

Biological Activity Estimation

Results of *Tanacetum parthenium*

Feverfew compounds:(Hordiei K, Gontova T, Trumbeckaite S, Yaremenko M, Raudone L. Phenolic Composition and Antioxidant Activity of *Tanacetum parthenium* Cultivated in Different Regions of Ukraine: Insights into the Flavonoids and Hydroxycinnamic Acids Profile. Plants (Basel). 2023 Aug 14;12(16):2940. doi: 10.3390/plants12162940. PMID: 37631152; PMCID: PMC10458129.)

Parthenolide

C/C/1=C\CC[C@@]2([C@H](O2)[C@@H]3[C@@H](CC1)C(=C)C(=O)O3)C

Artecenin

C[C@]1(CC[C@@H]2[C@@H]([C@@H]3[C@]14[C@H](O4)[C@H]5[C@@]3(O5)C)OC(=O)C2=C)O

Germacranolide

C/C/1=C\CC/C(=C/[C@@H]2[C@@H](CC1)C(=C)C(=O)O2)/C

chlorogenic acid

C1[C@H]([C@H]([C@@H](C[C@@]1(C(=O)O)O)OC(=O)/C=C/C2=CC(=C(C(=C2)O)O)O)O

dicafeoylquinic acids

C1[C@H]([C@H]([C@@H](C[C@@]1(C(=O)O)O)OC(=O)/C=C/C2=CC(=C(C(=C2)O)O)OC(=O)/C=C/C3=CC(=C(C(=C3)O)O)O

chicoric acid

C1=CC(=C(C(=C1/C=C/C(=O)O[C@@H](C(=O)O)[C@@H](OC(=O)/C=C/C2=CC(=C(C(=C2)O)O)C(=O)O)O)O

6-hydroxykaempferol-3,6-dimethyl ether

COC1=C(C2=C(C=C1O)OC(=C(C2=O)O)C3=CC=C(C(=C3)O)OC

6-hydroxykaempferol-3,7,4'-trimethyl ether (tanetin)

COC1CCC(CC1)C1OC2CC(OC)C(O)C(O)C2C(=O)C1OC

quercetagenin-3,6-dimethyl ether COC1=C(C2=C(C(=C1O)OC(=C(C2=O)OC)C3=CC(=C(C(=C3)O)O)O

quercetagenin-3,6,3'-trimethyl ether

COC1=C(C(=C(C(=C1)C2=C(C(=O)C3=C(O2)C=C(C(=C3O)OC)O)O)OC

Quercetin

C1=CC(=C(C=C1C2=C(C(=O)C3=C(C=C(C=C3O2)O)O)O)O)O

Apigenin

C1=CC(=CC=C1C2=CC(=O)C3=C(C=C(C=C3O2)O)O)O

apigenin-7-glucuronide

C1=CC(=CC=C1C2=CC(=O)C3=C(C=C(C=C3O2)O[C@H]4[C@@H]([C@H]([C@@H]([C@H](O4)C(=O)O)O)O)O)O)O

luteolin

C1=CC(=C(C=C1C2=CC(=O)C3=C(C=C(C=C3O2)O)O)O)O

luteolin-7-glucuronide

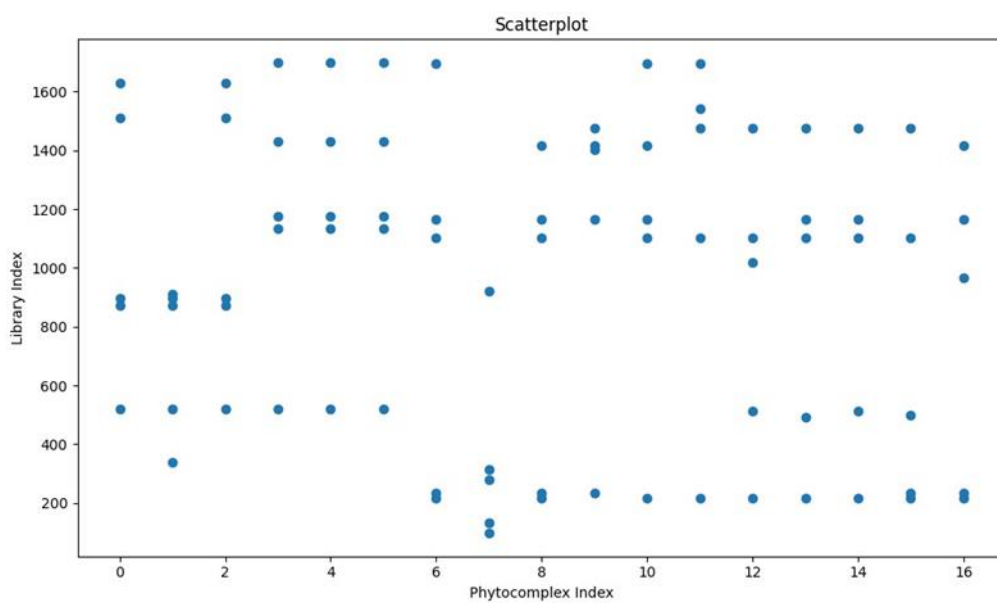
C1=CC(=C(C=C1C2=CC(=O)C3=C(C=C(C=C3O2)O[C@H]4[C@@H]([C@H]([C@@H]([C@H](O4)C(=O)O)O)O)O)O)O

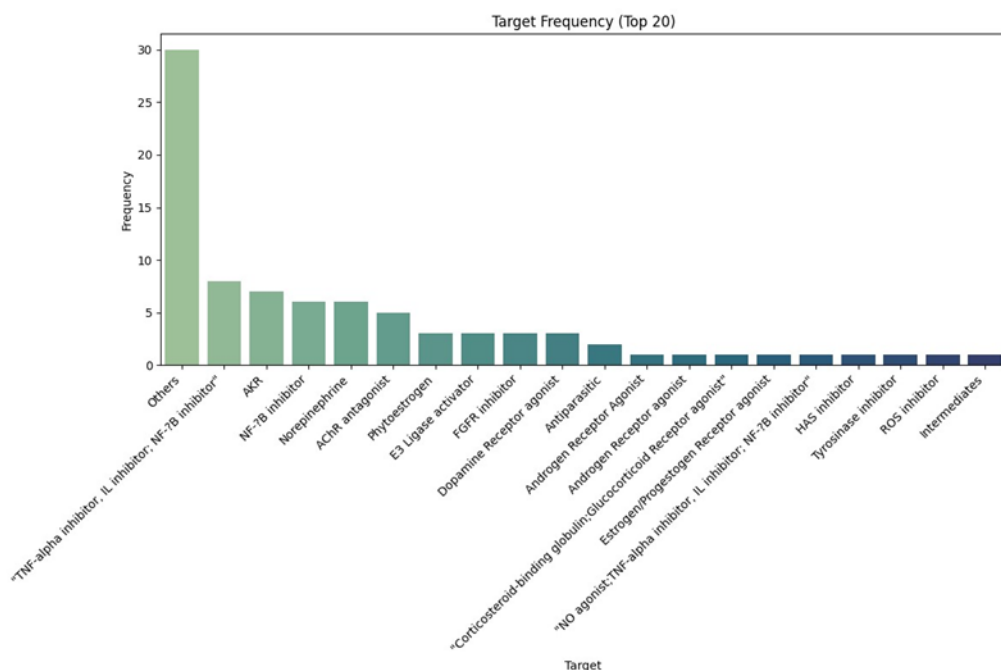
Chrysoeriol

COC1=C(C=CC(=C1)C2=CC(=O)C3=C(C=C(C=C3O2)O)O)O

Santin

COC1=CC=C(C=C1)C2=C(C(=O)C3=C(O2)C=C(C(=C3O)OC)O)OC





Analysis of TestBio Results vs. Traditional Use of Feverfew, by Gemini:

The image provided shows a bar graph representing the frequency of protein targets associated with compounds in Feverfew, compared to the TestBio library. Here are some key points:

- **"Others":**

This category is dominant, indicating the presence of compounds in feverfew that do not correspond to specific protein targets in the library.

An example is chlorogenic acid, a polyphenol with various biological activities (antioxidant, anti-inflammatory), but without a single, defined protein target.

This highlights the complexity of phytocomplexes, where many compounds act through multiple or unconventional mechanisms.

- **"TNF-alpha inhibitor, IL inhibitor; NF-7B inhibitor":**

This target suggests that feverfew may have strong anti-inflammatory properties.

Inhibition of TNF-alpha and IL (interleukin) is crucial in the treatment of chronic inflammatory diseases.

This supports the traditional use of feverfew for migraine and pain.

- **AKR (Aldo-Keto Reductase):**

AKRs are enzymes involved in the metabolism of various compounds, including toxins and drugs.

Interaction with AKRs may indicate that feverfew has detoxifying properties or may affect the metabolism of other compounds.

Some AKRs have been linked to chronic diseases such as diabetes and cardiovascular disease.

- **NF-κB** is a key transcription factor in the inflammatory and immune response.

Inhibition of NF-κB further enhances the anti-inflammatory properties of feverfew.

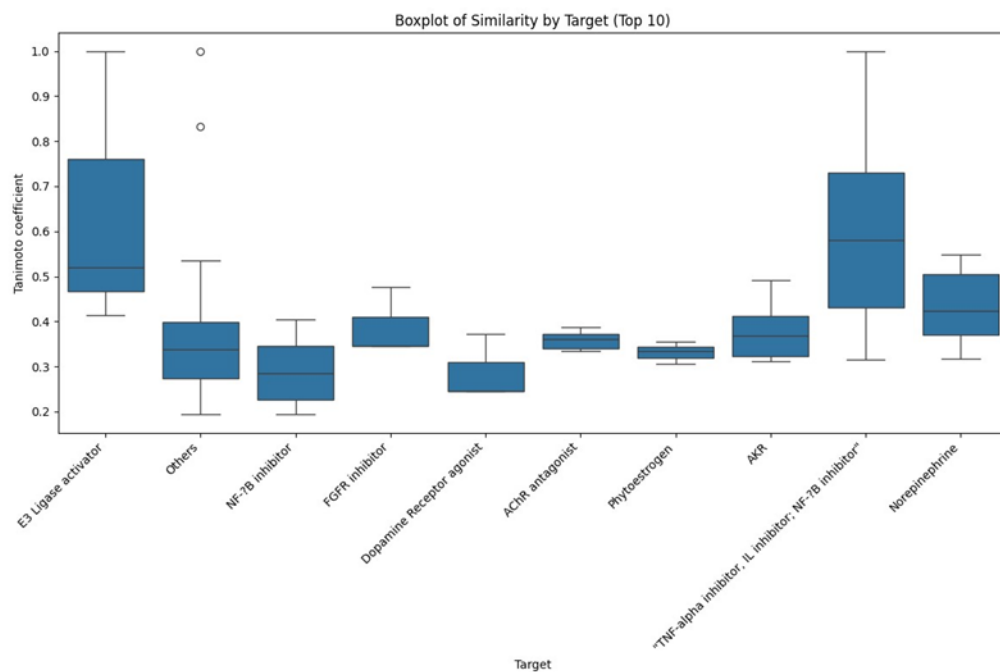
This target is relevant to feverfew's applications in inflammatory and autoimmune diseases.

- **Norepinephrine:**

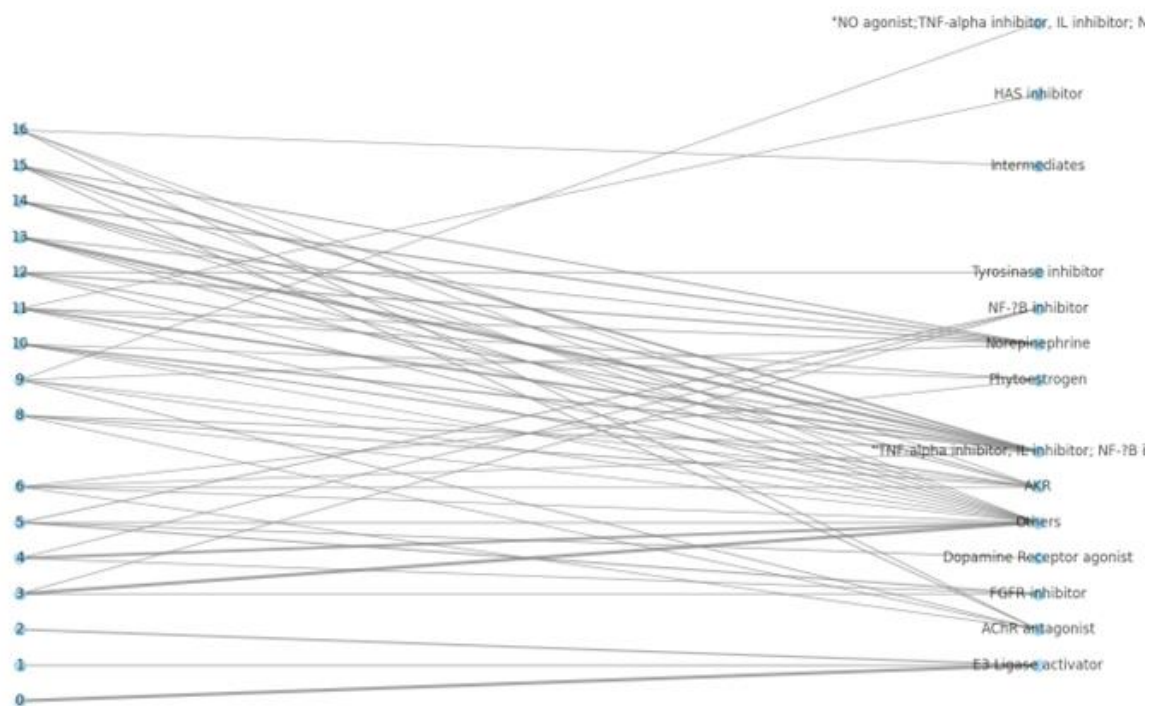
Norepinephrine is a neurotransmitter involved in the stress response and mood regulation.

Interaction with this target suggests that feverfew may have effects on the central nervous system.

This may explain some of the traditional uses of feverfew to relieve anxiety and improve mood.



Network Graph:



Comparison Results (Tanimoto coefficient):

Query Index	Library Index	Tanimoto Similarity	Target	Bioactivity
0	897	1.000	E3 Ligase activator	(-)-Parthenolide is a sesquiterpene lactone which occurs naturally in the plant feverfew(<i>Tanacetum parthenium</i>) and also promotes the ubiquitination of MDM2 and activates p53 cellular functions.
0	873	0.254	Others	Artemisinin is a drug used to treat multi-drug resistant strains of <i>falciparum</i> malaria (as well as increasingly <i>vivax</i> malaria). The compound is isolated from the plant <i>Artemisia annua</i> , a herb described in Chinese traditional medicine, though
0	1512	0.250	Others	Limonene is a colourless liquid hydrocarbon classified as a cyclic terpene. The more common d-isomer possesses a strong smell of oranges. It is used in chemical synthesis as a precursor to carvone and as a renewables-based solvent in clean
0	1630	0.231	Others	Nandrolone (19-nortestosterone) is an anabolic steroid that may be present naturally in the human body, albeit in minute quantities of less than 0.4 ng/ml.
0	521	0.227	NF- κ B inhibitor	Inhibitor of NF- κ B signaling; also attenuates concanavaline-induced IFN γ production in murine T cells (IC ₅₀ = 1.7 μ M). Blocks androgen receptor (AR) expression in AR-expressing C4-2 cells. Activates Nrf2 in BEAS-2B cells in response to ciga
1	897	0.414	E3 Ligase activator	(-)-Parthenolide is a sesquiterpene lactone which occurs naturally in the plant feverfew(<i>Tanacetum parthenium</i>) and also

Query Index	Library Index	Tanimoto Similarity	Target	Bioactivity
				promotes the ubiquitination of MDM2 and activates p53 cellular functions.
1	340	0.250	Androgen Receptor Agonist	Oxandrolone(SC11585) is a synthetic hormone with anabolic and androgenic properties.
1	912	0.234	Androgen Receptor agonist	17?-Methyltestosterone has similar binding affinity to AR and similar androgenic and anabolic activities as testosterone.
1	521	0.227	NF-?B inhibitor	Inhibitor of NF-?B signaling; also attenuates concanavline-induced IFN? production in murine T cells (IC50 = 1.7 ?M). Blocks androgen receptor (AR) expression in AR-expressing C4-2 cells. Activates Nrf2 in BEAS-2B cells in response to ciga
1	873	0.215	Others	Artemisinin is a drug used to treat multi-drug resistant strains of falciparum malaria (as well as increasingly vivax malaria). The compound is isolated from the plant Artemisia annua, a herb described in Chinese traditional medicine, though
2	897	0.520	E3 Ligase activator	(-)-Parthenolide is a sesquiterpene lactone which occurs naturally in the plant feverfew(Tanacetum parthenium) and also promotes the ubiquitination of MDM2 and activates p53 cellular functions.
2	1512	0.283	Others	Limonene is a colourless liquid hydrocarbon classified as a cyclic terpene. The more common d-isomer possesses a strong smell of oranges. It is used in chemical synthesis as a precursor to

Query Index	Library Index	Tanimoto Similarity	Target
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Bioactivity

carvone and as a renewables-based solvent in clean

2	1630	0.213	Others
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Nandrolone (19-nortestosterone) is an anabolic steroid that may be present naturally in the human body, albeit in minute quantities of less than 0.4 ng/ml.

2	873	0.197	Others
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Artemisinin is a drug used to treat multi-drug resistant strains of falciparum malaria (as well as increasingly vivax malaria). The compound is isolated from the plant *Artemisia annua*, a herb described in Chinese traditional medicine, though

2	521	0.194	NF- κ B inhibitor
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Inhibitor of NF- κ B signaling; also attenuates concanavaline-induced IFN γ production in murine T cells (IC₅₀ = 1.7 μ M). Blocks androgen receptor (AR) expression in AR-expressing C4-2 cells. Activates Nrf2 in BEAS-2B cells in response to ciga

3	520	1.000	Others
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Extracted from *Lonicera acuminata* Wall.; Suitability: Ethanol and acetone; Store the product in sealed, cool and dry condition

3	1698	0.345	FGFR inhibitor
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Ferulic Acid is a hydroxycinnamic acid and a type of organic compound found in the *Ferula assafoetida* L. or *Ligusticum chuanxiong*.

3	1432	0.345	NF- κ B inhibitor
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A yellow-orange dye obtained from tumeric, the powdered root of *CURCUMA longa*. It is used in the preparation of curcuma paper and the detection of boron. Curcumin appears to possess a

Query Index	Library Index	Tanimoto Similarity	Target	Bioactivity
				spectrum of pharmacological properties, due primarily to
3	1134	0.275	Others	: Actions Hydroxycinnamic acid found in many fruits and vegetables. Other Notes :Predominantly trans isomer. Packaging: 1,5,10,25 g in poly bottle
3	1175	0.246	Dopamine Receptor agonist	The naturally occurring form of DIHYDROXYPHENYLALANINE and the immediate precursor of DOPAMINE. Unlike dopamine itself, it can be taken orally and crosses the blood-brain barrier. It is rapidly taken up by dopaminergic neurons and converted
4	520	0.833	Others	Extracted from Lonicera acuminata.Wall.;Suitability:Ethanol and acetone;Store the product in sealed,cool and dry condition
4	1698	0.345	FGFR inhibitor	Ferulic Acid is a hydroxycinnamic acid and a type of organic compound found in the Ferula assafoetida L. or Ligusticum chuanxiong.
4	1432	0.345	NF- κ B inhibitor	A yellow-orange dye obtained from tumeric, the powdered root of CURCUMA longa. It is used in the preparation of curcuma paper and the detection of boron. Curcumin appears to possess a spectrum of pharmacological properties, due primarily to
4	1134	0.275	Others	: Actions Hydroxycinnamic acid found in many fruits and vegetables. Other Notes :Predominantly trans isomer. Packaging: 1,5,10,25 g in poly bottle
4	1175	0.246	Dopamine Receptor agonist	The naturally occurring form of DIHYDROXYPHENYLALANINE and the

Query Index	Library Index	Tanimoto Similarity	Target	Bioactivity
				immediate precursor of DOPAMINE. Unlike dopamine itself, it can be taken orally and crosses the blood-brain barrier. It is rapidly taken up by dopaminergic neurons and converted Ferulic Acid is a hydroxycinnamic acid and a type of organic compound found in the <i>Ferula assafoetida</i> L. or <i>Ligusticum chuanxiong</i>. Extracted from <i>Lonicera acuminata</i>. Wall.; Suitability: Ethanol and acetone; Store the product in sealed, cool and dry condition A yellow-orange dye obtained from tumeric, the powdered root of <i>CURCUMA longa</i>. It is used in the preparation of curcuma paper and the detection of boron. Curcumin appears to possess a spectrum of pharmacological properties, due primarily to : Actions Hydroxycinnamic acid found in many fruits and vegetables. Other Notes : Predominantly trans isomer. Packaging: 1,5,10,25 g in poly bottle The naturally occurring form of DIHYDROXYPHENYLALANINE and the immediate precursor of DOPAMINE. Unlike dopamine itself, it can be taken orally and crosses the blood-brain barrier. It is rapidly taken up by dopaminergic neurons and converted Plant growth factor derived from the root of <i>Scopolia carniolica</i> or <i>Scopolia japonica</i>.
5	1698	0.476	FGFR inhibitor	
5	520	0.462	Others	
5	1432	0.404	NF- κ B inhibitor	
5	1134	0.395	Others	
5	1175	0.372	Dopamine Receptor agonist	
6	234	0.340	AChR antagonist	

Query Index	Library Index	Tanimoto Similarity	Target	Bioactivity
6	1697	0.333	Phytoestrogen	Daidzein is a natural isoflavone phytoestrogen found in Leguminosae, used as a component of foods and dietary supplements.
6	1166	0.324	AKR	Rutin, a flavonol glycoside found in many plants including buckwheat; tobacco; forsythia; hydrangea; viola, etc., which possesses healthy effects for human.
6	218	0.324	Others	Extracted from CLUSIACEAE fruit;Suitability:Ethanol,methanol,acetone and pyridine;Store the product in sealed,cool and dry condition
6	1102	0.315	"TNF-alpha inhibitor, IL inhibitor; NF-?B inhibitor"	Luteolin is a flavone, a type of flavonoid. Like all flavonoids, it has a yellow crystalline appearance.
7	922	0.222	Antiparasitic	Doramectin is an antiparasitic agent.
7	278	0.205	"Corticosteroid-binding globulin;Glucocorticoid Receptor agonist"	Medrysone is a corticosteroid used in ophthalmology.
7	134	0.203	Estrogen/Progestogen Receptor agonist	A synthetic progestin that is derived from 17-hydroxyprogesterone. It is a long-acting contraceptive that is effective both orally or by intramuscular injection and has also been used to treat breast and endometrial neoplasms.
7	99	0.202	Antiparasitic	Selamectin is a topical parasiticide and antihelminthic used on dogs and cats, distributed by Zoetis. Selamectin disables parasites by activating glutamate-gated chloride channels at muscle synapses.
7	313	0.193	Others	A cardiac glycoside sometimes used in place of DIGOXIN. It has a longer half-life than digoxin; toxic effects, which are similar to those of digoxin, are longer

Query Index	Library Index	Tanimoto Similarity	Target	Bioactivity
				lasting. (From Martindale, The Extra Pharmacopoeia, 30th ed, p665
8	218	0.444	Others	Extracted from CLUSIACEAE fruit;Suitability:Ethanol,methanol,acetone and pyridine;Store the product in sealed,cool and dry condition
8	1166	0.414	AKR	Rutin, a flavonol glycoside found in many plants including buckwheat; tobacco; forsythia; hydrangea; viola, etc., which possesses healthy effects for human.
8	1102	0.385	"TNF-alpha inhibitor, IL inhibitor; NF-?B inhibitor"	Luteolin is a flavone, a type of flavonoid. Like all flavonoids, it has a yellow crystalline appearance.
8	234	0.333	AChR antagonist	Plant growth factor derived from the root of Scopolia carniolica or Scopolia japonica.
8	1415	0.313	Others	Troloxerutin, a natural bioflavonoid isolated from Sophora japonica., has been reported to have many benefits and medicinal properties.
9	234	0.373	AChR antagonist	Plant growth factor derived from the root of Scopolia carniolica or Scopolia japonica.
9	1415	0.338	Others	Troloxerutin, a natural bioflavonoid isolated from Sophora japonica., has been reported to have many benefits and medicinal properties.
9	1401	0.317	"NO agonist;TNF-alpha inhibitor, IL inhibitor; NF-?B inhibitor"	Bergenin monohydrate is an isocoumarin isolated from various medicinal plants. Shows mild anti-HIV activity,antihepatotoxic activity and antiulcer activity.

Query Index	Library Index	Tanimoto Similarity	Target	Bioactivity
9	1476	0.316	Norepinephrine	Diosmin is a semisynthetic phlebotropic agent and a member of the flavonoid family. Extracted from hesperidin;Store the product in sealed, cool and dry condition
9	1166	0.312	AKR	Rutin, a flavonol glycoside found in many plants including buckwheat; tobacco; forsythia; hydrangea; viola, etc., which possesses healthy effects for human.
10	1102	0.595	"TNF-alpha inhibitor, IL inhibitor; NF-?B inhibitor"	Luteolin is a flavone, a type of flavonoid. Like all flavonoids, it has a yellow crystalline appearance.
10	218	0.536	Others	Extracted from CLUSIACEAE fruit;Suitability:Ethanol, methanol, acetone and pyridine;Store the product in sealed, cool and dry condition
10	1166	0.492	AKR	Rutin, a flavonol glycoside found in many plants including buckwheat; tobacco; forsythia; hydrangea; viola, etc., which possesses healthy effects for human.
10	1415	0.316	Others	Troxeutin, a natural bioflavonoid isolated from Sophora japonica., has been reported to have many benefits and medicinal properties.
10	1697	0.306	Phytoestrogen	Daidzein is a natural isoflavone phytoestrogen found in Leguminosae, used as a component of foods and dietary supplements.
11	1102	0.778	"TNF-alpha inhibitor, IL inhibitor; NF-?B inhibitor"	Luteolin is a flavone, a type of flavonoid. Like all flavonoids, it has a yellow crystalline appearance.
11	1476	0.362	Norepinephrine	Diosmin is a semisynthetic phlebotropic agent and a member of the flavonoid family. Extracted from hesperidin;Store

Query Index	Library Index	Tanimoto Similarity	Target	Bioactivity
				the product in sealed, cool and dry condition
11	1697	0.356	Phytoestrogen	Daidzein is a natural isoflavone phytoestrogen found in Leguminosae, used as a component of foods and dietary supplements.
11	218	0.339	Others	Extracted from CLUSIACEAE fruit;Suitability:Ethanol,methanol,acetone and pyridine;Store the product in sealed,cool and dry condition
11	1543	0.318	HAS inhibitor	A coumarin derivative possessing properties as a spasmolytic, choleric and light-protective agent. It is also used in ANALYTICAL CHEMISTRY TECHNIQUES for the determination of NITRIC ACID.
12	1476	0.521	Norepinephrine	Diosmin is a semisynthetic phlebotropic agent and a member of the flavonoid family. Extracted from hesperidin;Store the product in sealed, cool and dry condition
12	1102	0.446	"TNF-alpha inhibitor, IL inhibitor; NF-?B inhibitor"	Luteolin is a flavone, a type of flavonoid. Like all flavonoids, it has a yellow crystalline appearance.
12	515	0.400	Others	Actions Daidzin is an isoflavone reported to have anti-oxidant,anti-carcinogenic,and anti-atherosclerotic activities. Daidzin is the major active component of the traditional Chinese medicine (TCM) derived from radix puerariae (Kudzu) that
12	218	0.389	Others	Extracted from CLUSIACEAE fruit;Suitability:Ethanol,methanol,acetone and pyridine;Store the product in sealed,cool and dry condition

Query Index	Library Index	Tanimoto Similarity	Target	Bioactivity
12	1019	0.362	Tyrosinase inhibitor	Arbutin is glucosylated hydroquinone, and may carry similar cancer risks, although there are also claims that arbutin reduces cancer risk. It prevents the formation of melanin.
13	1102	1.000	"TNF-alpha inhibitor, IL inhibitor; NF-?B inhibitor"	Luteolin is a flavone, a type of flavonoid. Like all flavonoids, it has a yellow crystalline appearance.
13	218	0.417	Others	Extracted from CLUSIACEAE fruit;Suitability:Ethanol,methanol,acetone and pyridine;Store the product in sealed,cool and dry condition
13	1476	0.391	Norepinephrine	Diosmin is a semisynthetic phlebotropic agent and a member of the flavonoid family. Extracted from hesperidin;Store the product in sealed, cool and dry condition
13	1166	0.368	AKR	Rutin, a flavonol glycoside found in many plants including buckwheat; tobacco; forsythia; hydrangea; viola, etc., which possesses healthy effects for human.
13	491	0.288	ROS inhibitor	Catechin is a flavan-3-ol, a type of natural phenol and antioxidant. It is a plant secondary metabolite. It belongs to the group of flavan-3-ols (or simply flavanols), part of the chemical family of flavonoids.
14	1102	0.566	"TNF-alpha inhibitor, IL inhibitor; NF-?B inhibitor"	Luteolin is a flavone, a type of flavonoid. Like all flavonoids, it has a yellow crystalline appearance.
14	1476	0.548	Norepinephrine	Diosmin is a semisynthetic phlebotropic agent and a member of the flavonoid family. Extracted from hesperidin;Store the product in sealed, cool and dry condition

Query Index	Library Index	Tanimoto Similarity	Target	Bioactivity
14	218	0.457	Others	Extracted from CLUSIACEAE fruit;Suitability:Ethanol, methanol, acetone and pyridine;Store the product in sealed, cool and dry condition
14	1166	0.410	AKR	Rutin, a flavonol glycoside found in many plants including buckwheat; tobacco; forsythia; hydrangea; viola, etc., which possesses healthy effects for human.
14	515	0.351	Others	Actions Daidzin is an isoflavone reported to have anti-oxidant, anti-carcinogenic, and anti-atherosclerotic activities. Daidzin is the major active component of the traditional Chinese medicine (TCM) derived from radix puerariae (Kudzu) that
15	1102	0.714	"TNF-alpha inhibitor, IL inhibitor; NF-?B inhibitor"	Luteolin is a flavone, a type of flavonoid. Like all flavonoids, it has a yellow crystalline appearance.
15	1476	0.457	Norepinephrine	Diosmin is a semisynthetic phlebotropic agent and a member of the flavonoid family. Extracted from hesperidin;Store the product in sealed, cool and dry condition
15	234	0.388	AChR antagonist	Plant growth factor derived from the root of Scopolia carniolica or Scopolia japonica.
15	498	0.346	Others	Etamivan (INN) or ethamivan (USAN), trade name Analepticon, is a respiratory stimulant drug related to nikethamide. It is no longer used in the United States.
15	218	0.338	Others	Extracted from CLUSIACEAE fruit;Suitability:Ethanol, methanol, acetone and pyridine;Store the product in sealed, cool and dry condition

Query Index	Library Index	Tanimoto Similarity	Target	Bioactivity
16	234	0.360	AChR antagonist	Plant growth factor derived from the root of <i>Scopolia carniolica</i> or <i>Scopolia japonica</i> .
16	218	0.338	Others	Extracted from CLUSIACEAE fruit;Suitability:Ethanol, methanol, acetone and pyridine;Store the product in sealed, cool and dry condition
16	967	0.327	Intermediates	Used as pharmaceutical intermediates
16	1166	0.320	AKR	Rutin, a flavonol glycoside found in many plants including buckwheat; tobacco; forsythia; hydrangea; viola, etc., which possesses healthy effects for human.
16	1415	0.313	Others	Troxeutin, a natural bioflavonoid isolated from <i>Sophora japonica</i> ., has been reported to have many benefits and medicinal properties.