

Supplementary

KERRA, Mixed Medicinal Plant Extracts, Inhibits SARS-CoV-2 Targets Enzymes and Feline Coronavirus

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Table S1. Phytochemical Profiles of KERRA extracts

List	Name	Formula	Molecular Weight (Da)	Area
1	2-Methoxy-9H-xanthen-9-one	C14 H10 O3	226.0594	7.43×10^9
2	Isorhapontigenin	C15 H14 O4	276.096	7.36×10^9
3	Betaine	C5 H11 N O2	117.0776	6.84×10^9
4	3-[(E)-2-[(1R,4aS,5R,6R,8aR)-6-hydroxy-5-(hydroxymethyl)-5,8a-dimethyl-2-methylidene-decahydronaphthalen-1-yl]ethenyl]-2,5-dihydrofuran-2-one	C20 H28 O4	314.1837	6.81×10^9
5	trans-Anethole	C10 H12 O	148.0869	4.82×10^9
6	Eicosatetraynoic acid	C20 H24 O2	296.1734	4.05×10^9
7	NP-020078	C17 H28 O3	302.1847	3.28×10^9
8	NP-003294	C18 H16 O7	344.085	3.09×10^9
9	9,16-dihydroxy-6-(hydroxymethyl)-2,6,11-trimethyl-15-oxatetracyclo[8.7.0.0.0]heptadec-12-en-14-one	C20 H30 O5	332.1946	2.88×10^9
10	N1-(3-chlorophenyl)-2-[2-(trifluoromethyl)-4-quinolyl]hydrazine-1-carboxamide	C17 H12 Cl F3 N4 O	380.0672	2.37×10^9
11	5-([3-chloro-5-(trifluoromethyl)-2-pyridyl]methyl)thio)-4-pentyl-4H-1,2,4-triazol-3-ol	C14 H16 Cl F3 N4 O S	380.0687	2.36×10^9
12	Choline	C5 H13 N O	103.0985	2.34×10^9
13	(1S,4S,5R,10S,13S,17S,19S,20R)-10-hydroxy-4,5,9,9,13,19,20-heptamethyl-24-oxahexacyclo[15.5.2.0.0.0.0]tetracos-15-en-23-one	C30 H46 O3	454.3393	2.20×10^9
14	NP-016928	C20 H28 O3	298.1892	1.92×10^9
15	NP-006862	C20 H32 O4	318.2154	1.49×10^9
16	DL-Stachydrine	C7 H13 N O2	143.0929	1.29×10^9
17	3-{2-[(1R,4aS,5R,6R,8aS)-6-hydroxy-5-(hydroxymethyl)-5,8a-dimethyl-2-methylidene-decahydronaphthalen-1-yl]-1-hydroxyethyl}-2,5-dihydrofuran-2-one	C20 H30 O5	332.1945	1.28×10^9
18	Apigenin 7-O-glucuronide	C21 H18 O11	446.0796	1.09×10^9
19	(1R,2R,5S,8R,10R,14R)-20-hydroxy-1,2,14,18,18-pentamethyl-17-oxo-8-(prop-1-en-2-yl)pentacyclo[11.8.0.0.0.0]henicosane-5-carboxylic acid	C30 H46 O4	492.3153	1.08×10^9

List	Name	Formula	Molecular Weight (Da)	Area
20	NP-004713	C15 H24 O2	218.1646	9.76 × 10 ⁸
21	Palmitoleic Acid	C16 H30 O2	276.2053	7.97 × 10 ⁸
22	7-hydroxy-1,4a-dimethyl-9-oxo-7-(propan-2-yl)-1,2,3,4,4a,4b,5,6,7,9,10,10a-dodecahydrophenanthrene-1-carboxylic acid	C20 H30 O4	316.1967	7.52 × 10 ⁸
23	11-(4-chloroanilino)-2,3-dihydro-1H-cyclopenta[4,5]pyrido[1,2-a]benzimidazole-4-carbonitrile	C21 H15 Cl N4	358.1008	7.07 × 10 ⁸
24	NP-009051	C17 H16 O5	300.0958	6.92 × 10 ⁸
25	NP-000615	C14 H12 O4	244.0704	6.60 × 10 ⁸
26	Oleamide	C18 H35 N O	281.2681	6.16 × 10 ⁸
27	Formononetin	C16 H12 O4	268.0696	5.94 × 10 ⁸
28	(1S,4aS,7aS)-7-(((2E)-3-phenylprop-2-enoyl)oxy)methyl)-1-(((2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl)oxy)-1H,4aH,5H,7aH-cyclopenta[c]pyran-4-carboxylic acid	C25 H28 O11	542.1191	5.73 × 10 ⁸
29	3',4'-Dimethoxyacetophenone	C10 H12 O3	180.0765	5.68 × 10 ⁸
30	NP-021050	C30 H48 O4	454.341	5.43 × 10 ⁸
31	Biochanin A	C16 H12 O5	284.0648	5.05 × 10 ⁸
32	Hexadecanamide	C16 H33 N O	255.2538	5.00 × 10 ⁸
33	(9R,10R)-10-hydroxy-8,8-dimethyl-9-(((2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl)oxy)-2H,8H,9H,10H-pyrano[2,3-h]chromen-2-one	C20 H24 O10	406.1218	4.79 × 10 ⁸
34	(4aR,5R,6R)-6-hydroxy-4a,5-dimethyl-3-(prop-1-en-2-yl)-2,4a,5,6,7,8-hexahydronaphthalen-2-one	C15 H20 O2	214.1332	4.43 × 10 ⁸
35	(1R,2S,3S,5S,11R,12R)-5-(furan-3-yl)-12-hydroxy-3,11-dimethyl-6,14-dioxatetracyclo[10.2.2.0.0.0]hexadec-15-ene-7,13-dione	C20 H22 O6	340.127	4.24 × 10 ⁸
36	ethyl 5-amino-3-(4-methoxyphenyl)-4-oxo-3,4-dihydrothieno[3,4-d]pyridazine-1-carboxylate	C16 H15 N3 O4 S	345.0813	4.23 × 10 ⁸
37	NP-014517	C14 H18 O9	352.0725	4.23 × 10 ⁸
38	4-(2,3-dihydro-1H-indol-1-yl)-1-phenyl-1H-pyrazolo[3,4-d]pyrimidine	C19 H15 N5	313.1276	4.21 × 10 ⁸

List	Name	Formula	Molecular Weight (Da)	Area
39	NP-020014	C15 H26 O3	276.1666	4.17 × 10 ⁸
40	Stearoyl Ethanolamide	C20 H41 N O2	309.2994	4.14 × 10 ⁸
41	D-(+)-Maltose	C12 H22 O11	364.0936	4.00 × 10 ⁸
42	NP-005821	C30 H46 O3	436.329	3.96 × 10 ⁸
43	2-(8-Hydroxy-4a,8-dimethyldecahydro-2-naphthalenyl)acrylic acid	C15 H24 O3	274.1533	3.87 × 10 ⁸
44	NP-000465	C17 H14 O6	314.0752	3.83 × 10 ⁸
45	Aflatoxin G2	C17 H14 O7	330.0696	3.48 × 10 ⁸
46	3-Hydroxy-2-methylpyridine	C6 H7 N O	109.0514	3.42 × 10 ⁸
47	1-(4-hydroxyphenyl)propane-1,2-diol	C9 H12 O3	190.061	3.22 × 10 ⁸
48	Agmatine	C5 H14 N4	130.1204	3.14 × 10 ⁸
49	Cinchonidine	C19 H22 N2 O	294.1768	3.09 × 10 ⁸
50	trans-3-Indoleacrylic acid	C11 H9 N O2	187.0613	2.96 × 10 ⁸
51	NP-012972	C14 H24 O3	222.1588	2.95 × 10 ⁸
52	5-[5-(methoxycarbonyl)-5,8a-dimethyl-2-methylidene-decahydronaphthalen-1-yl]-3-methylpentanoic acid	C21 H34 O4	350.2412	2.90 × 10 ⁸
53	4-Methylumbelliferone	C10 H8 O3	176.0454	2.84 × 10 ⁸
54	Trigonelline	C7 H7 N O2	96.01952	2.78 × 10 ⁸
55	D-(+)-Pyroglutamic Acid	C5 H7 N O3	129.0412	2.71 × 10 ⁸
56	(5S,6S)-5-Hydroxy-4-methoxy-6-[(E)-2-phenylvinyl]-5,6-dihydro-2H-pyran-2-one	C14 H14 O4	246.0866	2.49 × 10 ⁸
57	5-(4-carboxy-3-methylbutyl)-5,6,8a-trimethyl-3-oxo-3,4,4a,5,6,7,8,8a-octahydronaphthalene-1-carboxylic acid	C20 H30 O5	372.187	2.49 × 10 ⁸
58	Monoolein	C21 H40 O4	356.2886	2.41 × 10 ⁸
59	Ageratriol	C15 H24 O3	234.159	2.17 × 10 ⁸
60	5-hydroxy-6,7-dimethoxy-2-phenyl-4H-chromen-4-one	C17 H14 O5	298.0807	2.16 × 10 ⁸
61	NP-006105	C15 H16 O5	298.0799	2.15 × 10 ⁸
62	Cryptotanshinone	C19 H20 O3	296.1373	2.13 × 10 ⁸
63	4-Hydroxybenzaldehyde	C7 H6 O2	122.0354	2.09 × 10 ⁸
64	octadec-9-ynoic acid	C18 H32 O2	262.2267	2.08 × 10 ⁸
65	(1S,2R,9R,11R,12R,15R)-11-hydroxy-2,6,9,15-tetramethyl-13-	C18 H20 O5	338.1087	2.02 × 10 ⁸

List	Name	Formula	Molecular Weight (Da)	Area
	oxatetracyclo[10.2.1.0.0.0]pentadeca-4,6-diene-3,8,14-trione			
66	Harpagoside	C ₂₄ H ₃₀ O ₁₁	516.1549	2.01 × 10 ⁸
67	NP-008998	C ₁₆ H ₁₈ O ₆	328.0906	2.01 × 10 ⁸
68	Resorcinol monoacetate	C ₈ H ₈ O ₃	152.0455	1.86 × 10 ⁸
69	(+)-ar-Turmerone	C ₁₅ H ₂₀ O	216.1488	1.85 × 10 ⁸
70	Benzyl methacrylate	C ₁₁ H ₁₂ O ₂	158.0713	1.83 × 10 ⁸
71	Acetophenone	C ₈ H ₈ O	120.0555	1.76 × 10 ⁸
72	Avocadyne 1-acetate	C ₁₉ H ₃₄ O ₄	348.2256	1.73 × 10 ⁸
73	(3R,4R)-4-[(3,4-dimethoxyphenyl)methyl]-3-[(4-hydroxy-3-methoxyphenyl)methyl]oxolan-2-one	C ₂₁ H ₂₄ O ₆	394.1348	1.64 × 10 ⁸
74	[5-(2-methylimidazo[1,2-a]pyridin-3-yl)-1H-pyrazol-1-yl][4-(trifluoromethyl)phenyl]methanone	C ₁₉ H ₁₃ F ₃ N ₄ O	370.1053	1.62 × 10 ⁸
75	Apocynin	C ₉ H ₁₀ O ₃	166.0613	1.60 × 10 ⁸
76	1-Linoleoyl glycerol	C ₂₁ H ₃₈ O ₄	354.273	1.59 × 10 ⁸
77	NP-005146	C ₁₆ H ₁₈ O ₄	256.1068	1.52 × 10 ⁸
78	4-(4-methoxyphenyl)-2-(4-pyridyl)-1,3-thiazole hydrobromide	C ₁₅ H ₁₂ N ₂ O ₂ S	268.0698	1.48 × 10 ⁸
79	N ₂ -[[(3R,4S)-3-[[5-(4-methoxyphenyl)-1,2-oxazol-3-yl]methyl]-4-piperidinyl]acetyl]-N ₂ -methylglycinamide	C ₂₁ H ₂₈ N ₄ O ₄	422.1893	1.44 × 10 ⁸
80	Tridemorph	C ₁₉ H ₃₉ N ₂ O	297.3003	1.44 × 10 ⁸
81	Resveratrol	C ₁₄ H ₁₂ O ₃	228.0757	1.40 × 10 ⁸
82	L-Phenylalanine	C ₉ H ₁₁ N ₂ O ₂	165.077	1.36 × 10 ⁸
83	Tanshinone IIA	C ₁₉ H ₁₈ O ₃	294.1217	1.35 × 10 ⁸
84	(2S,3S,4S,5R,6S)-6-[[5,7-dihydroxy-2-(4-hydroxyphenyl)-4-oxo-4H-chromen-3-yl]oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	C ₂₁ H ₁₈ O ₁₂	462.0765	1.34 × 10 ⁸
85	Scutellarin	C ₂₁ H ₁₈ O ₁₂	462.0745	1.34 × 10 ⁸
86	Bicyclo Prostaglandin E ₂	C ₂₀ H ₃₀ O ₄	178.0962	1.30 × 10 ⁸
87	(4aS,9aR)-7-[2-(2,3-dimethoxyphenyl)ethyl]-2-[(4-methoxyphenyl)acetyl]decahydro-6H-pyrido[3,4-d]azepin-6-one	C ₂₈ H ₃₆ N ₂ O ₅	502.2485	1.29 × 10 ⁸

List	Name	Formula	Molecular Weight (Da)	Area
88	Apigenin	C15 H10 O5	270.0495	1.29 × 10 ⁸
89	15-Deoxy-Δ12,14-prostaglandin J2-2-glycerol ester	C23 H34 O5	390.234	1.24 × 10 ⁸
90	3-O-β-D-Glucopyranosylandrographolide	C26 H40 O10	534.2375	1.22 × 10 ⁸
91	Nalidixic acid	C12 H12 N2 O3	232.086	1.22 × 10 ⁸
92	methyl 2-ethyl-4-[(3R,4R,5S)-5-hydroxy-4,5-dimethyl-2-oxooxolan-3-yl]-2-methyl-3-oxobutanoate	C14 H22 O6	308.1196	1.21 × 10 ⁸
93	Vanillin	C8 H8 O3	152.0453	1.21 × 10 ⁸
94	(5S,6S)-5-hydroxy-4-methoxy-6-(2-phenylethyl)-5,6-dihydro-2H-pyran-2-one	C14 H16 O4	270.0855	1.17 × 10 ⁸
95	Ethylmorphine	C19 H23 N O3	313.164	1.15 × 10 ⁸
96	6-Methyl-2-pyridinemethanol	C7 H9 N O	123.0668	1.12 × 10 ⁸
97	NP-020214	C16 H32 O4	310.2107	1.12 × 10 ⁸
98	(1R,9S)-11-(Cyclohexylcarbonyl)-5-(2-methylphenyl)-7,11-diazatricyclo[7.3.1.0 ^{2,7}]trideca-2,4-dien-6-one	C25 H30 N2 O2	390.2329	1.10 × 10 ⁸
99	3',4'-Trimethylene-α-methylamino-valerophenone	C15 H21 N O	231.1596	1.10 × 10 ⁸
100	NP-018817	C15 H24 O4	290.146	1.10 × 10 ⁸
101	NP-002113	C20 H28 O4	354.1763	1.09 × 10 ⁸
102	NP-002322	C18 H32 O4	334.2082	1.09 × 10 ⁸
103	2-{4-[(1S,3aR,4R,6aR)-4-(3,4-dimethoxyphenyl)-hexahydrofuro[3,4-c]furan-1-yl]-2-methoxyphenoxy}-6-(hydroxymethyl)oxane-3,4,5-triol	C27 H34 O11	556.1855	1.06 × 10 ⁸
104	NP-020205	C11 H16 O4	234.0864	1.05 × 10 ⁸
105	(2S,3R,4S,5S,6R)-2-{3-hydroxy-5-[(E)-2-(4-hydroxy-3-methoxyphenyl)ethenyl]phenoxy}-6-(hydroxymethyl)oxane-3,4,5-triol	C21 H24 O9	442.1185	1.03 × 10 ⁸
106	3,3',5,5'-Tetramethyldiphenoquinone	C16 H16 O2	240.112	1.02 × 10 ⁸
107	3-Hydroxypyridine	C5 H5 N O	95.03605	1.02 × 10 ⁸
108	Rhamnetin	C16 H12 O7	316.0541	1.01 × 10 ⁸
109	4-Guanidinobutyric acid	C5 H11 N3 O2	145.0835	1.00 × 10 ⁸
110	Methoxyacetyl fentanyl	C22 H28 N2 O2	352.2184	99,759,859
111	(11E,15Z)-9,10,13-trihydroxyoctadeca-11,15-dienoic acid	C18 H32 O5	310.2108	96,929,532
112	2-(3,4-dihydroxyphenyl)-3,5,7-trihydroxy-6-methyl-4H-chromen-4-one	C16 H12 O7	316.0554	95,611,487
113	Chlorogenic acid	C16 H18 O9	376.0729	95,367,804

List	Name	Formula	Molecular Weight (Da)	Area
114	(2E)-3-(4-Hydroxyphenyl)-N-[2-(4-hydroxyphenyl)ethyl]acrylamide	C17 H17 N O3	283.1178	93,886,662
115	(3aS,5aS,9bR)-5a,9-dimethyl-3-methylidene-2H,3H,3aH,4H,5H,5aH,6H,7H,8H,9bH-naphtho[1,2-b]furan-2,5-dione	C15 H18 O3	228.1121	93,010,999
116	Daidzein	C15 H10 O4	254.055	92,720,175
117	N1-cyclooctyl-4-hydroxy-1-piperidinecarbothioamide	C14 H26 N2 O S	292.1622	92,451,286
118	N-[5-Hydroxy-4,8a-dimethyl-6-[1-oxo-1-(4-thiomorpholinyl)-2-propanyl]-4,4a,5,6,7,8,8a,9-octahydronaphtho[2,3-d][1,3]thiazol-2-yl]-1-methyl-1H-pyrrole-2-carboxamide	C26 H36 N4 O3 S2	516.227	91,472,896
119	T-2 Triol	C20 H30 O7	404.1788	88,975,025
120	5-((2R,3S)-6-Hydroxy-2-(4-hydroxyphenyl)-4-[(E)-2-(4-hydroxyphenyl)vinyl]-2,3-dihydro-1-benzofuran-3-yl)-1,3-benzenediol	C28 H22 O6	454.1364	88,307,788
121	NP-021293	C30 H48 O4	454.3399	88,067,373
122	15-(5-hydroxy-6-methylhept-6-en-2-yl)-7,7,12,16-tetramethylpentacyclo[9.7.0.0.0.0.0]octadecan-6-ol	C30 H50 O2	424.3658	87,922,433
123	Guanine	C5 H5 N5 O	151.0485	84,892,990
124	NP-005474	C21 H22 O9	418.1217	83,775,319
125	2,2,6,6-Tetramethyl-1-piperidinol (TEMPO)	C9 H19 N O	157.1448	82,866,884
126	NP-003141	C21 H20 O9	438.0873	82,431,805
127	Coumarin	C9 H6 O2	146.0348	82,355,781
128	Oleanolic acid	C30 H48 O3	438.3444	81,946,065
129	Carbaprostacyclin	C21 H34 O4	332.231	81,495,844
130	DL-Tryptophan	C11 H12 N2 O2	204.0875	80,563,233
131	Octylphosphonic acid	C8 H19 O3 P	194.1034	79,695,417
132	Trioxsalen	C14 H12 O3	228.0755	78,976,414
133	trans,trans-2,4-Heptadienal	C7 H10 O	110.0718	78,810,316
134	NP-014287	C18 H32 O3	318.213	77,233,880
135	(±)8-HEPE	C20 H30 O3	300.2053	75,941,839
136	Cholest-4-en-3-one	C27 H44 O	384.3348	75,360,861
137	Adenosine	C10 H13 N5 O4	267.0936	74,816,007
138	4-[2-(2-oxo-1-imidazolidinyl)ethyl]-1λ~6~,4-thiazinane-1,1-dione	C9 H17 N3 O3 S	269.0845	74,332,839

List	Name	Formula	Molecular Weight (Da)	Area
139	{(3S)-3-[5-(2-Fluorophenyl)-1,3,4-oxadiazol-2-yl]-1-pyrrolidinyl}(phenyl)methanone	C19 H16 F N3 O2	337.1273	74,001,254
140	4-Aminophenol	C6 H7 N O	109.0515	73,491,150
141	Lupeol	C30 H50 O	426.3811	72,201,114
142	Methyldienolone	C19 H26 O2	286.1891	72,082,535
143	4-phenoxyphenyl 4-hydroxypiperidine-1-carboxylate	C18 H19 N O4	335.1092	71,715,614
144	4-methoxy-6-(prop-2-en-1-yl)-2H-1,3-benzodioxole	C11 H12 O3	160.0504	71,158,053
145	NP-019848	C27 H46 N6 O7	566.3517	70,855,091
146	DL-Arginine	C6 H14 N4 O2	174.1096	70,649,859
147	1,4:3,6-Dianhydro-2-deoxy-5-O-[(4-phenoxyphenyl)carbamoyl]-2-[(2-pyrazinylcarbonyl)amino]-D-glucitol	C24 H22 N4 O6	484.1285	69,257,250
148	NP-020240	C14 H20 O3	186.1014	69,113,668
149	NP-019811	C6 H7 N O2	125.0464	68,696,381
150	1-{4-[2-(7-methoxy-2H-1,3-benzodioxol-5-yl)ethyl]phenoxy}-3-methylbutane-2,3-diol	C21 H26 O6	396.1502	65,453,635
151	NP-007909	C13 H20 O3	206.1285	64,617,637
152	Isobornyl methacrylate	C14 H22 O2	222.1598	63,603,104
153	Kanosamine	C6 H13 N O5	161.0671	63,573,239
154	NP-013210	C12 H14 O3	188.0817	63,140,447
155	Cyclo(leucylprolyl)	C11 H18 N2 O2	210.1347	60,426,370
156	12-Oxo phytodienoic acid	C18 H28 O3	292.1999	59,586,148
157	NP-003024	C12 H14 O5	260.0652	58,967,173
158	5,7-Dihydroxy-2-(4-hydroxyphenyl)-6,8-bis[3,4,5-trihydroxy-6-(hydroxymethyl)tetrahydro-2H-pyran-2-yl]-4H-chromen-4-one	C27 H30 O15	594.1521	58,459,871
159	(±)13-HpODE	C18 H32 O4	294.2159	58,317,690
160	Emodin	C15 H10 O5	270.0497	58,314,124
161	Maltol	C6 H6 O3	126.0303	57,637,035
162	(2R)-7-Methoxy-3-oxo-3,4-dihydro-2H-1,4-benzoxazin-2-yl β-D-glucopyranoside	C15 H19 N O9	379.0838	57,293,685
163	9-Oxo-ODE	C18 H30 O3	294.2153	57,068,495
164	6-[(2E,6E)-7-(5-hydroxy-3-methyl-2-oxocyclopent-3-en-1-yl)-6-methylhepta-2,6-dien-2-yl]-3-methyl-5,6-dihydro-2H-pyran-2-one	C20 H26 O4	330.1785	56,752,848

List	Name	Formula	Molecular Weight (Da)	Area
165	4a,5-dihydroxy-7-methyl-1-[[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy]-1H,4aH,5H,6H,7H,7aH-cyclopenta[c]pyran-7-yl acetate	C17 H26 O11	428.125	56,359,580
166	4-Amino-2-pyrazin-2-ylpyrimidine-5-carbonitrile	C9 H6 N6	198.0656	56,098,264
167	3-[4-methyl-1-(2-methylpropanoyl)-3-oxocyclohexyl]butanoic acid	C15 H24 O4	290.1454	55,375,637
168	5-hydroxy-2-(4-hydroxyphenyl)-6-methoxy-7-[[[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy]-4H-chromen-4-one	C22 H22 O11	462.111	55,103,926
169	Bis(4-ethylbenzylidene)sorbitol	C24 H30 O6	414.1994	55,038,320
170	NP-008274	C15 H20 O4	286.1169	54,710,900
171	Diosgenin	C27 H42 O3	396.2978	54,355,608
172	4-Indolecarbaldehyde	C9 H7 N O	145.0512	53,929,932
173	6-Hydroxy-1-(hydroxymethyl)-5-{2-[(4-methoxybenzyl)amino]-2-oxoethyl}-1,4a-dimethyldecahydro-2-naphthalenyl propylcarbamate	C27 H42 N2 O6	490.3	53,381,782
174	L-Tyrosine	C9 H11 N O3	181.0718	50,877,541
175	NP-013736	C10 H16 N2 O2	196.119	48,955,487
176	NP-013326	C15 H16 O4	242.091	48,052,999
177	3,5-di-tert-Butyl-4-hydroxybenzaldehyde	C15 H22 O2	234.1592	47,438,366
178	Aloe-emodin	C15 H10 O5	270.0495	45,963,974
179	(5E)-7-methylidene-10-oxo-4-(propan-2-yl)undec-5-enoic acid	C15 H24 O3	274.1514	45,813,299
180	[2-(hydroxymethyl)-5,5,8a-trimethyl-1,4,4a,5,6,7,8,8a-octahydronaphthalen-1-yl]methanol	C15 H26 O2	260.1722	45,422,507
181	NP-008993	C18 H34 O4	336.2236	44,613,421
182	NP-015559	C17 H14 O7	330.0699	44,353,657
183	Oleoyl ethanolamide	C20 H39 N O2	325.2943	43,929,483
184	4-Methoxybenzaldehyde	C8 H8 O2	136.051	43,889,807
185	1-adamantyl(1,4-thiazinan-4-yl)methanone	C15 H23 N O S	265.1494	43,135,442
186	4'-(Imidazol-1-yl)acetophenone	C11 H10 N2 O	186.0772	43,124,736
187	9-hydroxy-2,10,10-trimethyltricyclo[6.3.0.0.0]undec-6-ene-6-carboxylic acid	C15 H22 O3	232.1434	43,120,862
188	Tetranor-12(S)-HETE	C16 H26 O3	288.1691	43,117,886
189	N-Acetyloronithine	C7 H14 N2 O3	142.0763	42,842,000

List	Name	Formula	Molecular Weight (Da)	Area
190	Aloesin	C19 H22 O9	394.1197	42,676,729
191	NP-000308	C16 H12 O6	300.0597	42,565,135
192	NP-011220	C11 H18 N2 O2	210.1344	42,264,024
193	2-(3,4-Dihydroxyphenyl)ethyl 3-O-(6-deoxy-β-L-mannopyranosyl)-6-O-[(2E)-3-(3,4-dihydroxyphenyl)-2-propenoyl]-β-D-glucopyranoside	C29 H36 O15	646.1788	41,860,287
194	D-Raffinose	C18 H32 O16	526.1444	41,677,143
195	4-[(E)-2-[3-(β-D-Glucopyranosyloxy)-5-hydroxyphenyl]vinyl]-2-methoxyphenyl β-D-glucopyranoside	C27 H34 O14	582.1873	41,383,036
196	3-(propan-2-yl)-octahydropyrrolo[1,2-a]pyrazine-1,4-dione	C10 H16 N2 O2	196.1198	41,279,599
197	(2S,5aS,8aR)-6-Benzyl-1-methyl-2-[3-(4-morpholinyl)-3-oxopropyl]octahydropyrrolo[3,2-E][1,4]diazepin-5(2H)-one	C22 H32 N4 O3	422.2231	41,275,425
198	Nicotinic acid	C6 H5 N O2	123.0306	41,260,722
199	Betaxolol	C18 H29 N O3	307.211	40,881,749
200	2,6-Dimethyl-γ-pyrone	C7 H8 O2	124.051	40,804,739
201	(1aR,1bR,2R,3R,7R,7aS)-1b,2-dimethyl-7a-(prop-1-en-2-yl)-1aH,1bH,2H,3H,4H,5H,7H,7aH-naphtho[1,2-b]oxirene-3,7-diol	C15 H22 O3	232.1435	40,457,030
202	4-(2-methoxyphenyl)-1-(3-phenyl-1,2,4-thiadiazol-5-yl)piperidine	C20 H21 N3 O S	351.1428	39,297,321
203	SB236057A	C33 H34 N4 O3	534.2567	39,140,029
204	Indole	C8 H7 N	117.0563	39,050,503
205	Ambrosic acid	C15 H20 O4	286.115	38,842,262
206	Kynurenic acid	C10 H7 N O3	189.0406	38,727,203
207	8-{3-Oxo-2-[(2E)-2-penten-1-yl]-1-cyclopenten-1-yl}octanoic acid	C18 H28 O3	292.2001	38,683,339
208	NP-020327	C21 H24 O8	426.1237	38,580,877
209	2-Methoxyresorcinol	C7 H8 O3	140.0458	38,539,952
210	3-Methyl-4-[2-(4-morpholinophenyl)hydrazono]-1-phenyl-4,5-dihydro-1H-pyrazol-5-one	C20 H21 N5 O2	385.1483	38,526,023
211	9S,13R-12-Oxophytodienoic acid	C18 H28 O3	292.2012	38,119,466
212	Arachidonic acid	C20 H32 O2	286.2263	37,101,625
213	Cuminaldehyde	C10 H12 O	148.087	36,791,156
214	Pulegone	C10 H16 O	152.1181	36,137,196
215	NP-003399	C14 H12 O2	212.0813	36,003,314
216	NP-020112	C30 H48 O2	440.3605	35,225,004

List	Name	Formula	Molecular Weight (Da)	Area
217	(2R,3S,4S,5S,6R)-2-((7-hydroxy-4-((3Z)-5-hydroxy-3-methylpent-3-en-1-yl)-4a,8,8-trimethyl-3-methylidene-decahydronaphthalen-2-yl)oxy)-6-(hydroxymethyl)oxane-3,4,5-triol	C26 H44 O8	506.2946	35,207,040
218	Schaftoside	C26 H28 O14	564.1401	34,699,760
219	N-(2-(4-[5-(Acetylamino)-1H-benzimidazol-2-yl]phenyl)-1H-benzimidazol-5-yl)acetamide	C24 H20 N6 O2	424.1716	33,904,086
220	Salsolinol	C10 H13 N O2	179.0927	33,796,582
221	NP-008132	C20 H24 O9	430.1185	33,257,543
222	2,6-Dimethoxyphenol	C8 H10 O3	154.0613	33,068,750
223	3-{5-[(2S)-1-(4-Chlorobenzyl)-2-pyrrolidinyl]-1,2,4-oxadiazol-3-yl}-2-(2-methoxyethoxy)pyridine	C21 H23 Cl N4 O3	436.1296	32,810,671
224	NP-011548	C18 H34 O3	280.2369	32,694,515
225	5-fluoro AB-PINACA N-(4-hydroxypentyl) metabolite	C18 H25 F N4 O3	386.1811	31,861,743
226	6-Methylquinoline	C10 H9 N	143.0718	31,687,065
227	Nicotinuric acid	C8 H8 N2 O3	180.0556	31,203,244
228	NP-021018	C12 H18 O4	208.1077	31,035,152
229	(1S,2S,4R,7E,11S)-4,8-dimethyl-12-methylidene-3,14-dioxatricyclo[9.3.0.0.0]tetradec-7-en-13-one	C15 H20 O3	230.1279	30,944,116
230	10-Propoxydecanoic acid	C13 H26 O3	242.2005	30,925,139
231	Diphenylphosphine oxide	C12 H11 O P	202.0525	30,854,834
232	3-(3,4-dihydroxyphenyl)propanoic acid	C9 H10 O4	164.0456	29,678,071
233	Nicotinamide	C6 H6 N2 O	122.0466	29,612,560
234	(1S,3R,4S,5R)-3,5-bis(((2E)-3-(3,4-dihydroxyphenyl)prop-2-enoyl)oxy)-1,4-dihydroxycyclohexane-1-carboxylic acid	C25 H24 O12	516.1203	29,505,388
235	Penbutolol	C18 H29 N O2	291.2165	29,081,029
236	NP-004038	C16 H24 O3	246.159	28,950,112
237	Heptanophenone	C13 H18 O	190.1338	28,427,034
238	(3aR,5aR,9bR)-3a-hydroxy-5a,9-dimethyl-3-methylidene-2H,3H,3aH,4H,5H,5aH,6H,7H,8H,9bH-naphtho[1,2-b]furan-2-one	C15 H20 O3	270.1201	28,172,000
239	Diphenylamine	C12 H11 N	169.0874	27,885,206
240	Cyclo(phenylalanyl-prolyl)	C14 H16 N2 O2	244.1181	27,273,229
241	4-Isopropyl-9H-thioxanthen-9-one	C16 H14 O S	254.0734	27,187,080
242	Etiocholanolone	C19 H30 O2	272.2109	26,205,231
243	3-Methoxy prostaglandin F1 α	C21 H38 O6	408.2439	25,992,019

List	Name	Formula	Molecular Weight (Da)	Area
244	(3aR,4aS,5R,7aS,8S,9aR)-5-Hydroxy-4a,8-dimethyl-3-methyleneoctahydroazuleno[6,5-b]furan-2,6(3H,4H)-dione	C15 H20 O4	264.133	25,619,491
245	methyl 3-ethenyl-4-((6-[2-(4-hydroxyphenyl)ethyl]-4-oxooxan-2-yl)methyl)-2-[[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy]-3,4-dihydro-2H-pyran-5-carboxylate	C29 H38 O12	600.209	25,528,060
246	Luteolin	C15 H10 O6	286.0441	25,158,891
247	2-(tert-butyl)-6-(4-chlorophenyl)-4-(methylthio)pyridine	C16 H18 Cl N S	291.086	25,029,791
248	Ethyl paraben	C9 H10 O3	166.0611	24,772,472
249	(3S,4aR,5R,6R)-3,6-dihydroxy-4a,5-dimethyl-3-(prop-1-en-2-yl)-2,3,4,4a,5,6,7,8-octahydronaphthalen-2-one	C15 H22 O3	232.1433	24,707,449
250	4-Hydroxyephedrine	C10 H15 N O2	163.0979	24,340,907
251	(2S)-4-Oxo-2-phenyl-3,4-dihydro-2H-chromen-7-yl beta-D-glucopyranoside	C21 H22 O8	402.1266	24,304,502
252	(2E)-2-(hydroxymethyl)-3-[3-oxo-5-(propan-2-yl)-1,3,4,5,6,7-hexahydro-2-benzofuran-4-yl]prop-2-enoic acid	C15 H20 O5	302.1095	24,025,622
253	5-(6-hydroxy-6-methyloctyl)-2,5-dihydrofuran-2-one	C13 H22 O3	208.1439	23,986,648
254	6-(tert-butyl)pyridazin-3(2H)-one	C8 H12 N2 O	152.0932	23,904,057
255	2-sec-Butyl-3-methoxypyrazin	C9 H14 N2 O	166.1087	23,840,812
256	Acetylcholine	C7 H15 N O2	145.1085	23,731,706
257	Linoleoyl ethanolamide	C20 H37 N O2	323.2785	23,629,153
258	(2S,3R,4S,5S,6R)-2-((4a,5,7-trihydroxy-7-methyl-1H,4aH,5H,6H,7H,7aH-cyclopenta[c]pyran-1-yl)oxy)-6-(hydroxymethyl)oxane-3,4,5-triol	C15 H24 O10	386.1142	23,535,839
259	NP-001798	C16 H17 N O2	255.1231	23,489,644
260	4-decyl-3-hydroxy-5-oxoolane-2,3-dicarboxylic acid	C16 H26 O7	352.1449	23,400,192
261	2-Isobutyl-3-methoxypyrazine	C9 H14 N2 O	166.1086	23,015,572
262	Pipecolic acid	C6 H11 N O2	129.0775	22,973,316
263	N-Benzyl-2-[(3R,4S)-3-[[5-(cyclohexylmethyl)-1,2-oxazol-3-yl]methyl]-4-piperidinyl]-N-methylacetamide	C26 H37 N3 O2	445.2748	22,533,662
264	NP-020705	C17 H24 O8	378.1245	22,533,166

List	Name	Formula	Molecular Weight (Da)	Area
265	Norharman	C11 H8 N2	168.0669	22,381,368
266	γ -Linolenic acid ethyl ester	C20 H34 O2	312.2628	22,291,201
267	(2E)-3-[(1R,4S,7R,7aR)-1-hydroxy-3,7-dimethyl-2,4,5,6,7,7a-hexahydro-1H-inden-4-yl]-2-methylprop-2-enoic acid	C15 H22 O3	232.1435	22,288,124
268	6,7-Dihydroxy-4-methylcoumarin	C10 H8 O4	192.0402	21,460,057
269	NP-002336	C23 H36 O5	409.2773	21,340,698
270	α -Pinene-2-oxide	C10 H16 O	152.1185	21,322,644
271	1,2,3,4-Tetramethyl-1,3-cyclopentadiene	C9 H14	122.1085	21,086,160
272	Diundecyl phthalate	C30 H50 O4	496.3496	20,861,702
273	NP-016721	C15 H16 O4	282.0863	20,469,729
274	[4-(2-methoxyphenyl)piperazino](4-methylphenyl)methanone	C19 H22 N2 O2	310.1729	20,357,449
275	Uracil	C4 H4 N2 O2	112.026	20,227,338
276	NP-008198	C26 H32 O13	574.1752	20,115,132
277	8Z,11Z,14Z-Eicosatrienoic acid	C20 H34 O2	306.2525	19,964,197
278	6-Methoxyquinoline	C10 H9 N O	159.0669	19,903,165
279	4,8-dihydroxy-6,6,8-trimethyl-1H,3H,4H,4aH,5H,6H,7H,7aH,8H,9H-azuleno[5,6-c]furan-1-one	C15 H22 O4	288.1328	19,869,631
280	Methylhippuric acid	C10 H11 N O3	193.0719	19,711,927
281	Palmitoyl ethanolamide	C18 H37 N O2	299.2787	19,705,843
282	3-(2,6-Dioxocyclohexyl)propanenitrile	C9 H11 N O2	165.0769	19,583,327
283	2-Methoxybenzaldehyde	C8 H8 O2	136.0515	19,349,457
284	NP-016437	C15 H24 O5	306.1405	19,214,653
285	NP-020713	C20 H26 O4	330.1766	18,891,579
286	(1R,3R,4S,5R)-3,4-bis([(2E)-3-(3,4-dihydroxyphenyl)prop-2-enoyl]oxy)-1,5-dihydroxycyclohexane-1-carboxylic acid	C25 H24 O12	498.1113	18,870,286
287	5,10,15-trimethyl-4,9,13-trioxatetracyclo[10.3.0.0.0]penta-1(15)-en-14-one	C15 H20 O4	246.1226	18,681,670
288	(-)-Epicatechin	C15 H14 O6	290.0756	18,476,297
289	PD 0200347	C10 H17 N3 O2	211.1335	18,436,988
290	1-(3,4-dimethoxyphenyl)ethan-1-one oxime	C10 H13 N O3	177.077	18,405,606
291	Prolylleucine	C11 H20 N2 O3	228.1445	18,386,393
292	Benzyl 6-O-beta-D-glucopyranosyl-beta-D-glucopyranoside	C19 H28 O11	454.1381	18,341,336
293	4,6-Dimethyl-2(1H)-pyrimidinone	C6 H8 N2 O	124.0622	18,255,886
294	Tetranor-12R-HETE	C16 H26 O3	248.1746	18,178,612
295	NP-008882	C27 H48 O9	538.3046	17,867,532

List	Name	Formula	Molecular Weight (Da)	Area
296	Scoparone	C11 H10 O4	206.0553	17,852,271
297	N-{4-[(2R,3R)-3-(Hydroxymethyl)-5-oxo-4-(4-pyridinylmethyl)-2-morpholinyl]phenyl}-4-(trifluoromethyl)benzamide	C25 H22 F3 N3 O4	507.1317	17,687,990
298	Dulcitol	C6 H14 O6	182.0823	17,408,410
299	Azobenzene	C12 H10 N2	182.0831	17,159,521
300	4-[[5-(6-Hydroxy-5,5,8a-trimethyl-2-methylenedecahydro-1-naphthalenyl)-3-methylpentyl]oxy]-4-oxobutanoic acid	C24 H40 O5	390.2729	17,091,735
301	4'-Methoxyacetophenone	C9 H10 O2	150.0663	16,893,301
302	Esculetin	C9 H6 O4	178.0245	16,749,625
303	3-(4-Nitrophenyl)imidazo[1,5-a]pyridine	C13 H9 N3 O2	239.0682	16,479,751
304	NP-002089	C15 H22 O3	272.1361	16,444,281
305	N-(2,4-Dimethylphenyl)formamide	C9 H11 N O	149.0825	16,154,582
306	Zaleplon	C17 H15 N5 O	305.1237	15,997,293
307	6-Acetylmorphine	C19 H21 N O4	327.1431	15,965,597
308	13(S)-HOTrE	C18 H30 O3	294.2158	15,954,057
309	NP-000295	C17 H22 O4	312.1325	15,767,872
310	Heroin	C21 H23 N O5	369.1528	15,501,729
311	(3aR,7aS,8S,9aR)-5,8-dimethyl-3-methylidene-2H,3H,3aH,4H,6H,7H,7aH,8H,9H,9aH-azuleno[6,5-b]furan-2,6-dione	C15 H18 O3	246.1227	15,419,277
312	4-Methylumbelliferyl- α -D-glucopyranoside	C16 H18 O8	338.0955	15,357,162
313	2-[[2-(1H-indol-3-yl)ethyl]ethanimidoyl]phenol	C18 H18 N2 O	278.1463	15,344,890
314	N-{4-[(2R,3R)-3-(Hydroxymethyl)-4-methyl-5-oxo-2-morpholinyl]phenyl}-2-methylbenzamide	C20 H22 N2 O4	392.1191	15,237,300
315	2-[(5R,8S,8aS)-3,8-dimethyl-2-oxo-1,2,4,5,6,7,8,8a-octahydroazulen-5-yl]prop-2-enoic acid	C15 H20 O3	230.1281	15,047,930
316	8,8-dimethyl-2H,8H-pyrano[3,2-g]chromen-2-one	C14 H12 O3	228.0758	15,022,886
317	Buspirone	C21 H31 N5 O2	385.2422	15,015,423
318	1-(2,4-dihydroxyphenyl)-2-(3,5-dimethoxyphenyl)propan-1-one	C17 H18 O5	324.0947	14,833,751
319	Thymine	C5 H6 N2 O2	126.0416	14,704,546
320	3',4'-Dimethyl- α -ethylaminovalerophenone	C15 H23 N O	233.1751	14,531,645
321	Dehydroepiandrosterone (DHEA)	C19 H28 O2	288.2053	14,390,832
322	NP-021868	C15 H14 O4	240.0759	14,314,532
323	N-Acetylhistamine	C7 H11 N3 O	153.0884	13,978,793

List	Name	Formula	Molecular Weight (Da)	Area
324	NP-021085	C17 H26 O3	260.1741	13,528,614
325	2-(piperidinomethylidene)malononitrile	C9 H11 N3	161.0936	13,422,221
326	mesityl(piperidin-4-yl)methanone hydrochloride	C15 H21 N O	231.1597	13,411,287
327	2-[4-(3-Amino-2-hydroxypropoxy)phenyl]acetamide	C11 H16 N2 O3	224.1135	13,259,920
328	3-(4-hydroxyphenyl)-5-methoxy-7-[[[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy]-4H-chromen-4-one	C22 H22 O10	468.0976	13,076,977
329	3-(5-Cyclopropyl-1,3,4-oxadiazol-2-yl)-2-[(4-methylphenyl)thio]pyridine	C17 H15 N3 O S	309.0964	13,068,237
330	8-(2,3-dihydroxy-3-methylbutyl)-7-methoxy-2H-chromen-2-one	C15 H18 O5	300.0958	12,941,355
331	2-[(1S,4S,5S)-4-{{[(Ethylcarbamoyl)amino]methyl}-5-isopropyl-2-methyl-2-cyclohexen-1-yl]-N-(4-methoxybenzyl)acetamide	C24 H37 N3 O3	415.2824	12,878,588
332	NP-020293	C7 H14 N2 O3	196.0827	12,867,566
333	N-(4-piperidinophenyl)-2-thiophenecarboxamide	C16 H18 N2 O S	308.099	12,768,996
334	(-)-Strychnine	C21 H22 N2 O2	334.1717	12,744,644
335	3-[(4-hydroxyphenyl)methyl]-octahydropyrrolo[1,2-a]pyrazine-1,4-dione	C14 H16 N2 O3	260.1126	12,742,909
336	NP-022238	C20 H22 N2 O	306.1771	12,620,869
337	Sedanolide	C12 H18 O2	176.1179	12,503,179
338	4-hydroxy-6-[2-(2-methyl-1,2,4a,5,6,7,8,8a-octahydronaphthalen-1-yl)ethyl]oxan-2-one	C18 H28 O3	314.1821	12,399,291
339	6,7,8-trimethoxy-2-(2-phenoxy-3-pyridyl)-4H-3,1-benzoxazin-4-one	C22 H18 N2 O6	428.1028	12,157,122
340	2-[(4-cyclopropyl-5-hydroxy-4H-1,2,4-triazol-3-yl)sulfanyl]-1-(2,3-dihydro-1,4-benzodioxin-6-yl)-1-ethanone	C15 H15 N3 O4 S	333.0798	11,972,567
341	Benzoguanamine	C9 H9 N5	187.0822	11,890,538
342	Rilmenidine	C10 H16 N2 O	180.1245	11,681,064
343	NP-019401	C11 H15 N O2	193.1082	11,526,016
344	N-[[[(2R,4S,5S)-5-Ethynyl-1-azabicyclo[2.2.2]oct-2-yl]methyl]-2-naphthamide	C21 H22 N2 O	318.1768	11,439,391
345	3-(3-pyridylamino)-2-[4-(trifluoromethoxy)benzoyl]acrylonitrile	C16 H10 F3 N3 O2	333.0781	11,133,019
346	3-Succinoylpyridine	C9 H9 N O3	179.0563	11,040,457
347	1-Phenyl-3-methyl-5-pyrazolone	C10 H10 N2 O	174.0774	10,858,965

List	Name	Formula	Molecular Weight (Da)	Area
348	Pyrimethamine	C12 H13 Cl N4	248.0807	10,710,465
349	Artemisinin	C15 H22 O5	264.1307	10,662,530
350	2-(2-acetyl-3,5-dihydroxyphenyl)acetic acid	C10 H10 O5	192.0402	10,443,016
351	Carbofuran	C12 H15 N O3	221.1026	10,442,463
352	Ergocalciferol	C28 H44 O	396.3354	10,414,786
353	10-Nitrooleate	C18 H33 N O4	349.2207	10,152,263
354	(2S,3R)-2-(3,4-dihydroxyphenyl)-3,5-dihydroxy-3,4-dihydro-2H-1-benzopyran-7-yl 3,4,5-trihydroxybenzoate	C22 H18 O10	442.0846	10,078,644
355	Naringenin	C15 H12 O5	272.0653	10,027,835
356	Irganox 1035	C38 H58 O6 S	664.3885	10,003,353
357	(3aR,4aS,5R,6S,8S,9aR)-5,6-dihydroxy-4a,8-dimethyl-3-methylidene-dodecahydroazuleno[6,5-b]furan-2-one	C15 H22 O4	248.1382	9,961,772
358	(1R,4aS,5R,8aS)-5-(5-hydroxy-3-methylpentyl)-1,4a-dimethyl-6-methylidene-decahydronaphthalene-1-carboxylic acid	C20 H34 O3	339.273	9,842,456
359	7-hydroxy-6-methoxy-2H-chromen-2-one	C10 H8 O4	192.0402	9,832,967
360	(3R,4R)-4-Hydroxy-3-((4-[2-(4-morpholinyl)ethoxy]benzoyl)amino)-N-phenyl-1-azepanecarboxamide	C26 H34 N4 O5	504.2305	9,782,871
361	N-Feruloyloctopamine	C18 H19 N O5	311.1121	9,774,591
362	Maltotetraose	C24 H42 O21	688.1966	9,733,988
363	(1S,2S,4aR,7R,8aR)-1-[(3Z)-5-hydroxy-3-methylpent-3-en-1-yl]-2,5,5,8a-tetramethyl-decahydronaphthalene-2,7-diol	C20 H36 O3	346.2443	9,652,952
364	11(Z),14(Z),17(Z)-Eicosatrienoic acid	C20 H34 O2	306.2521	9,365,538
365	Debrisoquine	C10 H13 N3	175.1097	9,185,763
366	5,7-dihydroxy-2-(3-hydroxy-4-methoxyphenyl)-3,6-dimethoxy-4H-chromen-4-one	C18 H16 O8	360.0801	9,130,052
367	4-morpholinobenzoic acid	C11 H13 N O3	207.0871	8,968,512
368	HET0016	C12 H18 N2 O	228.1236	8,940,585
369	5-[(1E)-3-hydroxy-3-methylbut-1-en-1-yl]-2-methylcyclohex-5-ene-1,2,4-triol	C12 H20 O4	250.1153	8,915,535
370	NP-000124	C12 H20 O4	250.1156	8,915,535
371	NP-007111	C35 H58 O9	639.4208	8,802,503
372	Phloroglucinol	C6 H6 O3	126.0302	8,687,334
373	NP-006888	C13 H24 O4	266.1465	8,608,883
374	ethyl 4-[(4-methylphenyl)sulfonyl]amino}tetrahydro-1(2H)-pyridinecarboxylate	C15 H22 N2 O4 S	364.09	8,589,136

List	Name	Formula	Molecular Weight (Da)	Area
375	[(2R,3S,4S,5R,6R)-6-[2-(3,4-dihydroxyphenyl)ethoxy]-3,4,5-trihydroxyoxan-2-yl]methyl (2E)-3-(3,4-dihydroxyphenyl)prop-2-enoate	C23 H26 O11	478.1426	8,463,364
376	Wogonin	C16 H12 O5	284.0651	8,367,490
377	2-Hydroxyquinoline	C9 H7 N O	145.0511	8,300,054
378	3-Phenylpropionitrile	C9 H9 N	90.0452	8,179,167
379	NP-011878	C15 H26 O5	308.1563	8,129,868
380	NP-011150	C22 H24 O8	454.103	8,079,253
381	5 α -Dihydrotestosterone glucuronide	C25 H38 O8	466.2496	7,982,458
382	Mepanipyrim	C14 H13 N3	223.1082	7,916,105
383	NP-019748	C30 H48 O5	510.3252	7,826,258
384	N-((1S,4S,6S)-6-Isopropyl-3-methyl-4-[2-oxo-2-(1-pyrrolidiny)ethyl]-2-cyclohexen-1-yl)methyl)-2-pyrazinecarboxamide	C22 H32 N4 O2	406.2281	7,451,731
385	Apigetrin	C21 H20 O10	432.1003	7,450,390
386	(2R)-5-hydroxy-7-methoxy-2-phenyl-3,4-dihydro-2H-1-benzopyran-4-one	C16 H14 O4	270.0858	7,400,693
387	7-Aminoflunitrazepam	C16 H14 F N3 O	283.1174	7,288,007
388	Albendazole-2-aminosulfone	C10 H13 N3 O2 S	239.0679	7,198,178
389	Aflatoxin B2	C17 H14 O6	314.0751	6,996,550
390	(4aS,5R,6S,8aS)-5-[(3E)-5-methoxy-3-methyl-5-oxopent-3-en-1-yl]-5,6,8a-trimethyl-3,4,4a,5,6,7,8,8a-octahydronaphthalene-1-carboxylic acid	C21 H32 O4	348.2265	6,963,068
391	NP-016596	C19 H30 O8	408.1713	6,871,022
392	Cytisine	C11 H14 N2 O	190.1082	6,802,962
393	(3E,12E)-3,12-Dimethyl-8-methylene-6,18-dioxatricyclo[14.2.1.05,9]nonadeca-3,12,16(19)-triene-7,17-dione	C20 H24 O4	310.153	6,786,418
394	(2R)-1-(5-hydroxy-3-methylpentyl)-2,5,5,8a-tetramethyl-decahydronaphthalen-2-ol	C20 H38 O2	292.2733	6,650,316
395	(9cis)-Retinal	C20 H28 O	284.2107	6,564,013
396	2-[6-(1H-benzo[d]imidazol-2-yl)-2-pyridyl]-1H-benzo[d]imidazole	C19 H13 N5	311.1125	6,489,108
397	[3-((3-((Cyclopropylmethyl)amino)-3-oxetanyl)methyl)-1,2-oxazol-5-yl]methanol	C12 H18 N2 O3	238.1286	6,455,610
398	2-{3-hydroxy-5-[(E)-2-(4-hydroxyphenyl)ethenyl]phenoxy}-6-(hydroxymethyl)oxane-3,4,5-triol	C20 H22 O8	390.1264	6,452,913
399	NP-001928	C19 H18 O8	374.0954	6,436,781
400	JWH 018 adamantyl carboxamide	C24 H32 N2 O	386.239	6,384,503

List	Name	Formula	Molecular Weight (Da)	Area
401	AL 8810 Methyl ester	C25 H33 F O4	438.2205	6,361,755
402	5-Methoxyindole	C9 H9 N O	147.0666	6,089,400
403	4-(anilinomethylidene)-3-methyl-4,5-dihydroisoxazol-5-one	C11 H10 N2 O2	202.0722	5,938,247
404	N5-methyl-3-(1-adamantyl)-1,2,4-thiadiazol-5-amine	C13 H19 N3 S	249.1335	5,772,940
405	PV8	C17 H25 N O	259.19	5,722,026
406	2-{2-[(6-methoxy-2-morpholinopyridin-3-yl)amino]-2-oxoethoxy}acetic acid	C14 H19 N3 O6	325.1275	5,289,956
407	(3aR,4S,6R,11aR)-6,9-Dihydroxy-6,10-dimethyl-3-methylene-2,7-dioxo-2,3,3a,4,5,6,7,8,9,11a-decahydrocyclodeca[b]furan-4-yl methacrylate	C19 H24 O7	386.1308	5,105,020
408	2-[(2S,3R,4S,5R)-5-(Aminomethyl)-3,4-dihydroxytetrahydro-2-furanyl]-N-(4-methoxybenzyl)acetamide	C15 H22 N2 O5	348.1151	4,772,110
409	Testosterone enanthate	C26 H40 O3	400.3013	4,675,684
410	4,6-dihydroxy-5a-methyl-3-methylidene-2-oxo-dodecahydronaphtho[1,2-b]furan-9-carbaldehyde	C15 H20 O5	280.1274	4,265,171
411	Codeine	C18 H21 N O3	299.1481	4,239,551
412	Testosterone cypionate	C27 H40 O3	412.2944	3,940,585
413	5-[(4-methoxyphenyl)methylene]-3-phenyl-2,5-dihydro-1,2,4-triazin-6(1H)-one	C17 H15 N3 O2	293.1233	3,606,741
414	2-Arachidonoyl glycerol	C23 H38 O4	378.2723	2,962,038