

# Supplementary Materials

**Table S1.** Compound information and their medicinal plants.

No.	Constituent	PubChem CID	Medicinal Plant
1	Catechin	9064	<i>Acacia catehu</i> (L.f.) Willd.
2	Epicatechin	72,276	<i>Acacia catehu</i> (L.f.) Willd.
3	sesamin	72,307	<i>Acanthopanax gracilistylus</i> W. W. Smith
4	Eleutheroside E	3,084,742	<i>Acanthopanax senticosus</i> (Rupr.et Maxim.) Harms
5	Ciwujianoside B	71,571,445	<i>Acanthopanax senticosus</i> (Rupr.et Maxim.) Harms
6	hyaconitine	23,337	<i>Aconitum carmichaeli</i> Debx.
7	Mesaconitine	416,228	<i>Aconitum carmichaeli</i> Debx.
8	Lappaconitine	3886	<i>Aconitum carmichaelii</i> Debx.
9	8-O-Acetylharpagide	5,459,146	<i>Ajuga ciliata</i> Bunge.
10	Calceolarioside B	5,273,567	<i>Akebia quinata</i> (Thunb.) Decne.
11	Cardamonin	641,785	<i>Alpinia katsumadai</i> Hayata
12	Andrographolide	5,318,517	<i>Andrographis paniculata</i> (Burm.f.) Nees
13	mangiferin	5,281,647	<i>Anemarrhena asphodeloides</i> Bge.
14	Isoimperatorin	68,081	<i>Angelica dahurica</i> (Fisch. Ex Hoffm) Benth. et Hook.f
15	Imperatorin	10,212	<i>Angelica dahurica</i> (Fisch. Ex Hoffm) Benth. et Hook.f
16	Byakangelicin	10,211	<i>Angelica sinensis</i> (Oliv.) Diels
17	Columbianadin	6,436,246	<i>Angelica sinensis</i> (Oliv.) Diels
18	Succinic acid	1110	<i>Angelica sinensis</i> (Oliv.) Diels
19	Notoginsenoside R1	441,934	<i>Angelica sinensis</i> (Oliv.) Diels
20	Arctigenin	64,981	<i>Arctium lappa</i> L.
21	Arctiin	100,528	<i>Arctium lappa</i> L.
22	Aristolochic Acid I	2236	<i>Aristolochia manshuriensis</i> Kom.
23	Artemisinin	2240	<i>Artemisia annua</i> L.
24	Astragaloside	45,006,101	<i>Astragalus membranaceus</i> (Fisch.) Bge
25	Folic acid	6037	<i>Astragalus membranaceus</i> (Fisch.) Bge
26	Betaine	247	<i>Astragalus membranaceus</i> (Fisch.) Bge
27	Atractylenolide I	5,321,018	<i>Atractylodes macrocephala</i> Koidz.
28	Atractylenolide III	155,948	<i>Atractylodes macrocephala</i> Koidz.
29	Atractylenolide II	14,448,070	<i>Atractylodes macrocephala</i> Koidz.
30	Oleuropein	5,281,544	<i>Canavium album</i> Raeuseh
31	Hydroxysafflor yellow A	6,443,665	<i>Carthamus tinctorius</i> L.
32	Crocin	5,281,233	<i>Carthamus tinctorius</i> L.
33	Tracheloside	169,511	<i>Carthamus tinctorius</i> L.
34	asiaticoside	108,062	<i>Centella asiatica</i> (L.)Urb.
35	Isoferulic acid	736,186	<i>Cimicifuga heracleifolia</i> Kom.
36	Neohesperidin	442,439	<i>Citrus aurantium</i> L.
37	Nobiletin	72,344	<i>Citrus aurantium</i> L.
38	Limonin	179,651	<i>Citrus aurantium</i> L.
39	Rutin	5,280,805	<i>Citrus aurantium</i> L.
40	Hesperidin	10,621	<i>Citrus aurantium</i> L.
41	naringin	442,428	<i>Citrus aurantium</i> L.
42	Coptisine	72,322	<i>Coptis chinensis</i> Franch.
43	Berbamine dihydrochloride	56,845,155	<i>Coptis chinensis</i> Franch.

Table S1. Cont.

No.	Constituent	PubChem CID	Medicinal Plant
44	berbamine	10,170	<i>Coptis chinensis</i> Franch.
45	Loganin	87,691	<i>Cornus officinalis</i> Sieb. et Zucc.
46	Tetrahydropalmatine	72,301	<i>Corydalis yanhusuo</i> W. T. Wang
47	Hyperoside	5,281,643	<i>Crataegus pinnatifida</i> Bge.
48	Protopine	4970	<i>Daphne genkwa</i> Sieb. et Zucc.
49	Genkwanin	5,281,617	<i>Daphne genkwa</i> Sieb. et Zucc.
50	Ephedrine Hydrochloride	65,326	<i>Ephedra sinica</i> Stapf
51	Icariin	5,471,129	<i>Epimedium brevicornu</i> Maxim.
52	Chlorogenic acid	1,794,427	<i>Eucommia ulmoides</i> Oliv.
53	Eugenol	3314	<i>Eugenia caryophyllata</i> Thunb.
54	Phillyrin	44,584,288	<i>Forsythia suspensa</i> (Thunb.) Vahl
55	Forsythoside B	44,429,859	<i>Forsythia suspensa</i> (Thunb.) Vahl
56	Esculin hydrate	44,134,702	<i>Fraxinus rhychophylla</i> Hance
57	fraxetin	5,273,569	<i>Fraxinus rhychophylla</i> Hance
58	Peimine	131,900	<i>Fritillaria cirrhosa</i> D. Don
59	Peiminine	167,691	<i>Fritillaria cirrhosa</i> D. Don
60	Sipeimine	442,977	<i>Fritillaria cirrhosa</i> D. Don
61	Gardenoside	442,423	<i>Gardenia jasminoides</i> Ellis
62	Genipin	442,424	<i>Gardenia jasminoides</i> Ellis
63	Geniposidic acid	443,354	<i>Gardenia jasminoides</i> Ellis
64	Gentiobiose	441,422	<i>Gentiana manshurica</i> Kitag.
65	gentiopicroside	88,708	<i>Gentiana manshurica</i> Kitag.
66	Ginkgolide B	65,243	<i>Ginkgo biloba</i> L.
67	Ginkgolide C	16,211,418	<i>Ginkgo biloba</i> L.
68	Ginkgolide A	9,909,368	<i>Ginkgo biloba</i> L.
69	Daidzin	107,971	<i>Glycine max</i> (L.) Merr.
70	Genistin	5,281,377	<i>Glycine max</i> (L.) Merr.
71	Liquiritin	503,737	<i>Glycyrrhiza uralensis</i> Fisch.
72	Isoliquiritin	5,318,591	<i>Glycyrrhiza uralensis</i> Fisch.
73	Liquiritigenin	114,829	<i>Glycyrrhiza uralensis</i> Fisch.
74	Glycyrrhizic acid	656,656	<i>Glycyrrhiza uralensis</i> Fisch.
75	glycyrrhetic acid	10,114	<i>Glycyrrhiza uralensis</i> Fisch.
76	Monoammonium glycyrrhizinate	62,074	<i>Glycyrrhiza uralensis</i> Fisch.
77	Narcissoside	5,481,663	<i>Hedyotis chrysotricha</i> (Palib.) Merr.
78	Isorhamnetin	5,281,654	<i>Hippophae rhamnoides</i> L.
79	Allantoin	204	<i>Hordeum vulgare</i> L.
80	colchicine	6167	<i>Iphigenia indica</i> A. Gray
81	Ligustrazine HCl	156,709	<i>Ligusticum chuanxiong</i> Hort.
82	Senkyunolide A	3,085,257	<i>Ligusticum chuanxiong</i> Hort.
83	ferulic acid	445,858	<i>Ligusticum chuanxiong</i> Hort.
84	neochlorogenic acid	5,280,633	<i>Lonicera japonica</i> Thunb.
85	Isochlorogenic acid A	6,474,310	<i>Lonicera japonica</i> Thunb.

Table S1. Cont.

No.	Constituent	PubChem CID	Medicinal Plant
86	Luteoloside	5,280,637	<i>Lonicera japonica</i> Thunb.
87	Isochlorogenic acid C	6,474,309	<i>Lonicera japonica</i> Thunb.
88	3,4-Dicaffeoylquinic acid	5,281,780	<i>Lonicera japonica</i> Thunb.
89	Cryptochlorogenic acid	9,798,666	<i>Lonicera japonica</i> Thunb.
90	Tormentic acid	73,193	<i>Mosla chinensis</i> Maxim.
91	Nardosinone	168,136	<i>Nardostachys chinensis</i> Batal.
92	Neferine	159,654	<i>Nelumbo nucifera</i> Gaertn.
93	Liensinine	160,644	<i>Nelumbo nucifera</i> Gaertn.
94	Isoliensinine	5,274,591	<i>Nelumbo nucifera</i> Gaertn.
95	Liensinine perchlorate	71,307,566	<i>Nelumbo nucifera</i> Gaertn.
96	Ruscogenin	441,893	<i>Ophiopogon japonicus</i> (Thunb.) Ker-Gawl.
97	Paeoniflorin	442,534	<i>Paeonia lactiflora</i> Pall.
98	Paeonolum	11,092	<i>Paeonia suffruticosa</i> Andr.
99	Protopanaxadiol	11,213,350	<i>Panax ginseng</i> C. A. Mey.
100	Protopanaxatriol	22,392,424	<i>Panax ginseng</i> C. A. Mey.
101	Ginsenoside Rb1	9,898,279	<i>Panax ginseng</i> C. A. Mey.
102	Ginsenoside Rg1	441,923	<i>Panax ginseng</i> C. A. Mey.
103	Ginsenoside Re	73,149	<i>Panax ginseng</i> C. A. Mey.
104	Ginsenoside Rg2	6,441,009	<i>Panax ginseng</i> C. A. Mey.
105	Ginsenoside Rh2	119,307	<i>Panax ginseng</i> C. A. Mey.
106	beta-D-Glucopyranoside	3,811,495	<i>Panax ginseng</i> C. A. Mey.
107	Panaxadiol	328,778	<i>Panax ginseng</i> C. A. Mey.
108	panaxotriol	93,484	<i>Panax ginseng</i> C. A. Mey.
109	Perillene	9142	<i>Perilla frutescens</i> (L.) Britt.
110	Patchouli alcohol	521,903	<i>Pogostemon cablin</i> (Blanco) Benth.
111	Senegenin	200,662	<i>Polygala tenuifolia</i> Willd.
112	Amygdalin	656,516	<i>Prunus armeniaca</i> L. var. <i>ansu</i> Maxim.
113	Angelicin	10,658	<i>Psoralea corylifolia</i> L.
114	Puerarin	5,281,807	<i>Pueraria lobata</i> (Willd.) Ohwi
115	Catalpol	91,520	<i>Rehmannia glutinosa</i> Libosch.
116	Polydatin	5,281,718	<i>Reynoutria japonica</i> Houtt.
117	Aloe emodin	10,207	<i>Rheum palmatum</i> L.
118	Sennoside A	73,111	<i>Rheum palmatum</i> L.
119	Sennoside B	91,440	<i>Rheum palmatum</i> L.
120	Physcion	10,639	<i>Rheum palmatum</i> L.
121	Emodin	3220	<i>Rheum palmatum</i> L.
122	Chrysophanol	10,208	<i>Rheum palmatum</i> L.
123	Pyrogallic Acid	1057	<i>Rhus chinensis</i> Mill.
124	Purpurin	6683	<i>Rubia cordifolia</i> L.
125	Protocatechuic acid	72	<i>Salvia miltiorrhiza</i> Bge.
126	Tanshinone II A	164,676	<i>Salvia miltiorrhiza</i> Bge.
127	Lithospermic acid	6,441,498	<i>Salvia miltiorrhiza</i> Bge.
128	Caffeic acid	689,043	<i>Salvia miltiorrhiza</i> Bge.

Table S1. Cont.

No.	Constituent	PubChem CID	Medicinal Plant
129	Salvianolic acid A	5,281,793	<i>Salvia miltiorrhiza</i> Bge.
130	Salvianolic acid B	6,441,188	<i>Salvia miltiorrhiza</i> Bge.
131	Tanshinone I	114,917	<i>Salvia miltiorrhiza</i> Bge.
132	Cryptotanshinone	160,254	<i>Salvia miltiorrhiza</i> Bge.
133	Carnosol	2579	<i>Salvia officinalis</i> L.
134	Ursolic acid	64,945	<i>Salvia officinalis</i> L.
135	Carnosic acid	65,126	<i>Salvia officinalis</i> L.
136	Schisantherin A	151,529	<i>Schisandra chinensis</i> (Turcz.)
137	Schizandrin B	108,130	<i>Schisandra chinensis</i> (Turcz.)
138	Schisandrin	3,001,664	<i>Schisandra chinensis</i> (Turcz.)
139	schisandrin C	119,112	<i>Schisandra chinensis</i> (Turcz.)
140	Schizandrol B	68,781	<i>Schisandra chinensis</i> (Turcz.)
141	Baicalin	64,982	<i>Scutellaria baicalensis</i> Georgi
142	Wogonin	5,281,703	<i>Scutellaria baicalensis</i> Georgi
143	scutellarin	185,617	<i>Scutellaria baicalensis</i> Georgi
144	Sesamolin	101,746	<i>Sesamum indicum</i> L.
145	Sinomenine	5,459,308	<i>Sinomenium acutum</i> (Thunb.) Rehd. Et Wils.
146	Astilbin	119,258	<i>Smilax glabra</i> Roxb.
147	quercetin-3-rhamnoside	5,280,459	<i>Sophora japonica</i> L.
148	Tetrandrine	73,078	<i>Stephania tetrandra</i> S. Moore
149	Fangchinoline	73,481	<i>Stephania tetrandra</i> S. Moore
150	Triptolide	107,985	<i>Tripterygium wilfordii</i> Hook. f.
151	Dhydrodiisoeugenol	5,379,033	<i>Vaccaria segetalis</i> (Neck.) Garcke.
152	6-Gingerol	442,793	<i>Zingiber officinale</i> Rosc.
153	Bisdemethoxycurcumin	5,315,472	<i>Zingiber officinale</i> Rosc.
154	curcumenol	387,977	<i>Zingiber officinale</i> Rosc.
155	Borneol	64,685	<i>Zingiber officinale</i> Rosc.
156	Betulinic acid	64,971	<i>Ziziphus jujuba</i> Mill.var. <i>spinosa</i> (Bunge) Hu ex H.F.Chow
157	Betulin	72,326	<i>Ziziphus jujuba</i> Mill.var. <i>spinosa</i> (Bunge) Hu ex H.F.Chow
158	Jujuboside A	171,446	<i>Ziziphus jujuba</i> Mill.var. <i>spinosa</i> (Bunge) Hu ex H.F.Chow