

Supplementary material

Table S1. Untargeted metabolomics of duckweed.

Compound	Class	Abundance duckweed extract replicate 1	Abundance duckweed extract replicate 1	Abundance duckweed extract replicate 1	Composite Spectrum (mass and abundance combinations)	Retention Time
Dimethylselenoniopropanoate	Small Molecule	74478	84886	70276	(178.98517, 2464.5198)(187.99007, 2270.72)(182.9608, 5211.15)(183.96167, 801.4133)(184.95905, 939.35)	1.39
2-[(2'-Methylsulfanyl)Ethyl]Maleate	(methylsulfanyl)Alkyl]Maleate	77559	71230	75845	(171.01503, 6177.4233)(216.01082, 572.87665)	1.48
Diethyldithiocarbamate	Small Molecule	77559	71230	75845	(152.01387, 1155.0533)(171.01503, 6177.4233)	1.48
Oxalosuccinate	Small Molecule	77174	76844	77449	(186.99101, 4130.89)(187.99007, 2209.4434)	1.41
Calystegine A3	Small Molecule	81856	83794	80684	(142.08484, 2377.8699)(183.0825, 3850.78)	2.11
Geranylgeranyl Diphosphate	All-Trans-Polyisoprenyl Diphosphate	86123	87273	84622	(447.17734, 6150.0864)(429.16687, 917.5533)(431.18222, 3778.7034)	6.05
Sophoraflavanone G	Small Molecule	86123	87273	84622	(447.17734, 6150.0864)(429.16687, 917.5533)	6.05
Ajmaline	Small Molecule	92050	81597	88761	(309.2019, 3661.43)(350.1971, 3145.5168)	11.20
(9Z)-12,13-Dihydroxyoctadeca-9-Enoate	Long-Chain 2,3,4-Saturated Fatty Acid // Monounsaturated Fatty Acid	101798	95040	90053	(313.23108, 339.27)(318.20792, 5584.3066)	15.27
N,N-Dihydroxy-L-Dihomomethionine	L-N,N- Dihydroxypolyhomomethionine	98217	96772	92779	(195.0663, 3020.1367)(231.0471, 6451.267)	6.16

N-Benzoyl-L-Glutamate	Monocarboxylic Acid Amide	98217	96772	92779	(231.0471, 6451.267)(252.0836, 1720.1)(274.06537, 3447.4268)	6.16
O-Methylandrocymbine	Alkaloid	97848	95347	97791	(385.18433, 6376.547)(409.17734, 2426.6902)	6.16
7-Methylxanthosine	Modified Nucleoside	99750	106340	98144	(299.09546, 6249.813)(286.1096, 590.14667)	3.73
Antheraxanthin	Xanthophyll	165712	132244	100843	(567.42096, 77819.625)(568.4239, 22485.781)(568.4261, 5712.5103)(589.4079, 408151.5)(590.4094, 67175.31)(591.4106, 6176.3794)	14.73
Porphobilinogen	Small Molecule	175189	184376	101341	(248.07793, 10690.073)(249.08516, 1270.9033)	8.50
(2E)-Hexadecenal	Small Molecule	108944	106092	104421	(261.21814, 6611.8267)(243.20782, 1080.2933)	11.08
Plaunotol	Isoprenoid Derivative	104281	101141	105327	(307.25943, 4410.75)(329.2407, 3446.4434)	21.14
Dimethylselenopropanoate-Amine	Organosulfur Compound	118389	89238	106531	(168.0489, 8417.394)(169.05003, 843.27997)(201.0546, 1007.095)	1.39
3-Ureido-Isobutyrate	Ureidocarboxylate	118389	89238	106531	(168.0489, 8417.394)(169.05003, 843.27997)	1.39
1-Naphthaldehyde	Aromatic Aldehyde	118876	119861	107585	(140.0556, 1599.13)(157.0695, 8059.755)	1.39
3,5-Di-C-Glucosyl-2,4,4',6-Tetrahydroxydibenzoylmethane	Small Molecule	129509	112303	114434	(611.1779, 14230.013)(595.1574, 8364.227)(596.16034, 901.25665)(612.17596, 9758.246)(613.1755, 1982.7767)	15.32
Cyanidin 3-(P-Coumaroyl)-Glucoside	Small Molecule	129509	112303	114434	(595.1574, 8364.227)(596.16034, 901.25665)	5.38

3-Oxo-2-(Cis-2'-Pentenyl)-Cyclopentane-1-(3-Oxo-octanoyl)-CoA	Coenzyme A-Activated Compound	117065	116800	115968	(1054.2856, 4003.3333)(1055.2865, 4273.058)(1056.2852, 3978.8018)(1057.2845, 965.99335)	29.29
Rhamnetin	Flavonol // Flavone	118697	116413	116717	(299.043, 9927.094)(300.04398, 3061.5266)	1.39
Chlorophyll-B	Chlorophyll // Organometallic Compound	152281	127151	116984	(909.53955, 7655.0566)(910.54297, 2982.43)	28.48
(-)-Jasmonoyl-1-Aminocyclopropane-1 Carboxylate	Jasmonoyl-1-Aminocyclopropane-1 Carboxylate	135462	123673	117560	(275.15726, 3353.3867)(297.1387, 4715.8135)	2.38
7,8-Dimethoxy-Flavone	Methoxyflavone	136562	125467	117784	(265.07642, 7197.2266)(268.10068, 301.57666)	2.68
(2E,7Z,10Z,13Z,16Z,19Z)-Docosahexaenoyl-CoA	Small Molecule	133088	137109	120725	(1055.2865, 4323.815)(1056.2852, 4092.625)(1057.2837, 950.25)(1056.2852, 3989.6924)(1057.2849, 986.16754)	29.28
4-Sinapoyloxybutylglucosinolate	Small Molecule	143042	126874	121278	(602.1202, 8376.609)	4.96
C ₁₁ H ₁₇ N ₃ O	Nitroso Compound	119318	116104	123645	(189.12181, 3588.9797)(217.12703, 1954.14)	1.71
Gibberellin A8	Gibberellin	123608	124921	123702	(345.13773, 4178.23)(367.15463, 10226.27)(349.14453, 2678.2566)(386.12866, 5451.4033)	6.16
Tricoumaroyl Spermidine	Amide	130201	119931	125188	(585.2796, 7257.0)	9.33
N-Hydroxy DAP	Small Molecule	130597	120844	125323	(188.06934, 199676.42)(189.0718, 20374.412)	4.28
Palmitoleoyl-CoA	Long-Chain 2,3,4-Saturated Fatty Acyl Co// Hexadecenoyl-Co(N-C16:1coa)	155273	120218	129132	(981.2685, 4647.8335)(982.2669, 4149.7266)(983.26654, 663.55505)	28.68

L-Dopa	Catechol // Non-Proteinogenic A-Amino Acid	131433	130065	129391	(180.0611, 6715.44)(203.05048, 7303.6367)	2.74
Ancymidol	Small Molecule	136265	135564	129840	(256.1263, 4600.573)(238.11346, 1696.5366)(261.14188, 2375.03)	1.98
Cyanidin 3-O-[2\O-(Xylosyl)-6\O-(P-Coumaroyl) Glucoside] 5-O-Malonylglucoside"	Anthocyanin	161778	123837	130966	(980.2678, 4863.7866)(981.2685, 4535.267)(982.2669, 4051.3118)	28.68
(9Z,12Z)-Hexadeca-9,12-Dienoyl-Coa	Long-Chain Fatty Acyl-Coa	161778	138778	130966	(980.2678, 4863.7866)(981.2685, 4535.267)(982.2669, 4051.3118)(983.26654, 638.255)	28.69
C ₂₁ H ₂₉ O ₄	A Terpenophenolic	129480	129040	133074	(327.1968, 4151.2)(350.1821, 5750.1665)	4.06
1,3,7,9-Tetramethylurate	Small Molecule	142591	126274	133123	(206.0789, 9017.34)(230.07607, 2467.3267)	5.96
Pumiloside	Alkaloid	144339	141284	135382	(536.15845, 7439.793)(537.1589, 2144.2185)	24.46
2'-Hydroxy 3,6,7,4'-Tetramethylquercetagen 3'-O-D-Glucoside	Flavonol Derivative	144339	141284	135382	(536.1587, 7427.62)(537.15906, 2172.255)(538.1581, 292.58502)	24.46
C ₂₇ H ₃₀ O ₁₁	Polyketide // Phenol // Phenylpropanoid	144339	141284	135382	(536.15845, 7439.793)(537.1589, 2144.2185)(538.15717, 297.92502)	24.46
Peonidin 3,5-Diglucoside	Anthocyanin	142099	138302	138286	(625.16754, 9068.923)(626.17053, 1017.37665)	5.61
Kaempferol 3-O-(6\O-Feruloyl)-Glucoside"	Flavonol Derivative	147729	138302	138286	(647.1483, 427.02)(625.1673, 9825.37)(626.1703, 953.67)	5.61
2,4-Dihydroxycinnamoyl-Coa	Coenzyme A-Activated Compound	134824	133727	138939	(927.1021, 9818.313)(928.10455, 3321.0066)(911.124, 2012.2266)(913.117, 1497.8265)	5.98
9-(Methylsulfanyl)-2-Oxononanoate	Ω(Methylsulfanyl)-2-Oxoalkanoate	161652	165388	143966	(218.0996, 1281.1567)(240.0815, 7799.4004)	4.69

1-O-Malyl-D-Glucose	C4-Dicarboxylate	142507	150967	145658	(296.0625, 4938.677)(300.04398, 1622.4)	1.54
D,L-5-Fluorotryptophan	Small Molecule	165291	162382	145753	(222.08049, 1490.1733)(205.06667, 2784.5635)(223.09154, 5200.346)	4.18
(E)-9-(Methylsulfanyl)Nonanal Oxime	(E)- Ω (Methylsulfanyl)Alkanal Oxime	159562	155446	146105	(203.13689, 7331.9595)(189.12154, 719.9733)	2.19
(4ar,10bs)-Noroxomaritidine	Noroxomaritidine	152170	150779	146292	(253.10962, 8686.25)(256.1261, 394.82333)	2.19
4-Methylsalicylate	Small Molecule	156974	150325	150589	(151.03748, 10750.716)(135.04266, 2963.7537)	5.83
N, N-Dihydroxytrihomomethionine	L-N,N-Dihydroxypolyhomomethionine	206420	180690	151272	(222.08049, 1345.2001)(205.0667, 2876.4631)(223.09154, 4699.77)	4.18
Coniferaldehyde	Phenylpropanoid	153636	148461	154157	(204.06067, 2738.8633)(205.06624, 5933.5034)	7.36
(S)-Scoulerine	Small Molecule	158542	162430	156041	(332.13016, 11749.964)(333.133, 838.12665)	1.73
1-Alpha;-Linolenoyl-2-Linoleoyl-Phosphatidylcholine	Phosphatidylcholine-36:5	162548	162834	158785	(764.5551, 1356.0034)(803.5339, 11367.724)(804.5368, 4681.1035)	21.96
4-Aminobenzoate	Benzoate	142069	134746	161036	(137.0451, 5859.77)(119.0325, 3259.1)(140.05554, 1384.305)(123.0483, 2824.99)(145.0327, 499.28)	1.43
Trigonelline	Small Molecule	169093	156192	161036	(137.04506, 5744.857)(123.04824, 2567.867)(123.05404, 53031.176)(124.0553, 2578.6833)(165.05305, 13206.007)(147.0419, 2517.76)	2.08

(E)-1-(L-Cysteinyglycin---Yl)-N-Hydroxy-Omega;-(Methylsulfanyl)Hexan-1-Imine	(E)-1-(L-Cysteinyglycin-S-Yl)-N-Hydroxy-Ω(Methylsulfanyl)Alkan-1-Imine	168471	167117	161326	(319.11096, 10013.68)(365.10678, 4947.8135)	4.49
2,7-Dihydroxycadalene	Terpenoid	182067	176152	163675	(213.1211, 1403.96)(216.1319, 1860.35)(236.14673, 1216.7233)(216.13199, 1968.6849)(256.12625, 1743.5732)(238.11346, 1753.3232)	2.19
Hypoxanthine	Purine Base // Nucleic Acid Component	169093	162077	166452	(119.03253, 3388.25)(137.04506, 5539.11)	2.08
3,5-Dihydroxybiphenyl	Organic Aromatic Compound	177912	176998	166845	(186.0661, 16456.342)(187.06401, 12130.876)(168.06123, 10504.943)(173.07695, 851.5234)	1.83
Allysine	Small Molecule	177912	176998	166908	(168.06123, 10504.943)(152.0557, 174875.7)(153.05707, 9151.134)	2.26
Gibberellin A24	Gibberellin	165301	164208	167079	(367.15463, 9237.667)(349.14453, 2421.6833)	6.16
Delphinidin 3-O-Rutinoside-7-O-(6-O-(4-O-(Glucosyl)-Oxybenzoyl)-Glucoside)	Anthocyanidin-3-O-B-D-Glucoside	174820	175251	167443	(1054.2856, 4003.3333)(1055.2865, 4249.165)(1055.2866, 4320.8447)(1056.2852, 3957.02)(1057.2837, 925.645)	29.29
3-Carboxy-7-(Methylsulfanyl)-2-Oxoheptanoate	3-Carboxy-Ω(Methylsulfanyl)-2-Oxoalkanoate	166736	172757	168652	(237.02582, 13919.153)(238.02693, 2091.5764)	1.43
L-Hexahomomethionine	L-Polyhomomethionine	175881	175264	169785	(216.13196, 1929.09)(261.14188, 2452.2234)(236.14668, 5338.0103)	2.06
Dimp	Purine 2'-Deoxyribonucleoside 5'-Monophosphate // Nucleic Acid Component	177356	151890	170035	(316.03024, 3151.2568)(335.00964, 7409.867)	5.98

9,10-Epoxy-10,12Z,15Z-Octadecatrienoate	Small Molecule	167624	170248	171278	(291.192, 8808.353)(293.2073, 998.9167)(275.19742, 3340.1868)	13.07
3,7,3',4'-Tetramethylquercetin 2'-O-D-Glucoside	Flavonol Derivative	192955	187330	174395	(536.15845, 7875.565)(537.1589, 2269.1335)(538.15717, 315.0625)	24.46
3-Benzoyloxypropyl-Glucosinolate	Aliphatic Glucosinolate	181282	175095	174416	(464.05447, 12462.399)	5.98
4'-Hydroxyadonixanthin	Ketocarotenoid	178743	176735	174707	(604.3746, 9439.19)(605.377, 1535.5101)	6.96
N-(2-Methoxy-4-Pyridyl)-N'-Phenylurea	Phenylurea-Type Cytokinin	98055	184376	180824	(248.0779, 10273.101)(249.08527, 1353.0499)	8.50
Pimeloyl-Coa	Small Molecule	180983	179777	184659	(927.1021, 10303.329)(928.10455, 3487.54)(911.124, 2114.38)(913.117, 1577.5332)	5.98
Methylsalicylate	Phenylpropanoid	189723	185864	187687	(137.04506, 3735.11)(153.05693, 8292.696)	2.16
3-Phenylpropanoate	Aromatic Carboxylate // Monocarboxylate // Phenylalkanoate // Phenylpropanoid	189788	188061	194672	(149.0581, 6252.15)(131.04767, 5045.14)	2.73
Uroporphyrinogen-III	Porphyrin	235160	217694	194940	(832.2315, 9443.009)(833.2321, 6981.237)(834.23047, 5569.015)	27.41
Cis-Zeatin	Adenine-Type Cytokinin // Secondary Metabolite	190802	194747	197066	(242.09727, 5748.0566)(220.11566, 5669.505)	2.61
Coniferin	D-Glucoside	201826	195493	198987	(345.13858, 1545.5199)	5.95
Galactinol	Galactinol-Type-Disaccharide-Sugar-Alcohol // Galactosyl Inositol	201826	195493	198987	(343.12228, 14000.55)(344.12476, 1283.2034)	5.95
(Indol-3-yl)Acetyl-L-Tryptophan	Indole Derivative // Modified Amino Acid	201826	195493	198987	(343.12228, 14000.55)(344.12476, 1283.2034)(345.13858, 1545.5199)	5.95

2,4-Diamino-6-Methyl-5,3'-(3-Trifluoromethylphenoxy)Prop-1'-Yloxypyrimidine	Small Molecule	201826	195493	198987	(344.80087, 1405.1266)(345.1381, 1663.95)(345.1388, 1486.3049)	5.95
Gibberellin A8-Catabolite	Gibberellin	200769	195523	199096	(343.12228, 13067.18)(344.12476, 1197.6566)	5.95
L-Homoarginine	Amino Acid	204543	197597	200117	(192.13617, 993.99664)(172.13127, 9898.243)	3.54
Acetylserine	O-Acetylated Amino Acid	197822	187426	203252	(130.04866, 6344.6665)(148.0589, 6352.39)(156.0405, 3555.0369)	1.68
(+)-Catechin	(2r,3s)-Flavan-3-Ol	208873	195930	204294	(291.09396, 7694.814)(313.07535, 5652.69)	7.11
Cryptoxanthin	Xanthophyll	228982	200656	204624	(536.43097, 16082.023)(537.4338, 5794.25)	27.61
N,N-Dihydroxy-L-Valine	Small Molecule	226622	187426	205028	(148.05898, 5053.4165)(130.0487, 7149.9136)(150.0755, 8841.923)(154.0838, 1338.09)(133.05946, 3844.1035)	1.93
16-Hydroxypalmitate	Ω hydroxy Long-Chain Fatty Acid	199879	195044	206796	(294.21094, 10443.86)(276.2006, 1667.9233)	14.95
3-Hydroxy-9-Apo-Delta;-Caroten-9-One	9-Apo-Carotenone	214204	209951	210872	(209.15108, 3363.0632)(191.14076, 8685.637)	8.48
3S-(4-Hydroxyphenyl)-3-Hydroxy-Propanoyl-Coa	Small Molecule	210376	206947	211719	(911.124, 2114.38)(913.117, 1577.5332)	5.98
4alpha;-Carboxy-4methyl-5alpha;-Cholesta-8,24-Dien-3ol	3 β -Hydroxy-4 α -Carboxy-4 β -Methylsteroid	221312	222038	217682	(464.32773, 13078.581)(465.32846, 805.85333)	8.41
(22R,23R)-28-Homobrassinolide 22-Sulfate	(22R,23R)-28-Homobrassinolide Sulfate	240801	228582	218894	(579.2851, 14139.894)(580.288, 3422.41)	17.29
(S)-Nicotine	Alkaloid	255226	233730	237564	(163.12126, 9303.237)(189.1216, 790.12665)	2.03
Glutathione	Thiol // Glutathione And Derivatives	254288	241684	238439	(306.07642, 6539.0938)(307.07956,	2.16

					2188.2966)(290.08243, 1268.6967)	
Lutein	Xanthophyll	255484	247226	239005	(568.42584, 7420.3535)(591.4103, 8137.0347)	6.96
Phosphocholine	Small Molecule	237124	253769	243069	(185.06384, 9106.32)(165.05305, 14771.997)	2.13
(4-Hydroxyphenyl)Acetaldehyde	Aromatic Aldehyde	260664	260261	253899	(119.047264, 2669.4768)(123.05404, 40229.035)(137.0617, 7518.096)	2.13
3-Aminopropyl-Methyl-Phosphinate	Small Molecule	260664	260261	253899	(137.0617, 7518.096)(119.047264, 2669.4768)(143.08012, 14766.527)(121.0635, 388.8667)	2.13
13(S)-Hpote	Hydroperoxy Octadecatrienoate	269345	264662	261813	(309.202, 4671.35)(291.192, 8969.46)(293.2073, 1016.63666)(332.18655, 385.85)	13.07
C ₁₇ H ₂₆ O ₄	Phenylpropanoid	272450	278324	264962	(317.17496, 13871.684)(318.1784, 778.4567)	18.54
Dopamine Quinone	Small Molecule	280215	276339	265590	(152.069, 17273.877)(177.06783, 901.39667)	5.98
Moiramide B	Small Molecule	287956	270514	269764	(455.2415, 10607.367)	2.54
Methoxydihydrosorgoleone	Small Molecule	249183	260687	270156	(358.24008, 11827.906)(359.23886, 2344.6965)	2.06
(7Z,10Z,13Z,16Z,19Z)-Docosa- 7,10,13,16,19-Pentenoate	Long-Chain 2,3,4-Saturated Fatty Acid // Polyunsaturated Fatty Acid	275731	278115	272648	(331.2499, 904.7233)(352.23926, 17242.744)	7.58
71-Hydroxychlorophyll A	Organometallic Compound	366399	303616	277415	(909.53955, 7956.654)(910.54297, 3094.4402)	28.48
1-L-Myo-Inositol-1-P	Myo-Inositol Monophosphate	303926	280168	284249	(241.00218, 16799.184)(242.00298, 4429.8633)	1.40
Dihydrogeranylgeranyl Diphosphate	Small Molecule	309664	290302	285417	(431.18265, 13694.043)(432.186, 493.61)(473.192, 5508.5405)	6.43

Dimethylsulfonio-2-Hydroxybutanoate	Monocarboxylate // Organosulfur Compound	280101	302421	286450	(165.05305, 16083.914)(147.0419, 2958.5967)	2.13
Caffealdehyde	Phenylpropanoid	280101	302421	286450	(165.05305, 16083.914)(168.06136, 3322.867)(147.0419, 2958.5967)	2.13
S-Sulfanylgutathione	Perthiol // Glutathione-S-Conjugate	301388	290986	291147	(320.0419, 17607.883)(321.04028, 543.1467)	5.98
Dtmp	Pyrimidine 2'-Deoxyribonucleoside 5'-Monophosphate // Pyrimidine	301388	290986	291147	(320.0419, 17607.883)(321.04028, 543.1467)(307.0376, 339.43)	5.98
5-(Methylsulfanyl)-2,3-Dioxopentyl 1-Phosphate	Small Molecule	320216	292057	295251	(242.00304, 5403.555)(244.00064, 552.75)(223.98726, 1843.37)(225.98691, 743.12)(246.961, 507.12)	1.40
Melilotate	Aromatic Compound	106925	310391	295276	(165.0531, 9839.504)(148.71303, 6172.0396)(150.0569, 1194.25)	2.13
3-Carboxy-6-(Methylsulfanyl)-2-Oxohexanoate	3-Carboxy- Ω (Methylsulfanyl)-2-Oxoalkanoate	290899	267437	295627	(219.02428, 411.75)(222.027, 1124.14)	1.39
(S)-Laudanosine	Alkaloid	316045	304443	295889	(359.2145, 15060.899)(360.21765, 915.8833)(363.20987, 1191.2833)	16.00
L-Proline	Proteinogenic Amino Acid // Non-Polar Amino Acid // Neutral Amino Acid // L-Amino Acid	328297	289426	300265	(116.069496, 9727.293)(124.05526, 1281.8534)	1.66
2,4-Dinitrobenzenesulfonyl Chloride	C-Nitro Compound	315111	317304	305855	(268.94333, 15580.423)(270.94205, 1107.08)	1.74
Picrocrocin	Apocarotenoid // D-Glucoside	317358	308695	311899	(335.17892, 365.76)(331.18365, 14486.21)(332.18655, 335.87332)	13.07
C ₂₂ H ₃₁ O ₄	A Terpenophenolic	338639	320981	312483	(359.22214, 80795.63)(360.2246, 6347.5522)(361.22635,	11.78

					1753.11)(361.23038, 17998.852)(362.23337, 1989.8633)(367.21472, 1765.7601)	
2-[(5'-Methylsulfanyl)Pentyl]Malate	2-[(Ω methylsulfanyl)Alkyl]Malate	298130	299378	312651	(248.07796, 10368.217)(249.08525, 992.1433)	8.50
Gibberellin A12	Gibberellin	323351	320697	315232	(331.1827, 12112.144)(315.18918, 30034.904)(316.19238, 3266.6335)	15.35
4-Isopropylbenzyl Alcohol	Phenol	347013	282785	317232	(133.104, 17294.5)(177.1002, 2758.5234)	2.08
Gibberellin A14-Aldehyde	Gibberellin	329414	313805	317235	(331.18365, 14708.3)(332.18655, 339.67)(333.2, 24026.771)(334.2028, 3532.3965)(335.21194, 246.73)	13.07
Pelargonidin-3,5-Diglucoside-5-O-Caffeoylgucoside	Small Molecule	337827	329484	322112	(758.21356, 12720.977)(759.21405, 7676.28)(760.21234, 5762.725)(761.2116, 1627.8082)	26.69
3,6-Dihydronicotinate	Vitamin	603169	359389	325856	(129.02092, 29977.682)(130.0231, 527.5)	1.39
Mercuriphenyl Acetate	Small Molecule	344899	336670	326407	(341.01947, 441.485)(315.0104, 2503.09)(321.0174, 6827.44)(321.01752, 7075.1553)	5.98
Triketide Pyrone	Polyketide	339995	294949	326546	(186.06609, 20388.055)(187.06401, 14977.72)(188.06792, 731.03)	1.40
Gossyol-6,6'-Dimethyl Ether	Sesquiterpenoid	367658	354196	353011	(547.2439, 18856.697)(548.2465, 3710.57)	11.93
3-(Indol-3-Yl)Acrylate	Indole Derivative	381570	310489	357023	(168.04892, 6797.305)(169.05003, 843.27997)(187.06401, 15647.742)(188.06792, 779.6533)	1.39

2-Amino-4-Methyl-5-Hydroxyethylthiazole	Thiazole	375100	371337	360717	(164.06673, 752.9067)(164.0407, 18520.76)	5.98
Tetrahydropteroyl-Alpha;-Glutamylglutamate	Tetrahydrofolate	391672	368579	361081	(573.18695, 28352.74)(574.18945, 6278.5493)	7.46
1-Hydroxyglucobrassicin	Indolic Glucosinolate	369149	364791	361407	(464.05447, 10904.603)(469.02234, 11598.173)	5.98
Kaempferol-3-O-Gentiobioside-7-O-Alpha;-L-Rhamnoside	Flavonol-3-O-[D-Glucopyranosyl(1->6)D-Glucopyranoside]-7-O-L-Rhamnopyranoside	379289	367652	362814	(758.21356, 12976.849)(759.21405, 7940.65)(760.21234, 5961.029)(761.2116, 1684.1034)	26.69
Imidazole Acetol-Phosphate	Small Molecule	322194	295960	362891	(222.02693, 1949.6234)(241.00218, 13537.944)(242.00298, 3513.0283)(224.15733, 1111.91)(224.9951, 1720.25)	1.40
4-Coumaroylhexanoylmethane	Small Molecule	367414	370320	372320	(261.1417, 21385.906)(262.1445, 746.75336)	3.64
L-Pipecolate	Pipecolate	406380	384357	378988	(130.08643, 14044.91)(156.07504, 881.48)(136.06084, 61000.887)(137.06163, 2034.9468)	1.69
(S)-2-Hydroxyglutarate	(2S)-2-Hydroxycarboxylate // 2-Hydroxyglutarate	440871	466540	379084	(147.02177, 6662.763)(129.0209, 23436.146)(130.0231, 406.34402)(171.01503, 1512.3467)	1.39
(9Z,12Z)-Octadecadien-6-Ynoate	Long-Chain 2,3,4-Saturated Fatty Acid // Polyunsaturated Fatty Acid	384084	387467	383630	(275.1975, 17163.863)(276.2006, 1343.2533)	14.95
13-Apo-Carotenone	Apocarotenoid // Ketone	412517	393968	390543	(259.2029, 20195.85)(260.20596, 2260.1533)(241.19238, 4177.15)	11.93
6-Methyl-H2-Pterin	Small Molecule	1421871	473063	390719	(177.0674, 5854.8965)(160.05531,	4.49

					10893.087)(205.06633, 3695.3167)	
5-Methyl-Tetrahydropteroyl-Alpha;- Glutamylglutamate	Small Molecule	422297	401020	391928	(591.1972, 24750.225)(592.1999, 4966.6035)	5.80
P-Nitrophenyl-Chitobiose	Chitodextrin // P-Nitrophenyl-Modified Glycoside // C-Nitro Compound	411336	417328	401909	(545.1921, 22531.266)(546.19476, 4434.98)	6.73
(9Z)-12,13,17-Trihydroxyoctadeca-9-Enoate	Long-Chain 2,3,4-Saturated Fatty Acid // Monounsaturated Fatty Acid	408715	405069	409730	(311.21802, 6841.11)(334.20255, 9367.167)(335.214, 1706.8301)	13.43
Estrone	Estrogen-Like Compound	446005	419364	412184	(270.1542, 169156.14)(271.15637, 17916.18)(272.15805, 462.79498)(252.15448, 31423.14)(253.15741, 2411.9475)	7.68
Deoxycholate	Bile Acid	480591	449857	415932	(391.27795, 3374.5266)(414.26425, 14399.946)(415.26672, 213.97)	21.96
Pyropheophorbide A	Chlorin	448707	440420	432594	(533.2647, 19206.514)(534.26715, 4089.1565)	3.81
L-Homomethionine	L-Polyhomomethionine	449046	376112	434388	(164.07256, 20600.463)(165.07542, 547.36334)(187.06401, 15447.953)(168.0489, 6884.3364)(169.05003, 683.4467)	1.46
Deoxypumiloside	Alkaloid	473649	461269	447719	(479.1819, 21809.625)(480.1846, 3290.1033)(481.19565, 1852.0101)	8.48
1-(3,4-Dihydroxyphenyl)-5-Hydroxy-3-Decanone	Phenylpropanoid	483124	466122	464674	(281.1694, 31692.344)(282.17245, 2827.91)	16.04
3,6,7,2',4'-Pentamethylquercetagenin	Flavonol Derivative	488765	469655	468895	(405.10477, 27493.773)(406.10754, 2730.7532)	6.16

(E)-Glutaconate	Small Molecule	392474	371641	471308	(129.02092, 28934.646)(130.0231, 573.85)(114.015076, 1844.8184)	1.39
6-O-D-Glucosyl-6-Hydroxyflavone	Flavone	494147	477627	474146	(386.12866, 3830.0032)(405.10477, 25966.344)(406.10754, 2579.0466)	6.16
Bixin	Carboxylic Ester // Carotenoate // Monocarboxylate	489371	494288	475146	(393.20444, 26483.727)(394.2073, 3149.5)	4.49
Olivetol	Polyketide	520883	507250	488995	(181.1204, 12121.641)(203.10207, 16648.857)	11.05
Isatin	Indole Derivative	414102	396012	491552	(129.02095, 32845.406)(130.0231, 580.02997)(152.01387, 1109.1333)	1.39
N-Acetyl-Farnesylcysteine	N α -Acetylated Amino Acid // L-Cysteine-S-Conjugate	513794	506527	493913	(349.1941, 20502.0)(350.1971, 1689.7201)	11.20
Chlorophyll-A	Chlorophyll A	600451	544958	518258	(893.54535, 9173.577)(894.5484, 3507.2634)	29.00
D-Erythro-Imidazole-Glycerol-Phosphate	Small Molecule	543919	506335	520541	(237.02582, 10636.5)(238.02693, 1594.3701)(239.02397, 1680.68)(237.02673, 8569.72)(238.02773, 891.01)(239.02464, 1033.6066)(222.027, 1983.7965)(241.00218, 12888.825)(242.00298, 3394.72)	1.41
Ajmaline	Ajmalan-Type Monoterpenoid Indole Alkaloid	562086	552147	531386	(309.2019, 2014.7367)(349.1941, 21008.475)(350.1971, 1735.4867)	11.20
3''-Hydroxy-Geranylhydroquinone	Quinol	551684	559686	531761	(263.1575, 31451.26)(264.16058, 2582.5732)(290.16763, 1792.0067)	2.04

16-Methoxytabersonine	Small Molecule	555037	542139	538492	(349.1941, 20797.227)(350.1971, 1710.9268)	11.20
Indole-3-Lactate	Indole Derivative	408421	604590	539416	(187.064, 8303.636)(188.06815, 238.185)(205.066, 8309.0205)	1.39
L-Dehydro-Ascorbate	Small Molecule	4433724	4175755	564423	(175.01651, 24108.172)(158.35303, 199.97667)(160.02051, 86.395)(197.00375, 22525.979)	0.53
(-)-Jasmonoyl-L-Valine	Jasmonoyl-L-Valine	577073	567836	567521	(309.202, 4354.8066)(331.18365, 15169.37)(332.18655, 356.65665)	13.07
Cycloheximide	Small Molecule	599155	605102	572440	(281.16968, 41226.543)(282.17264, 4029.3367)(263.1575, 31451.26)(264.16058, 2582.5732)	9.04
Lotaustralin	D-Glucoside // Nitrile	276837	384175	574422	(247.126, 422.96)(268.10233, 358236.28)(269.1042, 35386.49)(270.10574, 2757.0566)	2.16
(4Z,7Z,10Z,13Z,16Z,19Z)-Docosahexaenoate	Ω3 Fatty Acid // Long-Chain Fatty Acid	590436	588791	574482	(332.21417, 22312.787)(333.21545, 2743.9167)	2.04
7-O-Methylmyricetin	Flavonol Derivative	578414	583762	576627	(333.05386, 25717.719)(334.05685, 1767.1533)	7.36
Dimethylsulfoniopropanoate-Amine	Organosulfur Compound	618771	591559	581600	(144.07933, 30345.053)(145.08244, 1637.7965)	5.14
S-Methyl-L-Methionine	Methylated Amino Acid // Organosulfur Compound	606368	513623	591039	(164.07256, 19312.932)(165.07542, 513.1533)(187.06401, 14482.457)(188.06792, 593.9667)(169.05003, 640.73334)	1.41

Myristate	Long-Chain 2,3,4-Saturated Fatty Acid // Saturated Fatty Acid	631332	612728	603705	(250.18855, 17206.033)(251.19078, 800.68335)	3.04
3,3'-Di(Indol-3-Yl)Methane	Indole-Phytoalexin	626423	630681	613055	(247.12593, 1645.2567)(269.1042, 23367.248)(270.10577, 1656.8033)	2.09
Lacinilene C	Terpenoid	626423	630681	613055	(247.12593, 1645.2567)(252.10718, 59644.668)(253.10962, 6152.7563)	2.09
2,3-Dioctanoylglyceramide	Small Molecule	661873	628119	617404	(339.2482, 552.9033)(340.25497, 564.9033)(362.2352, 12837.691)(363.24106, 581.64667)	10.67
Nicotinamide D-Ribonucleotide	Nicotinamide Mononucleotide	616149	621434	619496	(333.05386, 25717.719)(334.05685, 1767.1533)	7.36
Methyl (2E,6E)-Farnesoate	Methyl Farnesoate	666094	640384	626543	(250.18855, 17619.615)(251.19078, 828.11005)	3.04
Glycyrrhetaldehyde	Triterpenoid	641445	626308	629247	(454.34085, 22108.445)(455.34302, 1566.3151)(477.3252, 20202.008)(478.3274, 989.27)	6.11
N-Acetyl-S-Geranylgeranyl-L-Cysteine	N-Acetyl L-Amino Acid // L-Cysteine-S-Conjugate	654872	644730	642171	(416.27164, 33778.32)(417.2723, 293.38)(419.28003, 63334.71)(420.28174, 1996.6232)	8.04
(4S)-4-(5,5-Dimethylcyclohex-1-En-1-Yl)Cyclohex-1-Ene-1-Carbaldehyde	Sesquiterpenoid	660044	661527	644612	(241.15234, 22943.225)(242.15497, 571.29004)	2.18
(13S,14R)-13-O-Acetyl-1,8-Dihydroxy-N-Methylcanadine	Alkaloid	705903	696367	689437	(390.14014, 33177.02)(391.13205, 5615.94)	6.16
Nicotinamide	Aliphatic Amide // B Vitamin	1053836	804759	707998	(107.042755, 11957.7)(123.05413,	1.70

					61244.453)(124.0553, 2886.8098)(147.04207, 1292.8334)(127.02316, 109531.54)(128.02443, 30842.924)(129.02097, 26217.133)	
4-Prenylphlorisovalerophenone	2-Acyl-4-Prenylphloroglucinol	760959	725978	710005	(277.13828, 35098.92)(278.14114, 3319.33)	13.70
N-Hydroxypentahomomethionine	L-N-Hydroxypolyhomomethionine	749253	744051	736941	(217.10265, 29541.139)(218.10559, 504.435)(220.11559, 2911.1367)(239.09747, 4565.6504)	2.44
Geranyl D-Glucopyranoside	Monoterpenol // Monosaccharide	756942	737548	739583	(316.1923, 2519.2366)(317.205, 31454.154)(318.20792, 4201.7603)(339.18607, 1921.1268)	15.25
Kauralexin A3	Kauralexin	773052	744429	743811	(317.205, 34724.31)(318.20792, 4655.2095)	15.25
Dihydrozeatin-7-N-Glucose	Adenine-Type Cytokinin Glucoside	763634	762380	771287	(384.1818, 43779.062)(385.18433, 5626.3667)(409.17734, 2141.1965)	6.16
L-Tyrosine	Uncharged Polar Amino Acid // Aromatic L-Amino Acid // Proteinogenic Amino Acid // L-Amino Acid	825680	785040	785849	(182.07953, 42852.066)(183.0825, 2786.1301)(187.05681, 2512.0366)	2.13
Harmalol	Alkaloid	761574	800374	806701	(182.07942, 33861.082)(183.0825, 2946.2136)(201.1078, 139.57)	2.53
Serotonin	2-Arylethylamine	873648	839623	833044	(177.10027, 3808.5667)(179.11617, 14485.953)(182.07933, 22611.43)(183.0825, 2886.5735)	2.07
L-Canavanine	Small Molecule	873648	839623	833044	(177.1002, 2861.8733)(182.07953, 44339.03)(183.0825, 2886.5735)	2.13

(+)-7-Epi-12-Hydroxy-12-Oxojasmonoyl-L-Isoleucine	12-Hydroxy-12-Oxojasmonoyl-L-Amino Acid	887684	874072	850897	(333.1481, 41046.99)(334.15088, 3996.9434)	3.41
D-Mannitol	Hexitol	610660	882441	878272	(182.07942, 35506.867)(183.0825, 3127.7402)(166.0707, 260.2)(205.066, 7229.35)(187.05731, 2194.16)	2.11
Lathyrine	Small Molecule	760962	882441	878272	(182.07942, 33281.65)(183.0825, 2893.7703)(166.0707, 260.2)(205.0659, 4983.72)(187.05952, 4989.5234)	2.11
Chlorophyllide B	Chlorophyllide // Organometallic Compound	922765	890914	879628	(610.17737, 20327.559)(611.1778, 9600.599)	25.26
2-Decarboxy-Cyclo-Dopa	Alkaloid	975322	915531	886076	(136.07213, 62966.676)(137.0749, 1718.8383)(177.06828, 6064.928)	3.47
2-Phenylacetamide	Small Molecule	975322	915531	886076	(136.07213, 62966.676)(137.0749, 1718.8383)	3.47
(4E,6E)-1-(4-Hydroxyphenyl)-7-Phenylhepta-4,6-Dien-3-One	Secondary Metabolite	929921	883884	891674	(261.1283, 44606.53)(262.13132, 3054.077)	3.03
Quinidinone	Alkaloid	896789	890346	901173	(305.1539, 51173.94)(306.15677, 4709.4634)	3.56
Delta;-Carotene	Carotene	1019100	990557	921972	(536.43115, 29312.17)(537.4339, 10507.3125)	27.80
3-Methylthiopropylhydroxamic-Acid	(E)-Ω(Methylsulfanyl)Alkyl-Thiohydroximate // Aliphatic Aldoxime	964747	916131	922496	(152.01384, 89.579994)	0.09
8',10-Diapocarotene-8',10-Dial	Aldehyde	974962	952885	929980	(239.14604, 4205.6167)(261.1283, 46120.168)(262.13132, 3171.0566)	3.03

3,8-Divinyl Protochlorophyllide A	Chlorophyllide // Organometallic Compound	986179	945245	933800	(610.1774, 20799.129)(611.1778, 9922.528)(613.17535, 1347.225)	25.26
Kaempferide 3-O-D-Glucopyranosyl -(1->2)-O-Alpha;-L-Rhamnoside	Flavonol 3-O-Glycoside	986179	945245	933800	(610.1774, 20799.129)(611.1778, 9922.528)(612.1758, 6447.187)(613.17535, 1347.225)	25.26
10',6-Diapocarotene-10',6-Dial	Apocarotenoid // Aldehyde	987198	972529	985338	(283.1716, 4964.5664)(305.1539, 51173.94)(306.15677, 4709.4634)	3.56
8'-Hydroxyabscisate	Absciscic Acid Derivative	1020677	995420	991407	(284.0962, 50348.113)(285.09818, 4614.947)	2.14
5-Methylthioadenosine	Small Molecule	1018254	1018696	1020552	(298.09363, 47515.184)(299.09546, 4999.8535)(320.07462, 1557.7433)	3.73
2-Methyl-6-Farnesyl-1,4-Benzoquinol	Quinol	1023131	1034972	1025049	(352.23926, 14796.983)(331.2499, 778.12177)	7.58
10hydroxytaxa-4(20),11-Dien-5alpha;-Yl Acetate	Small Molecule	1023131	1034972	1025049	(331.2499, 778.12177)(352.23926, 14796.983)	7.58
5-(Hydroxymethyl)-2-Methyl-4(1H)-Pyrimidinone	Pyrimidine	1085914	1059885	1026306	(123.05404, 52645.188)(124.0553, 2403.1633)(165.05315, 8697.897)(147.04196, 1778.6167)	1.99
4-Nitrophenol	C-Nitro Compound // Phenol	1.28E+07	2063492	1041228	(143.00046, 128095.65)(144.0017, 5599.4624)	2.02
Dopamine	Catechol	1278816	1012290	1088909	(136.0721, 54786.59)(137.0749, 1443.0518)	3.47
Benzoyl-D-Glucopyranose	Glycosyl Ester // Aromatic Compound	1171431	1140574	1130778	(284.0962, 48499.047)(285.09818, 4462.3833)(307.07968, 1163.3)	2.14

(Indol-3-yl)Acetyl-L-Glutamine	Indole Derivative // Modified Amino Acid	1171431	1140574	1130778	(284.0962, 48499.047)(285.09818, 4462.3833)	2.14
Tolcapone	C-Nitro Compound	1187543	1172960	1151551	(274.06613, 81466.445)(275.06857, 8197.147)	5.96
Guanosine	Purine Ribonucleoside	1207329	1176965	1167587	(284.0962, 51099.926)(285.09818, 4701.8164)(306.07654, 9602.907)(307.07968, 908.0234)(290.0825, 1887.1234)	2.14
3''-Deamino-3''-Oxonicotianamine	Small Molecule	1202276	1177207	1167759	(284.0962, 51099.926)(285.09818, 4701.8164)(306.07654, 9602.907)(307.07968, 908.0234)	2.14
Nicotinate D-Ribonucleotide	Small Molecule	1279036	1225260	1259864	(335.03598, 5989.5234)(315.0107, 15480.91)	0.26
(3Z,6Z)-Nonadienal	Aldehyde	1333055	1317822	1277203	(143.08028, 38877.9)(144.08281, 860.33)	1.66
Alpha;-Linolenate	Long-Chain 2,3,4-Saturated Fatty Acid // Ω3 Fatty Acid	1338949	1311732	1285502	(277.2134, 53025.754)(278.2164, 7186.1997)	15.27
Kaempferol 3-O-D-Glucosylgalactoside	Flavonol 3-O-Glycoside	1348089	1300396	1287902	(612.1758, 7721.223)(613.17535, 1612.9067)	25.26
(2S,3E)-2-Amino-4-(2-Aminoethoxy)But-3-Enoate	Oxyvinylglycine	1359988	1337209	1297544	(143.08028, 38877.9)(144.08281, 860.33)(146.0912, 250.73502)(170.0792, 167.63)	1.66
N2,N2-Dihydroxy-L-Tryptophan	N-Hydroxylated L-Amino Acid	1509149	1459639	1436466	(240.04817, 70419.13)(241.0509, 6154.6934)	2.94
D-Tryptophan	Aromatic D-Amino Acid	1496799	1452068	1448922	(205.09528, 70349.12)(206.09813, 6634.3164)(227.07664, 4658.5503)	4.28
2-Amino-6-Hydroxymethyl-7,7-Dimethyl-7,8-Dihydropteridin-4-One	Small Molecule	1539996	1483914	1486314	(205.09528, 70349.12)(206.09813, 6634.3164)	4.28

5'-Deoxyadenosine	Modified Nucleoside	1547551	1569544	1529231	(252.10718, 72485.195)(253.10962, 7264.22)(238.11346, 1751.39)	2.19
1-Stearoyl-Sn-Glycerol	1-Acyl-Sn-Glycerol	1973201	1710755	1531469	(381.29297, 26002.463)(382.29587, 3363.4348)	20.05
S-(2-Aminoethyl)-L-Cysteine	L-Cysteine-S-Conjugate	2191968	2175395	1533925	(149.0581, 3869.5632)(152.05504, 3318.0066)	2.83
Cyanidin 3,7-Di-O-D-Glucoside	Anthocyanidin 3,7-Di-O-B-D-Glucoside	1623560	1570777	1542372	(612.1758, 8434.604)(613.17535, 1762.6201)(611.1778, 12953.5205)	25.26
Hesperidin	Flavanone Glycoside	1623560	1570777	1542372	(610.1774, 24965.875)(611.1778, 12953.5205)	25.26
Alizarin	Hydroxyanthraquinone	1637438	1586061	1556236	(240.04817, 70419.13)(241.0509, 6154.6934)(250.0359, 582.39)	2.94
Tetraketide Pyrone	Polyketide	1650819	1590943	1595201	(223.09154, 4907.3003)(206.09813, 6518.1665)	4.28
(7S)-Trans-Hinokiresinol	Trans-Hinokiresinol	1678194	1742529	1682502	(252.10718, 73427.56)(253.10962, 7383.31)(238.11346, 1781.3633)(255.12871, 1176.7167)(256.1261, 335.60336)(275.10672, 4003.1565)	2.19
Diisopropyl Fluorophosphate	Small Molecule	1866821	1682309	1826159	(184.73358, 77937.664)(186.06607, 19109.182)(189.0423, 845.38666)	1.39
2,4-Diamino-6-Ethyl-5,3'-(2-Cyclohexylphenoxy)Prop-1'-Yloxy pyrimidine	Small Molecule	2273787	2144875	1998013	(413.26138, 29248.43)(414.2642, 4829.777)(415.26672, 125.240005)	21.96

(22R,23R)-22,23-Dihydroxy-Campest-4-En-3-One	Brassinosteroid	2065308	2012244	2061785	(453.33862, 93793.98)(454.34082, 20998.096)(455.34302, 1476.7201)	6.10
6-Diazo-5-Oxonorleucine	Modified Amino Acid	2108148	2082312	2078806	(177.05347, 83174.09)(178.05617, 6248.8696)	7.36
3,5-Dimethoxyphenol	Small Molecule	2124202	2087590	2084042	(177.05347, 83174.09)(178.05617, 6248.8696)	7.36
Hypoglycin B	Amino Acid Or Its Derivative	2114356	2148647	2089439	(252.10718, 60363.312)(253.10962, 6070.1567)	2.18
Alliin	S-Alkyl-L-Cysteine S-Oxide // Organosulfur Compound	2171221	2178487	2164211	(178.05617, 6520.56)(201.04121, 10886.9795)	7.36
4-Methoxycinnamate	Small Molecule	2299443	2246989	2243461	(177.05347, 83174.09)(178.05617, 6248.8696)(203.38716, 2096.3633)(204.06064, 2165.13)	7.36
C ₂₆ H ₃₇ O ₄	Terpenoid Derivative	2606761	2447689	2268650	(413.26138, 32618.123)(414.2642, 5758.3496)(415.26672, 153.53)	21.96
Dalcochinin-8'-O-Glucoside	Isoflavone	2500173	2460247	2366759	(575.2037, 119381.055)(576.206, 28796.867)(577.2063, 4438.41)	6.70
5 Alpha;-Carboxystrictosidine	Small Molecule	2500173	2460247	2366759	(575.2037, 119381.055)(576.206, 28796.867)	6.70
Delta;-Tocotrienol	Tocotrienol	2398458	2381700	2373953	(419.2799, 54042.98)(420.28174, 1657.07)(397.29855, 60526.0)(398.30032, 1539.3033)	8.04
N,N-Dihydroxy-L-Isoleucine	N-Hydroxylated L-Amino Acid	1905260	325222	2430921	(166.0853, 45848.22)(167.0879, 3519.1602)(185.06439, 83703.04)(186.0661, 19499.04)(187.064, 14371.038)(188.0674,	1.86

					886.59)(168.06125, 2628.305)(170.0581, 156.15)	
Dihydroconiferyl Aldehyde	Small Molecule	1905260	325222	2430921	(182.07956, 11061.445)(183.0824, 799.325)(164.07236, 9954.865)(165.0757, 515.06)(166.0853, 45848.22)(167.0879, 3519.1602)(206.0789, 61.92)(186.73332, 15367.487)(187.46553, 11754.587)(188.0674, 886.59)	1.86
Kauralexin A2	Kauralexin	2716898	2592367	2646366	(333.19986, 45602.594)(334.20267, 6650.31)(335.2138, 1066.27)	13.58
5-Amino-1-(5-Phospho-D-Ribosyl)Imidazole-4-Carboxamide	Carboxamide	2790476	2724843	2714678	(319.03937, 149745.45)(320.0419, 16677.469)(321.04034, 508.075)(341.01947, 616.77)	5.98
5z13e-15s-1115-Dihydroxy-9-Oxopros	Prostaglandin-Like Compound	3106714	1913953	3035916	(333.19992, 51452.25)(334.20273, 7519.314)(335.21402, 1064.1533)(377.2254, 27828.56)(378.2282, 4831.28)	13.58
(3R)-Phenylalanine	Aromatic L-Amino Acid // B Amino Acid // Phenylpropanoid	3461268	8464896	3304427	(166.0854, 373521.16)(167.088, 29894.58)(188.06819, 115248.27)(189.07175, 17600.02)(170.05804, 2145.665)	3.76
1,2-Dioctanoyl-1,2,4-Butanetriol	Small Molecule	3545045	3514131	3525200	(340.25638, 171385.7)(341.2584, 13469.09)	7.58
3-(1H-Indol-3-Yl)Propanoate	Indole Derivative	3796730	3867673	3628546	(188.06927, 174342.47)(189.0718, 18017.588)(170.0581, 2147.2)	4.28
6-O-Methylnorlaudanoline	6-O-Methylnorlaudanoline	4076098	3986453	3846893	(303.13882, 204779.75)(304.1414, 20757.79)(305.141, 2395.39)	4.49
Sphingosine 1-Phosphate	Sphingoid 1-Phosphate	4150799	3961988	3862403	(360.7312, 30939.82)(361.7299, 4805.5366)(363.24258,	11.90

					268.83667)(362.23697, 18779.89)	
2,4-Diamino-6-Methyl-5,3'-(3-Nitrophenoxy)Prop-1'-Yloxypyrimidine	C-Nitro Compound	4475343	4370948	4220868	(303.13882, 207849.92)(304.1414, 21141.521)(305.141, 2443.6033)	4.49
(E)-5-(Methylsulfanyl)Pentanal Oxime	(E)- Ω (Methylsulfanyl)Alkanal Oxime	4308349	4352712	4272274	(133.05933, 1098.6034)(150.0756, 4448.8403)(153.05693, 5445.61)	2.14
Guanine	Purine // Purine Base	4308349	4352712	4272274	(137.04506, 2986.8933)(152.05563, 118473.98)(153.05693, 5445.61)	2.14
Kauralexin B3	Kauralexin	4452581	4359015	4328898	(315.19022, 155219.02)(316.19272, 23125.523)(317.1997, 2150.9834)	14.95
3,7,3',4',5'-Pentamethylmyricetin	Flavonol Derivative	4420335	4430267	4356132	(411.11725, 3089.9)(391.13205, 5498.9766)	6.16
Secologanin	Secoiridoid // Terpene Glycoside	4420335	4430267	4356132	(389.13794, 241257.11)(390.14014, 32490.709)(391.13205, 5498.9766)(411.1173, 2971.41)	6.16
Hederagenin	Triterpenoid	4575966	4457774	4500366	(453.33862, 91577.04)(454.34082, 20404.953)(455.34302, 1435.48)(476.32382, 160675.36)(477.3252, 18823.715)(478.3274, 934.31)	6.11
Adenine	Purine // Purine Base	4767036	4816992	4663748	(136.06136, 101441.27)(137.0617, 4176.72)	2.13
(2 _; OH)-Gibberellin28	Gibberellin	4947154	4944879	4859287	(390.14014, 32490.709)(391.13205, 5498.9766)	6.16
2-R-Hydroperoxy-Linolenate	(2R)-2-Hydroperoxy Fatty Acid // Long-Chain Fatty Acid	5222312	5096016	5084620	(293.2081, 52210.81)(294.21094, 7526.457)(333.19907, 1030.2032)(315.19022, 153396.38)(316.19272, 22869.9)(317.2001, 2352.58)	14.95

Heptanedioate	Small Molecule	5623987	5467105	5419568	(163.03793, 220429.38)(164.0407, 16307.753)	5.98
4-Hydroxycoumarin	Aromatic Compound	5654984	5498468	5457679	(163.03793, 220429.38)(164.0407, 16307.753)(145.02684, 1476.3766)(168.04893, 5177.217)(167.01064, 5883.1704)(168.0107, 874.29663)	3.70
3,5-Dihydroxyanisole	Small Molecule	5654984	5498468	5457679	(124.03806, 3650.3567)(163.03793, 220429.38)(164.0407, 16307.753)(145.02684, 1476.3766)	5.98
(R)-3-(4-Hydroxyphenyl)Lactate	3-(4-Hydroxyphenyl)Lactate // (R)-3-(Aryl)Lactate	5999088	5838442	5764221	(185.06374, 8170.0234)(163.03793, 226040.94)(164.0407, 16798.727)	5.98
4-Coumarate	3-(Aryl)Acrylate // Hydroxylated Carboxylate // Phenylpropanoid	6030084	5869805	5802331	(163.03793, 226040.94)(164.0407, 16798.727)(145.02684, 1528.25)	5.98
Hemanthamine	Small Molecule	6207315	6036241	5852777	(301.13828, 95739.164)(302.14108, 12807.519)(303.14304, 1322.0634)(289.144, 1310.3999)	17.31
2-Trans-Abscisate	Abscisic Acid	6063617	6078504	5935946	(268.1023, 310469.0)(269.1042, 30313.14)(270.10577, 2209.0735)	2.09
2'-Deoxyguanosine	Purine 2'-Deoxyribonucleoside // Nucleic Acid Component	6147224	6167132	6010439	(268.1023, 296796.03)(269.1042, 29040.11)(270.10577, 2092.8035)(290.0823, 539.0)	2.09
L-Isoleucine	Proteinogenic Amino Acid // Branched-Chain Amino Acid // Non-Polar Amino Acid // L-Amino Acid	6709382	4319604	6214181	(132.10126, 291880.06)(133.104, 15970.189)(114.0907, 163275.75)(115.09364, 8705.596)(154.08365, 1916.4299)(136.07217,	3.02

					71861.836)(137.07501, 2271.885)	
Triethanolamine	Non-Metabolic Compound	6994564	5797757	6495629	(132.10088, 144032.48)(133.104, 15293.399)(160.10646, 3315.7366)	2.07
Salicin	B-D Glucoside	6630422	6657607	6496154	(269.1042, 30313.14)(270.10577, 2209.0735)	2.09
Dioleoyl Phosphatidate	Phosphatidate-36:2	7268635	7074680	6929909	(698.4764, 3334.0469)(699.4783, 628.1883)	7.58
Geranyl Acetate	Ester	8985524	8849909	8596631	(178.13261, 155662.08)(179.13512, 14189.239)	3.95
Difluoromethylornithine	Small Molecule	8438432	8464896	8615269	(166.08534, 359770.66)(167.08794, 28909.057)(208.09447, 2556.14)	2.73
Pheophytin A	Pheophytin	9904414	9247602	8910259	(871.5639, 10006.641)(872.56696, 4303.1196)(871.5666, 147209.67)(872.56915, 82135.586)(873.5708, 19711.652)(874.5727, 1409.4733)(893.54535, 6375.013)(894.5484, 2440.3567)	29.02
2-(2-Methylpyridin-3-Yl)Ethanol	Pyridine	1.02E+07	9801032	9619782	(120.0803, 416368.78)(121.08304, 30765.797)	2.73
Tyramine	Aralkylamine	1.09E+07	1.05E+07	1.03E+07	(120.08033, 421962.9)(121.08304, 31168.062)	2.73
Gypsogenin	Triterpenoid	1.08E+07	1.06E+07	1.06E+07	(453.33862, 88106.52)(454.34082, 19505.984)(455.34302, 1371.2133)(475.3212, 615162.2)(476.32382, 154402.86)(477.3252, 17947.717)(478.3274, 885.13666)	6.11

3-Chlorobenzaldehyde	Aromatic Aldehyde // Chloroaromatic Compound	1.28E+07	4816246	1.16E+07	(143.0006, 172752.53)(144.00212, 7906.652)(147.02177, 9185.592)	0.95
Cinchonidine	Alkaloid	1.24E+07	1.19E+07	1.19E+07	(296.19427, 182339.69)(297.19656, 24887.938)(298.1984, 440.55664)	2.63
Choline	Quaternary Amine	1.86E+07	1.79E+07	1.72E+07	(104.1067, 513081.75)(105.1095, 22823.766)	1.63
Canthaxanthin	Ketocarotenoid	3.13E+07	3.05E+07	3.00E+07	(566.42194, 150616.03)(567.4242, 44119.387)(568.42584, 5710.2817)(588.40424, 1269720.9)(589.40753, 415177.4)(590.4092, 68645.9)(591.4103, 6260.0864)	6.96