

Supplementary

KERRA, mixed medicinal plant extracts, inhibits SARS-CoV-2 targets enzymes and feline corona virus

Supaphorn Seetaha^{1,4}, Phatcharin Khamplong¹, Panatda Wanaragthai², Thitinan Aiebchun¹, Siriluk Ratanabunyong¹, Sucheewin Krobthongand², Yodying Yingchutrakul⁵, Jatuporn Rattanasrisomporn³ and Kiattawee Choowongkomon^{1,2,4*}

¹ Department of Biochemistry, Faculty of Science, Kasetsart University, Bangkok 10900, Thailand; supaporn.se@ku.th

² Interdisciplinary of Genetic Engineering and Bioinformatics, Graduate School, Kasetsart University, Bangkok 10900, Thailand; sucheewin82@gmail.com

³ Department of Companion Animal Clinical Sciences, Faculty of Veterinary Medicine, Kasetsart University, Bangkok 10900, Thailand; fvetjpn@ku.ac.th

⁴ Kasetsart University Institute for Advanced Studies, Kasetsart University, Bangkok 10900, Thailand; kiattawee.c@ku.th

⁵ National Omics Center, National Science and Technology Development Agency, Pathumtani, 10110, Thailand; yodying.yin@nstda.or.th

*Correspondence: kiattawee.c@ku.th ; Tel.: (66) 2-562-5555 ext. 647729; Fax: (+66)2-561-4627

Supplementary Table 1: Phytochemical Profiles of KERRA extracts

List	Name	Formula	Molecular Weight (Da)	Area
1	2-Methoxy-9H-xanthen-9-one	C14 H10 O3	226.0594	7.43E+09
2	Isorhapontigenin	C15 H14 O4	276.096	7.36E+09
3	Betaine	C5 H11 N O2	117.0776	6.84E+09
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	6.81E+09
5	trans-Anethole	C10 H12 O	148.0869	4.82E+09
6	Eicosatetraynoic acid	C20 H24 O2	296.1734	4.05E+09
7	NP-020078	C17 H28 O3	302.1847	3.28E+09
8	NP-003294	C18 H16 O7	344.085	3.09E+09
9	9,16-dihydroxy-6-(hydroxymethyl)-2,6,11-trimethyl-15-oxatetracyclo[8.7.0.0.0.0.0]heptadec-12-en-14-one	C20 H30 O5	332.1946	2.88E+09
10	N1-(3-chlorophenyl)-2-[2-(trifluoromethyl)-4-quinolyl]hydrazine-1-carboxamide	C17 H12 Cl F3 N4 O	380.0672	2.37E+09
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	2.36E+09
12	Choline	C5 H13 N O	103.0985	2.34E+09
13	(1S,4S,5R,10S,13S,17S,19S,20R)-10-hydroxy-4,5,9,9,13,19,20-heptamethyl-24-oxahexacyclo[15.5.2.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0]tetracos-15-en-23-one	C30 H46 O3	454.3393	2.20E+09
14	NP-016928	C20 H28 O3	298.1892	1.92E+09
15	NP-006862	C20 H32 O4	318.2154	1.49E+09
16	DL-Stachydrine	C7 H13 N O2	143.0929	1.29E+09
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	1.28E+09
18	Apigenin 7-O-glucuronide	C21 H18 O11	446.0796	1.09E+09
19	(1R,2R,5S,8R,10R,14R)-20-hydroxy-1,2,14,18,18-pentamethyl-17-oxo-8-(prop-1-en-2-yl)pentacyclo[11.8.0.0.0.0.0]henicosane-5-carboxylic acid	C30 H46 O4	492.3153	1.08E+09
20	NP-004713	C15 H24 O2	218.1646	9.76E+08

List	Name	Formula	Molecular Weight (Da)	Area
21	Palmitoleic Acid	C16 H30 O2	276.2053	7.97E+08
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	7.52E+08
23	11-(4-chloroanilino)-2,3-dihydro-1H-cyclopenta[4,5]pyrido[1,2-a]benzimidazole-4-carbonitrile	C21 H15 Cl N4	358.1008	7.07E+08
24	NP-009051	C17 H16 O5	300.0958	6.92E+08
25	NP-000615	C14 H12 O4	244.0704	6.60E+08
26	Oleamide	C18 H35 N O	281.2681	6.16E+08
27	Formononetin	C16 H12 O4	268.0696	5.94E+08
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	5.73E+08
29	3',4'-Dimethoxyacetophenone	C10 H12 O3	180.0765	5.68E+08
30	NP-021050	C30 H48 O4	454.341	5.43E+08
31	Biochanin A	C16 H12 O5	284.0648	5.05E+08
32	Hexadecanamide	C16 H33 N O	255.2538	5.00E+08
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	4.79E+08
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	4.43E+08
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	4.24E+08
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	4.23E+08
37	NP-014517	C14 H18 O9	352.0725	4.23E+08
38	4-(2,3-dihydro-1H-indol-1-yl)-1-phenyl-1H-pyrazolo[3,4-d]pyrimidine	C19 H15 N5	313.1276	4.21E+08

List	Name	Formula	Molecular Weight (Da)	Area
39	NP-020014	C15 H26 O3	276.1666	4.17E+08
40	Stearoyl Ethanolamide	C20 H41 N O2	309.2994	4.14E+08
41	D-(+)-Maltose	C12 H22 O11	364.0936	4.00E+08
42	NP-005821	C30 H46 O3	436.329	3.96E+08
43	2-(8-Hydroxy-4a,8-dimethyldecahydro-2-naphthalenyl)acrylic acid	C15 H24 O3	274.1533	3.87E+08
44	NP-000465	C17 H14 O6	314.0752	3.83E+08
45	Aflatoxin G2	C17 H14 O7	330.0696	3.48E+08
46	3-Hydroxy-2-methylpyridine	C6 H7 N O	109.0514	3.42E+08
47	1-(4-hydroxyphenyl)propane-1,2-diol	C9 H12 O3	190.061	3.22E+08
48	Agmatine	C5 H14 N4	130.1204	3.14E+08
49	Cinchonidine	C19 H22 N2 O	294.1768	3.09E+08
50	trans-3-Indoleacrylic acid	C11 H9 N O2	187.0613	2.96E+08
51	NP-012972	C14 H24 O3	222.1588	2.95E+08
52	5-[5-(methoxycarbonyl)-5,8a-dimethyl-2-methylidene-decahydronaphthalen-1-yl]-3-methylpentanoic acid	C21 H34 O4	350.2412	2.90E+08
53	4-Methylumbelliferone	C10 H8 O3	176.0454	2.84E+08
54	Trigonelline	C7 H7 N O2	96.01952	2.78E+08
55	D-(+)-Pyroglutamic Acid	C5 H7 N O3	129.0412	2.71E+08
56	(5S,6S)-5-Hydroxy-4-methoxy-6-[(E)-2-phenylvinyl]-5,6-dihydro-2H-pyran-2-one	C14 H14 O4	246.0866	2.49E+08
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	2.49E+08
58	Monoolein	C21 H40 O4	356.2886	2.41E+08
59	Ageratriol	C15 H24 O3	234.159	2.17E+08
60	5-hydroxy-6,7-dimethoxy-2-phenyl-4H-chromen-4-one	C17 H14 O5	298.0807	2.16E+08
61	NP-006105	C15 H16 O5	298.0799	2.15E+08
62	Cryptotanshinone	C19 H20 O3	296.1373	2.13E+08
63	4-Hydroxybenzaldehyde	C7 H6 O2	122.0354	2.09E+08
64	octadec-9-ynoic acid	C18 H32 O2	262.2267	2.08E+08
65	(1S,2R,9R,11R,12R,15R)-11-hydroxy-2,6,9,15-tetramethyl-13-	C18 H20 O5	338.1087	2.02E+08

List	Name	Formula	Molecular Weight (Da)	Area
	oxatetracyclo[10.2.1.0.0 ^{1,2} .0.0 ^{3,4}]pentadeca-4,6-diene-3,8,14-trione			
66	Harpagoside	C24 H30 O11	516.1549	2.01E+08
67	NP-008998	C16 H18 O6	328.0906	2.01E+08
68	Resorcinol monoacetate	C8 H8 O3	152.0455	1.86E+08
69	(+)-ar-Turmerone	C15 H20 O	216.1488	1.85E+08
70	Benzyl methacrylate	C11 H12 O2	158.0713	1.83E+08
71	Acetophenone	C8 H8 O	120.0555	1.76E+08
72	Avocadyne 1-acetate	C19 H34 O4	348.2256	1.73E+08
73	(3R,4R)-4-[(3,4-dimethoxyphenyl)methyl]-3-[(4-hydroxy-3-methoxyphenyl)methyl]oxolan-2-one	C21 H24 O6	394.1348	1.64E+08
74	[5-(2-methylimidazo[1,2-a]pyridin-3-yl)-1H-pyrazol-1-yl][4-(trifluoromethyl)phenyl]methanone	C19 H13 F3 N4 O	370.1053	1.62E+08
75	Apocynin	C9 H10 O3	166.0613	1.60E+08
76	1-Linoleoyl glycerol	C21 H38 O4	354.273	1.59E+08
77	NP-005146	C16 H18 O4	256.1068	1.52E+08
78	4-(4-methoxyphenyl)-2-(4-pyridyl)-1,3-thiazole hydrobromide	C15 H12 N2 O S	268.0698	1.48E+08
79	N2-{[(3R,4S)-3-{[5-(4-methoxyphenyl)-1,2-oxazol-3-yl]methyl}-4-piperidiny]acetyl}-N2-methylglycinamide	C21 H28 N4 O4	422.1893	1.44E+08
80	Tridemorph	C19 H39 N O	297.3003	1.44E+08
81	Resveratrol	C14 H12 O3	228.0757	1.40E+08
82	L-Phenylalanine	C9 H11 N O2	165.077	1.36E+08
83	Tanshinone IIA	C19 H18 O3	294.1217	1.35E+08
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	C21 H18 O12	462.0765	1.34E+08
85	Scutellarin	C21 H18 O12	462.0745	1.34E+08
86	Bicyclo Prostaglandin E2	C20 H30 O4	178.0962	1.30E+08
87	(4aS,9aR)-7-[2-(2,3-Dimethoxyphenyl)ethyl]-2-[(4-methoxyphenyl)acetyl]decahydro-6H-pyrido[3,4-d]azepin-6-one	C28 H36 N2 O5	502.2485	1.29E+08

List	Name	Formula	Molecular Weight (Da)	Area
88	Apigenin	C15 H10 O5	270.0495	1.29E+08
89	15-Deoxy- Δ 12,14-prostaglandin J2-2-glycerol ester	C23 H34 O5	390.234	1.24E+08
90	3-O- β -D-Glucopyranosylandrographolide	C26 H40 O10	534.2375	1.22E+08
91	Nalidixic acid	C12 H12 N2 O3	232.086	1.22E+08
92	methyl 2-ethyl-4-[(3R,4R,5S)-5-hydroxy-4,5-dimethyl-2-oxoxolan-3-yl]-2-methyl-3-oxobutanoate	C14 H22 O6	308.1196	1.21E+08
93	Vanillin	C8 H8 O3	152.0453	1.21E+08
94	(5S,6S)-5-hydroxy-4-methoxy-6-(2-phenylethyl)-5,6-dihydro-2H-pyran-2-one	C14 H16 O4	270.0855	1.17E+08
95	Ethylmorphine	C19 H23 N O3	313.164	1.15E+08
96	6-Methyl-2-pyridinemethanol	C7 H9 N O	123.0668	1.12E+08
97	NP-020214	C16 H32 O4	310.2107	1.12E+08
98	(1R,9S)-11-(Cyclohexylcarbonyl)-5-(2-methylphenyl)-7,11-diazatricyclo[7.3.1.02,7]trideca-2,4-dien-6-one	C25 H30 N2 O2	390.2329	1.10E+08
99	3',4'-Trimethylene- α -methylamino-valerophenone	C15 H21 N O	231.1596	1.10E+08
100	NP-018817	C15 H24 O4	290.146	1.10E+08
101	NP-002113	C20 H28 O4	354.1763	1.09E+08
102	NP-002322	C18 H32 O4	334.2082	1.09E+08
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	1.06E+08
104	NP-020205	C11 H16 O4	234.0864	1.05E+08
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	1.03E+08
106	3,3',5,5'-Tetramethyldiphenoquinone	C16 H16 O2	240.112	1.02E+08
107	3-Hydroxypyridine	C5 H5 N O	95.03605	1.02E+08
108	Rhamnetin	C16 H12 O7	316.0541	1.01E+08
109	4-Guanidinobutyric acid	C5 H11 N3 O2	145.0835	1.00E+08
110	Methoxyacetyl fentanyl	C22 H28 N2 O2	352.2184	99759859
111	(11E,15Z)-9,10,13-trihydroxyoctadeca-11,15-dienoic acid	C18 H32 O5	310.2108	96929532
112	2-(3,4-dihydroxyphenyl)-3,5,7-trihydroxy-6-methyl-4H-chromen-4-one	C16 H12 O7	316.0554	95611487
113	Chlorogenic acid	C16 H18 O9	376.0729	95367804

List	Name	Formula	Molecular Weight (Da)	Area
114	(2E)-3-(4-Hydroxyphenyl)-N-[2-(4-hydroxyphenyl)ethyl]acrylamide	C17 H17 N O3	283.1178	93886662
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	93010999
116	Daidzein	C15 H10 O4	254.055	92720175
117	N1-cyclooctyl-4-hydroxy-1-piperidinecarbothioamide	C14 H26 N2 O S	292.1622	92451286
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	91472896
119	T-2 Triol	C20 H30 O7	404.1788	88975025
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	88307788
121	NP-021293	C30 H48 O4	454.3399	88067373
122	15-(5-hydroxy-6-methylhept-6-en-2-yl)-7,7,12,16-tetramethylpentacyclo[9.7.0.0.0.0.0]nona-2,4,6,8-tetraene-10-ol	C30 H50 O2	424.3658	87922433
123	Guanine	C5 H5 N5 O	151.0485	84892990
124	NP-005474	C21 H22 O9	418.1217	83775319
125	2,2,6,6-Tetramethyl-1-piperidinol (TEMPO)	C9 H19 N O	157.1448	82866884
126	NP-003141	C21 H20 O9	438.0873	82431805
127	Coumarin	C9 H6 O2	146.0348	82355781
128	Oleanolic acid	C30 H48 O3	438.3444	81946065
129	Carbaprostacyclin	C21 H34 O4	332.231	81495844
130	DL-Tryptophan	C11 H12 N2 O2	204.0875	80563233
131	Octylphosphonic acid	C8 H19 O3 P	194.1034	79695417
132	Trioxsalen	C14 H12 O3	228.0755	78976414
133	trans,trans-2,4-Heptadienal	C7 H10 O	110.0718	78810316
134	NP-014287	C18 H32 O3	318.213	77233880
135	(±)8-HEPE	C20 H30 O3	300.2053	75941839
136	Cholest-4-en-3-one	C27 H44 O	384.3348	75360861
137	Adenosine	C10 H13 N5 O4	267.0936	74816007
138	4-[2-(2-oxo-1-imidazolidinyl)ethyl]-1λ~6~,4-thiazinane-1,1-dione	C9 H17 N3 O3 S	269.0845	74332839

List	Name	Formula	Molecular Weight (Da)	Area
139	{{(3S)-3-[5-(2-Fluorophenyl)-1,3,4-oxadiazol-2-yl]-1-pyrrolidiny}}(phenyl)methanone	C19 H16 F N3 O2	337.1273	74001254
140	4-Aminophenol	C6 H7 N O	109.0515	73491150
141	Lupeol	C30 H50 O	426.3811	72201114
142	Methyldienolone	C19 H26 O2	286.1891	72082535
143	4-phenoxyphenyl 4-hydroxypiperidine-1-carboxylate	C18 H19 N O4	335.1092	71715614
144	4-methoxy-6-(prop-2-en-1-yl)-2H-1,3-benzodioxole	C11 H12 O3	160.0504	71158053
145	NP-019848	C27 H46 N6 O7	566.3517	70855091
146	DL-Arginine	C6 H14 N4 O2	174.1096	70649859
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	69257250
148	NP-020240	C14 H20 O3	186.1014	69113668
149	NP-019811	C6 H7 N O2	125.0464	68696381
150	1-{4-[2-(7-methoxy-2H-1,3-benzodioxol-5-yl)ethyl]phenoxy}-3-methylbutane-2,3-diol	C21 H26 O6	396.1502	65453635
151	NP-007909	C13 H20 O3	206.1285	64617637
152	Isobornyl methacrylate	C14 H22 O2	222.1598	63603104
153	Kanosamine	C6 H13 N O5	161.0671	63573239
154	NP-013210	C12 H14 O3	188.0817	63140447
155	Cyclo(leucylprolyl)	C11 H18 N2 O2	210.1347	60426370
156	12-Oxo phytodienoic acid	C18 H28 O3	292.1999	59586148
157	NP-003024	C12 H14 O5	260.0652	58967173
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	58459871
159	(±)13-HpODE	C18 H32 O4	294.2159	58317690
160	Emodin	C15 H10 O5	270.0497	58314124
161	Maltol	C6 H6 O3	126.0303	57637035
162	(2R)-7-Methoxy-3-oxo-3,4-dihydro-2H-1,4-benzoxazin-2-yl β-D-glucopyranoside	C15 H19 N O9	379.0838	57293685
163	9-Oxo-ODE	C18 H30 O3	294.2153	57068495
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	56752848

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	56359580
166	4-Amino-2-pyrazin-2-ylpyrimidine-5-carbonitrile	C9 H6 N6	198.0656	56098264
167	3-[4-methyl-1-(2-methylpropanoyl)-3-oxocyclohexyl]butanoic acid	C15 H24 O4	290.1454	55375637
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	55103926
169	Bis(4-ethylbenzylidene)sorbitol	C24 H30 O6	414.1994	55038320
170	NP-008274	C15 H20 O4	286.1169	54710900
171	Diosgenin	C27 H42 O3	396.2978	54355608
172	4-Indolecarbaldehyde	C9 H7 N O	145.0512	53929932
173	6-Hydroxy-1-(hydroxymethyl)-5-{2-[(4-methoxybenzyl)amino]-2-oxoethyl}-1,4a-dimethyldecahydro-2-naphthalenyl propylcarbamate	C27 H42 N2 O6	490.3	53381782
174	L-Tyrosine	C9 H11 N O3	181.0718	50877541
175	NP-013736	C10 H16 N2 O2	196.119	48955487
176	NP-013326	C15 H16 O4	242.091	48052999
177	3,5-di-tert-Butyl-4-hydroxybenzaldehyde	C15 H22 O2	234.1592	47438366
178	Aloe-emodin	C15 H10 O5	270.0495	45963974
179	(5E)-7-methylidene-10-oxo-4-(propan-2-yl)undec-5-enoic acid	C15 H24 O3	274.1514	45813299
180	[2-(hydroxymethyl)-5,5,8a-trimethyl-1,4,4a,5,6,7,8,8a-octahydronaphthalen-1-yl]methanol	C15 H26 O2	260.1722	45422507
181	NP-008993	C18 H34 O4	336.2236	44613421
182	NP-015559	C17 H14 O7	330.0699	44353657
183	Oleoyl ethanolamide	C20 H39 N O2	325.2943	43929483
184	4-Methoxybenzaldehyde	C8 H8 O2	136.051	43889807
185	1-adamantyl(1,4-thiazinan-4-yl)methanone	C15 H23 N O S	265.1494	43135442
186	4'-(Imidazol-1-yl)acetophenone	C11 H10 N2 O	186.0772	43124736
187	9-hydroxy-2,10,10-trimethyltricyclo[6.3.0.0.0]undec-6-ene-6-carboxylic acid	C15 H22 O3	232.1434	43120862
188	Tetranor-12(S)-HETE	C16 H26 O3	288.1691	43117886
189	N-Acetylorlornithine	C7 H14 N2 O3	142.0763	42842000

List	Name	Formula	Molecular Weight (Da)	Area
190	Aloesin	C19 H22 O9	394.1197	42676729
191	NP-000308	C16 H12 O6	300.0597	42565135
192	NP-011220	C11 H18 N2 O2	210.1344	42264024
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	41860287
194	D-Raffinose	C18 H32 O16	526.1444	41677143
195	4-[(E)-2-[3-(β-D-Glucopyranosyloxy)-5-hydroxyphenyl]vinyl]-2-methoxyphenyl β-D-glucopyranoside	C27 H34 O14	582.1873	41383036
196	3-(propan-2-yl)-octahydropyrrolo[1,2-a]pyrazine-1,4-dione	C10 H16 N2 O2	196.1198	41279599
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	41275425
198	Nicotinic acid	C6 H5 N O2	123.0306	41260722
199	Betaxolol	C18 H29 N O3	307.211	40881749
200	2,6-Dimethyl-γ-pyrone	C7 H8 O2	124.051	40804739
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	40457030
202	4-(2-methoxyphenyl)-1-(3-phenyl-1,2,4-thiadiazol-5-yl)piperidine	C20 H21 N3 O S	351.1428	39297321
203	SB236057A	C33 H34 N4 O3	534.2567	39140029
204	Indole	C8 H7 N	117.0563	39050503
205	Ambrosic acid	C15 H20 O4	286.115	38842262
206	Kynurenic acid	C10 H7 N O3	189.0406	38727203
207	8-[3-Oxo-2-[(2E)-2-penten-1-yl]-1-cyclopenten-1-yl]octanoic acid	C18 H28 O3	292.2001	38683339
208	NP-020327	C21 H24 O8	426.1237	38580877
209	2-Methoxyresorcinol	C7 H8 O3	140.0458	38539952
210	3-Methyl-4-[2-(4-morpholinophenyl)hydrazono]-1-phenyl-4,5-dihydro-1H-pyrazol-5-one	C20 H21 N5 O2	385.1483	38526023
211	9S,13R-12-Oxophytodienoic acid	C18 H28 O3	292.2012	38119466
212	Arachidonic acid	C20 H32 O2	286.2263	37101625
213	Cuminaldehyde	C10 H12 O	148.087	36791156
214	Pulegone	C10 H16 O	152.1181	36137196
215	NP-003399	C14 H12 O2	212.0813	36003314
216	NP-020112	C30 H48 O2	440.3605	35225004

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	35207040
218	Schaftoside	C26 H28 O14	564.1401	34699760
219	N-(2-{4-[5-(Acetylamino)-1H-benzimidazol-2-yl]phenyl}-1H-benzimidazol-5-yl)acetamide	C24 H20 N6 O2	424.1716	33904086
220	Salsolinol	C10 H13 N O2	179.0927	33796582
221	NP-008132	C20 H24 O9	430.1185	33257543
222	2,6-Dimethoxyphenol	C8 H10 O3	154.0613	33068750
223	3-{5-[(2S)-1-(4-Chlorobenzyl)-2-pyrrolidiny]-1,2,4-oxadiazol-3-yl}-2-(2-methoxyethoxy)pyridine	C21 H23 Cl N4 O3	436.1296	32810671
224	NP-011548	C18 H34 O3	280.2369	32694515
225	5-fluoro AB-PINACA N-(4-hydroxypentyl) metabolite	C18 H25 F N4 O3	386.1811	31861743
226	6-Methylquinoline	C10 H9 N	143.0718	31687065
227	Nicotinuric acid	C8 H8 N2 O3	180.0556	31203244
228	NP-021018	C12 H18 O4	208.1077	31035152
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	30944116
230	10-Propoxydecanoic acid	C13 H26 O3	242.2005	30925139
231	Diphenylphosphine oxide	C12 H11 O P	202.0525	30854834
232	3-(3,4-dihydroxyphenyl)propanoic acid	C9 H10 O4	164.0456	29678071
233	Nicotinamide	C6 H6 N2 O	122.0466	29612560
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	29505388
235	Penbutolol	C18 H29 N O2	291.2165	29081029
236	NP-004038	C16 H24 O3	246.159	28950112
237	Heptanophenone	C13 H18 O	190.1338	28427034
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	28172000
239	Diphenylamine	C12 H11 N	169.0874	27885206
240	Cyclo(phenylalanyl-prolyl)	C14 H16 N2 O2	244.1181	27273229
241	4-Isopropyl-9H-thioxanthen-9-one	C16 H14 O S	254.0734	27187080
242	Etiocholanolone	C19 H30 O2	272.2109	26205231
243	3-Methoxy prostaglandin F1 α	C21 H38 O6	408.2439	25992019

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	25619491
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	25528060
246	Luteolin	C15 H10 O6	286.0441	25158891
247	2-(tert-butyl)-6-(4-chlorophenyl)-4-(methylthio)pyridine	C16 H18 Cl N S	291.086	25029791
248	Ethyl paraben	C9 H10 O3	166.0611	24772472
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	24707449
250	4-Hydroxyephedrine	C10 H15 N O2	163.0979	24340907
251	(2S)-4-Oxo-2-phenyl-3,4-dihydro-2H-chromen-7-yl beta-D-glucopyranoside	C21 H22 O8	402.1266	24304502
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	24025622
253	5-(6-hydroxy-6-methyloctyl)-2,5-dihydrofuran-2-one	C13 H22 O3	208.1439	23986648
254	6-(tert-butyl)pyridazin-3(2H)-one	C8 H12 N2 O	152.0932	23904057
255	2-sec-Butyl-3-methoxypyrazin	C9 H14 N2 O	166.1087	23840812
256	Acetylcholine	C7 H15 N O2	145.1085	23731706
257	Linoleoyl ethanolamide	C20 H37 N O2	323.2785	23629153
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	23535839
259	NP-001798	C16 H17 N O2	255.1231	23489644
260	4-decyl-3-hydroxy-5-oxooxolane-2,3-dicarboxylic acid	C16 H26 O7	352.1449	23400192
261	2-Isobutyl-3-methoxypyrazine	C9 H14 N2 O	166.1086	23015572
262	Pipecolic acid	C6 H11 N O2	129.0775	22973316
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	22533662
264	NP-020705	C17 H24 O8	378.1245	22533166

List	Name	Formula	Molecular Weight (Da)	Area
265	Norharman	C11 H8 N2	168.0669	22381368
266	γ -Linolenic acid ethyl ester	C20 H34 O2	312.2628	22291201
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	22288124
268	6,7-Dihydroxy-4-methylcoumarin	C10 H8 O4	192.0402	21460057
269	NP-002336	C23 H36 O5	409.2773	21340698
270	α -Pinene-2-oxide	C10 H16 O	152.1185	21322644
271	1,2,3,4-Tetramethyl-1,3-cyclopentadiene	C9 H14	122.1085	21086160
272	Diundecyl phthalate	C30 H50 O4	496.3496	20861702
273	NP-016721	C15 H16 O4	282.0863	20469729
274	[4-(2-methoxyphenyl)piperazino](4-methylphenyl)methanone	C19 H22 N2 O2	310.1729	20357449
275	Uracil	C4 H4 N2 O2	112.026	20227338
276	NP-008198	C26 H32 O13	574.1752	20115132
277	8Z,11Z,14Z-Eicosatrienoic acid	C20 H34 O2	306.2525	19964197
278	6-Methoxyquinoline	C10 H9 N O	159.0669	19903165
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	19869631
280	Methylhippuric acid	C10 H11 N O3	193.0719	19711927
281	Palmitoyl ethanolamide	C18 H37 N O2	299.2787	19705843
282	3-(2,6-Dioxocyclohexyl)propanenitrile	C9 H11 N O2	165.0769	19583327
283	2-Methoxybenzaldehyde	C8 H8 O2	136.0515	19349457
284	NP-016437	C15 H24 O5	306.1405	19214653
285	NP-020713	C20 H26 O4	330.1766	18891579
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	18870286
287	5,10,15-trimethyl-4,9,13-trioxatetracyclo[10.3.0.0.0 Δ^1 , $\hat{\alpha}$ μ .0 $\hat{\alpha}$, $\hat{A}\hat{\alpha}$ ω]pentadec-1(15)-en-14-one	C15 H20 O4	246.1226	18681670
288	(-)-Epicatechin	C15 H14 O6	290.0756	18476297
289	PD 0200347	C10 H17 N3 O2	211.1335	18436988
290	1-(3,4-dimethoxyphenyl)ethan-1-one oxime	C10 H13 N O3	177.077	18405606
291	Prolylleucine	C11 H20 N2 O3	228.1445	18386393
292	Benzyl 6-O-beta-D-glucopyranosyl-beta-D-glucopyranoside	C19 H28 O11	454.1381	18341336
293	4,6-Dimethyl-2(1H)-pyrimidinone	C6 H8 N2 O	124.0622	18255886
294	Tetranor-12R-HETE	C16 H26 O3	248.1746	18178612
295	NP-008882	C27 H48 O9	538.3046	17867532

List	Name	Formula	Molecular Weight (Da)	Area
296	Scoparone	C11 H10 O4	206.0553	17852271
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	17687990
298	Dulcitol	C6 H14 O6	182.0823	17408410
299	Azobenzene	C12 H10 N2	182.0831	17159521
300	4-[[5-(6-Hydroxy-5,5,8a-trimethyl-2-methylenedecahydro-1-naphthalenyl)-3-methylpentyl]oxy]-4-oxobutanoic acid	C24 H40 O5	390.2729	17091735
301	4'-Methoxyacetophenone	C9 H10 O2	150.0663	16893301
302	Esculetin	C9 H6 O4	178.0245	16749625
303	3-(4-Nitrophenyl)imidazo[1,5-a]pyridine	C13 H9 N3 O2	239.0682	16479751
304	NP-002089	C15 H22 O3	272.1361	16444281
305	N-(2,4-Dimethylphenyl)formamide	C9 H11 N O	149.0825	16154582
306	Zaleplon	C17 H15 N5 O	305.1237	15997293
307	6-Acetylmorphine	C19 H21 N O4	327.1431	15965597
308	13(S)-HOTrE	C18 H30 O3	294.2158	15954057
309	NP-000295	C17 H22 O4	312.1325	15767872
310	Heroin	C21 H23 N O5	369.1528	15501729
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	15419277
312	4-Methylumbelliferyl- α -D-glucopyranoside	C16 H18 O8	338.0955	15357162
313	2-[[2-(1H-indol-3-yl)ethyl]ethanimidoyl]phenol	C18 H18 N2 O	278.1463	15344890
314	N-{4-[(2R,3R)-3-(Hydroxymethyl)-4-methyl-5-oxo-2-morpholinyl]phenyl}-2-methylbenzamide	C20 H22 N2 O4	392.1191	15237300
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	15047930
316	8,8-dimethyl-2H,8H-pyrano[3,2-g]chromen-2-one	C14 H12 O3	228.0758	15022886
317	Buspirone	C21 H31 N5 O2	385.2422	15015423
318	1-(2,4-dihydroxyphenyl)-2-(3,5-dimethoxyphenyl)propan-1-one	C17 H18 O5	324.0947	14833751
319	Thymine	C5 H6 N2 O2	126.0416	14704546
320	3',4'-Dimethyl- α -ethylaminovalerophenone	C15 H23 N O	233.1751	14531645
321	Dehydroepiandrosterone (DHEA)	C19 H28 O2	288.2053	14390832
322	NP-021868	C15 H14 O4	240.0759	14314532
323	N-Acetylhistamine	C7 H11 N3 O	153.0884	13978793

List	Name	Formula	Molecular Weight (Da)	Area
324	NP-021085	C17 H26 O3	260.1741	13528614
325	2-(piperidinomethylidene)malononitrile	C9 H11 N3	161.0936	13422221
326	mesityl(piperidin-4-yl)methanone hydrochloride	C15 H21 N O	231.1597	13411287
327	2-[4-(3-Amino-2-hydroxypropoxy)phenyl]acetamide	C11 H16 N2 O3	224.1135	13259920
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	13076977
329	3-(5-Cyclopropyl-1,3,4-oxadiazol-2-yl)-2-[(4-methylphenyl)thio]pyridine	C17 H15 N3 O S	309.0964	13068237
330	8-(2,3-dihydroxy-3-methylbutyl)-7-methoxy-2H-chromen-2-one	C15 H18 O5	300.0958	12941355
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	12878588
332	NP-020293	C7 H14 N2 O3	196.0827	12867566
333	N-(4-piperidinophenyl)-2-thiophenecarboxamide	C16 H18 N2 O S	308.099	12768996
334	(-)-Strychnine	C21 H22 N2 O2	334.1717	12744644
335	3-[(4-hydroxyphenyl)methyl]-octahydropyrrolo[1,2-a]pyrazine-1,4-dione	C14 H16 N2 O3	260.1126	12742909
336	NP-022238	C20 H22 N2 O	306.1771	12620869
337	Sedanolid	C12 H18 O2	176.1179	12503179
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	12399291
339	6,7,8-trimethoxy-2-(2-phenoxy-3-pyridyl)-4H-3,1-benzoxazin-4-one	C22 H18 N2 O6	428.1028	12157122
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	11972567
341	Benzoguanamine	C9 H9 N5	187.0822	11890538
342	Rilmenidine	C10 H16 N2 O	180.1245	11681064
343	NP-019401	C11 H15 N O2	193.1082	11526016
344	N-[[[(2R,4S,5S)-5-Ethynyl-1-azabicyclo[2.2.2]oct-2-yl]methyl]-2-naphthamide	C21 H22 N2 O	318.1768	11439391
345	3-(3-pyridylamino)-2-[4-(trifluoromethoxy)benzoyl]acrylonitrile	C16 H10 F3 N3 O2	333.0781	11133019
346	3-Succinoylpyridine	C9 H9 N O3	179.0563	11040457
347	1-Phenyl-3-methyl-5-pyrazolone	C10 H10 N2 O	174.0774	10858965

List	Name	Formula	Molecular Weight (Da)	Area
348	Pyrimethamine	C12 H13 Cl N4	248.0807	10710465
349	Artemisinin	C15 H22 O5	264.1307	10662530
350	2-(2-acetyl-3,5-dihydroxyphenyl)acetic acid	C10 H10 O5	192.0402	10443016
351	Carbofuran	C12 H15 N O3	221.1026	10442463
352	Ergocalciferol	C28 H44 O	396.3354	10414786
353	10-Nitrooleate	C18 H33 N O4	349.2207	10152263
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	10078644
355	Naringenin	C15 H12 O5	272.0653	10027835
356	Irganox 1035	C38 H58 O6 S	664.3885	10003353
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	9961772
358	(1R,4aS,5R,8aS)-5-(5-hydroxy-3-methylpentyl)-1,4a-dimethyl-6-methylidene-decahydronaphthalene-1-carboxylic acid	C20 H34 O3	339.273	9842456
359	7-hydroxy-6-methoxy-2H-chromen-2-one	C10 H8 O4	192.0402	9832967
360	(3R,4R)-4-Hydroxy-3-({4-[2-(4-morpholinyl)ethoxy]benzoyl}amino)-N-phenyl-1-azepanecarboxamide	C26 H34 N4 O5	504.2305	9782871
361	N-Feruloyloctopamine	C18 H19 N O5	311.1121	9774591
362	Maltotetraose	C24 H42 O21	688.1966	9733988
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	9652952
364	11(Z),14(Z),17(Z)-Eicosatrienoic acid	C20 H34 O2	306.2521	9365538
365	Debrisoquine	C10 H13 N3	175.1097	9185763
366	5,7-dihydroxy-2-(3-hydroxy-4-methoxyphenyl)-3,6-dimethoxy-4H-chromen-4-one	C18 H16 O8	360.0801	9130052
367	4-morpholinobenzoic acid	C11 H13 N O3	207.0871	8968512
368	HET0016	C12 H18 N2 O	228.1236	8940585
369	5-[(1E)-3-hydroxy-3-methylbut-1-en-1-yl]-2-methylcyclohex-5-ene-1,2,4-triol	C12 H20 O4	250.1153	8915535
370	NP-000124	C12 H20 O4	250.1156	8915535
371	NP-007111	C35 H58 O9	639.4208	8802503
372	Phloroglucinol	C6 H6 O3	126.0302	8687334
373	NP-006888	C13 H24 O4	266.1465	8608883
374	ethyl 4-[(4-methylphenyl)sulfonyl]amino}tetrahydro-1(2H)-pyridinecarboxylate	C15 H22 N2 O4 S	364.09	8589136

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	8463364
376	Wogonin	C16 H12 O5	284.0651	8367490
377	2-Hydroxyquinoline	C9 H7 N O	145.0511	8300054
378	3-Phenylpropionitrile	C9 H9 N	90.0452	8179167
379	NP-011878	C15 H26 O5	308.1563	8129868
380	NP-011150	C22 H24 O8	454.103	8079253
381	5 α -Dihydrotestosterone glucuronide	C25 H38 O8	466.2496	7982458
382	Mepanipirim	C14 H13 N3	223.1082	7916105
383	NP-019748	C30 H48 O5	510.3252	7826258
384	N-(((1S,4S,6S)-6-Isopropyl-3-methyl-4-[2-oxo-2-(1-pyrrolidinyl)ethyl]-2-cyclohexen-1-yl)methyl)-2-pyrazinecarboxamide	C22 H32 N4 O2	406.2281	7451731
385	Apigetrin	C21 H20 O10	432.1003	7450390
386	(2R)-5-hydroxy-7-methoxy-2-phenyl-3,4-dihydro-2H-1-benzopyran-4-one	C16 H14 O4	270.0858	7400693
387	7-Aminoflunitrazepam	C16 H14 F N3 O	283.1174	7288007
388	Albendazole-2-aminosulfone	C10 H13 N3 O2 S	239.0679	7198178
389	Aflatoxin B2	C17 H14 O6	314.0751	6996550
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	6963068
391	NP-016596	C19 H30 O8	408.1713	6871022
392	Cytisine	C11 H14 N2 O	190.1082	6802962
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	6786418
394	(2R)-1-(5-hydroxy-3-methylpentyl)-2,5,5,8a-tetramethyl-decahydronaphthalen-2-ol	C20 H38 O2	292.2733	6650316
395	(9cis)-Retinal	C20 H28 O	284.2107	6564013
396	2-[6-(1H-benzo[d]imidazol-2-yl)-2-pyridyl]-1H-benzo[d]imidazole	C19 H13 N5	311.1125	6489108
397	[3-({3-[(Cyclopropylmethyl)amino]-3-oxetanyl)methyl}-1,2-oxazol-5-yl]methanol	C12 H18 N2 O3	238.1286	6455610
398	2-{3-hydroxy-5-[(E)-2-(4-hydroxyphenyl)ethenyl]phenoxy}-6-(hydroxymethyl)oxane-3,4,5-triol	C20 H22 O8	390.1264	6452913
399	NP-001928	C19 H18 O8	374.0954	6436781
400	JWH 018 adamantyl carboxamide	C24 H32 N2 O	386.239	6384503

List	Name	Formula	Molecular Weight (Da)	Area
401	AL 8810 Methyl ester	C25 H33 F O4	438.2205	6361755
402	5-Methoxyindole	C9 H9 N O	147.0666	6089400
403	4-(anilinomethylidene)-3-methyl-4,5-dihydroisoxazol-5-one	C11 H10 N2 O2	202.0722	5938247
404	N5-methyl-3-(1-adamantyl)-1,2,4-thiadiazol-5-amine	C13 H19 N3 S	249.1335	5772940
405	PV8	C17 H25 N O	259.19	5722026
406	2-[2-[(6-methoxy-2-morpholinopyridin-3-yl)amino]-2-oxoethoxy]acetic acid	C14 H19 N3 O6	325.1275	5289956
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	5105020
408	2-[(2S,3R,4S,5R)-5-(Aminomethyl)-3,4-dihydroxytetrahydro-2-furanyl]-N-(4-methoxybenzyl)acetamide	C15 H22 N2 O5	348.1151	4772110
409	Testosterone enanthate	C26 H40 O3	400.3013	4675684
410	4,6-dihydroxy-5a-methyl-3-methylidene-2-oxo-dodecahydronaphtho[1,2-b]furan-9-carbaldehyde	C15 H20 O5	280.1274	4265171
411	Codeine	C18 H21 N O3	299.1481	4239551
412	Testosterone cypionate	C27 H40 O3	412.2944	3940585
413	5-[(4-methoxyphenyl)methylene]-3-phenyl-2,5-dihydro-1,2,4-triazin-6(1H)-one	C17 H15 N3 O2	293.1233	3606741
414	2-Arachidonoyl glycerol	C23 H38 O4	378.2723	2962038