₂₄ H ₄₈ O ₃	[M-H]-	383.35307	383.35312	0.13	1.2E+07	2.9E+07	1.6E+06	3.8E+06	8.9E+06	1.4E+07	1.7E+07	8.3E+06
330	Carboxy-tocotrienol	C ₂₄ H ₃₃ O ₄	[M-H]-	384.23061	384.23083	0.57		1.9E+06						
331	N-palmitoyl glutamic acid	C ₂₁ H ₃₉ NO ₅	[M-H]-	384.27555	384.27555	0.00		2.8E+06			2.1E+06		1.7E+06	

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332	6-Deoxyerythronolide B	C ₂₁ H ₃₈ O ₆	[M-H]-	385.25956	385.25962	0.16		6.0E+06			4.7E+06		3.5E+06	1.6E+06
333	Tuberonic acid glucoside	C ₁₈ H ₂₈ O ₉	[M-H]-	387.16606	387.16611	0.13	5.7E+06		3.0E+06				7.2E+06	
334	Rehmaionoside C	C ₁₉ H ₃₂ O ₈	[M-H]-	387.20244	387.20243	-0.03		1.6E+06						
335	Amino-tetrahydroxyeicosenoic acid	C ₂₀ H ₃₉ NO ₆	[M-H]-	388.27046	388.27049	0.08		3.4E+06			3.2E+06		2.0E+06	
336	Hydroxy-dihydrojasmonic acid glucoside	C ₁₈ H ₃₀ O ₉	[M-H]-	389.18171	389.18172	0.03		2.0E+06					1.9E+06	
337	Dehydrorotenone	C ₂₃ H ₂₀ O ₆	[M-H]-	391.11871	391.11885	0.36	2.9E+06							
338	Hexacosadienoic acid	C ₂₆ H ₄₈ O ₂	[M-H]-	391.35815	391.35822	0.18		3.0E+06			1.7E+06		2.0E+06	1.6E+06
339	Miraxanthin-I	C ₁₄ H ₁₈ N ₂ O ₇ S	[M+Cl]-	393.05287	393.05255	-0.81	1.0E+08		3.5E+07		2.1E+07		9.2E+07	
340	MG(0:0/18:0/0:0)	C ₂₁ H ₄₂ O ₄	[M+Cl]-	393.27771	393.27776	0.13					3.9E+06		2.5E+06	
341	Hexacosenoic acid	C ₂₆ H ₅₀ O ₂	[M-H]-	393.37380	393.37386	0.15	8.7E+06	1.7E+07		4.6E+06	6.9E+06	7.7E+06	1.1E+07	7.7E+06
342	PGF2alpha isopropyl ester	C ₂₃ H ₄₀ O ₅	[M-H]-	395.28030	395.28034	0.10		2.6E+06					2.0E+06	
343	Hydroxynervonic acid	C ₂₅ H ₄₈ O ₃	[M-H]-	395.35307	395.35306	-0.03							1.7E+06	
344	Methyl-hexacosanoic acid	C ₂₆ H ₅₂ O ₂	[M-H]-	395.38945	395.38950	0.13	4.5E+07	9.3E+07	2.5E+06	2.5E+07	3.9E+07	4.3E+07	7.0E+07	4.4E+07
345	Trihydroxy-prostadienoyl-ethanolamine	C ₂₂ H ₃₉ NO ₅	[M-H]-	396.27555	396.27562	0.18		1.9E+06						
346	Auramycinone	C ₂₁ H ₁₈ O ₈	[M-H]-	397.09289	397.09325	0.91			8.3E+06				2.4E+06	
347	Tetracosanedioic acid	C ₂₄ H ₄₆ O ₄	[M-H]-	397.33233	397.33238	0.13	2.1E+07	2.0E+07		5.4E+06	7.0E+06	9.7E+06	1.2E+07	1.6E+07
348	Hydroxy-pentacosanoic acid	C ₂₅ H ₅₀ O ₃	[M-H]-	397.36872	397.36877	0.13	9.4E+06	1.5E+07			5.9E+06	6.3E+06	9.3E+06	5.4E+06
349	Aurachin D	C ₂₅ H ₃₃ NO	[M+Cl]-	398.22562	398.22598	0.90		2.3E+06						
350	Oxo-hydroxydimethylprostadienoic acid	C ₂₂ H ₃₆ O ₄	[M+Cl]-	399.23076	399.23081	0.13							1.9E+06	
351	Didecanoylglycerol	C ₂₃ H ₄₄ O ₅	[M-H]-	399.31160	399.31164	0.10		4.8E+06			2.7E+06		3.6E+06	
352	Hydroxyvitamin D3	C ₂₇ H ₄₄ O ₂	[M-H]-	399.32685	399.32691	0.15		6.8E+06		2.2E+06	2.9E+06	2.9E+06	4.4E+06	2.7E+06

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353	Salicin 6-phosphate	C ₁₃ H ₁₉ O ₁₀ P	[M+Cl]-	401.04099	401.04131	0.80	1.1E+07		7.4E+06		3.8E+06		1.3E+07	
354	Dihydroxy-diperoxyeicosadienoic acid	C ₂₀ H ₃₄ O ₈	[M-H]-	401.21809	401.21811	0.05							2.6E+06	
355	Erythronolide B	C ₂₁ H ₃₈ O ₇	[M-H]-	401.25448	401.25453	0.12		2.3E+06					2.2E+06	
356	Hydroxy-mercapto-pregnenedione acetate	C ₂₃ H ₃₂ O ₄ S	[M-H]-	403.19485	403.19490	0.12	7.6E+06	1.5E+07			2.9E+06		5.7E+06	
357	Octacosaoctaenoic acid	C ₂₈ H ₄₀ O ₂	[M-H]-	407.29555	407.29559	0.10		8.6E+06		4.1E+06			5.3E+06	
358	Methyl-hexacosenoic acid	C ₂₇ H ₅₂ O ₂	[M-H]-	407.38945	407.38951	0.15		4.2E+06			2.9E+06		3.3E+06	2.1E+06
359	Palmitoylglycerol phosphate	C ₁₉ H ₃₉ O ₇ P	[M-H]-	409.23606	409.23619	0.32		2.7E+06						
360	Gama-Tocotrienol	C ₂₈ H ₄₂ O ₂	[M-H]-	409.31120	409.31127	0.17		1.8E+07						
361	MG(22:2/0:0/0:0)	C ₂₅ H ₄₆ O ₄	[M-H]-	409.33233	409.33242	0.22		2.2E+06						1.7E+06
362	Oxohexacosanoic acid	C ₂₆ H ₅₀ O ₃	[M-H]-	409.36872	409.36877	0.12		2.3E+06					2.0E+06	
363	Methyl-hexacosanoic acid	C ₂₇ H ₅₄ O ₂	[M-H]-	409.40510	409.40515	0.12	2.4E+07	2.5E+07		6.4E+06	1.4E+07	1.1E+07	2.6E+07	1.1E+07
364	N-oleoyl glutamic acid	C ₂₃ H ₄₁ NO ₅	[M-H]-	410.29120	410.29124	0.10		2.8E+06					1.9E+06	
365	MG(0:0/22:1/0:0)	C ₂₅ H ₄₈ O ₄	[M-H]-	411.34798	411.34802	0.10	1.6E+07	1.4E+07		3.5E+06	7.8E+06	5.8E+06	9.0E+06	1.0E+07
366	Hydroxyhexacosanoic acid	C ₂₆ H ₅₂ O ₃	[M-H]-	411.38437	411.38442	0.12	1.0E+07	1.2E+07			5.8E+06	6.2E+06	1.1E+07	5.2E+06
367	N-stearoyl glutamic acid	C ₂₃ H ₄₃ NO ₅	[M-H]-	412.30685	412.30681	-0.10		2.3E+06						
368	Methyl hydroperoxy bisepidioxy eicosadienoate	C ₂₁ H ₃₄ O ₈	[M-H]-	413.21809	413.21812	0.07							2.2E+06	
369	MG(0:0/22:0/0:0)	C ₂₅ H ₅₀ O ₄	[M-H]-	413.36363	413.36365	0.05		2.8E+06						
370	(Deoxy-gluc-4-enuronosyl)-N-acetyl-D- glucosamine	C ₁₄ H ₂₁ NO ₁₁	[M+Cl]-	414.08086	414.08071	-0.36	2.9E+06							
371	Calcitriol	C ₂₇ H ₄₄ O ₃	[M-H]-	415.32177	415.32180	0.07		3.0E+06					2.6E+06	
372	Dihydroxy-azavitamin D3	C ₂₆ H ₄₃ NO ₃	[M-H]-	416.31702	416.31701	-0.02		3.5E+06						

[illegible]

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393	Tridecyl oleate	C ₂₉ H ₅₆ O ₂	[M-H]-	435.42075	435.42079	0.09		3.8E+06			4.5E+06	3.6E+06	2.2E+06	3.4E+06
394	Deoxythymidine 5'-diphosphate	C ₁₀ H ₁₆ N ₂ O ₁₁ P ₂	[M+Cl]-	436.99233	436.99232	-0.02					3.7E+06		1.9E+07	
395	(Methyl-butanoyloxy)-villanovanediol	C ₂₅ H ₄₂ O ₆	[M-H]-	437.29086	437.29093	0.16						2.2E+06		3.0E+06
396	Norcholestanepentol	C ₂₆ H ₄₆ O ₅	[M-H]-	437.32725	437.32733	0.18								2.5E+06
397	Nonacosanoic acid	C ₂₉ H ₅₈ O ₂	[M-H]-	437.43640	437.43646	0.14		6.0E+06		4.5E+06	7.6E+06	7.6E+06	7.2E+06	8.2E+06
398	MG(24:1/0:0/0:0)	C ₂₇ H ₅₂ O ₄	[M-H]-	439.37928	439.37933	0.11	1.9E+07	1.4E+07		1.3E+07	9.5E+06	2.1E+07	1.1E+07	3.4E+07
399	Hydroxy-octacosanoic acid	C ₂₈ H ₅₆ O ₃	[M-H]-	439.41567	439.41573	0.14		2.3E+06			3.2E+06		2.0E+06	3.2E+06
400	N-linolenoyl-glutamine	C ₂₃ H ₃₈ N ₂ O ₄	[M+Cl]-	441.25256	441.25280	0.54	4.7E+07		1.1E+07	6.9E+07	3.7E+07	1.3E+08	6.9E+07	2.2E+08
401	MG(24:0/0:0/0:0)	C ₂₇ H ₅₄ O ₄	[M-H]-	441.39493	441.39497	0.09		6.5E+06		4.4E+06	6.2E+06	8.4E+06	5.4E+06	9.9E+06
402	Dihydrophaseic acid 4-O-beta-D-glucoside	C ₂₁ H ₃₂ O ₁₀	[M-H]-	443.19227	443.19229	0.05	1.5E+07		5.2E+06				4.9E+06	
403	Geranylgeranyl-glycerol phosphate	C ₂₃ H ₄₁ O ₆ P	[M-H]-	443.25680	443.25707	0.61		2.5E+06				2.8E+06		
404	Trihydroxycholanoic acid	C ₂₄ H ₄₀ O ₅	[M+Cl]-	443.25698	443.25707	0.20		2.5E+06				2.8E+06		
405	Glyceryl-keto-PGF1	C ₂₃ H ₄₀ O ₈	[M-H]-	443.26504	443.26509	0.11	5.4E+06				3.1E+06	2.2E+06	4.8E+06	3.1E+06
406	Dynorphin A	C ₁₈ H ₃₉ N ₉ O ₄	[M-H]-	444.30522	444.30485	-0.83		3.1E+06				2.7E+06		4.5E+06
407	Trihydroxy-oxovitamin D3	C ₂₇ H ₄₂ O ₅	[M-H]-	445.29595	445.29600	0.11						2.8E+06		4.3E+06
408	Grayanotoxin I	C ₂₂ H ₃₆ O ₇	[M+Cl]-	447.21551	447.21557	0.13							2.4E+06	
409	Methyl-octacosadienoic acid	C ₃₀ H ₅₆ O ₂	[M-H]-	447.42075	447.42079	0.09		3.2E+06			3.9E+06		2.5E+06	2.7E+06
410	Tetrahydroxyflavanone glucoside	C ₂₁ H ₂₂ O ₁₁	[M-H]-	449.10894	449.10902	0.18	4.2E+06							
411	Estratrienetriol triacetate	C ₂₄ H ₃₀ O ₆	[M+Cl]-	449.17364	449.17367	0.07		5.4E+06		4.2E+06		5.3E+06		
412	Coprocholic acid	C ₂₇ H ₄₆ O ₅	[M-H]-	449.32725	449.32728	0.07						2.7E+06		2.9E+06
413	Myristyl oleate	C ₃₀ H ₅₈ O ₂	[M-H]-	449.43640	449.43644	0.09	1.5E+07	1.4E+07		8.5E+06	1.5E+07	1.6E+07	1.3E+07	1.6E+07

ESI(-) FTICR-MS

No.	Plausible compound ^a	Molecular formula (M)	Ion	Theor . m/z ^b	Exp. m/z ^c	Δppm ^d	SM _R H ^e	SM _R O ^e	SM _P H ^e	SM _P O ^e	TF _R H ^e	TF _R O ^e	TF _P H ^e	TF _P O ^e
414	6-C-Glucopyranosylcatechin	C ₂₁ H ₂₄ O ₁₁	[M-H]-	451.12459	451.12466	0.16				4.8E+06			8.0E+06	
415	Cyprinol	C ₂₇ H ₄₈ O ₅	[M-H]-	451.34290	451.34294	0.09								2.6E+06
416	Tetradecyl-hexadecanoate	C ₃₀ H ₆₀ O ₂	[M-H]-	451.45205	451.45208	0.07	9.2E+06	7.8E+06		6.0E+06	9.4E+06	1.1E+07	9.8E+06	1.1E+07
417	Glucoerysolin	C ₁₂ H ₂₃ NO ₁₁ S ₃	[M-H]-	452.03605	452.03641	0.80	2.7E+06		3.6E+06				2.8E+06	
418	Pentamethoxy-prenyloxyflavone	C ₂₅ H ₂₈ O ₈	[M-H]-	455.17114	455.17125	0.24	3.4E+06							
419	Volicitin	C ₂₃ H ₃₈ N ₂ O ₅	[M+Cl]-	457.24747	457.24773	0.57								2.4E+06
420	Glucosyl sphingosine	C ₂₄ H ₄₇ NO ₇	[M-H]-	460.32798	460.32797	-0.02								3.3E+06
421	Tephrocin A	C ₂₄ H ₂₆ O ₇	[M+Cl]-	461.13725	461.13756	0.67	2.7E+06							
422	Hydroxypropyl-dihydroxy-norvitamin D3	C ₂₉ H ₅₀ O ₄	[M-H]-	461.36363	461.36371	0.17	7.4E+06				2.7E+06			
423	D-Glucosyldihydrosphingosine	C ₂₄ H ₄₉ NO ₇	[M-H]-	462.34363	462.34371	0.17								2.3E+06
424	Pentadecyl oleate	C ₃₁ H ₆₀ O ₂	[M-H]-	463.45205	463.45210	0.11	6.6E+06	5.2E+06	3.0E+06	3.5E+06	5.3E+06	5.0E+06	5.5E+06	5.6E+06
425	Cholesterol sulfate	C ₂₇ H ₄₆ O ₄ S	[M-H]-	465.30440	465.30443	0.06	1.9E+08	1.4E+08	5.9E+07	9.4E+07	1.3E+08	2.6E+08	1.3E+08	2.5E+08
426	Methyl-triacontanoic acid	C ₃₁ H ₆₂ O ₂	[M-H]-	465.46770	465.46778	0.17							2.6E+06	2.4E+06
427	Oxethazaine	C ₂₈ H ₄₁ N ₃ O ₃	[M-H]-	466.30752	466.30779	0.58	5.7E+07	4.1E+07	1.8E+07	2.8E+07	3.9E+07	7.7E+07	4.0E+07	7.1E+07
428	Catechinol O-galactopyranoside	C ₂₁ H ₂₄ O ₁₂	[M-H]-	467.11950	467.11956	0.13	2.8E+06							
429	Hydroxy-triacontanoic acid	C ₃₀ H ₆₀ O ₃	[M-H]-	467.44697	467.44706	0.19	2.7E+06					3.6E+06		3.3E+06
430	TG(8:0/8:0/8:0)	C ₂₇ H ₅₀ O ₆	[M-H]-	469.35346	469.35352	0.13	4.1E+06	2.8E+06			3.2E+06	4.3E+06		4.7E+06
431	Proteacin	C ₂₀ H ₂₇ NO ₁₂	[M-H]-	472.14605	472.14607	0.04	5.2E+06							
432	Formyltetrahydrofolate	C ₂₀ H ₂₃ N ₇ O ₇	[M-H]-	472.15862	472.15829	-0.70	2.7E+06							
433	Dihydroxy-dimethyl-hexadehydrovitamin D3	C ₂₉ H ₄₂ O ₃	[M+Cl]-	473.28280	473.28266	-0.30		1.5E+08	1.2E+07	7.4E+07	2.8E+07	5.1E+07	3.4E+07	5.1E+07
434	Glucocheirolin	C ₁₁ H ₂₁ NO ₁₁ S ₃	[M+Cl]-	473.99708	473.99669	-0.82	4.0E+06							

ESI(-) FTICR-MS														
No.	Plausible compound ^a	Molecular formula (M)	Ion	Theor. m/z ^b	Exp. m/z ^c	Δppm ^d	SM _R H ^e	SM _R O ^e	SM _P H ^e	SM _P O ^e	TF _R H ^e	TF _R O ^e	TF _P H ^e	TF _P O ^e
435	Punaglandin 8	C ₂₃ H ₃₃ ClO ₆	[M+Cl]-	475.16597	475.16591	-0.13				2.5E+06				
436	Kanokoside A	C ₂₁ H ₃₂ O ₁₂	[M-H]-	475.18210	475.18217	0.15	3.6E+06	2.6E+06				3.0E+06		4.7E+06
437	Trihydroxy-dimethoxychalcone-O-glucoside	C ₂₃ H ₂₆ O ₁₁	[M-H]-	477.14024	477.14051	0.57	2.7E+06							
438	Lusitanicoside	C ₂₁ H ₃₀ O ₁₀	[M+Cl]-	477.15330	477.15320	-0.21	3.0E+06							
439	Palmityl oleate	C ₃₂ H ₆₂ O ₂	[M-H]-	477.46770	477.46774	0.08	1.8E+07	1.3E+07	5.0E+06	8.7E+06	2.0E+07	1.6E+07	1.8E+07	1.6E+07
440	Hexahydroxyflavone 3-glucoside	C ₂₁ H ₂₀ O ₁₃	[M-H]-	479.08311	479.08314	0.06	5.0E+06							
441	Dihydroxyvitamin D3 sulfur dioxide adduct	C ₂₇ H ₄₄ O ₅ S	[M-H]-	479.28367	479.28369	0.04	5.3E+06	2.7E+06	3.2E+06		2.9E+06	3.9E+06	2.8E+06	7.6E+06
442	Hydroxyecdysone	C ₂₇ H ₄₄ O ₇	[M-H]-	479.30143	479.30146	0.06	3.9E+06		3.7E+06			2.6E+06		3.6E+06
443	Hexadecyl hexadecanoate	C ₃₂ H ₆₄ O ₂	[M-H]-	479.48335	479.48339	0.08					3.5E+06		3.0E+06	
444	Fusicoccin H	C ₂₆ H ₄₂ O ₈	[M-H]-	481.28069	481.28074	0.10	4.1E+06						2.6E+06	
445	Hydroxycholesterol sulfate	C ₂₇ H ₄₆ O ₅ S	[M-H]-	481.29932	481.29935	0.06	7.8E+06	4.9E+06	3.7E+06	3.6E+06	4.2E+06	6.6E+06	4.1E+06	1.1E+07
446	Triacantanedioic acid	C ₃₀ H ₅₈ O ₄	[M-H]-	481.42623	481.42626	0.06	5.7E+07	8.6E+07	8.4E+06	4.1E+07	8.9E+07	1.2E+08	8.4E+07	1.3E+08
447	Digalloyl-glucose	C ₂₀ H ₂₀ O ₁₄	[M-H]-	483.07803	483.07801	-0.04	3.0E+06							
448	Diospyrin	C ₂₁ H ₂₄ O ₁₃	[M-H]-	483.11441	483.11441	0.00	3.3E+06							
449	Cholestan-heptol	C ₂₇ H ₄₈ O ₇	[M-H]-	483.33273	483.33280	0.14		2.7E+06						2.9E+06
450	Cabergoline	C ₂₆ H ₃₇ N ₅ O ₂	[M+Cl]-	486.26413	486.26437	0.49								3.1E+06
451	Fucosyllactose	C ₁₈ H ₃₂ O ₁₅	[M-H]-	487.16684	487.16688	0.08		3.3E+06						4.0E+06
452	Ubiquinone Q4	C ₂₉ H ₄₂ O ₄	[M+Cl]-	489.27771	489.27756	-0.31	5.3E+07	3.6E+07	2.5E+07	3.0E+07	4.8E+07	6.5E+07	3.0E+07	6.7E+07
453	Heptadecyl oleate	C ₃₃ H ₆₄ O ₂	[M-H]-	491.48335	491.48340	0.10	4.1E+06	3.4E+06			5.7E+06	3.6E+06	3.7E+06	2.9E+06
454	Pentahydroxy-dimethoxyflavone L-arabinopyranoside	C ₂₂ H ₂₂ O ₁₃	[M-H]-	493.09876	493.09879	0.06	1.8E+07		4.4E+06		3.6E+06			

ESI(-) FTICR-MS

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455	N-(benzenesulfonamide) arachidonoyl amine	C ₂₆ H ₃₈ N ₂ O ₃ S	[M+Cl]-	493.22972	493.22933	-0.79					4.0E+06		4.6E+06	
456	Prednisolone tebutate	C ₂₇ H ₃₈ O ₆	[M+Cl]-	493.23624	493.23626	0.04	3.3E+06		3.9E+06				2.9E+06	
457	Hydroxy-dimethoxyflavone glucoside	C ₂₃ H ₂₄ O ₁₀	[M+Cl]-	495.10635	495.10590	-0.91	3.1E+06							
458	Arachidonoyl Serotonin	C ₃₀ H ₄₂ N ₂ O ₂	[M+Cl]-	497.29403	497.29427	0.48								3.4E+06
459	Cholestanoctol	C ₂₇ H ₄₈ O ₈	[M-H]-	499.32764	499.32772	0.16	3.8E+06							3.2E+06
460	Tetratriacontatetraenoic acid	C ₃₄ H ₆₀ O ₂	[M-H]-	499.45205	499.45210	0.10	4.4E+06	4.3E+06	2.6E+06		5.4E+06	5.3E+06	4.8E+06	3.6E+06
461	Fabatriose	C ₁₈ H ₃₀ O ₁₆	[M-H]-	501.14611	501.14611	0.00	3.6E+07		1.4E+07		2.8E+06		1.0E+07	
462	Trihydroxy-methoxy-phenylcoumarin O-acetylgalactoside	C ₂₄ H ₂₄ O ₁₂	[M-H]-	503.11950	503.11952	0.04	3.4E+06							
463	(Benzodioxolyl)-tetramethoxy-[(methyl- butenyl)oxy]-benzopyranone	C ₂₅ H ₂₆ O ₉	[M+Cl]-	505.12708	505.12741	0.65	1.1E+07		5.4E+06					
464	Stearyl oleate	C ₃₄ H ₆₆ O ₂	[M-H]-	505.49900	505.49903	0.06	6.7E+06	5.0E+06			8.0E+06	4.2E+06	7.2E+06	4.8E+06
465	Tetrahydroxy-dimethoxyflavone glucoside	C ₂₃ H ₂₄ O ₁₃	[M-H]-	507.11441	507.11470	0.57	4.5E+06							
466	DG(14:0/14:0/0:0)	C ₃₁ H ₆₀ O ₅	[M-H]-	511.43680	511.43682	0.04					3.3E+06			4.7E+06
467	Apigenin-(diacetylglucoside)	C ₂₅ H ₂₄ O ₁₂	[M-H]-	515.11950	515.11949	-0.02	1.1E+07		8.0E+06				1.1E+07	
468	Glucosyloxydocosanoate	C ₂₈ H ₅₄ O ₈	[M-H]-	517.37459	517.37461	0.04	1.1E+07		3.9E+06		4.1E+06		9.8E+06	
469	Hydrocortisone cypionate	C ₂₉ H ₄₂ O ₆	[M+Cl]-	521.26754	521.26763	0.17			4.0E+06					
470	DG(14:1/15:0/0:0)	C ₃₂ H ₆₀ O ₅	[M-H]-	523.43680	523.43681	0.02					3.6E+06			
471	Hexatriacontatetraenoic acid	C ₃₆ H ₆₄ O ₂	[M-H]-	527.48335	527.48339	0.08	5.6E+06	3.4E+06			5.6E+06		4.9E+06	3.5E+06
472	Luteolin glucoside-4'-(methyl-butenolate)	C ₂₆ H ₂₆ O ₁₂	[M-H]-	529.13515	529.13518	0.06	3.2E+06							
473	Epoxymurin-A	C ₃₅ H ₆₂ O ₃	[M-H]-	529.46262	529.46267	0.09					4.3E+07		1.8E+07	
474	Cefsulodin	C ₂₂ H ₂₀ N ₄ O ₈ S ₂	[M-H]-	531.06498	531.06479	-0.36	1.0E+07							

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475	Mayolene	C ₃₄ H ₆₀ O ₄	[M-H]-	531.44188	531.44191	0.06	6.8E+06	5.2E+06		4.3E+06	6.7E+06	7.6E+06	6.3E+06	5.1E+06
476	Nocardicin B	C ₂₃ H ₂₄ N ₄ O ₉	[M+Cl]-	535.12373	535.12326	-0.88			4.7E+06					5.3E+06
477	D-Glucan	C ₁₈ H ₃₂ O ₁₈	[M-H]-	535.15159	535.15160	0.02	4.1E+06							
478	Cellotriose	C ₁₈ H ₃₂ O ₁₆	[M+Cl]-	539.13844	539.13856	0.22			2.4E+06					
479	DG(14:0/16:0/0:0)	C ₃₃ H ₆₄ O ₅	[M-H]-	539.46810	539.46812	0.04	5.3E+06	4.2E+06			6.6E+06	1.1E+07	5.6E+06	7.5E+06
480	CMP-3-deoxy-manno-octulosonate	C ₁₇ H ₂₆ N ₃ O ₁₅ P	[M-H]-	542.10288	542.10329	0.76	7.4E+06							
481	Polyoxin B	C ₁₇ H ₂₅ N ₅ O ₁₃	[M+Cl]-	542.11429	542.11417	-0.22	5.7E+06							
482	Estriol 3-sulfate 16-glucuronide	C ₂₄ H ₃₂ O ₁₂ S	[M-H]-	543.15417	543.15432	0.28						8.5E+06		5.2E+06
483	Bacteriohopane-tetrol	C ₃₅ H ₆₂ O ₄	[M-H]-	545.45753	545.45755	0.04		4.0E+06					4.0E+06	
484	DG(15:0/16:1/0:0)	C ₃₄ H ₆₄ O ₅	[M-H]-	551.46810	551.46810	0.00		4.7E+06			4.5E+06		5.9E+06	6.8E+06
485	TG(10:0/10:0/10:0)	C ₃₃ H ₆₂ O ₆	[M-H]-	553.44736	553.44739	0.05		4.0E+06			3.6E+06			4.2E+06
486	DG(15:0/16:0/0:0)	C ₃₄ H ₆₆ O ₅	[M-H]-	553.48375	553.48375	0.00	4.5E+06	5.1E+06			5.4E+06	9.3E+06	5.2E+06	6.7E+06
488	Methylbacteriohopane-tetrol	C ₃₆ H ₆₄ O ₄	[M-H]-	559.47318	559.47318	0.00	9.4E+06	9.6E+06		5.9E+06	1.3E+07	1.4E+07	1.3E+07	1.2E+07
489	Cholesterol glucuronide	C ₃₃ H ₅₄ O ₇	[M-H]-	561.37968	561.37964	-0.07	6.8E+06				4.6E+06			4.3E+06
490	DG(18:2/14:0/0:0)	C ₃₅ H ₆₄ O ₅	[M-H]-	563.46810	563.46825	0.27								3.7E+06
491	N-Stearoylsphingosine	C ₃₆ H ₇₁ NO ₃	[M-H]-	564.53612	564.53616	0.07						6.5E+06		
492	Uridine diphosphategalactose	C ₁₅ H ₂₄ N ₂ O ₁₇ P ₂	[M-H]-	565.04774	565.04770	-0.07	2.4E+07		1.1E+07		7.5E+06		1.0E+07	
493	DG(14:0/18:0/0:0)	C ₃₅ H ₆₈ O ₅	[M-H]-	567.49940	567.49939	-0.02	5.8E+06	4.8E+06			6.5E+06	1.1E+07	6.2E+06	9.4E+06
494	DG(14:1/16:1/0:0)	C ₃₃ H ₆₀ O ₅	[M+Cl]-	571.41348	571.41352	0.07	4.1E+06							
495	N-Palmitoylsphingosine	C ₃₄ H ₆₇ NO ₃	[M+Cl]-	572.48150	572.48146	-0.07	4.6E+06							
496	DG(16:1/14:0/0:0)	C ₃₃ H ₆₂ O ₅	[M+Cl]-	573.42913	573.42912	-0.02	9.9E+06	6.3E+06	3.2E+06	5.6E+06	7.2E+06			9.1E+06

ESI(-) FTICR-MS

No.	Plausible compound ^a	Molecular formula (M)	Ion	Theor . m/z ^b	Exp. m/z ^c	Δppm ^d	SM _R H ^e	SM _R O ^e	SM _P H ^e	SM _P O ^e	TF _R H ^e	TF _R O ^e	TF _P H ^e	TF _P O ^e
497	(O-glucopyranosyl)-keto-hexacosanediol	C ₃₂ H ₆₂ O ₈	[M-H]-	573.43719	573.43719	0.00	1.1E+07		3.5E+06				9.7E+06	
498	Proanthocyanidin A2	C ₃₀ H ₂₄ O ₁₂	[M-H]-	575.11950	575.12006	0.97	3.1E+07		1.2E+07				1.6E+07	
499	(Glucopyranosyl)-hexacosanetriol	C ₃₂ H ₆₄ O ₈	[M-H]-	575.45284	575.45286	0.03	6.5E+07		2.1E+07		1.4E+07		5.4E+07	
500	Isochamaejasmin	C ₃₀ H ₂₂ O ₁₀	[M+Cl]-	577.09070	577.09015	-0.95			5.1E+06					
501	DG(15:0/18:2/0:0)	C ₃₆ H ₆₆ O ₅	[M-H]-	577.48375	577.48382	0.12					4.0E+06			3.8E+06
502	Cer(d18:1/19:0)	C ₃₇ H ₇₃ NO ₃	[M-H]-	578.55177	578.55176	-0.02						7.8E+06		4.1E+06
503	DG(15:0/18:1/0:0)	C ₃₆ H ₆₈ O ₅	[M-H]-	579.49940	579.49942	0.03		4.0E+06			4.7E+06		4.5E+06	5.6E+06
504	DG(O-16:0/18:1)	C ₃₇ H ₇₂ O ₄	[M-H]-	579.53578	579.53579	0.02	1.2E+07	1.5E+07		7.6E+06	1.8E+07	2.1E+07	1.9E+07	1.9E+07
506	Coixenolide	C ₃₈ H ₇₀ O ₄	[M-H]-	589.52013	589.52013	0.00	8.1E+06	1.2E+07		6.9E+06	1.4E+07	1.7E+07	1.5E+07	1.5E+07
507	Cer(d18:2/20:0)	C ₃₈ H ₇₃ NO ₃	[M-H]-	590.55177	590.55172	-0.08					3.8E+06	8.8E+06		
508	DG(16:0/18:2/0:0)	C ₃₇ H ₆₈ O ₅	[M-H]-	591.49940	591.49937	-0.05	4.5E+06				4.6E+06	8.3E+06	3.9E+06	5.1E+06
509	Cer(d16:1/22:0)	C ₃₈ H ₇₅ NO ₃	[M-H]-	592.56742	592.56743	0.02			3.0E+06		5.5E+06	1.7E+07		
510	DG(16:0/18:1/0:0)	C ₃₇ H ₇₀ O ₅	[M-H]-	593.51505	593.51507	0.03		3.8E+06					3.8E+06	4.5E+06
511	PI(18:2/0:0)	C ₂₇ H ₄₉ O ₁₂ P	[M-H]-	595.28889	595.28877	-0.20			3.7E+06					
512	[D-glucopyranosyl]-furostantriol	C ₃₃ H ₅₆ O ₉	[M-H]-	595.38516	595.38519	0.05	6.8E+06						3.8E+06	
513	DG(16:0/18:0/0:0)	C ₃₇ H ₇₂ O ₅	[M-H]-	595.53070	595.53080	0.17	3.8E+06				4.3E+06			
514	Catechin 3-O-rutinoside	C ₂₇ H ₃₄ O ₁₅	[M-H]-	597.18249	597.18253	0.07	1.1E+07						4.1E+06	
515	Cyanidin 3-(6"-malylglucoside)	C ₂₅ H ₂₅ O ₁₅	[M+Cl]-	600.08875	600.08879	0.07	4.1E+06		8.6E+06				9.8E+06	
516	DG(16:0/16:1/0:0)	C ₃₅ H ₆₆ O ₅	[M+Cl]-	601.46043	601.46041	-0.03			4.1E+06	9.6E+06				
517	(O-glucopyranosyl)-keto-octacosanediol	C ₃₄ H ₆₆ O ₈	[M-H]-	601.46849	601.46848	-0.02	8.4E+06						6.2E+06	
518	(O-galactopyranosyl)-octacosanetriol	C ₃₄ H ₆₈ O ₈	[M-H]-	603.48414	603.48413	-0.02	1.6E+07		6.0E+06		6.2E+06		1.4E+07	

ESI(-) FTICR-MS

No.	Plausible compound ^a	Molecular formula (M)	Ion	Theor . m/z ^b	Exp. m/z ^c	Δppm ^d	SM _R H ^e	SM _R O ^e	SM _P H ^e	SM _P O ^e	TF _R H ^e	TF _R O ^e	TF _P H ^e	TF _P O ^e
519	Kinetensin	C ₂₆ H ₃₈ N ₉ O ₆	[M+Cl]-	607.26391	607.26411	0.33		4.6E+06				5.2E+06	4.7E+06	
520	Pentahydroxyflavone neohesperidoside	C ₂₇ H ₃₀ O ₁₆	[M-H]-	609.14611	609.14609	-0.03	1.5E+07		6.1E+06		5.4E+06		3.2E+07	
521	Glutathione disulfide	C ₂₀ H ₃₂ N ₆ O ₁₂ S ₂	[M-H]-	611.14469	611.14472	0.05	5.2E+06		3.7E+06					
522	Evasterioside D	C ₃₃ H ₅₈ O ₁₀	[M-H]-	613.39572	613.39571	-0.02	1.4E+07	9.4E+06	5.7E+06	7.1E+06	5.8E+06	7.9E+06	6.7E+06	1.4E+07
523	Dimethyl-pentadecanoyl-(ladderane-octanyl)-sn- glycerol	C ₄₀ H ₇₂ O ₄	[M-H]-	615.53578	615.53578	0.00		4.1E+06					4.3E+06	
524	DG(15:0/18:0/0:0)	C ₃₆ H ₇₀ O ₅	[M+Cl]-	617.49173	617.49178	0.08				4.1E+06				
525	Cer(d18:1/22:1)	C ₄₀ H ₇₇ NO ₃	[M-H]-	618.58307	618.58313	0.10						4.9E+06		
526	Kanokoside D	C ₂₇ H ₄₄ O ₁₆	[M-H]-	623.25566	623.25564	-0.03	1.0E+07		5.0E+06					
527	DG(16:0/18:3/0:0)	C ₃₇ H ₆₆ O ₅	[M+Cl]-	625.46043	625.46037	-0.10	5.8E+06							
528	Kurilensoside F	C ₃₃ H ₅₈ O ₁₁	[M-H]-	629.39064	629.39063	-0.02	6.5E+06							
529	TG(12:0/12:0/12:0)	C ₃₉ H ₇₄ O ₆	[M-H]-	637.54126	637.54126	0.00	6.3E+06				5.2E+06	6.1E+06	5.5E+06	6.3E+06
530	Myricetin 3,3'-digalactoside	C ₂₇ H ₃₀ O ₁₈	[M-H]-	641.13594	641.13592	-0.03	4.2E+06							
531	Galactosylceramide (d18:1/12:0)	C ₃₆ H ₆₉ NO ₈	[M-H]-	642.49504	642.49500	-0.06	6.2E+06	4.1E+06			7.6E+06	6.1E+06	6.5E+06	6.9E+06
532	DG(15:0/20:1/0:0)	C ₃₈ H ₇₂ O ₅	[M+Cl]-	643.50738	643.50743	0.08	4.5E+06							
533	Didecanoyl-docosanediol	C ₄₂ H ₈₂ O ₄	[M-H]-	649.61403	649.61400	-0.05	2.1E+07	2.3E+07		1.1E+07	3.5E+07	3.5E+07	3.5E+07	2.8E+07
534	DG(16:1/20:3/0:0)	C ₃₉ H ₆₈ O ₅	[M+Cl]-	651.47608	651.47605	-0.05	3.6E+06							
535	Tetraacetoxy-cholestenol	C ₃₅ H ₅₄ O ₉	[M+Cl]-	653.34618	653.34602	-0.24	8.9E+06		3.8E+06		3.5E+06		8.7E+06	
536	DG(16:0/20:3/0:0)	C ₃₉ H ₇₀ O ₅	[M+Cl]-	653.49173	653.49176	0.05	4.9E+06							
537	DG(14:0/22:2/0:0)	C ₃₉ H ₇₂ O ₅	[M+Cl]-	655.50738	655.50719	-0.29		5.3E+06		3.6E+06				
538	DG(16:0/20:1/0:0)	C ₃₉ H ₇₄ O ₅	[M+Cl]-	657.52303	657.52281	-0.33		4.4E+06		3.4E+06				

ESI(-) FTICR-MS														
No.	Plausible compound ^a	Molecular formula (M)	Ion	Theor. m/z ^b	Exp. m/z ^c	Δppm ^d	SM _R H ^e	SM _R O ^e	SM _P H ^e	SM _P O ^e	TF _R H ^e	TF _R O ^e	TF _P H ^e	TF _P O ^e
539	Maltotetraose	C ₂₄ H ₄₂ O ₂₁	[M-H]-	665.21458	665.21419	-0.59	3.9E+06							
540	Ikarisoside F	C ₃₁ H ₃₆ O ₁₄	[M+Cl]-	667.17991	667.18025	0.51	3.6E+06							
541	Pandaroside B	C ₃₅ H ₅₄ O ₁₀	[M+Cl]-	669.34110	669.34104	-0.09	4.4E+06		4.2E+06					
542	PA(16:0/18:3)	C ₃₇ H ₆₇ O ₈ P	[M-H]-	669.45008	669.45000	-0.12						3.8E+06		
543	GlcCer(d18:1/14:0)	C ₃₈ H ₇₃ NO ₈	[M-H]-	670.52634	670.52624	-0.15							3.7E+06	
544	PA(16:0/18:2)	C ₃₇ H ₆₉ O ₈ P	[M-H]-	671.46573	671.46567	-0.09		4.7E+06		1.1E+07		7.6E+06		9.7E+06
545	Quercetin glucoside-glucuronide	C ₂₇ H ₂₈ O ₁₈	[M+Cl]-	675.09697	675.09701	0.06	5.9E+06		5.2E+06				5.8E+06	
546	Sophorosyloxydocosanoic acid	C ₃₄ H ₆₄ O ₁₃	[M-H]-	679.42742	679.42733	-0.13	7.0E+06							
547	Cer(d18:1/24:0)	C ₄₂ H ₈₃ NO ₃	[M+Cl]-	684.60670	684.60692	0.32	4.0E+06							
548	Glucopyranosyl-(tetradecanoyloxy)-eicosanol	C ₄₀ H ₇₈ O ₈	[M-H]-	685.56239	685.56235	-0.06	4.8E+06				5.2E+06		5.1E+06	
549	PA(18:2/18:3)	C ₃₉ H ₆₇ O ₈ P	[M-H]-	693.45008	693.45016	0.12						3.6E+06		
550	Phylloflavanine	C ₃₅ H ₃₂ O ₁₃	[M+Cl]-	695.15369	695.15333	-0.52	4.8E+06							
551	PA(18:1/18:3)	C ₃₉ H ₆₉ O ₈ P	[M-H]-	695.46573	695.46570	-0.04				7.2E+06		4.2E+06		
552	Cer(t18:0/24:0)	C ₄₂ H ₈₅ NO ₄	[M+Cl]-	702.61726	702.61727	0.01	3.8E+06							
553	Ceramide (d18:1/26:0)	C ₄₄ H ₈₇ NO ₃	[M+Cl]-	712.63800	712.63799	-0.01	4.1E+06							
554	PC(O-16:0/O-18:1)	C ₄₂ H ₈₆ NO ₆ P	[M-H]-	730.61200	730.61202	0.03	4.3E+06							
555	Quercetin glucosyl-xylosyl-rhamnoside	C ₃₂ H ₃₈ O ₂₀	[M-H]-	741.18837	741.18828	-0.12	7.3E+06		4.4E+06				8.8E+06	
556	TG(16:0/14:0/16:1)	C ₄₉ H ₉₂ O ₆	[M-H]-	775.68211	775.68172	-0.50					3.9E+06			
557	Quercetin-(di-p-coumarylglucoside)	C ₃₉ H ₃₂ O ₁₆	[M+Cl]-	791.13844	791.13897	0.67			3.3E+06					
558	PI(16:0/18:3)	C ₄₃ H ₇₇ O ₁₃ P	[M-H]-	831.50290	831.50270	-0.24			3.9E+06					
559	PI(16:0/18:2)	C ₄₃ H ₇₉ O ₁₃ P	[M-H]-	833.51855	833.51838	-0.20	5.9E+06		5.3E+06	4.0E+06			3.1E+06	

ESI(-) FTICR-MS														
No.	Plausible compound ^a	Molecular formula (M)	Ion	Theor. m/z ^b	Exp. m/z ^c	Δppm ^d	SM _R H ^e	SM _R O ^e	SM _P H ^e	SM _P O ^e	TF _R H ^e	TF _R O ^e	TF _P H ^e	TF _P O ^e
560	Diguanosine tetraphosphate	C ₂₀ H ₂₈ N ₁₀ O ₂₁ P ₄	[M-H]-	867.03082	867.03164	0.95				2.9E+06				
561	Malonyl-CoA semialdehyde	C ₂₄ H ₃₈ N ₇ O ₁₈ P ₃ S	[M+Cl]-	872.09009	872.08952	-0.65	3.6E+06			3.8E+06				

^a Cer: Ceramide; GalCer: Galactosylceramide; GlcCer: Glucosylceramide; LacCer: Lactosylceramide; MG: Monoacylglycerol; DG: Diacylglycerol; TG: Triacylglycerol; MGDG: Monoacyldiacylglycerol; PA:

Phosphatidic acid; PC: Phosphatidylcholine; PE: Phosphatidylethanolamine; PG: Glycerophospholipids; PI: Phosphatidylinositol; PS: Phosphatidylserine;; SM: Sphingomyelin

^b Theor. stands for calculated exact mass to charge ratio

^c Exp. stands for experimental m/z value

^d The error expressed in parts per million (ppm)

^e SM_RH and SM_RO stand for hydroalcoholic and organic portions of red San Marzano extracts, respectively; SM_PH and SM_PO stand for hydroalcoholic and organic portions of pink San Marzano extracts, respectively. TF_RH and TF_RO stand for hydroalcoholic and organic portions of red Torpedino di Fondi extracts, respectively; TF_PH and TF_PO stand for hydroalcoholic and organic portions of pink Torpedino di Fondi extracts, respectively.

Table 5. Antifungal activity of tomato fruit extracts against 4 *C. albicans* strains (ATCC10231, ATCC24433, 3153A, PMC1033), 3 *C. glabrata* strains (PMC0822, PMC0851, PMC0807) and 2 *C. krusei* strains (PMC0631, PMC0624). ^{a, b.}

<i>Candida</i>	MIC ₅₀ (µg/mL)															
	ORGANIC				HYDROALCOHOLIC				ORGANIC				HYDROALCOHOLIC			
	SM _R		SM _P		SM _R		SM _P		TF _R		TF _P		TF _R		TF _P	
	Range	GM	range	GM	range	GM	range	GM	range	GM	range	GM	range	GM	range	GM
<i>albicans</i> ^a	1000->1000	1834	250->1000	771	1000->1000	1682	1000->1000	1682	250->1000	841	500->1000	1000	1000->1000	1682	500->1000	1297
<i>glabrata</i> ^b	500->1000	944	250-1000	630	500->1000	944	250->1000	891	250-500	281	250-1000	375	500-1000	794	250-1000	595
<i>krusei</i> ^c	500->1000	841	>1000	>1000	>1000	>1000	>1000	>1000	>1000	>1000	>1000	>1000	>1000	>1000	>1000	>1000

	MIC ₉₀ (µg/mL)															
	ORGANIC				HYDROALCOHOLIC				ORGANIC				HYDROALCOHOLIC			
	SM _R		SM _P		SM _R		SM _P		TF _R		TF _P		TF _R		TF _P	
	Range	GM	range	GM	range	GM	range	GM	range	GM	range	GM	range	GM	range	GM
<i>albicans</i> ^c	>1000	>1000	500->1000	1297	>1000	>1000	>1000	>1000	500->1000	1190	500->1000	1297	>1000	>1000	500->1000	1682
<i>glabrata</i> ^d	1000->1000	1498	1000->1000	1587	1000->1000	1498	500->1000	1059	500-1000	561	500-1000	707	1000->1000	1260	1000	1000
<i>krusei</i> ^e	1000>1000	1414	>1000	>1000	>1000	>1000	>1000	>1000	>1000	>1000	>1000	>1000	>1000	>1000	>1000	>1000

	MIC ₁₀₀ (µg/mL)															
	ORGANIC				HYDROALCOHOLIC				ORGANIC				HYDROALCOHOLIC			
	SM _R		SM _P		SM _R		SM _P		TF _R		TF _P		TF _R		TF _P	
	range	GM	range	GM	range	GM	range	GM	range	GM	range	GM	range	GM	range	GM
<i>albicans</i> ^c	>1000	>1000	>1000	>1000	>1000	>1000	>1000	>1000	1000->1000	1834	1000->1000	1834	>1000	>1000	>1000	>1000
<i>glabrata</i> ^d	>1000	>1000	>1000	>1000	>1000	>1000	>1000	>1000	>1000	>1000	>1000	>1000	>1000	>1000	>1000	>1000
<i>krusei</i> ^e	>1000	>1000	>1000	>1000	>1000	>1000	>1000	>1000	>1000	>1000	>1000	>1000	>1000	>1000	>1000	>1000

^{a)} MIC=minimal inhibitory concentration. ^{b)} GM= geometric mean MIC₅₀, MIC₈₀, MIC₉₀, and MIC₁₀₀ are the lowest concentration of extracts that caused growth inhibition ≥ 50%, ≥ 80%, ≥ 90% and 100%, respectively. ^{c)} 4 strains (ATCC10231, ATCC24433, 3153A, PMC1033); ^{d)} 3 strains (PMC0822, PMC0851, PMC0807); ^{e)} and 2 strains (PMC0631, PMC0624).