

Cluster Analysis of Medicinal Plants and Targets Based on Multipartite Network

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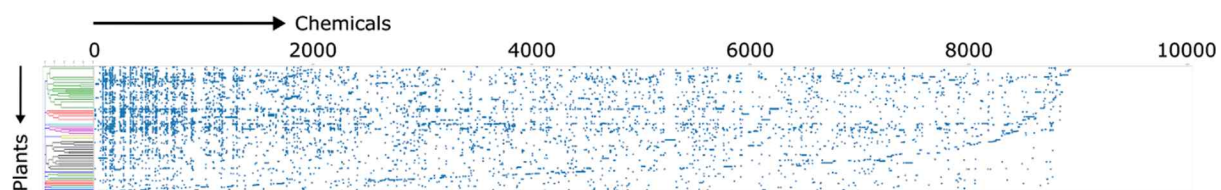


Figure S1. Visualization of non-zero values of the data matrix for the plants and chemicals, where the rows correspond to the plants and the columns correspond to the chemicals. The rows were permuted according to the order determined by the hierarchical clustering of the plants.

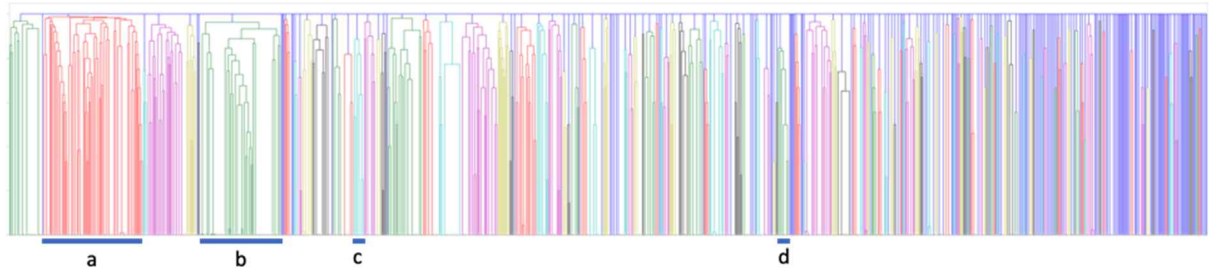
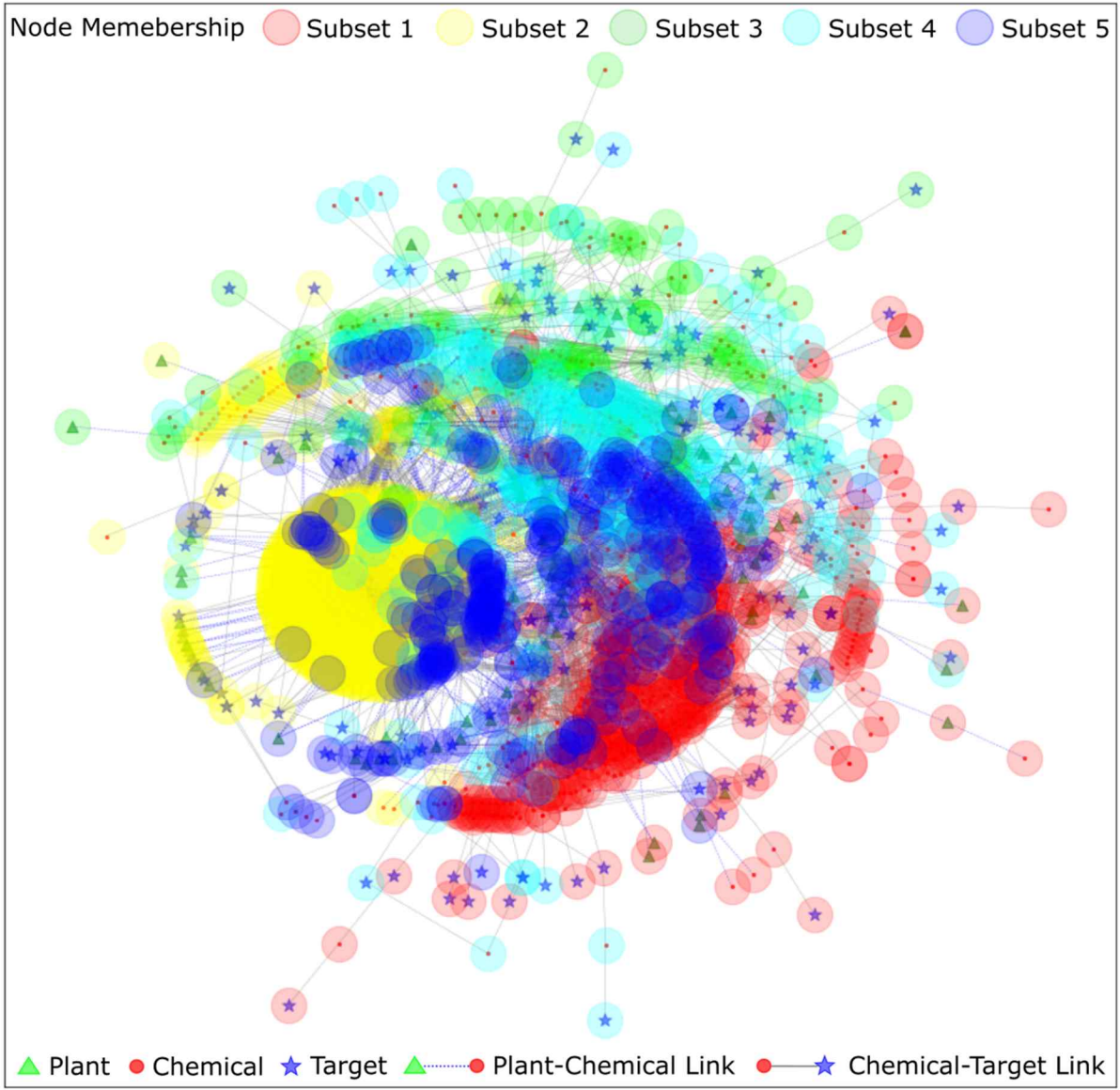
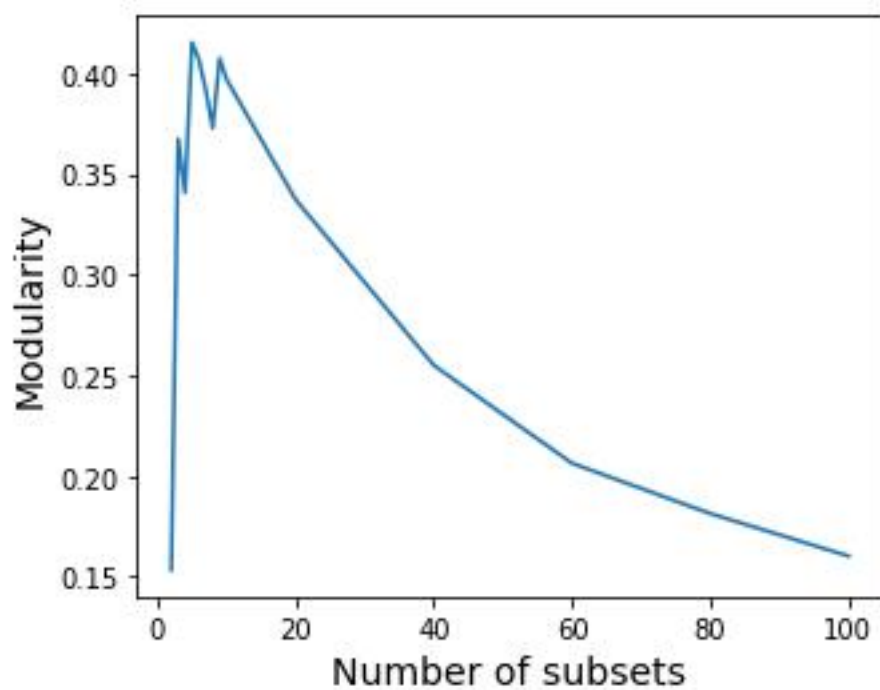


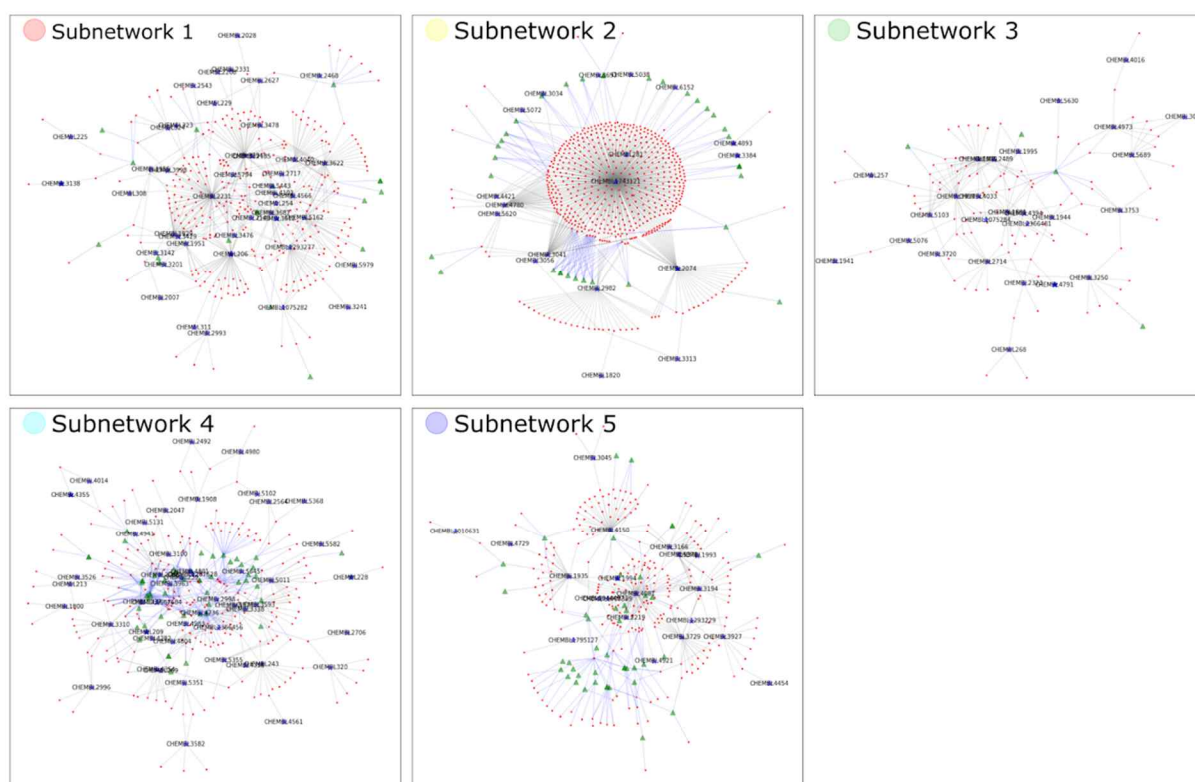
Figure S2. The whole dendrogram for clustering of plants obtained by the hierarchical clustering analysis. **a-d**: the dendrograms of **Figures 2A, 2C, 2E** and **2H**, respectively.



(A)



(B)



(C)

Figure S3. Visualization of the results of the spectral co-clustering. **(A)** Spectral co-clustering of the whole network. **(B)** The modularity values for the determination of the number of clusters for the spectral co-clustering algorithm. **(C)** The subnetworks induced by each of the

five subsets of nodes obtained by the spectral co-clustering. The 10% of the whole nodes were randomly selected for visualization.

Table S1. The structural properties of the whole network and the five subnetworks obtained by the spectral co-clustering algorithm.

Network	Number of Nodes				Number of Edges			Diameter	Average Bipartite Clustering Coefficient	Degree Assortativity
	Np	Nc	Nt	N	Epc	Ect	E			
Whole	1138	10051	1224	12413	34549	100290	134839	5	0.0946	-0.1954
Sub 1	276	3459	124	3859	3915	29493	33408	4	0.2116	-0.3936
Sub 2	327	2538	136	3001	3946	13456	17402	5	0.1595	-0.3672
Sub 3	34	676	177	887	205	5491	5696	5	0.1544	-0.4156
Sub 4	141	1907	361	2409	1564	14118	15682	4	0.1315	-0.3814
Sub 5	360	1471	426	2257	9751	5893	15644	5	0.1436	-0.2290

Np=number of plant nodes, Nc=number of chemical nodes, Nt=number of target nodes, N=total number of nodes, Epc=number of plant-chemical edges, Ect=number of chemical-target edges, E=total number of edges.

Table S2. List of plants illustrated in **Figures 2A** and **2B**.

Plant ID	Scientific Name	Latin Name	Family
M0000066	<i>Euphorbia kansui</i>	Euphorbiae Kansui Radix	Euphorbiaceae
M0000069	<i>Citrus suavissima</i>	Citri Suavissimae Exocarpium	Rutaceae
M0000072	<i>Glycyrrhiza uralensis</i>	Glycyrrhizae Praeparatus Pulvis	Leguminosae
M0000075	<i>Glycyrrhiza inflata</i>	Glycyrrhizae Radix	Leguminosae
M0000079	<i>Glycyrrhiza inflata</i>	Glycyrrhizae Resina	Leguminosae
M0000080	<i>Glycyrrhiza uralensis</i>	Glycyrrhizae Radicis Virgula	Leguminosae
M0000088	<i>Pinellia ternata</i>	Pinelliae Praeparatum cum Zingiberis	Araceae
M0000110	<i>Dianthus superbus</i>	Dianthi Herba	Caryophyllaceae
M0000127	<i>Zizyphus jujuba var. inermis</i>	Zizyphi Fructus	Rhamnaceae
M0000216	<i>Melia azedarach</i>	Meliae Cortex	Meliaceae
M0000222	<i>Melia azedarach</i>	Meliae Fructus	Meliaceae
M0000224	<i>Melia azed-arach var. japonica</i>	Meliae Cortex	Meliaceae
M0000262	<i>Cucumis melo</i>	Melo Pediculus	Cucurbitaceae
M0000264	<i>Sorghum vulgare</i>	Sorghum Acetum	Gramineae
M0000265	<i>Hordeum vulgare</i>	Hordei Acetum	Gramineae
M0000334	<i>Hordeum vulgare</i>	Hordei Fructus	Gramineae
M0000567	<i>Raphanus sativus</i>	Raphani Radix	Cruciferae
M0000581	<i>Kochia scoparia</i>	Kochiae Fructus	Chenopodiaceae
M0000607	<i>Strobilanthus flaccidifolia</i>	Strobilanthus Sedimentum	Acanthaceae
M0000646	<i>Raphanus sativus</i>	Raphani Semen	Cruciferae
M0000771	<i>Echinops latifolius</i>	Rhapontici Radix	Compositae
M0000816	<i>Lophatherum gracile</i>	Lophatheri Herba	Gramineae
M0000854	<i>Hordeum vulgare</i>	Hordei Semen	Gramineae
M0000855	<i>Hordeum vulgare</i>	Hordei Semen Pulvis	Gramineae
M0000856	<i>Hordeum vulgare</i>	Hordei Novella	Gramineae
M0000877	<i>Zizyphus vulgaris var. spinosus</i>	Jujubae Fructus	Rhamnaceae
M0000878	<i>Zizyphus jujuba var. inermis</i>	Jujubae Fructus	Rhamnaceae
M0000990	<i>Eucommia ulmoides</i>	Eucommiae Cortex	Eucommiaceae
M0001001	<i>Juncus effusus</i>	Junci Medulla	Juncaceae

M0001022	<i>Aristolochia contorta</i>	Aristolochiae Fructus	Aristolochiaceae
M0001046	<i>Calvatia gigantea</i>	Lasiosphaera Seu Calvatia	Rosacean
M0001069	<i>Portulaca oleracea</i>	Portulacae Herba	Portulacaceae
M0001089	<i>Vitex trifolia</i>	Viticis Fructus	Verbenaceae
M0001108	<i>Liriope platyphylla</i>	Liriopes Radix	Liliaceae
M0001114	<i>Hordeum vulgare var. hexastichon</i>	Hordei Fructus Germinatus	Gramineae
M0001115	<i>Hordeum vulgare</i>	Hordei Fructus Germinatus	Gramineae
M0001189	<i>Aralia elata</i>	Araliae Cortex Lignum seu Radicis	Araliaceae
M0001234	<i>Ficus carica</i>	Fici Fructus	Moraceae
M0001303	<i>Pinellia pedatisecta</i>	Pinelliae Rhizoma	Araceae
M0001305	<i>Pinellia ternata</i>	Pinelliae Rhizoma Fermentata	Araceae
M0001309	<i>Eleocharis dulcis</i>	Eleocharitis Tuber	Cyperaceae
M0001357	<i>vulgaris Lamarck var. spinosus</i>	Zizyphi Spina	Rhamnaceae
M0001377	<i>Ampelopsis japonica</i>	Ampelopsis Radix	Vitaceae
M0001523	<i>Ficus pumila</i>	Fici Pumilae Caulis	Moraceae
M0001541	<i>Psoralea corylifolia</i>	Psoraleae Fructus	Leguminosae
M0001581	<i>Ailanthus altissima</i> <i>Ailanthus glandulosa</i>	Ailanthi Herba	Simaroubaceae
M0001628	<i>Torreya nucifera</i>	Torreyae Semen	Taxaceae
M0001629	<i>Torreya grandis</i>	Torreyae Semen	Taxaceae
M0001663	<i>Adenophora triphylla var. japonica</i>	Adenophorae Radix	Campanulaceae
M0001710	<i>Sambucus javanica</i>	Sambuci Radix	Caprifoliaceae
M0001780	<i>Gardenia jasminoides</i>	Gardeniae Fructus	Rubiaceae
M0001808	<i>Morus alba</i>	Mori Cortex	Moraceae
M0001829	<i>Cynanchum atratum</i>	Cynanchi Radix	Asclepiadaceae
M0001836	<i>Morus alba</i>	Mori Favilla	Moraceae
M0001839	<i>Morus alba</i>	Mori Fructus	Moraceae
M0001855	<i>Morus alba</i>	Mori Ramulus	Moraceae
M0001940	<i>Dendrobium loddigesii</i>	Dendrobii Herba	Orchidaceae
M0002165	<i>Cynomorium songaricum</i>	Cynomorii Herba	Cynomoriaceae
M0002301	<i>Centipeda minima</i>	Centipedae Herba	Compositae
M0002470	<i>Hordeum vulgare</i>	Hordei Germinatus	Gramineae

M0002552	<i>Mirabilis jalapa</i>	Fucus cum Jalapae Tuber	Nyctaginaceae
M0002555	<i>Mirabilis jalapa</i>	Fucus cum Jalapae Embryo	Nyctaginaceae
M0002598	<i>Acanthopanax sessiliflorus</i>	Acanthopanax Cortex	Araliaceae
M0002661	<i>Lindera aggregata</i>	Linderae Radix	Lauraceae
M0002913	<i>Citrus suavissima</i>	Citri Suavissimae Fructus	Rutaceae
M0002915	<i>Artemisia anomala</i> <i>Artemisia viridissima</i>	Artemisiae Anomalae Herba	Compositae
M0002923	<i>Ulmus macrocarpa</i>	Ulmi Cortex	Ulmaceae
M0002991	<i>Coix lachryma-jobi</i> var. <i>ma-yeun</i>	Coicis Radix	Gramineae
M0002992	<i>Coix lachryma-jobi</i>	Coicis Radix	Gramineae
M0002993	<i>Coix lachryma-jobi</i> var. <i>ma-yeun</i>	Coicis Semen	Gramineae
M0002994	<i>Coix lachryma-jobi</i>	Coicis Semen	Gramineae
M0003064	<i>Glycyrrhiza uralensis</i>	Glycyrrhizae Radix Praeparata	Leguminosae
M0003088	<i>Spirodela polyrrhyza</i>	Spirodelae Herba	Lemnaceae
M0003284	<i>Tamarix chinensis</i>	Tamaricis Ramulus	Tamaricaceae
M0003373	<i>Adenophora trachelioides</i>	Trachelioidis Radix	Campanulaceae
M0003415	<i>Zizyphus jujuba</i> var. <i>inermis</i>	Zizyphi Radix	Rhamnaceae
M0003417	<i>Zizyphus jujuba</i> var. <i>inermis</i>	Zizyphi Folium	Rhamnaceae
M0003492	<i>Kochia scoparia</i>	Kochiae Herba	Chenopodiaceae
M0003630	<i>Euphorbia lathyris</i>	Euphorbiae Lathyridis Semen	Euphorbiaceae
M0003670	<i>Aristolochia contorta</i>	Aristolochiae Herba	Aristolochiaceae
M0003719	<i>Cucumis melo</i>	Melo Fructus	Cucurbitaceae
M0003720	<i>Cucumis melo</i>	Melo Semen	Cucurbitaceae
M0003721	<i>Cucumis melo</i>	Melonis Pedicelus	Cucurbitaceae
M0003731	<i>Baphicacanthus cusia</i>	Indigo Pulverata Levis	Acanthaceae
M0003752	<i>Morus alba</i>	Mori Radicis Cortex	Moraceae
M0003786	<i>Celosia argentea</i>	Celosiae Semen	Amaranthaceae
M0003830	<i>Sorghum vulgare</i>	Sorghu Radix	Gramineae
M0003831	<i>Dichroa febrifuga</i> <i>Orixa japonica</i>	Dichroae Arbor Novella	Saxifragaceae
M0003858	<i>Sorghum vulgare</i>	Sorghu Semen	Gramineae
M0003887	<i>Gardenia jasminoides</i>	Gardeniae Semen	Rubiaceae
M0003969	<i>Psoralea corylifolia</i>	Psoraleae Semen	Leguminosae

M0004009	<i>Patrinia scabiosaefolia</i>	Patriniae Radix	Valerianaceae
M0004073	<i>Prunella vulgaris</i>	Prunellae Spica	Labiatae
M0004247	<i>Cucumis sativus</i>	Cucumeris Fructus	Cucurbitaceae
M0004398	<i>Cudrania tricuspidata</i>	Cudraniae Folium	Moraceae

Table S3. List of plants illustrated in **Figures 2C** and **2D**.

Plant ID	Scientific Name	Latin Name	Family
M0000060	<i>Saccharum sinensis</i>	Sacchari Tuber	Gramineae
M0000124	<i>Caesalpinia sappan</i> <i>Cercis chinensis</i>	Fucus cum Caesalpiniae	Leguminosae
M0000179	<i>Areca catechu</i>	Arecae Semen	Palmae
M0000227	<i>Cannabis sativa</i>	Vetus Cannabis Solea	Cannabinaceae
M0000263	<i>Oryza sativa</i>	Oryzae Acetum	Gramineae
M0000286	<i>Oryza sativa</i>	Oryzae Fructus Germinatus	Gramineae
M0000557	<i>Oryza sativa</i>	Oryzae Glutinosa Medulla	Gramineae
M0000559	<i>Oryza sativa</i>	Oryzae Radix seu Rhizoma	Gramineae
M0000564	<i>Oryza sativa</i>	Oryzae Semen	Gramineae
M0000565	<i>Oryza sativa</i>	Alcohol cum Oryzae Semen	Gramineae
M0000803	<i>Santalum album</i>	Santali Albae Lignum	Santalaceae
M0000821	<i>Angelica sinensis</i>	Angelicae Gigantis Radix	Umbelliferae
M0000842	<i>Glycine max</i>	Glycinis Semen	Leguminosae
M0000844	<i>Glycine max</i>	Glycinis Semen Germinatum	Leguminosae
M0000846	<i>Glycine max</i>	Glycine Semen Germinatum	Leguminosae
M0000850	<i>Cannabis sativa</i>	Cannabis Herba	Cannabinaceae
M0000852	<i>Cannabis sativa</i>	Cannabis Semen	Cannabinaceae
M0000862	<i>Areca catechu</i>	Arecae Pericarpium	Palmae
M0000864	<i>Allium sativum</i>	Allii Bulbus	Liliaceae
M0000913	<i>Oryza sativa</i>	Oryzae Semen Germinatus	Gramineae
M0000938	<i>Benincasa cerifera</i> <i>Benincasa hispida</i>	Benincasae Fructus	Cucurbitaceae
M0000939	<i>Benincasa cerifera</i> <i>Benincasa hispida</i>	Benincasae Caulis	Cucurbitaceae
M0000940	<i>Benincasa cerifera</i> <i>Benincasa hispida</i>	Benincasae Folium	Cucurbitaceae
M0000984	<i>Glycine max</i>	Alcohol cum Glycinis Semen	Leguminosae
M0000986	<i>Glycine max</i>	Glycinis Semen Ptisanari	Leguminosae
M0000992	<i>Glycine max</i>	Glycinis Semen	Leguminosae
M0001013	<i>Agaricus campestris</i>	Agaricus Polyporus	Agaricaceae
M0001014	<i>Cannabis sativa</i>	Cannabis Radix	Cannabinaceae

M0001058	<i>Cannabis sativa</i>	Cannabis Folium	Cannabinaceae
M0001062	<i>Cannabis sativa</i>	Cannabis Fructus	Cannabinaceae
M0001191	<i>Auricularia auricula-judae</i>	Auriculariae Polyporus	Auriculariaceae
M0001197	<i>Auricularia auricula-judae</i>	Auriculariae Polyporus	Auriculariaceae
M0001359	<i>Santalum album</i>	Santali Albi Lignum	Santalaceae
M0001418	<i>Oryza sativa</i>	Oryzae Semen Pulvus	Gramineae
M0001422	<i>Saccharum sinensis</i>	Saccharum Alba	Gramineae
M0001473	<i>Oryza sativa</i>	Oryzae Ptisanari	Gramineae
M0001540	<i>Oryza sativa</i>	Alcohol Orizae cum Medico Fermento	Gramineae
M0001639	<i>Saccharum sinensis</i>	Saccharum Glacialis	Gramineae
M0001659	<i>Saccharum sinensis</i>	Saccharum	Gramineae
M0001901	<i>Scutellaria baicalensis</i>	Scutellariae Radix	Labiatae
M0002086	<i>Caesalpinia sappan</i> <i>Cercis chinensis</i>	Sappan Lignum	Anacardiaceae
M0002150	<i>Tricholoma matsutake</i>	Tricholomae Polyporus	Tricholomataceae
M0002185	<i>Polygonum hydropiper</i>	Polygoni Hydropiper Herba	Polygonaceae
M0002221	<i>Benincasa cerifera</i> <i>Benincasa hispida</i>	Benincasae Fructus	Cucurbitaceae
M0002476	<i>Glycine max</i>	Glycinis Semen	Leguminosae
M0002477	<i>Glycine max</i>	Glycinis Testa	Leguminosae
M0002568	<i>Oryza sativa</i>	Vinum Ferri	Gramineae
M0002573	<i>Glycine max</i>	Faba cum Sale Fermentoque Praeparata	Leguminosae
M0002721	<i>Pisum sativum</i>	Pisi Flos	Leguminosae
M0002742	<i>Polygonum hydropiper</i>	Polygoni Fructus	Polygonaceae
M0002806	<i>Cyathula capitata</i>	Achyranthis Radix	Amaranthaceae
M0002807	<i>Cyathula officinalis</i>	Achyranthis Radix	Amaranthaceae
M0002810	<i>Achyranthes bidentata</i>	Achyranthis Radix	Amaranthaceae
M0002870	<i>Glycine max</i>	Glycine Semen Nigrae	Leguminosae
M0003033	<i>Panax ginseng</i>	Ginseng Radix	Araliaceae
M0003035	<i>Panax ginseng</i>	Ginseng Nodus	Araliaceae
M0003066	<i>Sagittaria sagittifolia</i>	Sagittariae Tuber	Alismataceae
M0003235	<i>Oryza sativa</i>	Oryzae Testa	Gramineae
M0003380	<i>Capsella bursa-pastoris</i>	Capsellae Herba	Cruciferae

M0003381	<i>Capsella bursa-pastoris</i>	Capsellae Semen	Cruciferae
M0003559	<i>Oryza sativa</i>	Arida Oryza Distillata	Gramineae
M0003622	<i>Angelica sinensis</i>	Angelicae Sinensis Radix	Umbelliferae
M0003764	<i>Glycine max</i>	Liquor Salsus ex Faba	Leguminosae
M0003765	<i>Oryza sativa</i>	Purum Vinum Oryzae	Gramineae
M0003853	<i>Oryza sativa</i>	Vinum in Primo Vere	Gramineae
M0003864	<i>Oryza sativa</i>	Arida Oryza Praeparatum	Gramineae
M0004061	<i>Ricinus communis</i>	Ricini Folium	Euphorbiaceae
M0004062	<i>Ricinus communis</i>	Ricini Semen	Euphorbiaceae
M0004267	<i>Coriandrum sativum</i>	Coriandri Herba cum Radix	Umbelliferae
M0004268	<i>Coriandrum sativum</i>	Coriandri Herba cum Radix	Umbelliferae
M0004269	<i>Coriandrum sativum</i>	Coriandri Fructus	Umbelliferae
M0004270	<i>Glycine max</i>	Glycinis Semen Praeparatum	Leguminosae
M0004286	<i>Piper nigrum</i>	Pireris Nigri Fructus	Piperaceae
M0004303	<i>Alpinia galanga</i>	Galangae Fructus	Zingiberaceae
M0004460	<i>Glycine max</i>	Glycinis Semen Nigra	Leguminosae
M0004463	<i>Saccharum sinensis</i>	Saccharum Nigrum	Gramineae
M0004468	<i>Glycine max</i>	Glycinis Nigra Testa	Leguminosae

Table S4. List of plants illustrated in **Figures 2E** and **2F**.

Plant ID	Scientific Name	Latin Name	Family
M0000806	<i>Phellodendron amurense</i>	Phellodendri Caulis	Rutaceae
M0002558	<i>Corydalis ternata</i>	Corydalis (Tuber) Rhizoma	Papaveraceae
M0003700	<i>Coptis japonica</i>	Coptidis Rhizoma	Ranunculaceae
M0004375	<i>Coptis deltoidea</i>	Coptidis Rhizoma	Ranunculaceae
M0004376	<i>Coptis teetoides</i>	Coptidis Rhizoma	Ranunculaceae
M0004377	<i>Coptis japonica var. dissecta</i>	Coptidis Rhizoma	Ranunculaceae
M0004379	<i>Coptis japonica</i>	Alcohol cum Coptidis Rhizoma	Ranunculaceae
M0004380	<i>Coptis chinensis</i>	Alcohol cum Coptidis Rhizoma	Ranunculaceae
M0004387	<i>Phellodendron chinense</i>	Phellodendri Cortex	Rutaceae
M0004394	<i>Phellodendron amurense</i>	Phellodendri Radix	Rutaceae

Table S5. List of plants illustrated in **Figures 2G** and **2H**.

Plant ID	Scientific Name	Latin Name	Family
M0000112	<i>Prunus humilis</i>	Pruni Humilis Semen	Rosaceae
M0000501	<i>Apium graveolens var. dulce</i>	Apii Herba	Umbelliferae
M0001048	<i>Lasiosphaera nipponica</i>	Lasiosphaera Seu Calvatia	Lycoperdaceae
M0002838	<i>Prunus humilis</i>	Pruni Cortex	Rosaceae
M0002840	<i>Prunus humilis</i>	Pruni Folium	Rosaceae
M0003141	<i>Amaranthus mangostanus</i>	Amaranthi Herba	Amaranthaceae
M0003628	<i>Prunus humilis</i>	Pruni Lignum	Rosaceae
M0003833	<i>Allium fistulosum</i>	Allii Radix	Liliaceae
M0003836	<i>Allium fistulosum</i>	Allii Fistulosi Succus	Liliaceae
M0003852	<i>Ailanthus altissima</i> <i>Ailanthus glandulosa</i>	Ailanthi Folium	Simaroubaceae
M0004209	<i>Amaranthus mangostanus</i>	Amaranthi Semen	Amaranthaceae

Table S6. List of chemicals which are targeted on phosphodiesterase 10A in **Figure 3A**.

Chemical ID	Chemical Name	inchikey	Chemical Class				
			Kingdom	Superclass	Class	Subclass	Direct_parent
1570	1-(2'-Hydroxyethyl)-4-methoxy-beta-carboline	XAKXPUZLFGDHAO-UHFFFAOYSA-N	Organic compounds	Alkaloids and derivatives	Harmala alkaloids	None	Harmala alkaloids
5411	1-Hydroxycanthin-6-one	LWYFITNQEPSUDK-UHFFFAOYSA-N	Organic compounds	Alkaloids and derivatives	Indolonaphthyridine alkaloids	None	Indolonaphthyridine alkaloids
1574	1-Methoxycanthin-6-one	LEPXKGXTXIACRO-UHFFFAOYSA-N	Organic compounds	Alkaloids and derivatives	Indolonaphthyridine alkaloids	None	Indolonaphthyridine alkaloids
17289	1-Hydroxycanthin-6-one; Me ether	LEPXKGXTXIACRO-UHFFFAOYSA-N	Organic compounds	Alkaloids and derivatives	Indolonaphthyridine alkaloids	None	Indolonaphthyridine alkaloids
537	Canthin-6-one	ZERVJPYNQLONEK-UHFFFAOYSA-N	Organic compounds	Alkaloids and derivatives	Indolonaphthyridine alkaloids	None	Indolonaphthyridine alkaloids
629	2-Ethyl-3-methylpyrazine	LNIMMWYNSBZESE-UHFFFAOYSA-N	Organic compounds	Organoheterocyclic compounds	Diazines	Pyrazines	Pyrazines
1558	2-Hydroxycanthin-6-one	BDCOKQCMZJCYDY-UHFFFAOYSA-N	Organic compounds	Alkaloids and derivatives	Indolonaphthyridine alkaloids	None	Indolonaphthyridine alkaloids
631	2-Methylpyrazine	CAWHJQAVHZEVTJ-UHFFFAOYSA-N	Organic compounds	Organoheterocyclic compounds	Diazines	Pyrazines	Pyrazines
632	2-Methoxy-3-methylpyrazine	VKJIAEQRKBQLLA-UHFFFAOYSA-N	Organic compounds	Organoheterocyclic compounds	Diazines	Pyrazines	Methoxypyrazines
1561	5-Hydroxycanthin-6-one	HOTCTNQHGFRFLK-UHFFFAOYSA-N	Organic compounds	Alkaloids and derivatives	Indolonaphthyridine alkaloids	None	Indolonaphthyridine alkaloids
630	2-Ethylpyrazine	KVFIJWMDDBAGDP-UHFFFAOYSA-N	Organic compounds	Organoheterocyclic compounds	Diazines	Pyrazines	Pyrazines
1564	5-Hydroxymethylcanthin-6-one	NGLFCPGASUBUBB-UHFFFAOYSA-N	Organic compounds	Alkaloids and derivatives	Indolonaphthyridine alkaloids	None	Indolonaphthyridine alkaloids

Table S7. List of chemicals linked with the plant, *Morus alba* and the target, tyrosinase.

Chemical ID	Chemical Name	inchikey	Chemical Class				
			Kingdom	Superclass	Class	Subclass	Direct_parent
7808	Mulberrofuran A	MQYYTNPXQXSQGM-CAOOACKPSA-N	Organic compounds	Phenylpropano ids and polyketides	2-arylbenzofuran flavonoids	None	2-arylbenzofuran flavonoids
6657	Morachalcone A	NXBYIJSAISXPKJWEVVVXLNSA-N	Organic compounds	Phenylpropano ids and polyketides	Linear 1,3-diarylpropano ids	Chalcones and dihydrochalcones	3-prenylated chalcones
7809	Resorcinol	GHMLBKRAJXCXBS-UHFFFAOYSA-N	Organic compounds	Benzenoids	Phenols	Benzenediols	Resorcinols
7810	Oxydihydroresveratrol	IEOZKGCYMAJAHS-UHFFFAOYSA-N	Organic compounds	Phenylpropano ids and polyketides	Stilbenes	None	Stilbenes
7811	Dihydroresveratrol	HITJFUSPLYBJPE-UHFFFAOYSA-N	Organic compounds	Phenylpropano ids and polyketides	Stilbenes	None	Stilbenes
7812	Oxyresveratrol (E-form)	PDHAOJSHSJQANO-OWOJBTEDSA-N	Organic compounds	Phenylpropano ids and polyketides	Stilbenes	None	Stilbenes
7813	beta-Resorecylaldehyde	IUNJCFABHJZSKB-UHFFFAOYSA-N	Organic compounds	Organic oxygen compounds	Organooxygen compounds	Carbonyl compounds	Hydroxybenzaldehydes
788	Albafuran A	KGOOVUKZICPAIZ-FRKPEAEDSA-N	Organic compounds	Phenylpropano ids and polyketides	2-arylbenzofuran flavonoids	None	2-arylbenzofuran flavonoids
789	Albafuran B	ODASNNUHLRPEL-FRKPEAEDSA-N	Organic compounds	Phenylpropano ids and polyketides	2-arylbenzofuran flavonoids	None	2-arylbenzofuran flavonoids
791	Albanol A	MJJWBJFYRAYKU-UHFFFAOYSA-N	Organic compounds	Phenylpropano ids and polyketides	2-arylbenzofuran flavonoids	None	2-arylbenzofuran flavonoids
792	5,7-Dihydroxychromone	NYCXYKOXLNBYID-UHFFFAOYSA-N	Organic compounds	Organoheterocyclic compounds	Benzopyrans	1-benzopyrans	Chromones
793	Dimoracin	GKHRLTCUMXVTAV-UHFFFAOYSA-N	Organic compounds	Phenylpropano ids and polyketides	2-arylbenzofuran flavonoids	None	2-arylbenzofuran flavonoids
17947	1-(2,4-Dihydroxyphenyl)-2-(3,5-dihydroxyphenyl)ethylene; 3'-O-beta-D-Glucopyranoside	GGQVPULXXVQLRT-OWOJBTEDSA-N	Organic compounds	Phenylpropano ids and polyketides	Stilbenes	Stilbene glycosides	Stilbene glycosides
796	Moracin C	ZTGHWUWBQNCCOH-UHFFFAOYSA-N	Organic compounds	Phenylpropano ids and polyketides	2-arylbenzofuran flavonoids	None	2-arylbenzofuran flavonoids
797	Mulberrofuran F	SCNZCLDHJJSZBK-UHFFFAOYSA-N	Organic compounds	Phenylpropano ids and polyketides	2-arylbenzofuran flavonoids	None	2-arylbenzofuran flavonoids
17948	cis-Mulberroside A	HPSWAEGGWLOOKT-UPHRSURJSA-N	Organic compounds	Phenylpropano ids and polyketides	Stilbenes	Stilbene glycosides	Stilbene glycosides
799	Mulberrofuran P	WZXFDNVWWQJWRC-UHFFFAOYSA-N	Organic compounds	Phenylpropano ids and polyketides	2-arylbenzofuran flavonoids	None	2-arylbenzofuran flavonoids

7337	Mulberranol	FMKONXHUEWRD EL-UHFFFAOYSA-N	Organic compounds	Phenylpropano ids and polyketides	Flavonoids	Flavones	6-prenylated flavones
8623	Resveratrol	LUKBXSAWLPMM Z-OWOJBTEDSA-N	Organic compounds	Phenylpropano ids and polyketides	Stilbenes	None	Stilbenes
8369	Broussonin A	MSNVBURPCQDLE P-UHFFFAOYSA-N	Organic compounds	Phenylpropano ids and polyketides	Linear 1,3- diarylpropanoi ds	Cinnamylphe nols	Cinnamylphenols
8370	Broussonin B	CJJQWAYMRTLJT- UHFFFAOYSA-N	Organic compounds	Phenylpropano ids and polyketides	Linear 1,3- diarylpropanoi ds	Cinnamylphe nols	Cinnamylphenols
823	Moracin M	LHPRYOJTASOZGJ- UHFFFAOYSA-N	Organic compounds	Phenylpropano ids and polyketides	2- arylbenzofuran flavonoids	None	2-arylbenzofuran flavonoids
8887	Kuwanon Y	YYUHPJKWIHNMS V-NSCUHMNNSA-N	Organic compounds	Phenylpropano ids and polyketides	Diarylheptanoi ds	Linear diarylheptanoi ds	Linear diarylheptanoids
1215	omega- Hydroxymoracin N	GPKLNIVEGYWQJZ -BIIKFXOESA-N	Organic compounds	Phenylpropano ids and polyketides	2- arylbenzofuran flavonoids	None	2-arylbenzofuran flavonoids
1225	Moracin N	WBSCSIABHGPAM C-UHFFFAOYSA-N	Organic compounds	Phenylpropano ids and polyketides	2- arylbenzofuran flavonoids	None	2-arylbenzofuran flavonoids
10575	Dihydrooxyresverat rol	IEOZKGCYMAJHS -UHFFFAOYSA-N	Organic compounds	Phenylpropano ids and polyketides	Stilbenes	None	Stilbenes
6617	Mulberrin	UWQYBLOHTQWS QD-UHFFFAOYSA- N	Organic compounds	Phenylpropano ids and polyketides	Flavonoids	Flavones	8-prenylated flavones
6619	Kuwanon A	DBUNRZUFILGKHP -UHFFFAOYSA-N	Organic compounds	Phenylpropano ids and polyketides	Flavonoids	Flavones	3-prenylated flavones
6238	Chrysanthemine	RKWHWFONKJEU F-UHFFFAOYSA-O	Organic compounds	Phenylpropano ids and polyketides	Flavonoids	Flavonoid glycosides	Anthocyanidin-3-O- glycosides
6624	Kuwanon G	APPXYONGBIXGR O-UHFFFAOYSA-N	Organic compounds	Phenylpropano ids and polyketides	Flavonoids	Flavones	8-prenylated flavones
6625	Kuwanon H	DKBPTKFKCCNXN H-UHFFFAOYSA-N	Organic compounds	Phenylpropano ids and polyketides	Flavonoids	Flavones	8-prenylated flavones
6626	Kuwanon I	KBAPHKOHTBBCT O-AWNIVKPZSA-N	Organic compounds	Phenylpropano ids and polyketides	Diarylheptanoi ds	Linear diarylheptanoi ds	Linear diarylheptanoids
6627	Kuwanon J	KBAPHKOHTBBCT O-AWNIVKPZSA-N	Organic compounds	Phenylpropano ids and polyketides	Diarylheptanoi ds	Linear diarylheptanoi ds	Linear diarylheptanoids
6628	Kuwanon R	LSWPUMCBBKEXM W-VIZOYTHASA-N	Organic compounds	Phenylpropano ids and polyketides	Diarylheptanoi ds	Linear diarylheptanoi ds	Linear diarylheptanoids
6629	Kuwanon Q	WDCSNUYKXLXPB M-OVCLIPMQSA-N	Organic compounds	Phenylpropano ids and polyketides	Diarylheptanoi ds	Linear diarylheptanoi ds	Linear diarylheptanoids
6630	Kuwanon V	SUQUIVSLHDOSQP -REZTVBANSAN	Organic compounds	Phenylpropano ids and polyketides	Diarylheptanoi ds	Linear diarylheptanoi ds	Linear diarylheptanoids
6631	Kuwanon K	FEAIYAOTVUYWQ Z-UHFFFAOYSA-N	Organic compounds	Phenylpropano ids and polyketides	Flavonoids	Flavones	3'-prenylated flavones
6633	Albafuran C	SEUPIEHHWMMQ G-UHFFFAOYSA-N	Organic compounds	Phenylpropano ids and polyketides	2- arylbenzofuran flavonoids	None	2-arylbenzofuran flavonoids

6636	Morusinol	AFOKZNPZDXHDD-UHFFFAOYSA-N	Organic compounds	Phenylpropanoids and polyketides	Flavonoids	Flavones	3-prenylated flavones
6637	Mulberrofuran E	RQIKMRKKKIMUNB-UHFFFAOYSA-N	Organic compounds	Phenylpropanoids and polyketides	2-arylbenzofuran flavonoids	None	2-arylbenzofuran flavonoids
6638	Mulberrofuran T	XXMZFDZDVCIFKB-UHFFFAOYSA-N	Organic compounds	Phenylpropanoids and polyketides	2-arylbenzofuran flavonoids	None	2-arylbenzofuran flavonoids
6639	Mulberrofuran C	WTGKDESIYCVAOP-UHFFFAOYSA-N	Organic compounds	Phenylpropanoids and polyketides	2-arylbenzofuran flavonoids	None	2-arylbenzofuran flavonoids
6641	Sanggenon E	NJQZTHTXKPCAHD-UHFFFAOYSA-N	Organic compounds	Phenylpropanoids and polyketides	Stilbenes	None	Stilbenes
6643	Sanggenon P	CUJITBMGUHNKPO-UHFFFAOYSA-N	Organic compounds	Phenylpropanoids and polyketides	Diarylheptanoids	Linear diarylheptanoids	Linear diarylheptanoids
6644	Chalcomoracin	SEHVRKPXIDOTRX-UHFFFAOYSA-N	Organic compounds	Phenylpropanoids and polyketides	2-arylbenzofuran flavonoids	None	2-arylbenzofuran flavonoids
6646	Morusin	XFFOMNJDRDDLQ-UHFFFAOYSA-N	Organic compounds	Phenylpropanoids and polyketides	Flavonoids	Flavones	3-prenylated flavones
6647	Cyclomulberrin	SYFDWXWLRGHYAJ-UHFFFAOYSA-N	Organic compounds	Phenylpropanoids and polyketides	Flavonoids	Pyranoflavonoids	Pyranoflavonoids
6648	Moracenin D	PYXAHGLTSLDDJH-UHFFFAOYSA-N	Organic compounds	Phenylpropanoids and polyketides	Flavonoids	Flavones	8-prenylated flavones
7806	2,4-Dihydroxybenzoic acid ethyl ether	BRDIPNLKURUXCU-UHFFFAOYSA-N	Organic compounds	Benzenoids	Benzene and substituted derivatives	Benzoic acids and derivatives	p-Hydroxybenzoic acid alkyl esters
7807	Kuwanol E	HGFVVFTZYRFRI-AATRIKPKSA-N	Organic compounds	Phenylpropanoids and polyketides	Diarylheptanoids	Linear diarylheptanoids	Linear diarylheptanoids

Table S8. List of chemicals linked with the plants, *Carthamus tinctorius*, *Cudrania tricuspidata*, *Glycyrrhiza inflata* and *Glycyrrhiza uralensis* and the target, tyrosinase.

Chemical ID	Chemical Name	inchikey	Chemical Class				
			Kingdom	Superclass	Class	Subclass	Direct parent
<i>Carthamus tinctorius</i>							
7232	Safflomin C	CCEKPTFNQKNHKZ-XCVCLJGOSA-N	Organic compounds	Phenylpropanoids and polyketides	Diarylheptanoids	Linear diarylheptanoids	Curcuminoids
6187	Safflor Yellow B	WBKUQZJRZIYAJL-YDWXAUTNSA-N	None	None	None	None	None
17516	PRE	ITBPOPSLMGJTQH-YDWXAUTNSA-N	None	None	None	None	None
7231	Safflomin A	NNXHCBKOBDDJFM-ZZXKWWIFSA-N	None	None	None	None	None
920	N-(p-Coumaroyl)-5-hydroxytryptamine	WLZPAFGVOWCVMG-FPYGCLRLSA-N	Organic compounds	Organoheterocyclic compounds	Indoles and derivatives	Tryptamines and derivatives	N-acylserotonins
918	N-Feruloylserotonin	WGHKJYWENWLOMY-XVNBXDOJSA-N	Organic compounds	Organoheterocyclic compounds	Indoles and derivatives	Tryptamines and derivatives	N-acylserotonins
17495	4,4"-Bi(N-4-hydroxycinnamoylserotonin); (E,E)-form	OIUNULHHOJRJBIIAGONARPSA-N	Organic compounds	Organoheterocyclic compounds	Indoles and derivatives	Tryptamines and derivatives	N-acylserotonins
17496	4-[N-(p-Coumaroyl)serotonin-4"-yl]-N-feruloylserotonin	ZPNFTINOYMQICL-PWSZKDBUSA-N	Organic compounds	Organoheterocyclic compounds	Indoles and derivatives	Tryptamines and derivatives	N-acylserotonins
17497	4,4"-Bis(N-feruloyl)serotonin	URHRFQQPWDNDQE-ACFHMISVSA-N	Organic compounds	Organoheterocyclic compounds	Indoles and derivatives	Tryptamines and derivatives	N-acylserotonins
7261	Safflor yellow A	YKDBQWHZEDSTAI-ZZXKWWIFSA-N	Organic compounds	Phenylpropanoids and polyketides	Cinnamic acids and derivatives	Hydroxycinnamic acids and derivatives	Hydroxycinnamic acids and derivatives
1502	N-(p-Coumaroyl)serotonin	WLZPAFGVOWCVMG-FPYGCLRLSA-N	Organic compounds	Organoheterocyclic compounds	Indoles and derivatives	Tryptamines and derivatives	N-acylserotonins
1503	N-(p-Coumaroyl)serotonin mono-beta-D-glucopyranoside	LPGWQGDUKIPAME-FPYGCLRLSA-N	Organic compounds	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates	Phenolic glycosides
<i>Cudrania tricuspidata</i>							
7808	Mulberrofuran A	MQYYTNPXQXSQGM-CAOACKPSA-N	Organic compounds	Phenylpropanoids and polyketides	2-arylbenzofuran flavonoids	None	2-arylbenzofuran flavonoids

6657	Morachalcone A	NXBYJISAISXPKJ-WEVVVXLNSA-N	Organic compounds	Phenylpropanoids and polyketides	Linear 1,3-diarylpropanoids	Chalcones and dihydrochalcones	3-prenylated chalcones
7810	Oxydihydroresveratrol	IEOZKGCYMAJAH S-UHFFFAOYSA-N	Organic compounds	Phenylpropanoids and polyketides	Stilbenes	None	Stilbenes
7811	Dihydroresveratrol	HITJFUSPLYBJPE-UHFFFAOYSA-N	Organic compounds	Phenylpropanoids and polyketides	Stilbenes	None	Stilbenes
7812	Oxyresveratrol (E-form)	PDHAOJSHSJQANO-OWOJBTEDSA-N	Organic compounds	Phenylpropanoids and polyketides	Stilbenes	None	Stilbenes
7813	beta-Resorcyaldehyde	IUNJCFABHJZSKB-UHFFFAOYSA-N	Organic compounds	Organic oxygen compounds	Organooxygen compounds	Carbonyl compounds	Hydroxybenzaldehydes
7809	Resorcinol	GHMLBKRAJCXBS-UHFFFAOYSA-N	Organic compounds	Benzenoids	Phenols	Benzenediols	Resorcinols
788	Albafuran A	KGOOVUKZICPAIZ-FRKPEAEDSA-N	Organic compounds	Phenylpropanoids and polyketides	2-arylbenzofuran flavonoids	None	2-arylbenzofuran flavonoids
789	Albafuran B	ODASNNUHHLRPEL-FRKPEAEDSA-N	Organic compounds	Phenylpropanoids and polyketides	2-arylbenzofuran flavonoids	None	2-arylbenzofuran flavonoids
791	Albanol A	MJJWBJFYRAYKU-UHFFFAOYSA-N	Organic compounds	Phenylpropanoids and polyketides	2-arylbenzofuran flavonoids	None	2-arylbenzofuran flavonoids
792	5,7-Dihydroxychromone	NYCXYKOXLNBYID-UHFFFAOYSA-N	Organic compounds	Organoheterocyclic compounds	Benzopyrans	1-benzopyrans	Chromones
793	Dimoracin	GKHRLTCUMXVTAV-UHFFFAOYSA-N	Organic compounds	Phenylpropanoids and polyketides	2-arylbenzofuran flavonoids	None	2-arylbenzofuran flavonoids
17947	1-(2,4-Dihydroxyphenyl)-2-(3,5-dihydroxyphenyl)ethane; 3'-O-beta-D-Glucopyranoside	GGQVPULXXVQLRT-OWOJBTEDSA-N	Organic compounds	Phenylpropanoids and polyketides	Stilbenes	Stilbene glycosides	Stilbene glycosides
17948	cis-Mulberroside A	HPSWAEGGWLOOKT-UPHRSURJSA-N	Organic compounds	Phenylpropanoids and polyketides	Stilbenes	Stilbene glycosides	Stilbene glycosides

796	Moracin C	ZTGHWUWBQNCC OH-UHFFFAOYSA- N	Organic compoun ds	Phenylpropanoi ds and polyketides	2- arylbenzofura n flavonoids	None	2-arylbenzofuran flavonoids
797	Mulberrofuran F	SCNZCLDHJJSZBK- UHFFFAOYSA-N	Organic compoun ds	Phenylpropanoi ds and polyketides	2- arylbenzofura n flavonoids	None	2-arylbenzofuran flavonoids
799	Mulberrofuran P	WZXFDNVVWQJW RC-UHFFFAOYSA- N	Organic compoun ds	Phenylpropanoi ds and polyketides	2- arylbenzofura n flavonoids	None	2-arylbenzofuran flavonoids
7337	Mulberranol	FMKONXHUEWRD EL-UHFFFAOYSA- N	Organic compoun ds	Phenylpropanoi ds and polyketides	Flavonoids	Flavones	6-prenylated flavones
8623	Resveratrol	LUKBXSAWLPMM SZ-OWOJBTEDSA- N	Organic compoun ds	Phenylpropanoi ds and polyketides	Stilbenes	None	Stilbenes
8369	Broussonin A	MSNVBURPCQDLE P-UHFFFAOYSA-N	Organic compoun ds	Phenylpropanoi ds and polyketides	Linear 1,3- diarylpropano ids	Cinnamylphenols	Cinnamylphenols
8370	Broussonin B	CJJQWAYMRTLJT -UHFFFAOYSA-N	Organic compoun ds	Phenylpropanoi ds and polyketides	Linear 1,3- diarylpropano ids	Cinnamylphenols	Cinnamylphenols
823	Moracin M	LHPRYOJTASOZGJ -UHFFFAOYSA-N	Organic compoun ds	Phenylpropanoi ds and polyketides	2- arylbenzofura n flavonoids	None	2-arylbenzofuran flavonoids
8887	Kuwanon Y	YYUHPJKWIHNMS V-NSCUHMNNSA- N	Organic compoun ds	Phenylpropanoi ds and polyketides	Diarylheptan oids	Linear diarylheptanoids	Linear diarylheptanoids
1215	omega-Hydroxymoracin N	GPKLNIVEGYWQJ Z-BIIKFXOESA-N	Organic compoun ds	Phenylpropanoi ds and polyketides	2- arylbenzofura n flavonoids	None	2-arylbenzofuran flavonoids
1225	Moracin N	WBSCSIABHGPAM C-UHFFFAOYSA-N	Organic compoun ds	Phenylpropanoi ds and polyketides	2- arylbenzofura n flavonoids	None	2-arylbenzofuran flavonoids
10575	Dihydroxyresveratrol	IEOZKGCYMAJAH S-UHFFFAOYSA-N	Organic compoun ds	Phenylpropanoi ds and polyketides	Stilbenes	None	Stilbenes
6617	Mulberrin	UWQYBLOHTQWS QD-UHFFFAOYSA- N	Organic compoun ds	Phenylpropanoi ds and polyketides	Flavonoids	Flavones	8-prenylated flavones
6619	Kuwanon A	DBUNRZUFILGKH P-UHFFFAOYSA-N	Organic compoun ds	Phenylpropanoi ds and polyketides	Flavonoids	Flavones	3-prenylated flavones

6238	Chrysanthemim	RKWHWFONKJEU EF-UHFFFAOYSA- O	Organic compoun ds	Phenylpropanoi ds and polyketides	Flavonoids	Flavonoid glycosides	Anthocyanidin-3- O-glycosides
6624	Kuwanon G	APPXYONGBIXGR O-UHFFFAOYSA-N	Organic compoun ds	Phenylpropanoi ds and polyketides	Flavonoids	Flavones	8-prenylated flavones
6625	Kuwanon H	DKBPTKFKCCNXN H-UHFFFAOYSA-N	Organic compoun ds	Phenylpropanoi ds and polyketides	Flavonoids	Flavones	8-prenylated flavones
6626	Kuwanon I	KBAPHKOHTBBCT O-AWNIVKPZSA-N	Organic compoun ds	Phenylpropanoi ds and polyketides	Diarylheptan oids	Linear diarylheptanoids	Linear diarylheptanoids
6627	Kuwanon J	KBAPHKOHTBBCT O-AWNIVKPZSA-N	Organic compoun ds	Phenylpropanoi ds and polyketides	Diarylheptan oids	Linear diarylheptanoids	Linear diarylheptanoids
6628	Kuwanon R	LSWPUMCBBKEX MW-VIZOYTHASA- N	Organic compoun ds	Phenylpropanoi ds and polyketides	Diarylheptan oids	Linear diarylheptanoids	Linear diarylheptanoids
6629	Kuwanon Q	WDCSNUYKXLXP BM-OVCLIPMQSA- N	Organic compoun ds	Phenylpropanoi ds and polyketides	Diarylheptan oids	Linear diarylheptanoids	Linear diarylheptanoids
6630	Kuwanon V	SUQUIVSLHDOSQP -REZTVBANSAN	Organic compoun ds	Phenylpropanoi ds and polyketides	Diarylheptan oids	Linear diarylheptanoids	Linear diarylheptanoids
6631	Kuwanon K	FEAIYAOTVUYWQ Z-UHFFFAOYSA-N	Organic compoun ds	Phenylpropanoi ds and polyketides	Flavonoids	Flavones	3'-prenylated flavones
6633	Albafuran C	SEUPIEHHWMMM QG-UHFFFAOYSA- N	Organic compoun ds	Phenylpropanoi ds and polyketides	2- arylbenzofura n flavonoids	None	2-arylbenzofuran flavonoids
6636	Morusinol	AFOKZNPZDXHDH D-UHFFFAOYSA-N	Organic compoun ds	Phenylpropanoi ds and polyketides	Flavonoids	Flavones	3-prenylated flavones
6637	Mulberrofuran E	RQIKMRKKKIMUN B-UHFFFAOYSA-N	Organic compoun ds	Phenylpropanoi ds and polyketides	2- arylbenzofura n flavonoids	None	2-arylbenzofuran flavonoids
6638	Mulberrofuran T	XMZXFZDVCIFK B-UHFFFAOYSA-N	Organic compoun ds	Phenylpropanoi ds and polyketides	2- arylbenzofura n flavonoids	None	2-arylbenzofuran flavonoids
6639	Mulberrofuran C	WTGKDESIYCAVO P-UHFFFAOYSA-N	Organic compoun ds	Phenylpropanoi ds and polyketides	2- arylbenzofura n flavonoids	None	2-arylbenzofuran flavonoids

6641	Sanggenon E	NJQZTHTXKPCAH D-UHFFFAOYSA-N	Organic compoun ds	Phenylpropanoi ds and polyketides	Stilbenes	None	Stilbenes
6643	Sanggenon P	CUJJTBMGUHNKP O-UHFFFAOYSA-N	Organic compoun ds	Phenylpropanoi ds and polyketides	Diarylheptan oids	Linear diarylheptanoids	Linear diarylheptanoids
6644	Chalcomoracin	SEHVRKPXIDOTR X-UHFFFAOYSA-N	Organic compoun ds	Phenylpropanoi ds and polyketides	2- arylbenzofura n flavonoids	None	2-arylbenzofuran flavonoids
6646	Morusin	XFFOMNJDRDDL Q-UHFFFAOYSA-N	Organic compoun ds	Phenylpropanoi ds and polyketides	Flavonoids	Flavones	3-prenylated flavones
6647	Cyclomulberrin	SYFDWXWLRGHY AJ-UHFFFAOYSA- N	Organic compoun ds	Phenylpropanoi ds and polyketides	Flavonoids	Pyranoflavonoids	Pyranoflavonoids
6648	Moracenin D	PYXAHGLTSLDDJ H-UHFFFAOYSA-N	Organic compoun ds	Phenylpropanoi ds and polyketides	Flavonoids	Flavones	8-prenylated flavones
7806	2,4-Dihydroxybenzoic acid ethyl ether	BRDIPNLKURUXC U-UHFFFAOYSA-N	Organic compoun ds	Benzenoids	Benzene and substituted derivatives	Benzoic acids and derivatives	p-Hydroxybenzoic acid alkyl esters
7807	Kuwanol E	HGFVWFTZYRJFRI -AATRIKPKSA-N	Organic compoun ds	Phenylpropanoi ds and polyketides	Diarylheptan oids	Linear diarylheptanoids	Linear diarylheptanoids

Glycyrrhiza inflata

17792	Licochalcone C	WBDNTJSRHDSPS R-KPKJPENVSA-N	Organic compoun ds	Phenylpropanoi ds and polyketides	Linear 1,3- diarylpropano ids	Chalcones and dihydrochalcones	Retrochalcones
7300	5'-Prenyllicodione	VAWLLIOUAFRMH N-UHFFFAOYSA-N	Organic compoun ds	Phenylpropanoi ds and polyketides	Linear 1,3- diarylpropano ids	Chalcones and dihydrochalcones	Retro- dihydrochalcones
7301	Glycyrdione A	VDOHBGQSFOWY TB-UHFFFAOYSA- N	Organic compoun ds	Phenylpropanoi ds and polyketides	Linear 1,3- diarylpropano ids	Chalcones and dihydrochalcones	Retro- dihydrochalcones
7303	Glyinflanin A	VDOHBGQSFOWY TB-UHFFFAOYSA- N	Organic compoun ds	Phenylpropanoi ds and polyketides	Linear 1,3- diarylpropano ids	Chalcones and dihydrochalcones	Retro- dihydrochalcones
7317	Licochalcone C	WBDNTJSRHDSPS R-KPKJPENVSA-N	Organic compoun ds	Phenylpropanoi ds and polyketides	Linear 1,3- diarylpropano ids	Chalcones and dihydrochalcones	Retrochalcones

7318	Licochalcone D	RETRVWFVEFCGO K-RMKNXTFCSA-N	Organic compoun ds	Phenylpropanoi ds and polyketides	Linear 1,3- diarylpropano ids	Chalcones and dihydrochalcones	3-prenylated chalcones
5960	Isoliquiritigenin	DXDRHHKMWQZJ HT-FPYGCLRLSA- N	Organic compoun ds	Phenylpropanoi ds and polyketides	Linear 1,3- diarylpropano ids	Chalcones and dihydrochalcones	2'- Hydroxychalcones
8137	Glycoumarin	NZYSZZDSYIBYLC -UHFFFAOYSA-N	Organic compoun ds	Phenylpropanoi ds and polyketides	Isoflavonoids	Hydroxyisoflavon oids	Hydroxyisoflavono ids
10318	Licoflavone B	GLDVIKFETPAZNV -UHFFFAOYSA-N	Organic compoun ds	Phenylpropanoi ds and polyketides	Flavonoids	Flavones	6-prenylated flavones
10330	Licoflavone C	MEHHCBRXCIDGK Z-UHFFFAOYSA-N	Organic compoun ds	Phenylpropanoi ds and polyketides	Flavonoids	Flavones	8-prenylated flavones
5980	Echinatin	QJKMIJNRNLQSS- WEVVVXLNSA-N	Organic compoun ds	Phenylpropanoi ds and polyketides	Linear 1,3- diarylpropano ids	Chalcones and dihydrochalcones	Retrochalcones
5981	Licochalcone A	KAZSKMJFUPEHH W-DHZHZOJOSA-N	Organic compoun ds	Phenylpropanoi ds and polyketides	Linear 1,3- diarylpropano ids	Chalcones and dihydrochalcones	Retrochalcones
5982	Licochalcone B	DRDRYGIIYOPBBZ -XBXARRHUSA-N	Organic compoun ds	Phenylpropanoi ds and polyketides	Linear 1,3- diarylpropano ids	Chalcones and dihydrochalcones	Retrochalcones
5983	Isoliquiritin	YNWXJFQOCHMPC K-FPYGCLRLSA-N	Organic compoun ds	Phenylpropanoi ds and polyketides	Flavonoids	Flavonoid glycosides	Flavonoid glycosides
17774	Licoflavone B	GLDVIKFETPAZNV -UHFFFAOYSA-N	Organic compoun ds	Phenylpropanoi ds and polyketides	Flavonoids	Flavones	6-prenylated flavones
17777	Glyinflanin I; (R)-form	AFQCFVZKNRRL S-UHFFFAOYSA-N	Organic compoun ds	Phenylpropanoi ds and polyketides	Isoflavonoids	Pyranoisoflavonoi ds	Pyranoisoflavonoid s
17781	Glyinflanin E	YSMQGBBJPVUXE X-UHFFFAOYSA-N	Organic compoun ds	Phenylpropanoi ds and polyketides	Linear 1,3- diarylpropano ids	Chalcones and dihydrochalcones	Retro- dihydrochalcones
7162	Licoflavone A	HJGURBGBPIKRER -UHFFFAOYSA-N	Organic compoun ds	Phenylpropanoi ds and polyketides	Flavonoids	Flavones	6-prenylated flavones
17787	Inflacoumarin A	RNBLSJGPGNSIN- UHFFFAOYSA-N	Organic compoun ds	Phenylpropanoi ds and polyketides	Neoflavonoid s	Prenylated neoflavonoids	Prenylated neoflavonoids

17791	Licochalcone D	RETRVWFVEFCGO K-RMKNXTFCSA-N	Organic compounds	Phenylpropanoids and polyketides	Linear 1,3-diarylpropanoids	Chalcones and dihydrochalcones	3-prenylated chalcones
<i>Glycyrrhiza uralensis</i>							
17793	Uralennoeside	VWQASRWQZBVN EI-UHFFFAOYSA-N	Organic compounds	Benzenoids	Benzene and substituted derivatives	Benzoic acids and derivatives	p-Hydroxybenzoic acid alkyl esters
17794	6"-Acetylliquiritin	HKUBLIRXXFRGK E-UHFFFAOYSA-N	Organic compounds	Phenylpropanoids and polyketides	Flavonoids	Flavonoid glycosides	Flavonoid O-glycosides
17797	Kanzonol H	JRV DUBFSQWHYR J-UHFFFAOYSA-N	Organic compounds	Phenylpropanoids and polyketides	Isoflavonoids	O-methylated isoflavonoids	5-O-methylated isoflavonoids
17799	Kanzonol L	CLXMHBYPZWNJQ I-UHFFFAOYSA-N	Organic compounds	Phenylpropanoids and polyketides	Isoflavonoids	Isoflavans	6-prenylated isoflavanones
6280	2',4,4'-Trihydroxy-3'-prenylchalcone	DUWPGRAKHMEP CM-IZZDOVSWSA-N	Organic compounds	Phenylpropanoids and polyketides	Linear 1,3-diarylpropanoids	Chalcones and dihydrochalcones	3-prenylated chalcones
17800	Kanzonol N	ANRYVYXUTFJPO R-UHFFFAOYSA-N	Organic compounds	Phenylpropanoids and polyketides	Isoflavonoids	O-methylated isoflavonoids	5-O-methylated isoflavonoids
17801	Kanzonol M	KZQAGRHRFKIER V-UHFFFAOYSA-N	Organic compounds	Phenylpropanoids and polyketides	Isoflavonoids	O-methylated isoflavonoids	5-O-methylated isoflavonoids
17807	Kanzonol G	OWVFKLIUBOKW CT-UHFFFAOYSA-N	Organic compounds	Phenylpropanoids and polyketides	Isoflavonoids	Isoflavans	3'-prenylated isoflavanones
17808	Kanzonol K	UWUOGPWSIVRQ NM-UHFFFAOYSA-N	Organic compounds	Phenylpropanoids and polyketides	Isoflavonoids	Isoflavans	6-prenylated isoflavanones
17809	Glyurallin B	DPLWUTYEBRKBL I-UHFFFAOYSA-N	Organic compounds	Phenylpropanoids and polyketides	Isoflavonoids	Isoflav-2-enes	Isoflavones
17810	Kanzonol P	ZCGOJWAIXQAUM W-UHFFFAOYSA-N	Organic compounds	Phenylpropanoids and polyketides	Isoflavonoids	Furanisoflavonoids	Pterocarpan
7454	Gancaonin R	QFAPONVNJTUMH F-UHFFFAOYSA-N	Organic compounds	Phenylpropanoids and polyketides	Stilbenes	None	Stilbenes

7455	Gancaonin S	VLJOWGMLRJTND Q-UHFFFAOYSA-N	Organic compounds	Phenylpropanoids and polyketides	Stilbenes	None	Stilbenes
7456	Gancaonin U	YJXCOSDPIJFJR- UHFFFAOYSA-N	Organic compounds	Benzenoids	Phenanthrenes and derivatives	Hydrophenanthrenes	Hydrophenanthrenes
7457	Gancaonin V	UEXOPXIMQJMWK A-UHFFFAOYSA-N	Organic compounds	Benzenoids	Phenanthrenes and derivatives	Hydrophenanthrenes	Hydrophenanthrenes
7205	Gancaonin C	MEADLGUPYQNU NF-BIIKFXOESA-N	Organic compounds	Phenylpropanoids and polyketides	Isoflavonoids	Isoflav-2-enes	Isoflavones
7206	Gancaonin D	UCKSAYIMWMIZQ J-QDEBKDIKSA-N	Organic compounds	Phenylpropanoids and polyketides	Isoflavonoids	O-methylated isoflavonoids	3'-hydroxy,4'- methoxyisoflavonoids
7208	Gancaonin L	WSOHPJFMARQRF D-UHFFFAOYSA-N	Organic compounds	Phenylpropanoids and polyketides	Isoflavonoids	Isoflav-2-enes	Isoflavones
7209	Gancaonin M	DDLPIQXHEKZHQ X-UHFFFAOYSA-N	Organic compounds	Phenylpropanoids and polyketides	Isoflavonoids	O-methylated isoflavonoids	4'-O- methylisoflavones
7210	Gancaonin O	AFJYQKPCJLMHCC -UHFFFAOYSA-N	Organic compounds	Phenylpropanoids and polyketides	Flavonoids	Flavones	6-prenylated flavones
7212	Gancaonin Q	WGNIVAMNAWBY RO-UHFFFAOYSA- N	Organic compounds	Phenylpropanoids and polyketides	Flavonoids	Flavones	6-prenylated flavones
8896	Gancaonin T	OWBYJSNJVWQEQ X-UHFFFAOYSA-N	Organic compounds	Phenylpropanoids and polyketides	Stilbenes	None	Stilbenes
8134	Glycyrin	FWWGXZYURXJ LK-UHFFFAOYSA- N	Organic compounds	Phenylpropanoids and polyketides	Isoflavonoids	Hydroxyisoflavonoids	Hydroxyisoflavonoids
5960	Isoliquiritigenin	DXDRHHKMWQZJ HT-FPYGCLRLSA- N	Organic compounds	Phenylpropanoids and polyketides	Linear 1,3- diarylpropanoids	Chalcones and dihydrochalcones	2'- Hydroxychalcones
8137	Glycoumarin	NZYSZZDSYIBYLC -UHFFFAOYSA-N	Organic compounds	Phenylpropanoids and polyketides	Isoflavonoids	Hydroxyisoflavonoids	Hydroxyisoflavonoids
5980	Echinatin	QJKMIJNRNLQSS- WEVVVXLNSA-N	Organic compounds	Phenylpropanoids and polyketides	Linear 1,3- diarylpropanoids	Chalcones and dihydrochalcones	Retrochalcones

5981	Licochalcone A	KAZSKMJFUPEHH W-DHZHZOJOSA-N	Organic compoun ds	Phenylpropanoi ds and polyketides	Linear 1,3- diarylpropanoi ds	Chalcones and dihydrochalcones	Retrochalcones
5982	Licochalcone B	DRDRYGIIYOPBBZ -XBXARRHUSA-N	Organic compoun ds	Phenylpropanoi ds and polyketides	Linear 1,3- diarylpropanoi ds	Chalcones and dihydrochalcones	Retrochalcones
5983	Isoliquiritin	YNWXJFQOCHMPC K-FPYGCLRLSA-N	Organic compoun ds	Phenylpropanoi ds and polyketides	Flavonoids	Flavonoid glycosides	Flavonoid O- glycosides
8542	1-O-Protocatechuy- beta-D-xylose	VWQASRWQZBVN EI-UHFFFAOYSA-N	Organic compoun ds	Benzenoids	Benzene and substituted derivatives	Benzoic acids and derivatives	p-Hydroxybenzoic acid alkyl esters
5989	Licoflavonol	TVMHBSODLWMM MV-UHFFFAOYSA- N	Organic compoun ds	Phenylpropanoi ds and polyketides	Flavonoids	Flavones	6-prenylated flavones
5994	Licoricone	GGWMNTNDTRKE TA-UHFFFAOYSA- N	Organic compoun ds	Phenylpropanoi ds and polyketides	Isoflavonoids	O-methylated isoflavonoids	4'-O- methylisoflavones
5996	Gancaonin A	JQNSUDIGIIGIOL- UHFFFAOYSA-N	Organic compoun ds	Phenylpropanoi ds and polyketides	Isoflavonoids	Isoflavans	6-prenylated isoflavanones
5998	Gancaonin N	STFVTZQCNYBLN E-UHFFFAOYSA-N	Organic compoun ds	Phenylpropanoi ds and polyketides	Isoflavonoids	Isoflavans	6-prenylated isoflavanones
7162	Licoflavone A	HJGURBGBPIKRER -UHFFFAOYSA-N	Organic compoun ds	Phenylpropanoi ds and polyketides	Flavonoids	Flavones	6-prenylated flavones
7163	Lupiwighteone	YGCCASGFIOIXIN- UHFFFAOYSA-N	Organic compoun ds	Phenylpropanoi ds and polyketides	Isoflavonoids	Isoflav-2-enes	Isoflavones

Table S9. List of chemicals which are co-targeted on S5R1 and S5R2.

Chemical ID	Chemical Name	inchikey	Chemical Class				
			Kingdom	Superclass	Class	Subclass	Direct_parent
1925	Ergost-4-en-3-one	QQIOPZVFTIHASB-UHFFFAOYSA-N	Organic compounds	Lipids and lipid-like molecules	Steroids and steroid derivatives	Ergostane steroids	Ergosterols and derivatives
1926	Ergost-4-en-3,6-dione	HYALICAWSDCPS-UHFFFAOYSA-N	Organic compounds	Lipids and lipid-like molecules	Steroids and steroid derivatives	Ergostane steroids	Ergosterols and derivatives
1927	Stigmast-4-en-3,6-dione	UVFOCYGYACXLAY-UHFFFAOYSA-N	Organic compounds	Lipids and lipid-like molecules	Steroids and steroid derivatives	Stigmastanes and derivatives	Stigmastanes and derivatives
1928	Stigmasta-4,22-dien-3-one	MKGZDUKUQPPHFM-CMDGGOBGSA-N	Organic compounds	Lipids and lipid-like molecules	Steroids and steroid derivatives	Stigmastanes and derivatives	Stigmastanes and derivatives
10505	17-Deoxywithanone	ZTEVDTFJUUBLP-UHFFFAOYSA-N	Organic compounds	Lipids and lipid-like molecules	Steroids and steroid derivatives	Steroid lactones	Withanolides and derivatives
1929	Stigmasta-4,22-dien-3,6-dione	XWHBTBBUPBKDBB-CMDGGOBGSA-N	Organic compounds	Lipids and lipid-like molecules	Steroids and steroid derivatives	Stigmastanes and derivatives	Stigmastanes and derivatives
10632	24-Ethyl-24-dehydrocholesterol	YYLFLRIUDMIWTD-UHFFFAOYSA-N	Organic compounds	Lipids and lipid-like molecules	Steroids and steroid derivatives	Stigmastanes and derivatives	Stigmastanes and derivatives
10636	Ergostenone(24R)	QQIOPZVFTIHASB-UHFFFAOYSA-N	Organic compounds	Lipids and lipid-like molecules	Steroids and steroid derivatives	Ergostane steroids	Ergosterols and derivatives
10637	Stigmasta-4,22-dien-3-one	MKGZDUKUQPPHFM-CMDGGOBGSA-N	Organic compounds	Lipids and lipid-like molecules	Steroids and steroid derivatives	Stigmastanes and derivatives	Stigmastanes and derivatives
10638	Stigmasta-4,6-dien-3-one	KEAZWUZFBXOMV-UHFFFAOYSA-N	Organic compounds	Lipids and lipid-like molecules	Steroids and steroid derivatives	Stigmastanes and derivatives	Stigmastanes and derivatives
2702	Castasterone	VYUIKSFYFRVQLF-UHFFFAOYSA-N	Organic compounds	Lipids and lipid-like molecules	Steroids and steroid derivatives	Bile acids, alcohols and derivatives	Tetrahydroxy bile acids, alcohols and derivatives
9612	Kusunol	MQWIFDHBNGIVPO-UHFFFAOYSA-N	Organic compounds	Lipids and lipid-like molecules	Prenol lipids	Sesquiterpenoids	Eremophilane, 8,9-secoeremophilane and furoeremophilane sesquiterpenoids
10633	Stigmasta-5,24(28)-dien-3-ol	OSELKOCHBMDKEJ-QPSGOUHRSA-N	Organic compounds	Lipids and lipid-like molecules	Steroids and steroid derivatives	Stigmastanes and derivatives	Stigmastanes and derivatives
10635	Cholesta-4,6-dien-3-one	XIWMRKFKRSYIJ-UHFFFAOYSA-N	Organic compounds	Lipids and lipid-like molecules	Steroids and steroid derivatives	Cholestane steroids	Cholesterols and derivatives

1940	Isofucosterol	OSELKOCHBMDKEJ-YXSASFJKSA-N	Organic compounds	Lipids and lipid-like molecules	Steroids and steroid derivatives	Stigmastanes and derivatives	Stigmastanes and derivatives
11158	Dehydroabietinal	YCLCHPWGSDZKL-UHFFFAOYSA-N	Organic compounds	Lipids and lipid-like molecules	Prenol lipids	Diterpenoids	Diterpenoids
2585	Panax ginseng glycoside P1	DAPLORBFRRJHHY-UHFFFAOYSA-N	Organic compounds	Lipids and lipid-like molecules	Steroids and steroid derivatives	Steroidal glycosides	Steroidal glycosides
2330	alpha-Teresantallic acid	QHDPITNBVDSMQH-UHFFFAOYSA-N	Organic compounds	Lipids and lipid-like molecules	Prenol lipids	Monoterpenoids	Bicyclic monoterpenoids
1956	31-Norlanost-8-en-3-ol	IXVNEXDXGHWLS-UHFFFAOYSA-N	Organic compounds	Lipids and lipid-like molecules	Steroids and steroid derivatives	Cholestane steroids	Cholesterols and derivatives
1959	31-Norlanost-9(11)-enol	SZCKXGWHINUNKB-UHFFFAOYSA-N	Organic compounds	Lipids and lipid-like molecules	Steroids and steroid derivatives	Cholestane steroids	Cholesterols and derivatives
2345	Campesterol	SGNBVLWSZMBQTH-UHFFFAOYSA-N	Organic compounds	Lipids and lipid-like molecules	Steroids and steroid derivatives	Ergostane steroids	Ergosterols and derivatives
1961	Lophenol	LMYZQUNLYGJIHI-UHFFFAOYSA-N	Organic compounds	Lipids and lipid-like molecules	Steroids and steroid derivatives	Cholestane steroids	Cholesterols and derivatives
3118	Stigmastane-3,6-dione (5alpha H)	HMMVBVVQLUGQA-UHFFFAOYSA-N	Organic compounds	Lipids and lipid-like molecules	Steroids and steroid derivatives	Stigmastanes and derivatives	Stigmastanes and derivatives
1967	4-alpha-Methylcholest-8-en-3-ol	SCEZIHJVTBQOLS-UHFFFAOYSA-N	Organic compounds	Lipids and lipid-like molecules	Steroids and steroid derivatives	Cholestane steroids	Cholesterols and derivatives
9519	5-alpha-Stigmast-22-en-3-one	RTLUSWHIKFIQFU-CMDGGOBGSA-N	Organic compounds	Lipids and lipid-like molecules	Steroids and steroid derivatives	Stigmastanes and derivatives	Stigmastanes and derivatives
9520	Stigmast-5-en-3-beta-ol-7-one	ICFXJOAKQGDRCT-UHFFFAOYSA-N	Organic compounds	Lipids and lipid-like molecules	Steroids and steroid derivatives	Stigmastanes and derivatives	Stigmastanes and derivatives
1970	Withanolide B	ZTEVDTFJUUBLP-UHFFFAOYSA-N	Organic compounds	Lipids and lipid-like molecules	Steroids and steroid derivatives	Steroid lactones	Withanolides and derivatives
2226	Estradiol	VOXZDWNVPJITMN-UHFFFAOYSA-N	Organic compounds	Lipids and lipid-like molecules	Steroids and steroid derivatives	Estrane steroids	Estrogens and derivatives
9654	(-)-Ylangene	VLXDPFLIRFYIME-UHFFFAOYSA-N	Organic compounds	Lipids and lipid-like molecules	Prenol lipids	Sesquiterpenoids	Sesquiterpenoids
1847	(-)-alpha-Copaene	VLXDPFLIRFYIME-UHFFFAOYSA-N	Organic compounds	Lipids and lipid-like molecules	Prenol lipids	Sesquiterpenoids	Sesquiterpenoids
11070	Aromadendrane-4-beta,10-alpha-diol	DWNPMJOWAWGIMM-UHFFFAOYSA-N	Organic compounds	Lipids and lipid-like molecules	Prenol lipids	Sesquiterpenoids	5,10-cycloaromadendrane sesquiterpenoids

11076	Neointermedeol	DPQYOKVMVCQHMY-UHFFFAOYSA-N	Organic compounds	Lipids and lipid-like molecules	Prenol lipids	Sesquiterpenoids	Eudesmane, isoeudesmane or cycloeudesmane sesquiterpenoids
1863	3-beta-Hydroxystigmast-5-en-7-one	ICFXJOAKQGDRCT-UHFFFAOYSA-N	Organic compounds	Lipids and lipid-like molecules	Steroids and steroid derivatives	Stigmastanes and derivatives	Stigmastanes and derivatives
2001	Stigmastan-3-one (5-alpha)	BVVFRHKBULZQCQ-UHFFFAOYSA-N	Organic compounds	Lipids and lipid-like molecules	Steroids and steroid derivatives	Stigmastanes and derivatives	Stigmastanes and derivatives
4562	3,5-Acoradiene	ZQMYLSWMANINAL-UHFFFAOYSA-N	Organic compounds	Hydrocarbons	Unsaturated hydrocarbons	Branched unsaturated hydrocarbons	Branched unsaturated hydrocarbons
3032	Ledol	AYXPYQRXGNDJFU-UHFFFAOYSA-N	Organic compounds	Lipids and lipid-like molecules	Prenol lipids	Sesquiterpenoids	5,10-cycloaromadendrane sesquiterpenoids
4187	Stigmasterol	HCVXJBMSMIARIN-CMDGGOBGSA-N	Organic compounds	Lipids and lipid-like molecules	Steroids and steroid derivatives	Stigmastanes and derivatives	Stigmastanes and derivatives
1769	Stigmast-22-en-3-beta-ol	CSVWWLUMXNHWSU-CMDGGOBGSA-N	Organic compounds	Lipids and lipid-like molecules	Steroids and steroid derivatives	Stigmastanes and derivatives	Stigmastanes and derivatives
10630	24-Methylcholest-5,22-dien-3-ol; (3-beta,22E,24R)-form	OILXMJHPFNGGTO-BQYQJAHWSA-N	Organic compounds	Lipids and lipid-like molecules	Steroids and steroid derivatives	Ergostane steroids	Ergosterols and derivatives
1774	beta-Sitosterol	KZJWDPNRJALLNS-UHFFFAOYSA-N	Organic compounds	Lipids and lipid-like molecules	Steroids and steroid derivatives	Stigmastanes and derivatives	Stigmastanes and derivatives
10631	24-Ethyl-22-trans-dehydrocholesterol; (3-beta,22E,24R)-form	HCVXJBMSMIARIN-CMDGGOBGSA-N	Organic compounds	Lipids and lipid-like molecules	Steroids and steroid derivatives	Stigmastanes and derivatives	Stigmastanes and derivatives
1776	Brassicasterol	OILXMJHPFNGGTO-BQYQJAHWSA-N	Organic compounds	Lipids and lipid-like molecules	Steroids and steroid derivatives	Ergostane steroids	Ergosterols and derivatives
1777	Cholesterol	HVYWMOMLDIMFJA-UHFFFAOYSA-N	Organic compounds	Lipids and lipid-like molecules	Steroids and steroid derivatives	Cholestane steroids	Cholesterols and derivatives
2550	Campest-5-en-7-one-3-beta-ol	LTLKHSBYMNKWPFUHFFFAOYSA-N	Organic compounds	Lipids and lipid-like molecules	Steroids and steroid derivatives	Ergostane steroids	Ergosterols and derivatives

Table S10. List of chemicals which are co-targeted on S5R1 and AR.

Chemical ID	Chemical Name	inchikey	Chemical Class				
			Kingdom	Superclass	Class	Subclass	Direct_parent
1984	Dihydro-epideoxyarteannuin B	SXDUGGRDNCRRHY-UHFFFAOYSA-N	Organic compounds	Lipids and lipid-like molecules	Prenol lipids	Terpene lactones	Germacranolides and derivatives
9607	4-Hydroxy-4-methyl-5-dodecanylcyclopenten-2-one	HWMQXCKSSOGAEL-UHFFFAOYSA-N	Organic compounds	Organic oxygen compounds	Organoxygen compounds	Alcohols and polyols	Tertiary alcohols
3815	19(4-3)Abeo-12,14,15-trihydroxy-11-methoxyabiet-4(18),8,11,13-Tetraen-7-one	NHLQPIOUCQBSFL-UHFFFAOYSA-N	Organic compounds	Lipids and lipid-like molecules	Prenol lipids	Diterpenoids	Diterpenoids
9612	Kusunol	MQWIFDHBNGIVPO-UHFFFAOYSA-N	Organic compounds	Lipids and lipid-like molecules	Prenol lipids	Sesquiterpenoids	Eremophilane, 8,9-secoeremophilane and furoeremophilane sesquiterpenoids
1847	(-)-alpha-Copaene	VLXDPFLIRFYIME-UHFFFAOYSA-N	Organic compounds	Lipids and lipid-like molecules	Prenol lipids	Sesquiterpenoids	Sesquiterpenoids
10638	Stigmasta-4,6-dien-3-one	KEAZWUZFBXOMV-UHFFFAOYSA-N	Organic compounds	Lipids and lipid-like molecules	Steroids and steroid derivatives	Stigmastanes and derivatives	Stigmastanes and derivatives
2253	epsilon-Muurolene	NOLWRMQDWRAODO-UHFFFAOYSA-N	Organic compounds	Lipids and lipid-like molecules	Prenol lipids	Sesquiterpenoids	Sesquiterpenoids
2001	Stigmastan-3-one (5-alpha)	BVVFRHKBULZQCQ-UHFFFAOYSA-N	Organic compounds	Lipids and lipid-like molecules	Steroids and steroid derivatives	Stigmastanes and derivatives	Stigmastanes and derivatives
11158	Dehydroabietinal	YCLCHPWGSDZKL-UHFFFAOYSA-N	Organic compounds	Lipids and lipid-like molecules	Prenol lipids	Diterpenoids	Diterpenoids
9654	(-)-Ylangene	VLXDPFLIRFYIME-UHFFFAOYSA-N	Organic compounds	Lipids and lipid-like molecules	Prenol lipids	Sesquiterpenoids	Sesquiterpenoids

Table S11. List of chemicals which are co-targeted on S5R2 and AR.

Chemical ID	Chemical Name	inchikey	Chemical Class				
			Kingdom	Superclass	Class	Subclass	Direct_parent
12777	Zerumbone	GIHNTRQPEMKFO-SKTNYSRSSA-N	Organic compounds	Lipids and lipid-like molecules	Prenol lipids	Sesquiterpenoids	Sesquiterpenoids
9612	Kusunol	MQWIFDHBNGIVPO-UHFFFAOYSA-N	Organic compounds	Lipids and lipid-like molecules	Prenol lipids	Sesquiterpenoids	Eremophilane, 8,9-secoeremophilane and furoeremophilane sesquiterpenoids
1847	(-)-alpha-Copaene	VLXDPFLIRFYIME-UHFFFAOYSA-N	Organic compounds	Lipids and lipid-like molecules	Prenol lipids	Sesquiterpenoids	Sesquiterpenoids
10638	Stigmasta-4,6-dien-3-one	KEAZWUZFBXOMV-UHFFFAOYSA-N	Organic compounds	Lipids and lipid-like molecules	Steroids and steroid derivatives	Stigmastanes and derivatives	Stigmastanes and derivatives
2001	Stigmastan-3-one (5-alpha)	BVVFRHKBULZQCQ-UHFFFAOYSA-N	Organic compounds	Lipids and lipid-like molecules	Steroids and steroid derivatives	Stigmastanes and derivatives	Stigmastanes and derivatives
11158	Dehydroabietinal	YCLCHPWGRSDZKL-UHFFFAOYSA-N	Organic compounds	Lipids and lipid-like molecules	Prenol lipids	Diterpenoids	Diterpenoids
9654	(-)-Ylangene	VLXDPFLIRFYIME-UHFFFAOYSA-N	Organic compounds	Lipids and lipid-like molecules	Prenol lipids	Sesquiterpenoids	Sesquiterpenoids