Electronic Supporting Information

In Search of SARS CoV-2 Inhibitors as RNA Dependent RNA Polymerase and Main Protease inhibitors: Molecular Docking, ADMET Analysis and Molecular Dynamic Simulations

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[*]Corresponding Authors: E-mail: tejas.dhameliya@lmcp.ac.in (TMD), gaurang.shah@lmcp.ac.in (GBS). Tel: +91 79 2630 2746. Fax: +91 79 2630 4865.

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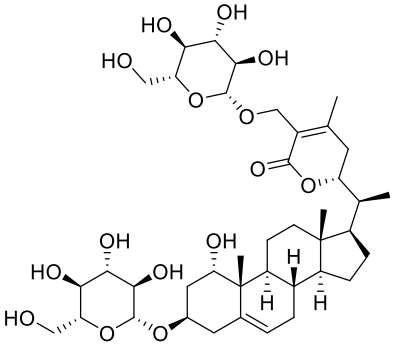
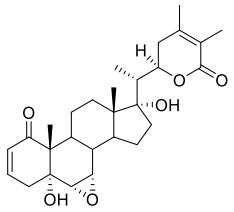
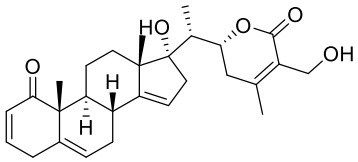
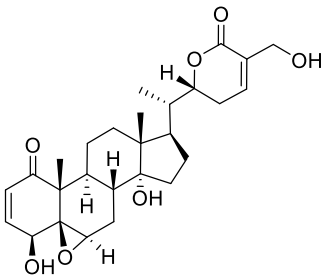
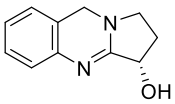
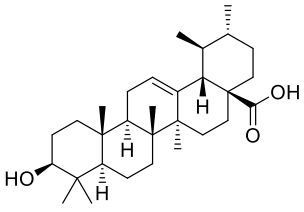
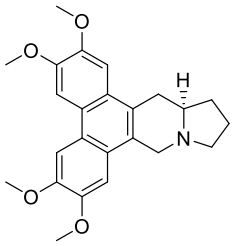
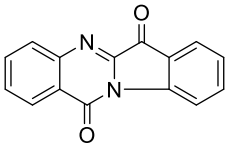
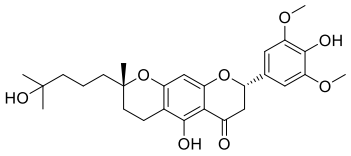
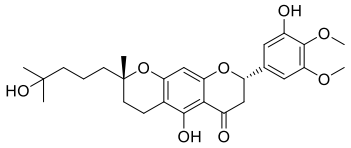
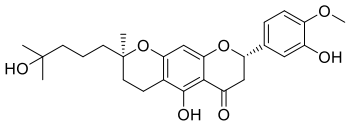
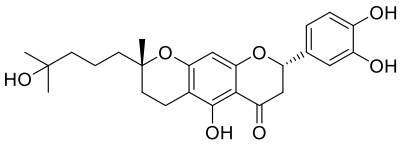
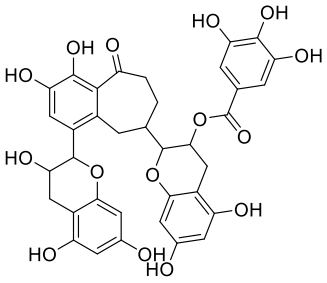
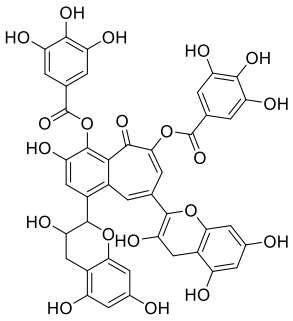
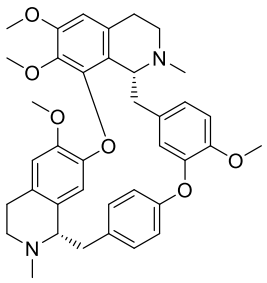
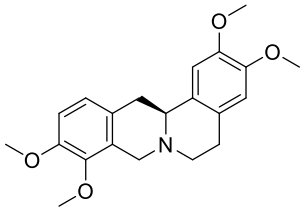
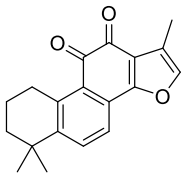
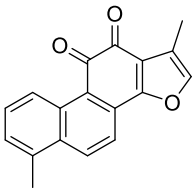
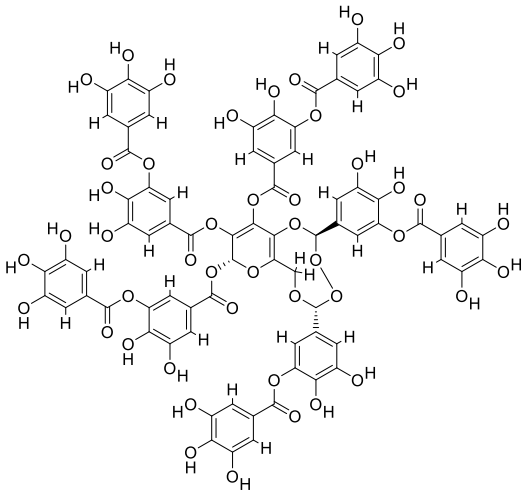
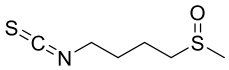
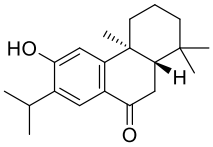
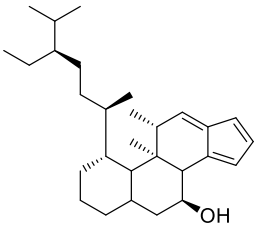
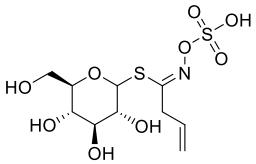
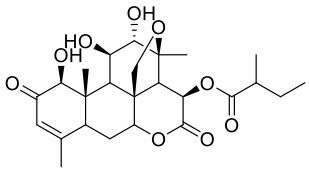
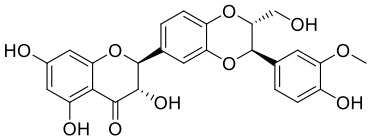
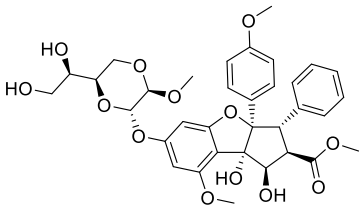
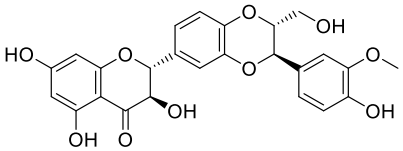
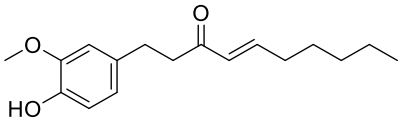
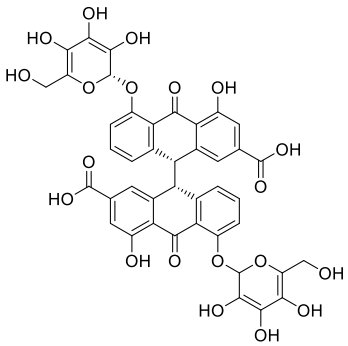
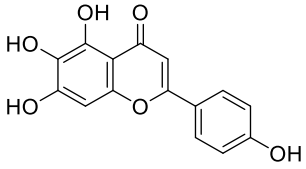
1. Dataset for Selected Natural Products and their Derivatives

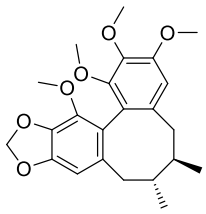
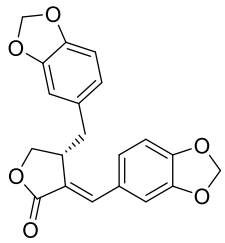
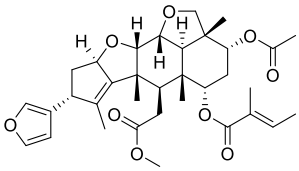
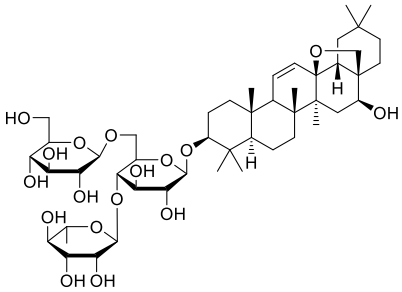
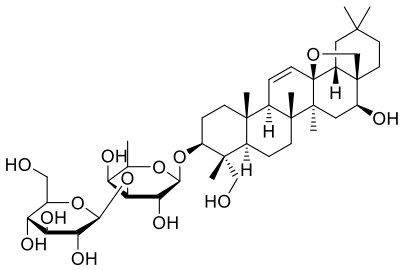
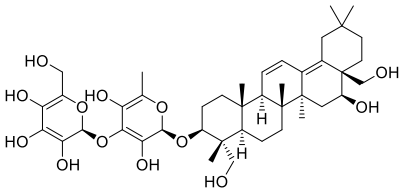
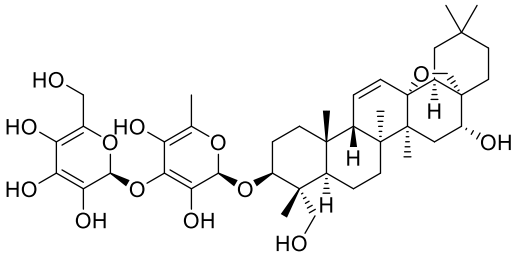
Table S1. Selected natural products and their derivatives as ligands for molecular modeling.

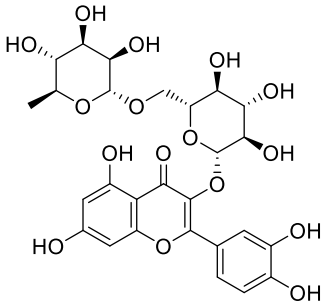
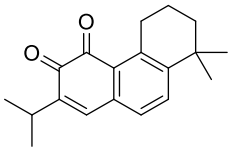
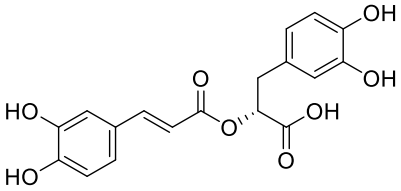
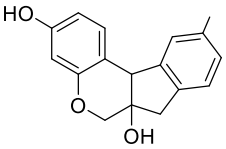
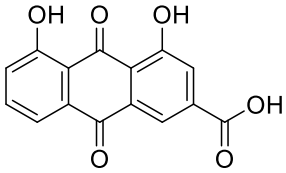
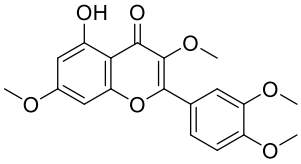
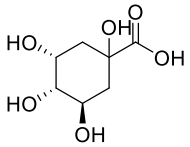
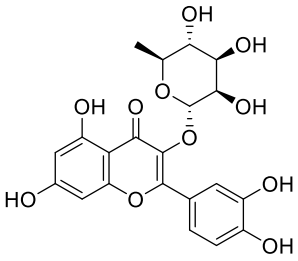
Entry	2-Dimensional Structure	Name	Biological source	Ref.
1		Withanoside X	*Withania somnifera*	[1]
2		Withanone	*Withania somnifera*	[1]
3		Withanolide N	*Withania somnifera*	[1]
4		Withaferin A	*Withania somnifera*	[1]
5		Vasicin	*Adhatoda vasaca*	[2]
6		Urosolic acid	*Ocimum tenuiflorum*	[1]

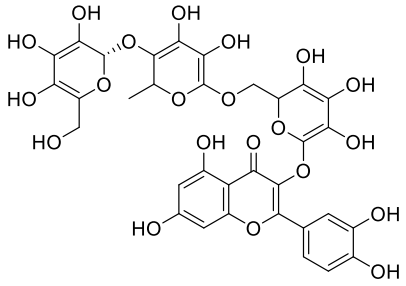
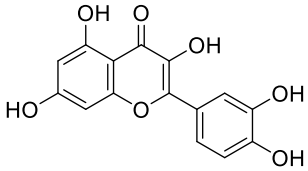
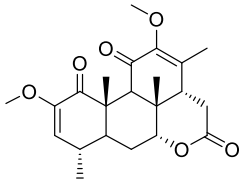
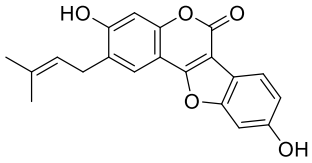
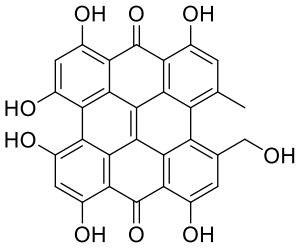
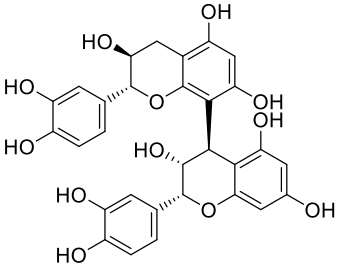
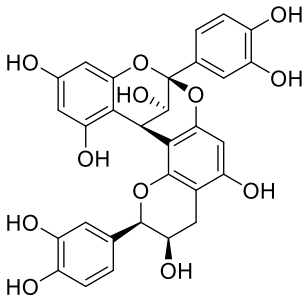
7		Tylophorine	*Tylophora indica*	[3]
8		Tryptanthrine	*Strobilanthes cusia*	[4]
9		Tomentin D	*Sphaeralcea angustifolia*	[3]
10		Tomentin C	*Sphaeralcea angustifolia*	[3]
11		Tomentin B	*Sphaeralcea angustifolia*	[3]
12		Tomentin A	*Sphaeralcea angustifolia*	[3]
13		Theaflavin-3`-o-gallate	*Camellia sinensis*	[3]
14		Theaflavin-3,3`-digallate	*Camellia sinensis*	[3]

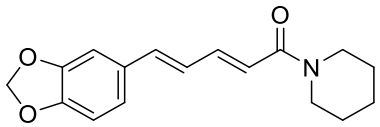
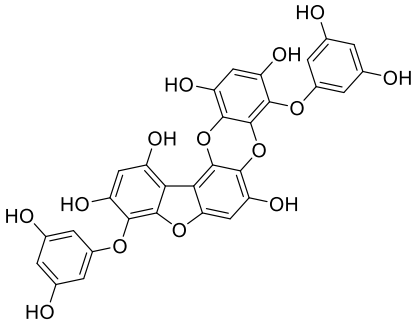
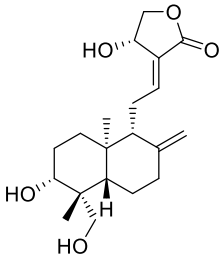
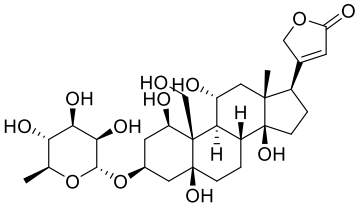
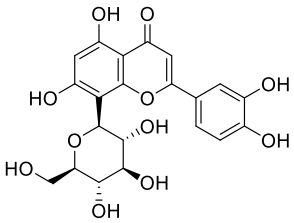
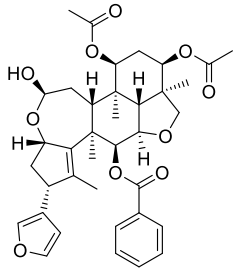
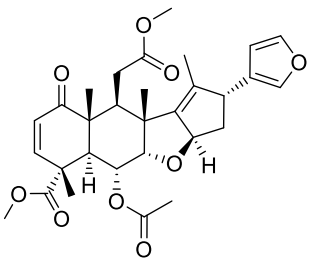
15		Tetrandrine	*Stephania tetrandra*	[3]
16		Tetrahydropalmatine	*Plants of corydalis genus*	[5]
17		Tanshinone IIA	*Salvia miltiorrhiza*	[6]
18		Tanshinone I	*Salvia miltiorrhiza*	[3]
19		Tannic acid	*Caesalpinia spinosa*	[3]
20		Sulforaphane	*Cruciferous vegetables*	[7]
21		Sugiol	*Metasequoia glyptostrobodies*	[8]

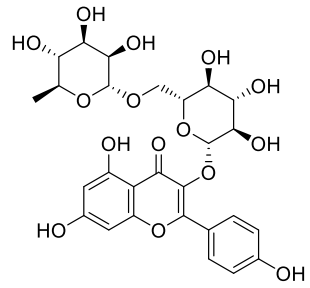
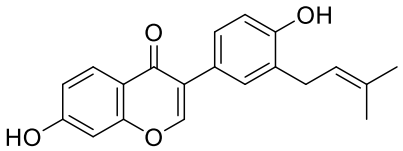
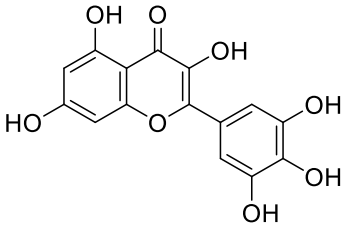
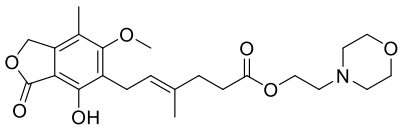
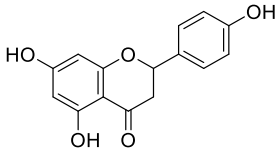
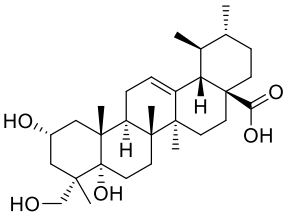
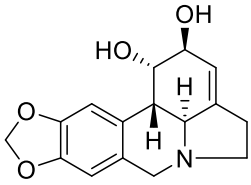
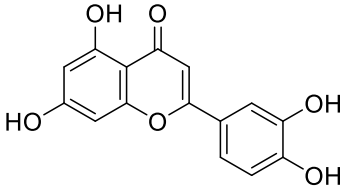
22		Sitosterol	*Tinospora cordifolia*	[3]
23		Sinigrin	*Seeds of Brassica nigra*	[3]
24		Simalikalactone D	*Simarouba tulae*	[9]
25		Silymarin	*Silybum marianum*	[10]
26		Silvestrol	*Aglaia silvestris*	[3]
27		Silibinin	*Silybum marianum*	[10]
28		Shogaol	*Zingiber officinale*	[1]
29		Sennoside A	*Rheum palmatum*	[11]
30		Scutellarein	*Erigeron breviscapus*	[12]

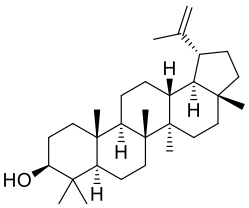
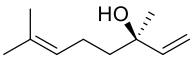
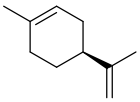
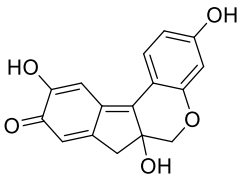
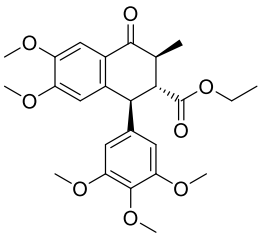
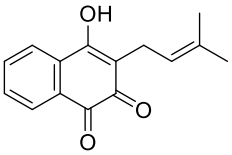
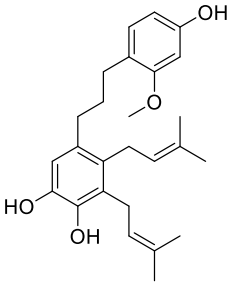
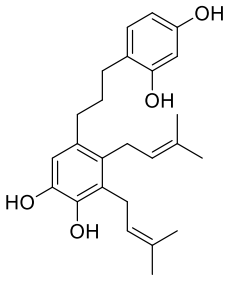
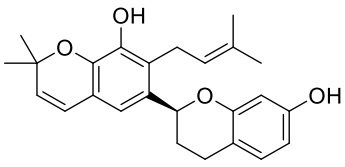
31		Schisandrin B	*Schisandra chinensis*	[10]
32		Savinin	*Pterocarpus santalinus*	[3]
33		Salannine	*Azadirachta indica*	[12]
34		Saikosaponin C	*Bupleuri Radix*	[3]
35		Saikosaponin D	*Bupleuri Radix*	[3]
36		Saikosaponin B2	*Bupleuri Radix*	[3]
37		Saikosaponin A	*Bupleuri Radix*	[3]

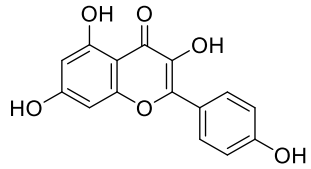
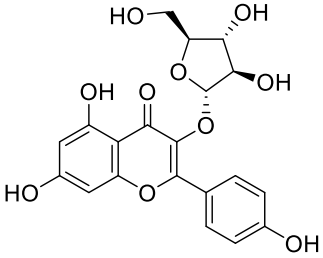
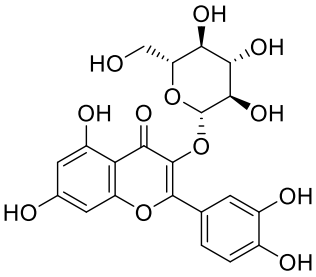
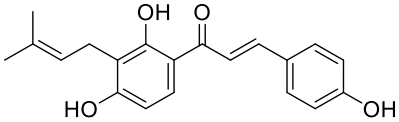
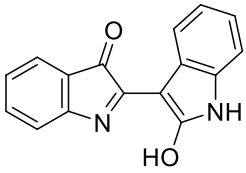
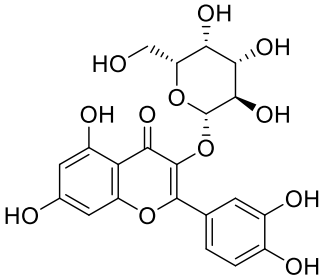
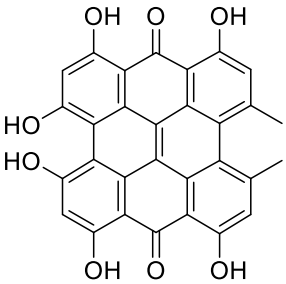
38		Rutin	*Ruta graveolens, Tephrosia purpurea, Eucalyptus sp.*	[3]
39		Rosmariquinone	*Rosmarinus officinalis*	[3]
40		Rosmarinic acid	*Rosmarinus officinalis*	[13]
41		Brazilin	*Caelsapinia sappan*	[14]
42		Rhein	*Rheum undulatum*	[3]
43		Retusin	*Dipteryx odorata*	[15]
44		Quinic acid	*Eucalyptus globulus*	[16]
45		Quercetrin	*Allium cepa*	[3]

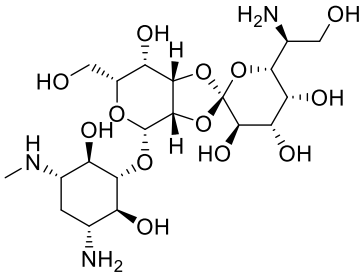
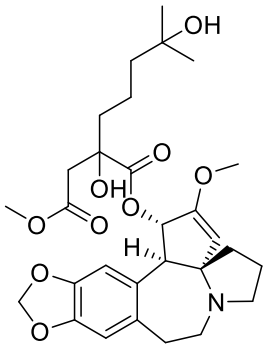
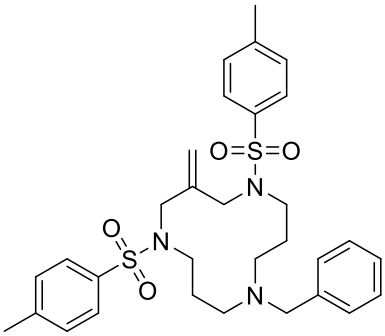
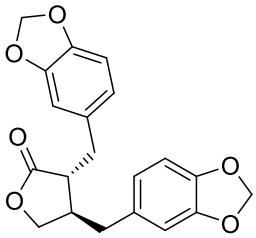
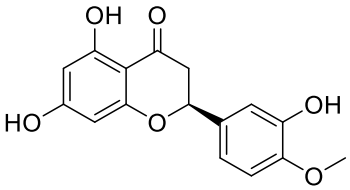
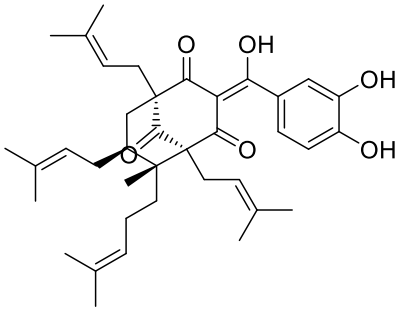
46		Quercetin-3-O-galactosyl-rhamnosyl-glucoside	*Allium cepa*	[17]
47		Quercetin	*Allium cepa*	[3]
48		Quassin	*Quassia amara*	[9]
49		Psoralidin	*Psoralea corylifolia*	[3]
50		Pseudohypericin	*Hypericum perforatum*	[18]
51		Procyanidin B1	*Vitis vinifera*	[3]
52		Procyanidin A2	*Vitis vinifera*	[3]

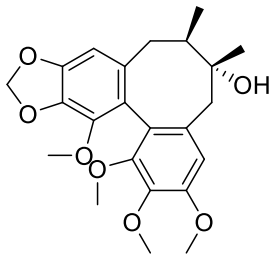
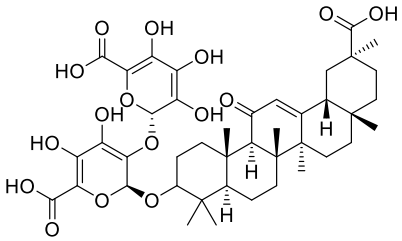
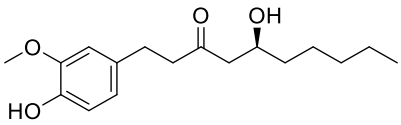
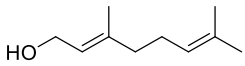
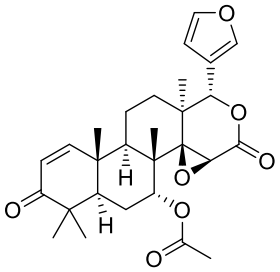
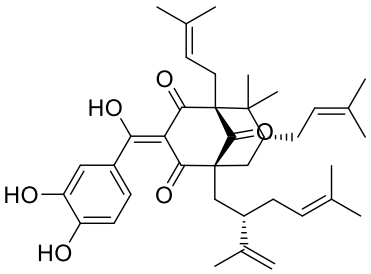
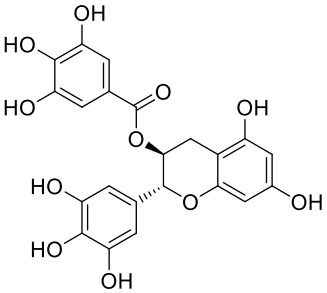
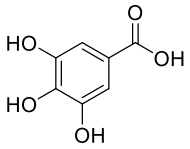
53		Piperine	*Piper nigrum*	[1]
54		Phlorofucofuroeckol A	*Eisenia bicyclis*	[3]
55		Andrographolide	*Andrographis paniculta*	[14]
56		Oubain	*Acokanthera schimperi*	[3]
57		Orientin	*Ocimum sanctum*	[19]
58		Octacosanol	*Saccharum officinarum*	[20]
59		Nimbolinin A	*Azadirachta indica*	[21]
60		Nimbin	*Azadirachta indica*	[1]

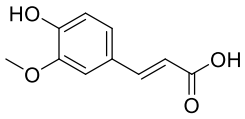
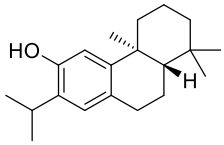
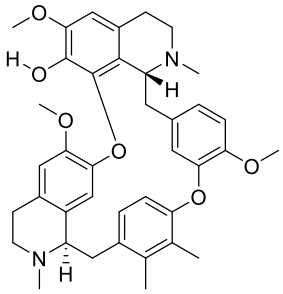
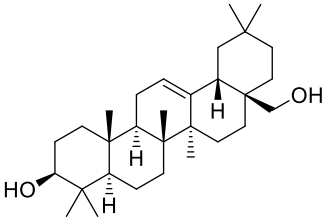
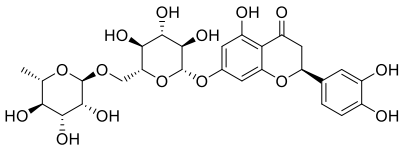
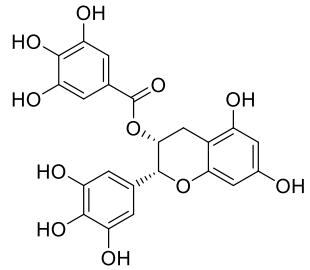
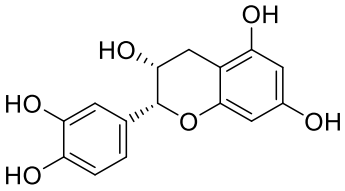
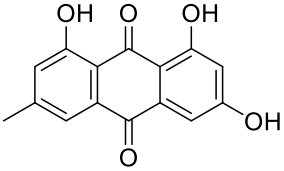
61		Nictoflorin	*Nyctanthes arbortristis*	[1]
62		Neobavaisoflavone	*Psoralia corylifolia*	[3]
63		Myricetin	*Solanum lycopersicum*	[14]
64		Mycophenolate mofetile	*Panicillium stoloniferum*	[3]
65		Naringenin	*Citrus sp*	[14]
66		Asiatic acid	*Centella asiatica*	[14]
67		Lycorine	*Lycoris radiata*	[3]
68		Luteolin	*Moringa oleifera*	[3]

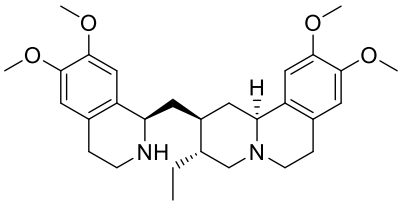
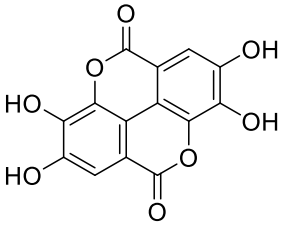
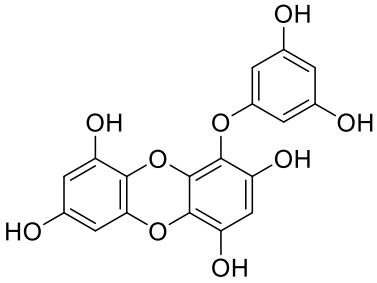
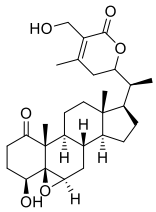
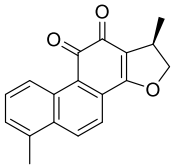
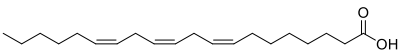
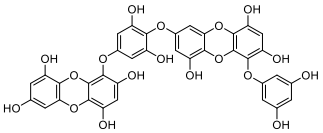
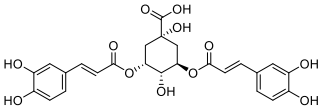
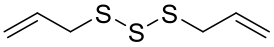
69		Lupeol	*Nyctanthes arbortristis*	[1]
70		Linalool	*Family Lamiaceae, Lauraceae, Rutaceae*	[22]
71		Limonin	*Citrus sp*	[23]
72		Brazilein	*Caesalpinia sappan*	[14]
73		Lignan	*Linum usitatissimum*	[6]
74		Lapachol	*Tabebuia avellanedae*	[24]
75		Kazinol J	*Broussonetia kazinoki*	[3]
76		Kazinol F	*Broussonetia kazinoki*	[3]
77		Kazinol B	*Broussonetia kazinoki*	[3]

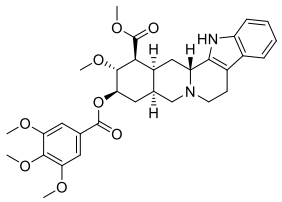
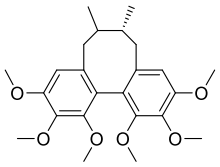
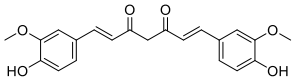
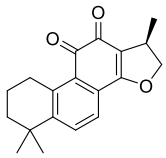
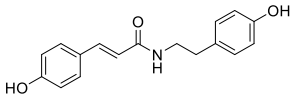
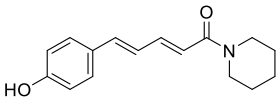
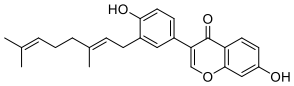
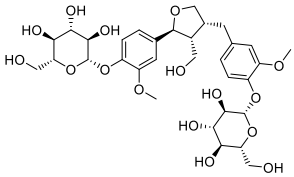
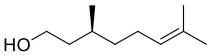
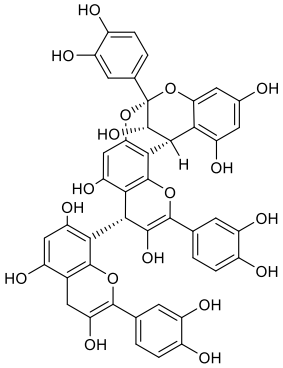
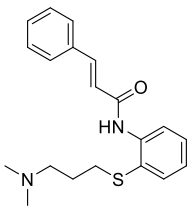
78		Kaempferol	*Psidium guajava*	[6]
79		Juglanin	*Polygonum aviculare*	[3]
80		Isoquercitrin	*Rheum nobile*	[25]
81		Isobavachalcone	*Psoralea corylifolia*	[3]
82		Indirubin	*Isatis tinctoria*	[26]
83		Hyperoside	*Hypericum perforatum*	[18]
84		Hypericin	*Hypericum perforatum*	[18]

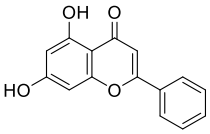
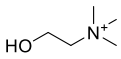
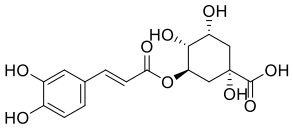
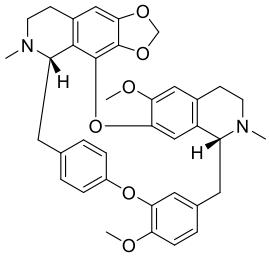
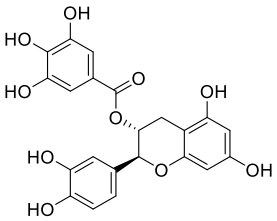
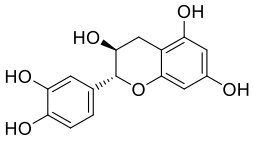
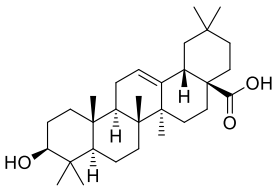
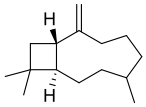
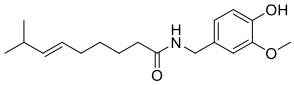
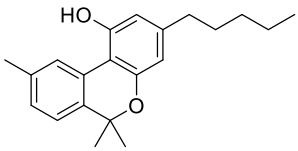
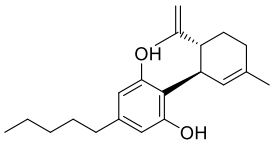
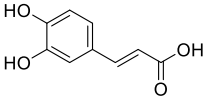
85		Hygromycin B	*Streptomyces hygroscopicus*	[3]
86		Homoharringtonine	*Cephalotaxus tree*	[3]
87		Hippeastrum hybrid agglutinin		[27]
88		Hinokinin	*Species of Chamaecyparis, Zanthoxylum*	[3]
89		Hesperatin	*Citrus sp.*	[3]
90		Guttiferone	*Allanblackia stuhlmannii*	[28]

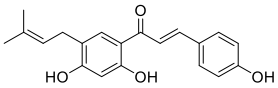
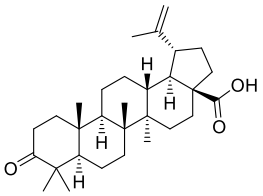
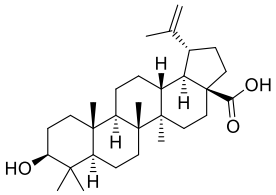
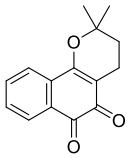
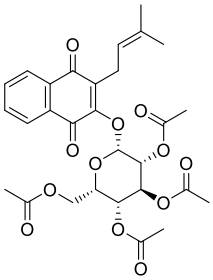
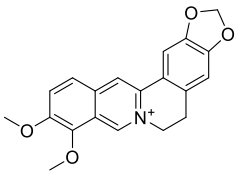
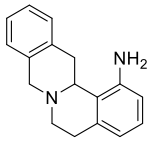
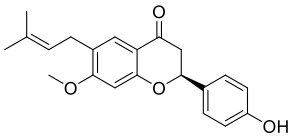
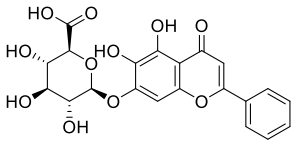
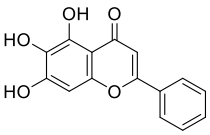
91		Gomisin A	*Schisandra chinensis*	[29]
92		Glycyrrhizin	*Lycoris radiata*	[30]
93		Gingerol	*Zingiber officinale*	[1]
94		Geraniol	*Rosa alba*	[31]
95		Gedunin	*Azadirachta indica*	[21]
96		Gracinol	*Garcinia parvifolia*	[32]
97		Gallocatechin gallate	*Camellia sinensis*	[3]
98		Gallic acid	*Rubus fruticosus*	[33]

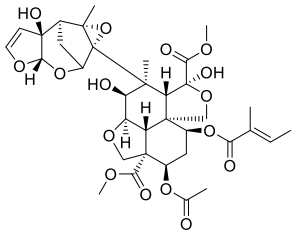
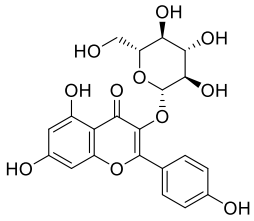
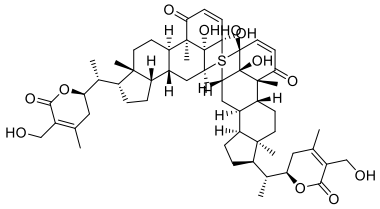
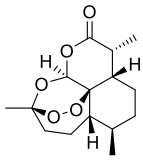
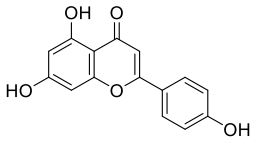
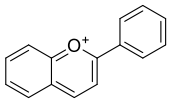
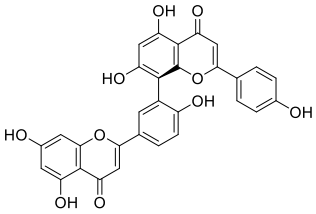
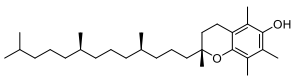
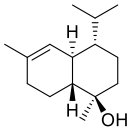
99		Ferulic acid	*Ananas comosus*	[34]
100		Ferruginol	*Sequoia sempervirens*	[3]
101		Fangchinoline	*Stephaniae tetrandrine*	[3]
102		Erythrodiol	*Tripterygium wilfordi*	
103		Eriocitrin	*Citrus grandis, Citrus limon, Mentha longifolia, Mentha piperita, Thymus vulgaris*	[35]
104		Epigallocatechin-3-gallate	*Camellia sinensis*	[36]
105		Epicatechin	*Camellia sinensis*	[36]
106		Emodin	*Polygonum cuspidatum*	[37]

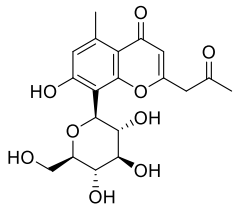
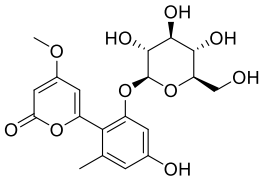
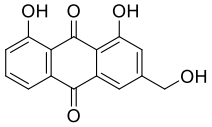
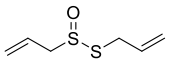
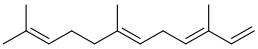
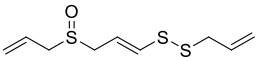
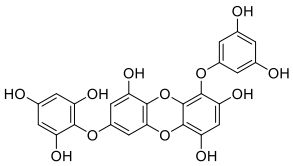
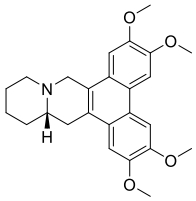
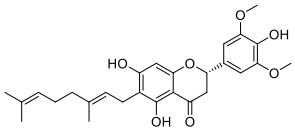
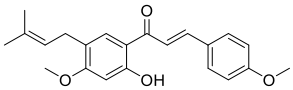
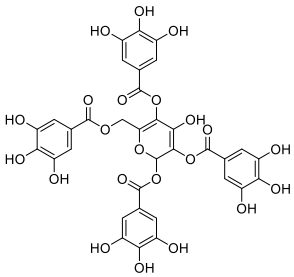
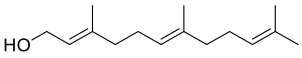
107		Emetin	*Lagerstroemia speciosa*	[38]
108		Ellagic acid	*Fragaria ananassa*	[39]
109		Eckol	*Ecklonia maxima*	[3]
110		Dihydrowithaferin A	*Withania somnifera*	[40]
111		Dihydrotanshinone I	*Salvia miltiorrhiza*	[6]
112		Dihydro-gamma-linolenic acid	*Durio graveolens*	[6]
113		Dieckol	*Ecklonia cava*	[3]
114		Dicaffeoylquinic acid	*plant of Asteraceae family, Coffea arabica*	[41]
115		Diallyl trisulfide	*Allium sativum*	[17]

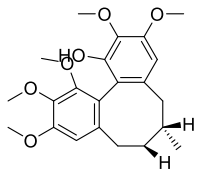
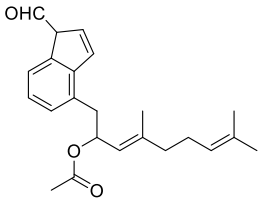
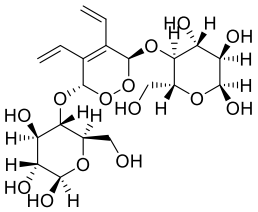
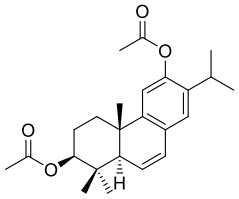
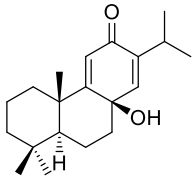
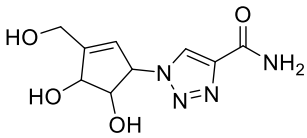
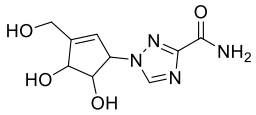
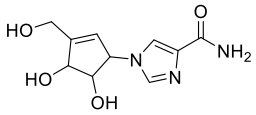
116		Desmethoxyreserpine	*Rauvolfia serpentina*	[6]
117		Deoxyschisandrin	*Schisandra chinensis*	[10]
118		Curcumin	*Curcuma longa*	[3]
119		Cryptotenshinone	*Salvia miltiorrhiza*	[6]
120		Coumaroyltyramine	*Exochorda racemosa*	[6]
121		Coumaperine	*Exochorda racemosa*	[42]
122		Corylifol A	*Psoralea corylifolia*	[3]
123		Clemastanin B	*Clematis stans, Isatis indigotica*	[43]
124		Citronellol	*citronella oils*	[22]
125		Cinnamatannin B1	*Cinnamomum zeylanicum*	[3]
126		Cinanserin		[3]

127		Chrysin	*Passiflora caerulea and Passiflora incarnata, Oroxylum indicum*	[3]
128		Choline	*Glycine max*	[44]
129		Chlorogenic acid	*Coffea arabica*	[41]
130		Cepharanthine	*Stephania cephalantha Hayata*	[3]
131		Catechin gallate	*Uncaria sinensis*, Cameria sinensis	[36]
132		Catechin	*Uncaria sinensis*, Cameria sinensis	[14, 36]
133		Caryophyllin	*Melissa officinalis*	[22]
134		Caryophyllene	*Melissa officinalis*	[22]
135		Capsaicin	*Capsicum annuum*	[45]
136		Cannabinol	*Cannabis sativa*	[46]
137		Cannabidiol	*Cannabis sativa*	[1]
138		Caffeic acid	*Coffea Arabica*	[41]

139		Broussochalcone B	*Broussonetia papyrifera*	[3]
140		Betulonic acid	*Betula pubescens*	[3]
141		Betulinic acid	*Betula pubescens*	[3]
142		Beta lapachone	*Tabebuia avellanedae*	[24]
143		Beta lapachol	*Tabebuia avellanedae*	[24]
144		Berberine	*Tinospora cordifolia*	[1]
145		Berbamine	*Tinospora cordifolia*	[3]
146		Bavachinin	*Psoralea corylifolia*	[3]
147		Baicalin	*Scutellaria baicalensis*	[47]
148		Baicalein	*Scutellaria baicalensis*	[47]

149		Azadirachtin	*Azadirachta indica*	[21]
150		Astragalin	*Nyctanthes arbortristis*	[1]
151		Ashwagandhanolide	*Withania somnifera*	
152		Artemisinin	*Artemisia annua*	[30]
153		Apigenin	*Ocimum tenuiflorum*	[3]
154		Anthocyanins	*Rubus fruticosus*	
155		Amentoflavone	*Cassia fistula*	[3]
156		Alpha-tocopherol	*Oils from corn, cottonseed, soybean, safflower, and wheat germ*	
157		Alpha-cadinol	*Schisandra chinensis*	[29]

158		Aloesin	*Aloe barbadensis*	[1]
159		Aloenin	*Aloe barbadensis*	[1]
160		Aloe emodin	*Barbados aloe*	[3]
161		Allicin	*Allium sativum*	[17]
162		Alpha fernesine	*oil of perilla*	[22]
163		Ajoene	*Allium Sativum*	[17]
164		7-Phloroeckol	*Ecklonia bicyclis*	[3]
165		7-Methoxycryptopleurine	*Boehmeria pannosa*	[3]
166		6-geranyl-4',5,7-trihydroxy-3',5'-dimethoxyflavanone		[3]
167		4'-O-Methylbavachalcone	*Psoralea corylifolia*	[3]
168		1,2,4,6-*tetra*-*O*-Galloyl-β-D-glucose	*Phyllanthus emblica*	[3]
169		(*E*,*E*)-farnesol	*Cymbopogon citratus*	[22]

170		Schisanthenol	*Schisandra chinensis*	[3]
171		Halituna	*Genus Cimicifuga*	[3]
172		Shuangkangsu	*Lonicera japonica*	[3]
173		(2*S*,4a*S*,10a*R*)-7-isopropyl-1,1,4a-trimethyl-1,2,3,4,4a,10a-hexahydrophenanthrene-2,6-diyl diacetate		[3]
174		(4b*S*,8a*S*,10a*R*)-10a-hydroxy-2-isopropyl-4b,8,8-trimethyl-5,6,7,8,8a,9,10,10a-octahydrophenanthren-3(4b*H*)-one		[3]
175		1-(4,5-dihydroxy-3-(hydroxymethyl)cyclopent-2-en-1-yl)-1*H*-1,2,3-triazole-4-carboxamide		[3]
176		1-(4,5-dihydroxy-3-(hydroxymethyl)cyclopent-2-en-1-yl)-1H-1,2,4-triazole-3-carboxamide		[3]
177		1-(4,5-dihydroxy-3-(hydroxymethyl)cyclopent-2-en-1-yl)-1H-imidazole-4-carboxamide		[3]

2. Molecular Docking

Table S2. Docking scores of compounds having docking score of ≤ -6.9 using SP module.

Entry	Compounds	Docking score	PDB ID
1	Dieckol	-9.0	**6M71**
2	Tannic acid	-8.4	
3	Theaflavin-3,3'-digallate	-7.2	
4	Phlorofucofuroeckol A1	-7.1	
5	Theaflavin-3,3'-digallate	-8.3	**6Y2E**
6	Rutin	-8.2	
7	7-Phloroeckol	-8.0	
8	Epigallocatechin-3-gallate	-7.7	
9	Catechin	-7.4	
10	Phlorofucofuroecko A	-7.4	
11	Procyanidin A2	-7.4	
12	Dieckol	-7.3	
13	Procyanidin B1	-7.2	
14	Nictoflorin	-7.2	
15	Astragalin	-7.1	
16	Juglanin	-7.1	
17	Eckol	-7.1	
18	1-(4,5-dihydroxy-3-(hydroxymethyl)cyclopent-2-en-1-yl)-1*H*-1,2,4-triazole-3-carboxamide	-7.0	
19	Silibinin	-7.0	
20	1-(4,5-dihydroxy-3-(hydroxymethyl)cyclopent-2-en-1-yl)-1*H*-1,2,3-triazole-4-carboxamide	-7.0	
21	Hyperoside	-7.0	
22	Neobavaisoflavone	-7.0	

3. Analysis of Drug likeness of identified hits.

Table S3. Lipinski rule analysis.[a]

Name of Compound	MW[b]	HBA[c]	HBD[d]	LogP[e]	RB[f]
Dieckol	742.55	11	11	0.994	6
Theaflavin-3,3'-digallate	866.69	18	13	-0.956	8
Phlorofurofucoeckol A	602.46	9	9	1.137	4
Rutin	610.52	16	10	-2.595	6
7-phloroeckol	496.38	8	8	0.649	4
Nictoflorin	594.52	15	9	-1.826	6
Procyanidin A2	576.51	12	9	0.301	2
Hyperoside	464.38	12	8	-1.397	4
Epigallocatechin-3-Gallate	458.37	10	8	-0.251	4
Juglanin	418.35	10	6	-0.318	4
Eckol	372.28	6	6	0.476	2
Astragalin	448.38	11	7	-0.748	4
Procyanidin B1	578.52	12	10	0.461	3

[a]The parameters have been calculated using QikProp [48]. [b]Molecular weight (<500 Da), [c]Number of hydrogen bond acceptors (<10), [d]Number of hydrogen bond donors (<5), [e]Partition coefficient in oil to water (<5), [f]Number of rotational bonds (<5)

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