

Supplementary Table S1. Identification of the major constituents of CFE in positive and negative ion modes by HPLC–MS/MS

No.	Classification	Analyte Name	R.T (min)	Molecular Formula	Molecular Weight	Adduct	Theoretical Mass	Measure d Mass	Mass error (ppm)
		Leucrose	1.06	C ₁₂ H ₂₂ O ₁₁	342.1	[M+Na] ⁺	365.1054322	365.105	0.969
		Itaconate	1.25	C ₅ H ₆ O ₄	130	[M-H] ⁻	129.0193322	129.018	11.468
		Citramalic acid	1.32	C ₅ H ₈ O ₅	148	[M-H] ⁻	147.0298969	147.029	8.643
		MEGLUTOL	1.51	C ₆ H ₁₀ O ₅	162.1	[M-H] ⁻	161.045547	161.044	7.579
		GLUTARYLCARNITINE	1.55	C ₁₂ H ₂₁ NO ₆	275.1	[M+H] ⁺	276.1441638	276.15	21.028
		(4R)-3-methylidene-4-[(E)-3-methyl-4-(4-methyl-5-oxooxolan-2-yl)but-2-enyl]oxolan-2-one	1.67	C ₁₅ H ₂₀ O ₄	264.1	[M-H-H ₂ O] ⁻	245.118318	245.114	18.308
		L-Propionylcarnitine	2.09	C ₁₀ H ₁₉ NO ₄	217.1	[M+H] ⁺	218.1386845	218.139	1.079
		MEVALONATE	2.4	C ₆ H ₁₂ O ₄	148.1	[M+HCO ₂] ⁻	193.0717617	193.071	4.775
		Adipate	5.03	C ₆ H ₁₀ O ₄	146.1	[M-H] ⁻	145.0506323	145.049	8.714
		Pimelate	8.86	C ₇ H ₁₂ O ₄	160.1	[M-H] ⁻	159.0662824	159.065	8.011
		FURFURYL BUTYRATE	9.21	C ₉ H ₁₂ O ₃	168.1	[M+HCO ₂] ⁻	213.0768471	213.073	156.337
		D-Leucic acid	9.58	C ₆ H ₁₂ O ₃	132.1	[M-H] ⁻	131.0713678	131.07	10.834

NONANOATE	13.0	3	C ₉ H ₁₈ O ₂	158.1	[M+Na] ⁺	181.1199005	181.122	14.059
Ethyl 3-phenylpropanoate	13.9	5	C ₁₁ H ₁₄ O ₂	178.1	[M+H] ⁺	179.1066561	179.107	0.732
(3S,5R,6R,7E)-3,5,6-Trihydroxy-7-megastigmen-9-one	17.2	2	C ₁₃ H ₂₂ O ₄	242.2	[M+H-H ₂ O] ⁺	225.148521	225.149	0.84
Valproate	17.7	7	C ₈ H ₁₆ O ₂	144.1	[M+HCO ₂] ⁻	189.1132326	189.112	4.53
AZELATE	17.7	8	C ₉ H ₁₆ O ₄	188.1	[M-H] ⁻	187.0975825	187.097	4.606
(3aR,4aS,5S,5aR,6aR)-5-(3-hydroxybutyl)-5a-methyl-3-methylidene-3a,4,4a,5,6,6a-hexahydrocyclopropa[f][1]benzofuran-2-one	20.0	8	C ₁₅ H ₂₂ O ₃	250.2	[M+H-H ₂ O] ⁺	233.1536063	233.154	0.761
Isoalantolactone	20.5	2	C ₁₅ H ₂₀ O ₂	232.1	[M+H] ⁺	233.1536063	233.154	0.944
2-[(3S)-3-hydroxy-4a,8-dimethyl-2,3,4,5,6,7-hexahydro-1H-naphthalen-2-yl]prop-2-enoic acid	21.5	5	C ₁₅ H ₂₂ O ₃	250.2	[M+HCO ₂] ⁻	295.1550974	295.155	0.621
Sebacate	22.2	4	C ₁₀ H ₁₈ O ₄	202.1	[M-H] ⁻	201.1132326	201.113	3.624
4-Hydroxynonenal alkyne	22.6		C ₉ H ₁₂ O ₂	152.1	[M+H-H ₂ O] ⁺	135.0804414	135.081	0.996
13,14-Dihydro-15-ketotetranorprostaglandin F1.beta.	22.6	9	C ₁₆ H ₂₈ O ₅	300.2	[M-H] ⁻	299.1863975	299.186	0.764
ESTRADIOL 3-(TRIMETHYLSILYL)	23.1		C ₂₁ H ₃₂ O ₂ Si	344.2	[M-H] ⁻	343.2098803	343.212	6.645

ETHER		8						
2,3-Dinor-8-isoprostaglandin-F2.alpha.	23.3	6	C ₁₈ H ₃₀ O ₅	326.2	[M+H] ⁺	327.2166005	327.217	0.844
18-Carboxydinorleukotriene B4	23.4	9	C ₁₈ H ₂₆ O ₆	338.2	[M+H- H ₂ O] ⁺	321.1696503	321.167	7.35
(2E,4E)-12-hydroxy-13-(hydroxymethyl)- 3,5,7-trimethyltetradeca-2,4-dienedioic acid	23.7		C ₁₈ H ₃₀ O ₆	342.2	[M+H- H ₂ O] ⁺	325.2009504	325.201	1.608
Rubescensin A	24.1	1	C ₂₀ H ₂₈ O ₆	364.2	[M+H] ⁺	365.1958651	365.193	6.744
A1-Phytostane-I	24.1	7	C ₁₈ H ₂₈ O ₄	308.2				
ESTRONE TRIMETHYL ETHER	24.2	3	C ₂₁ H ₃₀ O ₂ Si	342.2	[M-H] ⁻	341.1942303	341.196	6.628
Palmitic acid alkyne	25.5	3	C ₁₆ H ₂₈ O ₂	252.2	[M+Na] ⁺	275.1981508	275.201	9.108
Undecanedioic acid	26.5	1	C ₁₁ H ₂₀ O ₄	216.1	[M-H] ⁻	215.1288827	215.128	3.553
Dinor-12-oxophytodienoic acid	27.6	3	C ₁₆ H ₂₄ O ₃	264.2	[M+H] ⁺	265.1798211	265.18	1.547
Empenthrin	27.7	4	C ₁₈ H ₂₆ O ₂	274.2	[M+H] ⁺	275.2005565	275.201	0.676
Hymeglusin	27.8	7	C ₁₈ H ₂₈ O ₅	324.2	[M+H] ⁺	325.2009504	325.201	1.418
9-Hydroperoxy-10E,12Z,15Z-octadecatrienoic	27.9		C ₁₈ H ₃₀ O ₄	310.2	[M+H- H ₂ O] ⁻	293.2111212	293.211	0.507

acid	4			H2O]+			
(10E,15Z)-9,12,13-trihydroxyoctadeca-10,15-dienoic acid	27.9 7	C ₁₈ H ₃₂ O ₅	328.2	[M-H]-	327.2176977	327.218	1.054
8-[3-oxo-2-[(E)-pent-2-enyl]cyclopenten-1-yl]octanoic acid	28.2 4	C ₁₈ H ₂₈ O ₃	292.2	[M+H-H2O]+	275.2005565	275.201	0.797
Costunolide	28.3 2	C ₁₅ H ₂₀ O ₂	232.1	[M+H]+	233.1536063	233.154	0.914
cis-.DELTA.2-11-Methyldodecenoic acid	28.3 3	C ₁₃ H ₂₄ O ₂	212.2	[M+Na]+	235.1668507	235.169	10.272
h_92_oxabolone	28.5 7	C ₁₈ H ₂₆ O ₃	290.2	[M+H-H2O]+	273.1849065	273.185	0.448
16,16-Dimethyl-6-ketoprostaglandin E1	28.7 2	C ₂₂ H ₃₆ O ₆	396.3	[M-H]-	395.2439124	395.244	0.44
16-Hydroxyhexadecanoic acid	29.1 4	C ₁₆ H ₃₂ O ₃	272.2	[M+Na]+	295.2243656	295.227	8.503
(1R,4Z,9S)-4-(hydroxymethyl)-11,11-dimethyl-8-methylidenebicyclo[7.2.0]undec-4-en-3-one	29.2	C ₁₅ H ₂₂ O ₂	234.2	[M+HCO2]-	279.1601828	279.16	1.345
9,12-Octadecadiynoic acid	29.2 1	C ₁₈ H ₂₈ O ₂	276.2	[M+H]+	277.2162066	277.216	1.129
(Z)-9,12,13-trihydroxyoctadec-15-enoic acid	29.2 2	C ₁₈ H ₃₄ O ₅	330.2	[M+Na]+	353.2298449	353.231	2.894
ARTENIMOL	29.2 4	C ₁₅ H ₂₄ O ₅	284.2	[M-H-H2O]-	265.1445327	265.144	1.111

6,15-Diketo-13,14-dihydroprostaglandin F1.alpha.	29.3	1	C ₂₀ H ₃₄ O ₆	370.2	[M+H-H ₂ O] ⁺	353.2322506	353.231	4.638
Estriol	29.3	3	C ₁₈ H ₂₄ O ₃	288.2	[M+H] ⁺	289.1798211	289.18	0.993
Dodecanedioate	29.3	5	C ₁₂ H ₂₂ O ₄	230.2	[M-H] ⁻	229.1445327	229.144	2.873
3-[(E)-[(3aR,4S,5S,6aR)-4-[(E,3R)-3-cyclohexyl-3-hydroxyprop-1-enyl]-5-hydroxy-3,3a,4,5,6,6a-hexahydro-1H-pentalen-2-ylidene]methyl]benzoic acid	29.3	9	C ₂₅ H ₃₂ O ₄	396.2	[M-H] ⁻	395.2227831	395.227	10.548
Phytprostane A1 (PPA1)	29.4	3	C ₁₈ H ₂₈ O ₃	292.2	[M+H] ⁺	293.2111212	293.211	0.507
5-Isoprostaglandin-F2.alpha.-VI	29.4	4	C ₂₀ H ₃₄ O ₅	354.2	[M-H] ⁻	353.2333477	353.233	1.223
Chrysanthemic Acid, Ethyl Ester	29.6		C ₁₂ H ₂₀ O ₂	196.1	[M-H] ⁻	195.1390534	195.138	4.76
Prostaglandin D3	30.2	3	C ₂₀ H ₃₀ O ₅	350.2	[M+Na] ⁺	373.1985448	373.199	1.01
20-Trifluoroleukotriene B4	30.3		C ₂₀ H ₂₉ F ₃ O ₄	390.2	[M+H-H ₂ O] ⁺	373.1985058	373.199	0.876
12(13)Ep-9-KODE	30.4	9	C ₁₈ H ₃₀ O ₄	310.2	[M+H] ⁺	311.2216859	311.222	0.957
8-Iso-16-cyclohexyltetranorprostaglandin E2	30.6	3	C ₂₂ H ₃₄ O ₅	378.2	[M-H] ⁻	377.2333477	377.227	16.408
NCGC00180485-03_C21H32O4_(5beta,8alpha,9beta,10alpha,13alpha)-18-Methoxy-18-oxokauran-17-oic	31.0							

acid							
Valerenic acid	31.0 7	C ₁₅ H ₂₂ O ₂	234.2	[M+H] ⁺	235.1692564	235.169	0.873
15-Keto-prostaglandin F2a	31.1 7	C ₂₀ H ₃₂ O ₅	352.2	[M+H] ⁺	353.2322506	353.232	2.402
Ophiobolin A	31.2 8	C ₂₅ H ₃₆ O ₄	400.3	[M+H- H ₂ O] ⁺	383.2580714	383.259	70.657
7-[(2R)-2-[(E,3S,4S)-3-hydroxy-4-methylnon-1-en-6-ynyl]-5-oxopyrrolidin-1-yl]heptanoic acid	31.4 9	C ₂₁ H ₃₃ NO ₄	363.2	[M+H] ⁺	364.248235	364.248	1.031
Ingenol	31.6 1	C ₂₀ H ₂₈ O ₅	348.2	[M+H] ⁺	349.2009504	349.198	7.135
17-trans-Prostaglandin E3	31.6 3	C ₂₀ H ₃₀ O ₅	350.2	[M-H- H ₂ O] ⁻	331.1914829	331.191	1.969
Carveol	31.6 9	C ₁₀ H ₁₆ O	152.1	[M+Na] ⁺	175.1093358	175.112	13.831
Prostaglandin E2 serinolamide	31.7 2	C ₂₃ H ₃₉ NO ₆	425.3	[M+H] ⁺	426.2850144	426.272	31.768
methyl (2E)-2-[(4aR,8aS)-4a-methyl-8-methylidene-3,4,5,6,7,8a-hexahydro-1H-naphthalen-2-ylidene]-3-hydroxypropanoate	31.8 8	C ₁₆ H ₂₄ O ₃	264.2	[M+H- H ₂ O] ⁺	247.1692564	247.169	0.751
Traumatic acid	31.9 2	C ₁₂ H ₂₀ O ₄	228.1	[M-H] ⁻	227.1288827	227.128	2.973
13-HPODE	31.9 7	C ₁₈ H ₃₂ O ₄	312.2	[M-H] ⁻	311.2227831	311.222	1.947

9-Oxo-10E,12Z,15Z-octadecatrienoic acid	31.9 8	C ₁₈ H ₂₈ O ₃	292.2	[M+H- H ₂ O] ⁺	275.2005565	275.201	0.945
Dinorprostaglandin E1	32.0 1	C ₁₈ H ₃₀ O ₅	326.2	[M-H- H ₂ O] ⁻	307.1914829	307.191	0.866
13-KODE	32.1 2	C ₁₈ H ₃₀ O ₃	294.2	[M+H- H ₂ O] ⁺	277.2162066	277.217	1.247
10-Nitrooleic acid	32.1 6	C ₁₈ H ₃₃ NO ₄	327.2	[M+H] ⁺	328.248235	328.248	1.081
Prostaglandin A2	32.2 3	C ₂₀ H ₃₀ O ₄	334.2	[M+H- H ₂ O] ⁺	317.2111212	317.21	3.561
15-Deoxy-d-12,14-PGJ2	32.3 3	C ₂₀ H ₂₈ O ₃	316.2	[M+H] ⁺	317.2111212	317.211	0.739
13,14-Dihydro-15-ketoprostaglandin A2	32.3 5	C ₂₀ H ₃₀ O ₄	334.2	[M-H] ⁻	333.207133	333.207	1.172
NCGC00380425-01!1-(3,5-dihydroxyphenyl)- 12-hydroxytridecan-2-one	32.3 6	C ₁₉ H ₃₀ O ₄	322.2	[M+H] ⁺	323.2216859	323.222	2.169
5-trans-Prostaglandin D2	32.3 9	C ₂₀ H ₃₂ O ₅	352.2	[M+H- H ₂ O] ⁺	335.2216859	335.221	3.141
9-HPODE	32.4	C ₁₈ H ₃₂ O ₄	312.2	[M-H] ⁻	311.2227831	311.223	0.39
16a-Hydroxydehydroisoandrosterone	32.4 4	C ₁₉ H ₂₈ O ₃	304.2	[M+H] ⁺	305.2111212	305.211	1.294
Walleminone	32.6 8	C ₁₅ H ₂₄ O ₃	252.2	[M+H] ⁺	253.1798211	253.18	0.67
Tetranor 12-HETE	32.6	C ₁₆ H ₂₆ O ₃	266.2	[M+H] ⁺	267.1954711	267.196	0.461

	8							
PGB2-[d4]	32.7 1	C ₂₀ H ₃₀ O ₄	334.2	[M+Na] ⁺	357.2036301	357.204	0.747	
Bacillaene	32.7 1	C ₃₄ H ₄₈ N ₂ O ₆	580.4	[M+H- H ₂ O] ⁺	563.347949	563.349	1.375	
Parthenolide	32.7 1	C ₁₅ H ₂₀ O ₃	248.1	[M+H] ⁺	249.148521	249.149	0.742	
1-METHOXYCARBONYL-4-(1,5-DIMETHYL-3-OXOHEX-4-ENYL)-CYCLOHEXENE	32.7 1	C ₁₆ H ₂₄ O ₃	264.2	[M-H] ⁻	263.1652682	263.165	1.678	
MGMG 16:3	32.9 2	C ₂₅ H ₄₂ O ₉	486.3	[M+HCO 2] ⁻	531.2810858	531.28	2.019	
19-Nor-4-androstene-3,17-dione	32.9 7	C ₁₈ H ₂₄ O ₂	272.2	[M+H] ⁺	273.1849065	273.185	0.486	
1-(5Z,8Z,11Z,14Z-Eicosatetraenoyl)-sn-glycero-3-phospho-(1'-sn-glycerol)	33.0 6	C ₂₆ H ₄₅ O ₉ P	532.3	[M-H] ⁻	531.2728432	531.278	10.271	
1-(5Z,8Z,11Z,14Z-Eicosatetraenoyl)-sn-glycero-3-phosphate	33.1 6	C ₂₃ H ₃₉ O ₇ P	458.2	[M-H- H ₂ O] ⁻	439.2254991	439.225	0.907	
17-Keto-4(Z),7(Z),10(Z),13(Z),15(E),19(Z)-docosahexaenoic acid	33.2 8	C ₂₂ H ₃₀ O ₃	342.2	[M+H- H ₂ O] ⁺	325.2162066	325.219	7.227	
9-KODE	33.3 8	C ₁₈ H ₃₀ O ₃	294.2	[M+H] ⁺	295.2267713	295.227	1.842	
5,8,11-Eicosatriynoic acid	33.4	C ₂₀ H ₂₈ O ₂	300.2	[M+H] ⁺	301.2162066	301.217	3.819	
Bicyclo-prostaglandin E1	33.4	C ₂₀ H ₃₂ O ₄	336.2	[M+Na] ⁺	359.2192802	359.219	0.462	

	3						
Hellebrigenin-D-glucose	33.4 8	C ₃₀ H ₄₂ O ₁₁	578.3	[M-H]-	577.2654357	577.268	5.105
Roridin A	33.4 8	C ₂₉ H ₄₀ O ₉	532.3	[M+HCO 2]-	577.2654357	577.268	5.105
Tetrahydrocorticosterone	33.5 5	C ₂₁ H ₃₄ O ₄	350.2	[M+H]+	351.252986	351.253	0.914
Phosphatidylcholine lyso 20:5	33.5 7	C ₂₈ H ₄₈ NO ₇ P	541.3	[M+H]+	542.324116	542.327	5.347
Phosphatidylcholine lyso 18:3	33.5 7	C ₂₆ H ₄₈ NO ₇ P	517.3	[M+HCO 2]-	562.3150424	562.315	1.272
LPC(18:2)	33.6	C ₂₆ H ₅₀ NO ₇ P	519.3	[M+Na]+	542.3217103	542.329	14.151
15-keto-PGF1alpha	33.6 1	C ₂₀ H ₃₄ O ₅	354.2	[M+H- H2O]+	337.237336	337.243	18.091
(1S)-(+)-Camphorquinone	33.6 1	C ₁₀ H ₁₄ O ₂	166.1	[M+H- H2O]+	149.0960915	149.096	1.003
Stearidonic acid	33.7 4	C ₁₈ H ₂₈ O ₂	276.2	[M+H- H2O]+	259.2056419	259.206	0.637
LysoPC(16:0)	33.9 2	C ₂₄ H ₅₀ NO ₇ P	495.3	[M+Na]+	518.3217103	518.324	5.042
Docosahexaenoic acid methyl ester	33.9 8	C ₂₃ H ₃₄ O ₂	342.3	[M+Na]+	365.245101	365.24	73.761
(-)-Carvophyllene oxide	34.0	C ₁₅ H ₂₄ O	220.2	[M+H-	203.1794272	203.18	1.421

	4			H ₂ O]+			
13-HOTrE	34.0 6	C ₁₈ H ₃₀ O ₃	294.2	[M+H] ⁺	295.2267713	295.227	0.745
9-HOTrE	34.0 6	C ₁₈ H ₃₀ O ₃	294.2	[M+HCO 2] ⁻	339.2176977	339.217	1.479
(9Z,12E)-15,16-dihydroxyoctadeca-9,12-dienoic acid	34.1 1	C ₁₈ H ₃₂ O ₄	312.2	[M-H- H ₂ O] ⁻	293.2122184	293.212	1.153
13-Hydroperoxy-9Z,11E-octadecadienoic acid	34.2	C ₁₈ H ₃₂ O ₄	312.2	[M-H- H ₂ O] ⁻	293.2122184	293.212	1.389
5-[5-(acetyloxymethyl)-1,2,4a-trimethyl-7-oxo-3,4,8,8a-tetrahydro-2H-naphthalen-1-yl]-3-methylpentanoic acid	34.3	C ₂₂ H ₃₄ O ₅	378.2	[M-H- H ₂ O] ⁻	359.2227831	359.222	1.277
Cortisol	34.3 1	C ₂₁ H ₃₀ O ₅	362.2	[M+H] ⁺	363.2166005	363.231	46.57
Lipoxin B4	34.3 8	C ₂₀ H ₃₂ O ₅	352.2	[M-H] ⁻	351.2176977	351.217	1.318
Lyso-PC 18:1(9Z)	34.4 3	C ₂₆ H ₅₂ NO ₇ P	521.3	[M+H] ⁺	522.3554161	522.356	2.086
LysoPE(16:0/0:0)	34.4 8	C ₂₁ H ₄₄ NO ₇ P	453.3	[M-H] ⁻	452.2782629	452.28	4.707
Curcumol	34.5 8	C ₁₅ H ₂₄ O ₂	236.2	[M+H- H ₂ O] ⁺	219.1743418	219.174	0.566
(9Z,12Z,15Z)-9,12,15-Octadecatrienoic acid, 3-(hexopyranosyloxy)-2-hydroxypropyl ester	34.6	C ₂₇ H ₄₆ O ₉	514.3	[M-H] ⁻	513.3069066	513.305	3.409

LysoPC(17:0)	34.6 2	C ₂₅ H ₅₂ NO ₇ P	509.3	[M+Na] ⁺	532.3373603	532.347	18.882
Monopalmitolein (9c)	34.6 9	C ₁₉ H ₃₆ O ₄	328.3	[M+H- H ₂ O] ⁺	377.2686361	377.269	0.207
Manoalide	34.7 3	C ₂₅ H ₃₆ O ₅	416.3	[M+H] ⁺	417.2635507	417.265	20.256
2-(14,15-Epoxyeicosatrienoyl)glycerol	34.7 4	C ₂₃ H ₃₈ O ₅	394.3	[M+H- H ₂ O] ⁺	377.2686361	377.269	0.735
LPA(18:1(9Z)/0:0)	34.8 2	C ₂₁ H ₄₁ O ₇ P	436.3	[M+HCO 2] ⁻	481.2571931	481.257	1.576
Phosphatidylcholine lyso 16:0	34.8 7	C ₂₄ H ₅₀ NO ₇ P	495.3	[M+HCO 2] ⁻	540.3306924	540.334	6.503
METHYL RICINOLEATE	34.8 9	C ₁₉ H ₃₆ O ₃	312.3	[M+H] ⁺	313.2737215	313.274	0.428
LysoPC(0:0/18:0)	35.2 3	C ₂₆ H ₅₄ NO ₇ P	523.4	[M+H] ⁺	524.3710662	524.369	5.98
4-HDoHE	35.2 8	C ₂₂ H ₃₂ O ₃	344.2	[M+H] ⁺	345.2424213	345.242	0.602
Linoelaidic acid	35.2 9	C ₁₈ H ₃₂ O ₂	280.2	[M+Na] ⁺	303.229451	303.232	7.784
EPA	35.3 1	C ₂₀ H ₃₀ O ₂	302.2	[M+H- H ₂ O] ⁺	285.2212920	285.225	13.042
12(S)-HETE-d8	35.3 8	C ₂₀ H ₃₂ O ₃	320.2	[M+H- H ₂ O] ⁺	303.2318567	303.232	1.739

11-HETE	35.3 9	C ₂₀ H ₃₂ O ₃	320.2	[M+H- H ₂ O] ⁺	303.2318567	303.232	1.739
Dodeca-2(E),4(E)-dienoic acid	35.4 7	C ₁₂ H ₂₀ O ₂	196.1	[M+H- H ₂ O] ⁺	179.1430416	179.143	0.668
Ricinoleic acid	35.5	C ₁₈ H ₃₄ O ₃	298.3	[M-H] ⁻	297.2435185	297.243	1.402
[(1R,2S,3S,4R,4aS)-2,3-dihydroxy-3,4a,8,8-tetramethyl-4-[(E)-3-oxobut-1-enyl]-2,4,5,6,7,8a-hexahydro-1H-naphthalen-1-yl] acetate	35.5 3	C ₂₀ H ₃₂ O ₅	352.2	[M+HCO 2] ⁻	397.223177	397.226	7.232
1-Palmitoyl-2-hydroxy-sn-glycero-3-phospho-(1'-rac-glycerol)	35.6 3	C ₂₂ H ₄₄ NaO ₉ P	506.5	[M+Na] ⁺	507.2693404	507.27	1.428
3-Hydroxymyristic acid	35.7	C ₁₄ H ₂₈ O ₃	244.2	[M-H] ⁻	243.1965683	243.196	2.939
15S-Hydroxy-8Z,11Z,13E-eicosatrienoic acid	35.9	C ₂₀ H ₃₄ O ₃	322.3	[M-H] ⁻	321.2435185	321.242	4.206
Prostaglandin A1 ethyl ester	36.0 1	C ₂₂ H ₃₆ O ₄	364.3	[M+H] ⁺	365.2686361	365.268	10.492
O-Arachidonoylglycidol	36.1 2	C ₂₃ H ₃₆ O ₃	360.3	[M+Na] ⁺	383.2556657	383.25	55.057
MG(0:0/16:0/0:0)	36.1 6	C ₁₉ H ₃₈ O ₄	330.3	[M+H] ⁺	331.2842861	331.284	1.061
Dioctyl sulfosuccinate	36.1 7	C ₂₀ H ₃₈ O ₇ S	422.2	[M-H] ⁻	421.2265481	421.226	0.773
1-Oleoyl-2-hydroxy-sn-glycero-3-phospho-(1'-rac-glycerol)	36.3 3	C ₂₄ H ₄₇ O ₉ P	510.3	[M-H] ⁻	509.2884933	509.288	1.193
Prostaglandin F2.alpha. Ethanolamide	36.4	C ₂₂ H ₃₉ NO ₅	397.3	[M+H] ⁻	380.2795351	380.284	12.174

				H2O)+				
(Z)-3-Hydroxyhexadec-7-enoic acid	36.4	1	C ₁₆ H ₃₀ O ₃	270.2	[2M-H]-	539.4317132	539.431	1.402
9,10-DiHOME	36.4	7	C ₁₈ H ₃₄ O ₄	314.2	[M+H-H2O)+	297.2424213	297.243	0.812
Halocynthiaxanthin	36.6	1	C ₄₀ H ₅₄ O ₄	598.4	[M+H)+	599.4094867	599.408	4.148
MLS001076098-01!	36.6	3	C ₂₂ H ₃₂ O ₃	344.2	[M+H)+	345.2424213	345.241	5.219
Norgestrel	36.6	5	C ₂₁ H ₂₈ O ₂	312.2	[M-H]-	311.2016537	311.202	1.056
16,16-Dimethylprostaglandin A2	36.7	2	C ₂₂ H ₃₄ O ₄	362.2	[M+H)+	363.252986	363.253	0.536
Glyceryl linolenate	36.9	5	C ₂₁ H ₃₆ O ₄	352.3	[M+H)+	353.2686361	353.269	0.644
11-Hydroxy-12E,14Z-eicosadienoic acid	37	37	C ₂₀ H ₃₆ O ₃	324.3	[M-H]-	323.2591686	323.259	1.281
12'-Apozeaxanthin	37.0	3	C ₂₅ H ₃₄ O ₂	366.3	[M+H)+	367.2631568	367.256	22.433
Pacificanone A	37.3	8	C ₂₀ H ₃₄ O ₃	322.3	[M+Na)+	345.2400156	345.241	2.712
Pinolenic acid	37.3	8	C ₁₈ H ₃₀ O ₂	278.2	[M+H-H2O)+	261.221292	261.221	0.701
15S-Hydroperoxy-11Z,13E-eicosadienoic acid	37.4	8	C ₂₀ H ₃₆ O ₄	340.3	[M+H)+	341.2686361	341.266	6.837

1-Arachidonoylglycerol	37.7	C ₂₃ H ₃₈ O ₄	378.3	[M+H] ⁺	379.2842861	379.282	5.772
9(10)-Epoxy-12Z-octadecenoic acid	37.7 3	C ₁₈ H ₃₂ O ₃	296.2	[M+H- H ₂ O] ⁺	279.2318567	279.232	1.465
16(S)-HETE	37.8 6	C ₂₀ H ₃₂ O ₃	320.2	[M-H- H ₂ O] ⁻	301.2173037	301.217	1.232
8-HETE	38.0 7	C ₂₀ H ₃₂ O ₃	320.2	[M-H- H ₂ O] ⁻	301.2173037	301.217	1.232
[(2Z)-6-hydroxy-2,6-dimethylocta-2,7-dienyl] 2-(5-ethenyl-5-methyloxolan-2-yl)propanoate	38.1 2	C ₂₀ H ₃₂ O ₄	336.2	[M+HCO 2] ⁻	381.2282624	381.231	8.273
Kinoprene	38.1 7	C ₁₈ H ₂₈ O ₂	276.2	[M+H- H ₂ O] ⁺	259.2056419	259.206	1.055
Palmitamide	38.2 6	C ₁₆ H ₃₃ NO	255.3	[M+H] ⁺	256.2634911	256.264	0.687
Lichestylic acid	38.3 4	C ₁₈ H ₃₄ O ₃	298.3	[2M-H] ⁻	595.4943134	595.498	7.603
OLEATE	38.7 1	C ₁₈ H ₃₄ O ₂	282.3	[M+Na] ⁺	305.245101	305.248	8.062
Oleamide	38.7 3	C ₁₈ H ₃₅ NO	281.3	[M+H] ⁺	282.2791412	282.279	0.725
AA-[d8]	38.7 6	C ₂₀ H ₃₂ O ₂	304.2	[M+H] ⁺	305.2475067	305.248	0.74
14(15)-Epoxyeicosadienoic Acid	38.7 7	C ₂₀ H ₃₄ O ₃	322.3	[M+H] ⁺	323.2580714	323.258	1.235
Khivorin	39.3	C ₃₂ H ₄₂ O ₁₀	586.3	[M+Na] ⁺	609.2670182	609.267	11.397

	1						
25-Hydroxyvitamin D2	39.4						
	2	C ₂₈ H ₄₄ O ₂	412.3	[M+H] ⁺	413.3414071	413.327	35.596
Erucamide	41.7						
	7	C ₂₂ H ₄₃ NO	337.3	[M+H] ⁺	338.3417414	338.342	0.446
ACETOACETATE	1.03	C ₄ H ₆ O ₃	102	[2M+H] ⁺	205.0706646	205.071	17.854
L-Glu	1.05	C ₃ H ₉ NO ₄	147.1	[M+H] ⁺	148.0604342	148.06	0.535
Gln-Glu	1.1	C ₁₀ H ₁₇ N ₃ O ₆	275.1	[M-H] ⁻	274.1044588	274.104	0.743
METHYLMALONATE	1.11	C ₄ H ₆ O ₄	118	[M+HCO 2] ⁻	163.0248115	163.024	7.731
N-Methylthreonine	1.12	C ₅ H ₁₁ NO ₃	133.1	[M+H- H ₂ O] ⁺	116.070605	116.071	2.259
Valine	1.13	C ₅ H ₁₁ NO ₂	117.1	[M+H] ⁺	118.086255	118.087	2.087
Malate	1.13	C ₄ H ₆ O ₅	134	[M-H] ⁻	133.0142468	133.014	18.246
Pro	1.14	C ₃ H ₉ NO ₂	115.1	[M+H] ⁺	116.070605	116.071	2.659
AC-LYS-OH	1.16	C ₈ H ₁₆ N ₂ O ₃	188.1	[M+H] ⁺	189.1233688	189.124	4.029
Glu-Gln	1.17	C ₁₀ H ₁₇ N ₃ O ₆	275.1	[M+H- H ₂ O] ⁺	258.108447	258.109	5.136
Methyl 1-aminocyclopropanecarboxylate	1.17	C ₃ H ₉ NO ₂	115.1	[M+H] ⁺	116.070605	116.071	2.268
CITRATE	1.18	C ₆ H ₈ O ₇	192	[M+Na] ⁺	215.0162233	215.016	1.158
DL-Threonine methyl ester	1.18	C ₅ H ₁₁ NO ₃	133.1	[M+H- H ₂ O] ⁺	116.070605	116.071	2.268

Pro-Gly	1.19	C ₇ H ₁₂ N ₂ O ₃	172.1	[M+H-H ₂ O] ⁺	155.081504	155.082	0.65
Arginine	1.22	C ₆ H ₁₄ N ₄ O ₂	174.1	[M+H] ⁺	175.1189521	175.119	1.333
PIDOLATE	1.26	C ₃ H ₇ NO ₃	129	[M+H] ⁺	130.0498695	130.05	1.75
Leu-Gly	1.27	C ₈ H ₁₆ N ₂ O ₃	188.1	[M+H] ⁺	189.1233688	189.124	4.025
4-ACETAMIDOBUTANOATE	1.38	C ₆ H ₁₁ NO ₃	145.1	[M+H-H ₂ O] ⁺	128.070605	128.071	1.23
.alpha.-L-Glu-L-Asp	1.38	C ₉ H ₁₄ N ₂ O ₇	262.1	[M+H-H ₂ O] ⁺	245.0768126	245.078	4.022
Alanine-2,3,3,3-d ₄	1.49	C ₃ H ₇ NO ₂	93.1	[M+HCO ₂] ⁻	134.0458813	134.046	0.799
Ile-Ser	1.52	C ₉ H ₁₈ N ₂ O ₄	218.1	[M+H] ⁺	219.1339335	219.134	1.656
Leucenol	1.52	C ₈ H ₁₀ N ₂ O ₄	198.1	[M+HCO ₂] ⁻	243.0622597	243.062	2.151
N-Acetylglutamate	1.52	C ₇ H ₁₁ NO ₅	189.1	[M-H] ⁻	188.056446	188.056	4.372
PyroGlu-Val	1.55	C ₁₀ H ₁₆ N ₂ O ₄	228.1	[M+H] ⁺	229.1182834	229.119	1.449
N-Fructosyl isoleucine	1.57	C ₁₂ H ₂₃ NO ₇	293.1	[M+H] ⁺	294.1547285	294.125	145.85 5
Arg-Leu	1.59	C ₁₂ H ₂₅ N ₅ O ₃	287.2	[M+H] ⁺	288.2030161	288.201	8.78
Isovalerylglycine	1.61	C ₇ H ₁₃ NO ₃	159.1	[M+Na] ⁺	182.078764	182.08	20.477
Ile-Asp-Arg	1.61	C ₁₆ H ₃₀ N ₆ O ₆	402.2	[M-H] ⁻	401.2154062	401.218	7.034
Tyr	1.62	C ₉ H ₁₁ NO ₃	181.1	[M+H] ⁺	182.0811697	182.081	1.065

TYROSINE	1.62	C ₉ H ₁₁ NO ₃	181.1	[M-H]-	180.0666168	180.065	6.42
Ile-Asn	1.63	C ₁₀ H ₁₉ N ₃ O ₄	245.1	[M+H]+	246.1448325	246.145	0.676
Gln-Met	1.63	C ₁₀ H ₁₉ N ₃ O ₄ S	277.1	[M+H]+	278.1169035	278.117	7.115
ASUCCIN	1.67	C ₄ H ₆ O ₄	118	[M-H]-	117.0193322	117.018	12.694
Ile	1.75	C ₆ H ₁₃ NO ₂	131.1	[M+H]+	132.1019051	132.102	3.028
Ile-Met(O)	1.82	C ₁₁ H ₂₂ N ₂ O ₄ S	278.1	[M+H]+	279.1373046	279.137	1.499
Thr-Ile	1.99	C ₁₀ H ₂₀ N ₂ O ₄	232.1	[M+HCO 2]-	277.14051	277.144	13.136
Glutarate	2.41	C ₅ H ₈ O ₄	132	[M+HCO 2]-	177.0404616	177.039	5.826
Phe-Ser	2.47	C ₁₂ H ₁₆ N ₂ O ₄	252.1	[M+H]+	253.1182834	253.119	1.622
Ile-Glu	2.64	C ₁₁ H ₂₀ N ₂ O ₅	260.1	[M+H]+	261.1444982	261.145	1.238
Val-Val	2.79	C ₁₀ H ₂₀ N ₂ O ₃	216.1	[M+H]+	217.154669	217.155	1.546
Gln-Tyr	2.86	C ₁₄ H ₁₉ N ₃ O ₅	309.1	[M+H]+	310.1397472	310.136	14.218
Phe	3.06	C ₉ H ₁₁ NO ₂	165.1	[M+H]+	166.086255	166.086	1.355
Val-Pro	3.09	C ₁₀ H ₁₈ N ₂ O ₃	214.1	[M+H- H ₂ O]+	197.1284542	197.129	1.244
N-Fructosyl phenylalanine	3.42	C ₁₅ H ₂₁ NO ₇	327.1	[M+H]+	328.1390785	328.151	37.897
Ser-Leu	3.55	C ₉ H ₁₈ N ₂ O ₄	218.1	[M+H]+	219.1339335	219.134	1.656

Asn-Leu	3.63	C ₁₀ H ₁₉ N ₃ O ₄	245.1	[M+H] ⁺	246.1448325	246.143	8.446
L-Alanyl-L-norleucine	3.7	C ₉ H ₁₈ N ₂ O ₃	202.1	[M-H] ⁻	201.124466	201.124	3.765
Acetylproline	3.98	C ₇ H ₁₁ NO ₃	157.1	[M+H] ⁺	158.0811697	158.081	1.55
4-Oxohexanoate	4.04	C ₆ H ₁₀ O ₃	130.1	[M-H] ⁻	129.0557177	129.054	11.419
Gly-Leu	4.1	C ₈ H ₁₆ N ₂ O ₃	188.1	[M+H] ⁺	189.1233688	189.124	1.81
Ile-Asp	4.33	C ₁₀ H ₁₈ N ₂ O ₅	246.1	[M+H- H ₂ O] ⁺	229.1182834	229.119	1.449
Asp-Leu	4.33	C ₁₀ H ₁₈ N ₂ O ₅	246.1	[M-H] ⁻	245.1142952	245.114	1.542
Phe-Ala	4.45	C ₁₂ H ₁₆ N ₂ O ₃	236.1	[M+H] ⁺	237.1233688	237.124	1.591
Tyr-Pro	4.84	C ₁₄ H ₁₈ N ₂ O ₄	278.1	[M+H] ⁺	279.1339335	279.136	5.876
Leu-Glu	4.9	C ₁₁ H ₂₀ N ₂ O ₅	260.1	[M+H] ⁺	261.1444982	261.145	0.941
Ile-Val	5.21	C ₁₁ H ₂₂ N ₂ O ₃	230.2	[M+H] ⁺	231.170319	231.171	1.523
Pro-Leu	5.23	C ₁₁ H ₂₀ N ₂ O ₃	228.1	[M+H] ⁺	229.154669	229.155	1.315
Ser-Phe	5.34	C ₁₂ H ₁₆ N ₂ O ₄	252.1	[M+H] ⁺	253.1182834	253.119	1.666
Phe-Thr	5.77	C ₁₃ H ₁₈ N ₂ O ₄	266.1	[M+H] ⁺	267.1339335	267.134	1.658
Ala-Phe	5.98	C ₁₂ H ₁₆ N ₂ O ₃	236.1	[M+H] ⁺	237.1233688	237.124	1.233
Leu-Pro	6.14	C ₁₁ H ₂₀ N ₂ O ₃	228.1	[M+H] ⁺	229.154669	229.155	1.615
ASP-PHE	6.23	C ₁₃ H ₁₆ N ₂ O ₅	280.1	[M+H] ⁺	281.1131981	281.112	5.015
Val-Leu	6.94	C ₁₁ H ₂₂ N ₂ O ₃	230.2	[M+H] ⁺	231.170319	231.171	1.146

2-amino-9-methanesulfinylnonanoic acid	7.89	C ₁₀ H ₂₁ NO ₃ S	235.1	[M+H] ⁺	236.131491	236.128	13.074
Phe-Val	8.24	C ₁₄ H ₂₀ N ₂ O ₃	264.1	[M+H] ⁺	265.154669	265.155	1.79
L-Tyrosine, ethyl ester	8.32	C ₁₁ H ₁₅ NO ₃	209.1	[M+H] ⁺	210.1124698	210.113	1.64
Tyr-Leu	9.08	C ₁₅ H ₂₂ N ₂ O ₄	294.2	[M+H] ⁺	295.1652336	295.166	1.597
Val-Phe	9.31	C ₁₄ H ₂₀ N ₂ O ₃	264.1	[M+H] ⁺	265.154669	265.155	1.372
Thr-Val-Leu	9.39	C ₁₅ H ₂₉ N ₃ O ₅	331.2	[M+H] ⁺	332.2179975	332.218	0.992
Cyclo(L-Val-L-Pro)	9.87	C ₁₀ H ₁₆ N ₂ O ₂	196.1	[M+HCO 2] ⁻	241.1193806	241.119	2.177
Glu-Ile	9.91	C ₁₁ H ₂₀ N ₂ O ₅	260.1	[M+H- H ₂ O] ⁺	243.1339335	243.134	1.517
Ile-Leu	10.0 1	C ₁₂ H ₂₄ N ₂ O ₃	244.2	[M+H] ⁺	245.1859691	245.186	1.132
Leu-Leu	10.9 1	C ₁₂ H ₂₄ N ₂ O ₃	244.2	[M-H] ⁻	243.1714162	243.171	1.861
3-Oxo-1,8-octanedicarboxylic acid	10.9 4	C ₁₀ H ₁₆ O ₅	216.1	[M-H- H ₂ O] ⁻	197.0819325	197.081	4.258
N-Acetyl-D-norleucine	11.3 2	C ₈ H ₁₅ NO ₃	173.1	[M-H] ⁻	172.0979169	172.097	6.658
3-Methoxycyclohexanecarboxylic acid	11.7	C ₈ H ₁₄ O ₃	158.1	[M+H- H ₂ O] ⁺	141.0910061	141.091	0.999
Ile-Phe	12.6 3	C ₁₅ H ₂₂ N ₂ O ₃	278.2	[M+H] ⁺	279.170319	279.17	4.636

Glu-Phe	12.6 7	C ₁₄ H ₁₈ N ₂ O ₅	294.1	[M-H- H ₂ O]-	275.1037305	275.104	1.026
AC-PHE-OH	13.1 8	C ₁₁ H ₁₃ NO ₃	207.1	[M-H]-	206.0822668	206.082	3.256
Gly-Pro	13.2 3	C ₇ H ₁₂ N ₂ O ₃	174.1	[M-H]-	173.0819325	173.081	6.746
Leu-Gly-Leu	13.9 7	C ₁₄ H ₂₇ N ₃ O ₄	301.2	[M+H] ⁺	302.2074328	302.208	1.225
o-Tyrosine	14.0 6	C ₉ H ₁₁ NO ₃	181.1	[M+H- H ₂ O] ⁺	164.070605	164.071	0.665
3-Cyclohexyl-1,1-dimethylurea	18.1 7	C ₉ H ₁₈ N ₂ O	170.1	[M+H] ⁺	171.1491896	171.149	0.975
His-Thr-Lys	23.8 5	C ₁₆ H ₂₈ N ₆ O ₅	384.2	[M+H- H ₂ O] ⁺	367.2088298	367.21	2.359
IAA-Val	23.9 4	C ₁₅ H ₁₈ N ₂ O ₃	274.1	[M+H- H ₂ O] ⁺	257.1284542	257.129	0.906
Denatonium	25.2 5	C ₂₁ H ₂₈ N ₂ O	324.2	[M+H] ⁺	325.22744	325.226	6.07
Ser-Lys-Arg	26.7	C ₁₅ H ₃₁ N ₇ O ₅	389.2	[M-H- H ₂ O]-	370.220826	370.226	14.14
3-oxo-C12 homoserine lactone	29.4 7	C ₁₆ H ₂₇ NO ₄	297.2	[M+H] ⁺	298.2012848	298.201	1.016
Lys-Pro-Arg	29.5 1	C ₁₇ H ₃₃ N ₇ O ₄	399.3	[M+H- H ₂ O] ⁺	382.2561143	382.258	6.25

Texanol	30.9 5	C ₁₂ H ₂₄ O ₃	216.2	[M+Na] ⁺	239.1617653	239.164	10.567
Lauramidopropylbetaine	30.9 6	C ₁₉ H ₃₈ N ₂ O ₃	342.3	[M+H] ⁺	343.2955195	343.296	0.746
Lys-His-Lys	30.9 7	C ₁₈ H ₃₃ N ₇ O ₄	411.3	[M+H] ⁺	412.266679	412.269	6.586
Myristamidopropyl betaine	32.8 5	C ₂₁ H ₄₂ N ₂ O ₃	370.3	[M+H] ⁺	371.3268197	371.327	0.764
Lauryl sulfate	33.3 7	C ₁₂ H ₂₆ O ₄ S	266.2	[M-H] ⁻	265.1479039	265.147	1.721
C12-AE1S (TENTATIVE)	34.5 4	C ₁₄ H ₃₀ O ₅ S	310.2	[M-H] ⁻	309.1741186	309.174	1.16
Diethylene glycol dodecyl ether sulfate	35.0 6	C ₁₆ H ₃₄ O ₆ S	354.2	[M-H] ⁻	353.2003334	353.2	1.566
Palmitoylglycine	35.2 4	C ₁₈ H ₃₅ NO ₃	313.3	[M+H-H ₂ O] ⁺	296.2584057	296.244	50.501
Myristyl sulfate	35.7 1	C ₁₄ H ₃₀ O ₄ S	294.2	[M-H] ⁻	293.179204	293.182	26.37
N-Oleoyl-L-serine	36.1 9	C ₂₁ H ₃₉ NO ₄	369.3	[M-H] ⁻	368.2806323	368.28	1.477
Oleyl sarcosine	38.3 5	C ₂₁ H ₃₉ NO ₃	353.3	[M-H] ⁻	352.2857177	352.285	1.434
4-Pyridoxate	1.08	C ₈ H ₉ NO ₄	183.1	[M+H] ⁺	184.0604342	184.064	21.359
Vitamin C	1.14	C ₆ H ₈ O ₆	176	[2M-H] ⁻	351.0568995	351.058	5.338

.beta.-Homoproline	1.18	C ₆ H ₁₁ NO ₂	129.1	[M+H] ⁺	130.086255	130.086	1.253
Isonicotinate	1.44	C ₆ H ₅ NO ₂	123	[M+H] ⁺	124.0393049	124.039	1.555
Niacinamide	1.44	C ₆ H ₆ N ₂ O	122	[M+H] ⁺	123.0552893	123.056	1.787
Adenine	1.46	C ₅ H ₅ N ₅	135.1	[M+H] ⁺	136.0617716	136.062	1.295
Xanthine	1.46	C ₅ H ₄ N ₄ O ₂	152	[M-H] ⁻	151.0261489	151.025	9.251
2-Furoate	1.92	C ₅ H ₄ O ₃	112	[M+H] ⁺	113.0233204	113.024	3.494
5-HYDROXYTRYPTOPHAN	1.99	C ₁₁ H ₁₂ N ₂ O ₃	220.1	[M+H] ⁺	221.0920687	221.092	3.82
Hypoxanthine	2.77	C ₅ H ₄ N ₄ O	136	[M+H] ⁺	137.0457872	137.046	1.156
FAPy-adenine	2.81	C ₅ H ₇ N ₅ O	153.1	[M+H-H ₂ O] ⁺	136.0617716	136.062	2.949
Indoline	3.1	C ₈ H ₉ N	119.1	[M+H] ⁺	120.0807757	120.081	2.967
Guanine	3.1	C ₅ H ₅ N ₅ O	151	[M+H] ⁺	152.0566862	152.057	0.502
Indacaterol	3.1	C ₂₄ H ₂₈ N ₂ O ₃	392.4	[M+HCO ₂] ⁻	437.2081956	437.214	12.997
4-Chromanone	3.2	C ₉ H ₈ O ₂	148.1	[M+H-H ₂ O] ⁺	131.0491413	131.049	1.499
MEVALOLACTONE	4.07	C ₆ H ₁₀ O ₃	130.1	[M+H] ⁺	131.0702706	131.071	2.394
Serotonin	5.78	C ₁₀ H ₁₂ N ₂ O	176.1	[M+H-H ₂ O] ⁺	159.0916748	159.092	0.591
Indole	5.79	C ₈ H ₇ N	117.1	[M+H] ⁺	118.0651257	118.065	2.496
Indolelactic acid	5.82	C ₁₁ H ₁₁ NO ₃	205.1	[M+H] ⁻	188.070605	188.071	1.361

					H2O)+			
Trp	5.83	C ₁₁ H ₁₂ N ₂ O ₂	204.1	[M+H] ⁺	205.0971541	205.097	1.269	
2-TRIMETHYLSILYLOXY-N-(2-(DIETHYLAMINO)ETHYL)-4-QUINOLINECARBOXAMIDE	6.95	C ₁₉ H ₂₉ N ₃ O ₂ Si	359.2	[M+H] ⁺	360.2101802	360.213	8.463	
Lyxoflavin	11.9							
	9	C ₁₇ H ₂₀ N ₄ O ₆	376.1	[M+H] ⁺	377.1455608	377.146	0.884	
gamma-Undecalactone	13.0							
	8	C ₁₁ H ₂₀ O ₂	184.1	[M+Na] ⁺	207.1355506	207.138	12.476	
PYRIDOXINE	13.8							
	1	C ₈ H ₁₁ NO ₃	169.1	[M-H- H2O] ⁻	150.0560521	150.055	8.876	
Quinolin-7-ol	14.5							
	3	C ₉ H ₇ NO	145.1	[M-H] ⁻	144.0454874	144.044	9.172	
Indole-6-carboxaldehyde	14.6							
	7	C ₉ H ₇ NO	145.1	[M+H] ⁺	146.0600403	146.06	0.984	
Loliolide	15.3	C ₁₁ H ₁₆ O ₃	196.1	[M+H] ⁺	197.1172208	197.117	1.002	
3-ETHOXYCARBONYL-6-ISOPROPYL-1-OXA-3,3A,4,5,6,7,8,8A-OCTAHYDROAZULEN-2(1H)-ONE	15.5							
	3	C ₁₅ H ₂₄ O ₄	268.2	[M+HCO 2] ⁻	313.1656621	313.166	0.476	
1,5,6,7-TETRAHYDRO-4H-INDOL-4-ONE	21.1							
	3	C ₈ H ₉ NO	135.1	[M+HCO 2] ⁻	180.0666168	180.065	6.42	
tubermycin B	25.5							
	9	C ₁₃ H ₈ N ₂ O ₂	224.1	[M+H] ⁺	225.0658539	225.066	0.726	
2-Heptyl-4-hydroxyquinoline N-oxide	28.4	C ₁₆ H ₂₁ NO ₂	259.2	[M+H] ⁻	242.1539407	242.154	1.026	

				H2O)+			
Latanoprost lactone diol	29.4 8	C ₁₈ H ₂₄ O ₄	304.2	[M+H] ⁺	305.1747357	305.173	6.2
Sclareolide	29.6 3	C ₁₆ H ₂₆ O ₂	250.2	[M+Na] ⁺	273.1825008	273.185	9.091
2-heptylquinolin-4(1H)-one	30.3	C ₁₆ H ₂₁ NO	243.2	[M+H] ⁺	244.1695907	244.17	0.536
xi-5-Dodecanolide	31.2 1	C ₁₂ H ₂₂ O ₂	198.2	[M+Na] ⁺	221.1512006	221.154	11.43
Koninginin A	31.7 7	C ₁₆ H ₂₈ O ₄	284.2	[M+Na] ⁺	307.1879801	307.19	7.893
Koninginin E	31.8 2	C ₁₆ H ₂₆ O ₄	282.2	[M-H] ⁻	281.1758329	281.176	1.187
Andrographolide	32.0 3	C ₂₀ H ₃₀ O ₅	350.2	[M+H- H2O] ⁺	333.2060358	333.204	5.345
NCGC00380405-01_C24H35NO5_1H- Cycloundec[d]isoindole-1,12,15-trione, 2,3,3a,4,6a,9,10,11,13,14-decahydro-11,13- dihydroxy-4,5,8-trimethyl-3-(2- methylpropyl)-, (7E)-	32.3 2	C ₂₄ H ₃₅ NO ₅	417.3	[M+H] ⁺	418.2587997	418.248	26.739
Bisabolol oxide A	32.4 3	C ₁₅ H ₂₆ O ₂	238.2	[M+Na] ⁺	261.1825008	261.184	5.785
Sedanolide	32.4 5	C ₁₂ H ₁₈ O ₂	194.1	[M+H] ⁺	195.1379563	195.138	1.656
2,2,5,7,8-PENTAMETHYLCHROMAN-6- OL	32.5 7	C ₁₄ H ₂₀ O ₂	220.1	[M+H] ⁺	221.1536063	221.154	1.1

3,7-Epoxyecaryophyllan-6-One	34.0 6	C ₁₅ H ₂₄ O ₂	236.2	[M+HCO 2]-	281.1758329	281.176	1.187
Phthalic anhydride	35.1 4	C ₈ H ₄ O ₃	148	[M+H] ⁺	149.0233204	149.023	1.33
2-ETHYLHEXANAL ETHYLENE GLYCOL ACETAL	38.8 3	C ₁₀ H ₂₀ O ₂	172.1	[2M-H] ⁻	343.2853833	343.285	1.256
Deoxykhivorin	39.7 8	C ₃₂ H ₄₂ O ₉	570.3	[M+Na] ⁺	593.2721036	593.276	6.018
Pheophorbide a	40.2 7	C ₃₅ H ₃₆ N ₄ O ₅	592.3	[M+H] ⁺	593.2758467	593.276	0.767
Dopamine	1.36	C ₈ H ₁₁ NO ₂	153.1	[M+H- H ₂ O] ⁺	136.0756904	136.076	1.271
Phenylacetic acid	1.37	C ₈ H ₈ O ₂	136.1	[M+H- H ₂ O] ⁺	119.0491413	119.067	152.19 7
4-Aminobenzoic acid	1.45	C ₇ H ₇ NO ₂	136	[M+H] ⁺	137.0471299	137.046	8.712
p-Toluamide	1.63	C ₈ H ₉ NO	135.1	[2M-H] ⁻	269.1295514	269.131	5.052
Betaxolol	7.08	C ₁₈ H ₂₉ NO ₃	307.2	[M+Na] ⁺	330.2039645	330.203	2.125
5-Amino-2-methoxyphenol	7.71	C ₇ H ₉ NO ₂	139.1	[M-H] ⁻	138.0560521	138.055	8.695
3,5-Dihydroxybenzyl alcohol	8.68	C ₇ H ₈ O ₃	140	[M-H- H ₂ O] ⁻	121.029503	121.028	11.885
4-Methylhippuric acid	11.8 6	C ₁₀ H ₁₁ NO ₃	193.1	[M-H] ⁻	192.0666168	192.066	3.974
ANISYL ISOVALERATE	14.9	C ₁₃ H ₁₈ O ₃	222.1	[M+H] ⁺	223.1328709	223.133	0.916

	1						
2-(1-METHOXYBENZYL)CYCLOPENTANONE	14.9	C ₁₃ H ₁₆ O ₂	204.1	[M+H] ⁺	205.1223062	205.123	1.647
	1						
BENZALACETONE	17.9	C ₁₀ H ₁₀ O	146.1	[M+H] ⁺	147.0804414	147.081	0.453
	4						
Tyramine	21.1	C ₈ H ₁₁ NO	137.1	[M-H] ⁻	136.0767875	136.075	9.838
	5						
P-CRESOL	22.6	C ₇ H ₈ O	108.1	[M+H] ⁺	109.0647913	109.065	2.861
	22.6						
Pentamidine	23.9	C ₁₉ H ₂₄ N ₄ O ₂	340.2	[M-H] ⁻	339.1826496	339.181	4.97
	5						
NCGC00160195-01!2-(5-Hydroxymethyl-8-methyl-3-oxa-bicyclo[3.3.1]non-7-en-2-yl)-phenol	25.6	C ₁₆ H ₂₀ O ₃	260.1	[M+H] ⁺	261.148521	261.149	0.46
	25.6						
Bisoprolol	27.5	C ₁₈ H ₃₁ NO ₄	325.2	[M+HCO 2] ⁻	370.2235113	370.223	0.926
	5						
BENZALDEHYDE DIETHYLACETAL	27.8	C ₁₁ H ₁₆ O ₂	180.1	[M+H] ⁺	181.1223062	181.122	1.259
	1						
3,4-Dimethylbenzaldehyde	28.7	C ₉ H ₁₀ O	134.1	[M+H] ⁺	135.0804414	135.081	1.177
	9						
Olivetol	29.2	C ₁₁ H ₁₆ O ₂	180.1	[M+H] ⁺	181.1223062	181.122	0.827
	4						
4-Phenylbutyric acid	30.0	C ₁₀ H ₁₂ O ₂	164.1	[M+H- H ₂ O] ⁺	147.0804414	147.08	1.057
	6						
3,4-Dimethylbenzoic acid	30.0	C ₉ H ₁₀ O ₂	150.1	[M+H] ⁺	151.075356	151.075	0.792
	30.0						

	6						
Latanoprost lactol	30.7 3	C ₁₈ H ₂₆ O ₄	306.2	[M-H]-	305.1758329	305.176	0.989
2-(1-METHOXYBENZYL)CYCLOHEXANONE	31.1 9	C ₁₄ H ₁₈ O ₂	218.1	[M+H]+	219.1379563	219.138	0.749
shogaol	31.3 2	C ₁₇ H ₂₄ O ₃	276.2	[M+H]+	277.1798211	277.18	1.049
6-Gingerol	31.3 5	C ₁₇ H ₂₆ O ₄	294.2	[M+H]+	295.1903858	295.194	13.219
(3S,4S)-5-BENZYLOXY-3-METHOXYETHOXYMETHOXY-4-METHYLPENTAN-2-OL	31.3 8	C ₁₇ H ₂₈ O ₅	312.2	[M+Na]+	335.1828947	335.183	0.928
Nadolol	31.6	C ₁₇ H ₂₇ NO ₄	309.2	[M-H]-	308.1867319	308.193	18.787
3-PHENYLPROPANOL	31.8 9	C ₉ H ₁₂ O	136.1	[M+H-H ₂ O]+	119.0855268	119.086	1.186
1-Phenyl-1-hexyn-3-ol	31.9 3	C ₁₂ H ₁₄ O	174.1	[M+H-H ₂ O]+	157.1011768	157.101	0.368
Methyleugenol	31.9 4	C ₁₁ H ₁₄ O ₂	178.1	[M+H]+	179.1066561	179.107	0.766
4-BENZYLOXY-3-HYDROXY-2-METHYL-1-BUTENE	31.9 4	C ₁₂ H ₁₆ O ₂	192.1	[M+H]+	193.1223062	193.123	1.448
4-BENZYLOXY-2-METHYL-1,3-BUTADIENE	31.9 4	C ₁₂ H ₁₄ O	174.1	[M+H]+	175.1117415	175.112	0.896
2,4-dimethylphenylformamid	32.5	C ₉ H ₁₁ NO	149.1	[M+HCO	194.0822668	194.082	2.835

	4			2]-			
Methylgingerol	32.8 5	C ₁₈ H ₂₈ O ₄	308.2	[M-H]-	307.1914829	307.191	0.949
Cannabidiolic acid	33.4 5	C ₂₂ H ₃₀ O ₄	358.2	[M+H]+	359.2216859	359.219	6.815
6-Acetyl-1,1,2,4,4,7-hexamethyltetralin	33.7 8	C ₁₈ H ₂₆ O	258.2	[M+H]+	259.2056419	259.206	0.585
Dodecylbenzenesulfonic acid	35.7 8	C ₁₈ H ₃₀ O ₃ S	326.2	[M-H]-	325.1842894	325.184	1.212
MANNITOL	1.05	C ₆ H ₁₄ O ₆	182.1	[M+H- H ₂ O]+	165.0757499	165.076	1.079
Erythrose	1.06	C ₄ H ₈ O ₄	120	[M+HCO 2]-	165.0404616	165.038	16.296
Melezitose	1.07	C ₁₈ H ₃₂ O ₁₆	504.2	[M+Na]+	527.1582556	527.159	2.341
GLCA	1.08	C ₆ H ₁₀ O ₇	194	[M-H]-	193.0353762	193.034	4.663
4-Fluoro-.alpha.-pyrrolidinobutiophenone	1.09	C ₁₅ H ₂₀ FNO	249.3	[M+H]+	236.1445189	236.142	40.244
Sorbitol	1.09	C ₆ H ₁₄ O ₆	182.1	[M-H- H ₂ O]-	163.061197	163.06	10.162
Arabinonic acid	1.1	C ₅ H ₁₀ O ₆	166	[2M-H]-	331.0881996	331.084	13.526
Glycerate	1.1	C ₃ H ₆ O ₄	106	[M-H]-	105.0193322	105.018	14.384
Xylose	1.1	C ₅ H ₁₀ O ₅	150.1	[M-H- H ₂ O]-	131.0349823	131.034	10.141

Acetamidopropanal	1.11	C ₅ H ₉ NO ₂	115.1	[M-H]-	114.0560521	114.054	14.161
Threonic acid	1.14	C ₄ H ₈ O ₅	136	[2M-H]-	271.0670703	271.054	66.382
Sorbitol 6-phosphate	1.3	C ₆ H ₁₅ O ₉ P	262	[M-H]-	261.0380922	261.04	57.815
Salicylaldehyde	1.59	C ₇ H ₆ O ₂	122	[M+H]+	123.0440559	123.044	1.898
Ethyl glucuronide	1.64	C ₈ H ₁₄ O ₇	222.1	[M+HCO 2]-	267.0721556	267.073	3.168
D-Glucose	1.91	C ₆ H ₁₂ O ₆	180.1	[M-H- H ₂ O]-	161.045547	161.044	7.579
Phenethylamine glucuronide	3.06	C ₁₄ H ₁₉ N O ₆	297.1	[M-H- H ₂ O]-	278.1033962	278.107	11.908
N-Acetylmuramic Acid	3.12	C ₁₁ H ₁₉ NO ₈	293.1	[M-H]-	292.1037901	292.104	1.071
PANTOTHENATE	4.15	C ₉ H ₁₇ NO ₅	219.1	[M+H]+	220.1179491	220.118	1.417
VITAMIN B5	4.17	C ₉ H ₁₇ NO ₅	219.1	[M+H]+	220.1179491	220.118	1.417
2-(hydroxymethyl)-6-[[[(1R,4S)-2,2,4-trimethyl-3-oxabicyclo[2.2.2]octan-5-yl]oxy]oxane-3,4,5-triol	13.6 4	C ₁₆ H ₂₈ O ₇	332.2	[M-H- H ₂ O]-	313.1656621	313.165	0.788
Thymoquinone	17.9 1	C ₁₀ H ₁₂ O ₂	164.1	[M+H]+	165.0910061	165.091	0.565
4-Oxo-2-nonenal	20.4	C ₉ H ₁₄ O ₂	154.1	[M+H- H ₂ O]+	137.0960915	137.096	0.835
13,14-Dihydro-15-ketotetranorprostaglandin E2	21.6 3	C ₁₆ H ₂₆ O ₅	298.2	[M+Na]+	321.1672446	321.167	0.717

LY-255283	23.2 3	C ₁₉ H ₂₈ N ₄ O ₃	360.2	[M+H- H ₂ O] ⁺	343.2128525	343.212	2.732
JASMONE	25.5	C ₁₁ H ₁₆ O	164.1	[M+H] ⁺	165.1273916	165.128	1.207
13,14-Dihydro-15-ketotetranorprostaglandin D2	25.6 4	C ₁₆ H ₂₆ O ₅	298.2	[M-H- H ₂ O] ⁻	279.1601828	279.16	1.342
4-Methyl-.alpha.-ethylaminopentiophenone	28.4	C ₁₄ H ₂₁ NO	219.2	[M+Na] ⁺	242.151535	242.154	10.574
Polygodial	30.0 6	C ₁₅ H ₂₂ O ₂	234.2	[M+H] ⁺	235.1692564	235.169	0.776
4-Hydroxy-3-(3-methyl-2- butenyl)acetophenone	30.2 1	C ₁₃ H ₁₆ O ₂	204.1	[M+H] ⁺	205.1223062	205.123	1.329
Isophorone	31.8 6	C ₉ H ₁₄ O	138.1	[M+H- H ₂ O] ⁺	121.1011768	121.101	0.615
2-Adamantanone	31.9 7	C ₁₀ H ₁₄ O	150.1	[M+H- H ₂ O] ⁺	133.1011768	133.101	0.834
(4S,5S,6R)-5-methoxy-4-[(2R,3R)-2-methyl- 3-(3-methylbut-2-enyl)oxiran-2-yl]-1- oxaspiro[2.5]octan-6-ol	33.1 3	C ₁₆ H ₂₆ O ₄	282.2	[M+H- H ₂ O] ⁺	265.1798211	265.18	1.568
Acetildenafil	35.6 2	C ₂₅ H ₃₄ N ₆ O ₃	466.3	[M+H- H ₂ O] ⁺	449.2659507	449.266	1.105
Ethylene glycol tetradecyl ether sulfate	37.2 1	C ₁₆ H ₃₄ O ₅ S	338.2	[M-H] ⁻	337.2054187	337.205	1.892
Spiroxamine	37.5	C ₁₈ H ₃₅ NO ₂	297.3	[M+H- H ₂ O] ⁺	280.2634911	280.264	0.607
3.6.9.12-Tetraoxatetracosan-1-ol	37.5	C ₂₀ H ₄₂ O ₅	362.3	[M+H] ⁺	363.3105009	363.311	0.785

		1						
	Guanosine	1.15	C ₁₀ H ₁₃ N ₅ O ₅	283.1	[M+H] ⁺	284.098945	284.101	7.07
	Cytidine	1.32	C ₉ H ₁₃ N ₃ O ₅	243.1	[M+H] ⁺	244.092797	244.093	1.163
	URIDINE	1.43	C ₉ H ₁₂ N ₂ O ₆	244.1	[M+HCO 2] ⁻	289.067739	289.067	18.417
	CGMP	1.51	C ₁₀ H ₁₂ N ₅ O ₇ P	345	[M+H] ⁺	346.0547108	346.055	0.986
	Allopurinol riboside	1.65	C ₁₀ H ₁₂ N ₄ O ₅	268.1	[2M-H] ⁻	535.1542625	535.154	0.951
	Ado	1.7	C ₁₀ H ₁₃ N ₅ O ₄	267.1	[M+H] ⁺	268.1040303	268.104	0.684
	INO	1.8	C ₁₀ H ₁₂ N ₄ O ₅	268.1	[2M+H] ⁺	537.1688154	537.169	0.687
	dA	1.8	C ₁₀ H ₁₃ N ₅ O ₃	251.1	[M+H] ⁺	252.1091157	252.109	0.852
	Adenosine	1.88	C ₁₀ H ₁₃ N ₅ O ₄	267.1	[M+HCO 2] ⁻	312.0949567	312.095	1.068
6	Nucleosides, nucleotides, and analogues							
	Adenylyl(3'-5')cytidine	2.43	C ₁₉ H ₂₅ N ₈ O ₁ iP	572.1	[M-H] ⁻	571.1307638	571.131	0.316
	2-O-Methyladenosine	2.72	C ₁₁ H ₁₅ N ₅ O ₄	281.1	[M+H] ⁺	282.1196804	282.12	1.425
	2-O-Methylguanosine	3.12	C ₁₁ H ₁₅ N ₅ O ₅	297.1	[M-H] ⁻	296.1000421	296.1	0.987
	3'-O-Methylinosine	3.27	C ₁₁ H ₁₄ N ₄ O ₅	282.1	[M-H] ⁻	281.0891431	281.089	0.764
	1-Methyladenosine	3.45	C ₁₁ H ₁₅ N ₅ O ₄	281.1	[M+H] ⁺	282.1196804	282.12	1.206
	Thymidine	3.45	C ₁₀ H ₁₄ N ₂ O ₅	242.1	[M+HCO 2] ⁻	287.0884744	287.086	10.133

	N6-Succinyladenosine; LC-tDDA; CE10	4.94	C ₁₄ H ₁₇ N ₅ O ₈	383.1	[M-H]-	382.1004361	382.101	1.062	
	Flavin Mononucleotide	9.87	C ₁₇ H ₂₁ N ₄ O ₉ P	456.1	[M-H]-	455.0973384	455.097	0.937	
	M1dG	33.7 6	C ₁₃ H ₁₃ N ₅ O ₄	303.1	[2M-H]-	605.1862313	605.182	7.3	
	Pongamol	1.07	C ₁₈ H ₁₄ O ₄	294.1	[M+H- H ₂ O]+	277.0859207	277.092	23.267	
	HPLA	1.44	C ₉ H ₁₀ O ₄	182.1	[M+H- H ₂ O]+	165.0546206	165.055	2.081	
	4-COUMARATE	1.48	C ₉ H ₈ O ₃	164	[M+H]+	165.0546206	165.055	2.086	
	albocycline	24.8 5	C ₁₈ H ₂₈ O ₄	308.2	[M+H- H ₂ O]+	291.1954711	291.196	1.183	
	Brefeldin A	25.0 5	C ₁₆ H ₂₄ O ₄	280.2	[M+H]+	281.1747357	281.175	0.923	
7	Phenylpropa noids and polyketides	(E)-3-(4-methoxyphenyl)-1-[2,4,6-trimethoxy- 3-(3-methylbut-2-enyl)phenyl]prop-2-en-1- one	26.7 4	C ₂₄ H ₂₈ O ₅	396.2	[M-H- H ₂ O]-	377.1758329	377.173	6.845
	Octinoxate	28.4 5	C ₁₈ H ₂₆ O ₃	290.2	[M+H]+	291.1954711	291.195	0.515	
	(1S,2S,3E,7R,11E,13R)-2-Hydroxy-7-methyl 6-oxabicyclo[11.3.0]hexadecane-3,11-diene- 5,15-dione	29.1 8	C ₁₆ H ₂₂ O ₄	278.2	[M+H- H ₂ O]+	261.148521	261.149	1.634	
	ALPHA-HEXYLCINNAMALDEHYDE	31.8 6	C ₁₅ H ₂₀ O	216.2	[M+H- H ₂ O]+	199.148127	199.148	1.337	

		PHENYLETHANOLAMINE	3.1	C ₈ H ₁₁ NO	137.1	[M+H-H ₂ O] ⁺	120.0807757	120.081	2.967
		Octylamine	8.4	C ₈ H ₁₉ N	129.2	[M+H] ⁺	130.1590261	130.159	2.591
		4-(1-Phenylcyclohexyl)morpholine	30.2						
			6	C ₁₆ H ₂₃ NO	245.2	[M+Na] ⁺	268.1671851	268.169	8.606
		Lauryldiethanolamine	30.9						
			9	C ₁₆ H ₃₅ NO ₂	273.3	[M+H] ⁺	274.2740558	274.274	0.706
8	Organic nitrogen compounds	N-Methyldodecylamine	31.4						
			7	C ₁₃ H ₂₉ N	199.2	[M+H] ⁺	200.2372764	200.238	1.269
		Tetradecylamine	31.7						
			7	C ₁₄ H ₃₁ N	213.2	[M+H] ⁺	214.2529264	214.253	1.035
		Lauryldimethylamine Oxide	31.7						
			9	C ₁₄ H ₃₁ NO	229.2	[M+H] ⁺	230.2478411	230.246	8.836
		Oleoyl Ethanolamide	36.1						
			36.1	C ₂₀ H ₃₉ NO ₂	325.3	[M+H] ⁺	326.3053559	326.305	0.708
		Enterodiol	30.0						
			3	C ₁₈ H ₂₂ O ₄	302.2	[M+H] ⁺	303.1590856	303.157	7.558
9	Lignans, neolignans and related compounds	6-[3-[(3,4-dimethoxyphenyl)methyl]-4-methoxy-2-(methoxymethyl)butyl]-4-methoxy-1,3-benzodioxole	33.2						
			1	C ₂₄ H ₃₂ O ₇	432.2	[M+H-H ₂ O] ⁺	415.2115151	415.216	10.543
10	Alkaloids and derivatives	Hydromorphone	5.76						
			5.76	C ₁₇ H ₁₉ NO ₃	285.1	[M+H] ⁺	286.1437699	286.149	34.05
