

Biological Activity Estimation Results of lamb's lettuce

lamb's lettuce compounds: (Hernández V, Botella MÁ, Hellín P, Cava J, Fenoll J, Mestre T, Martínez V, Flores P. Phenolic and Carotenoid Profile of Lamb's Lettuce and Improvement of the Bioactive Content by Preharvest Conditions. Foods. 2021 Jan 18;10(1):188. doi: 10.3390/foods10010188. PMID: 33477681; PMCID: PMC7831921.)

Chlorogenic

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

Coumaroylquinic acid

C1[C@H](C([C@@H](CC1(C(=O)O)O)O)OC(=O)/C=C/C2=CC(=C(C(=C2)O)O)O

dicafeoylquinic

C1[C@H]([C@H]([C@@H](C[C@@H]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

feruloylquinic acid

COC1=C(C=CC(=C1)/C=C/C(=O)OC2[C@@H](CC(C[C@H]2O)(C(=O)O)O)O

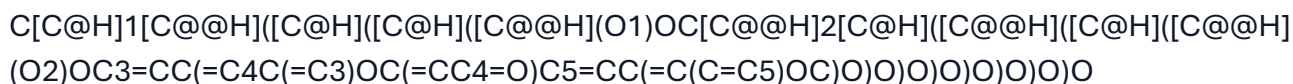
luteolin-7-rutinoside

C[C@H]1[C@@H]([C@H]([C@H]([C@@H](O1)OC[C@@H]2[C@H]([C@@H]([C@H]([C@@H](O2)OC3=CC(=C4C(=C3)OC(=CC4=O)C5=CC(=C(C(=C5)O)O)O)O)O)O)O)O

disomethine-apiosylglucoside

COC1=C(C=C(C(=C1)C2=CC(=O)C3=C(C=C(C(=C3O2)O)O)O[C@H]4[C@@H]([C@H]([C@@H]([C@H](O4)C(=O)O)O)O)O

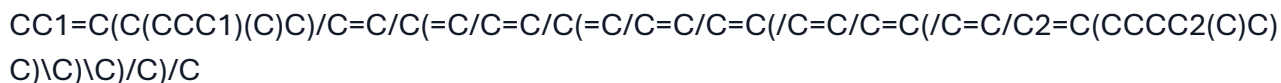
diosmin



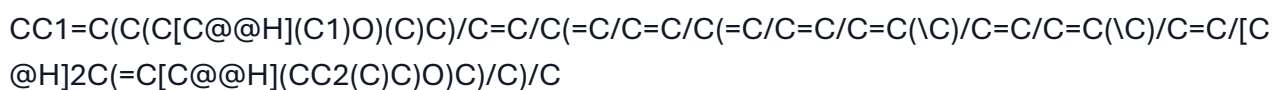
sinapic acid-hexosoide



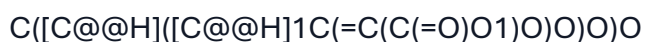
β -carotene



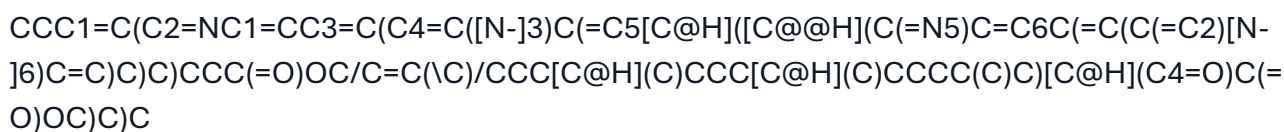
Lutein



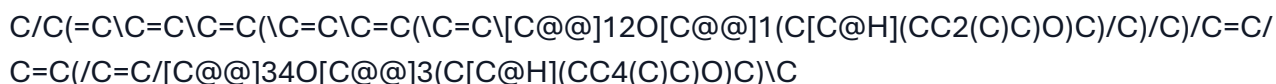
vitamin C



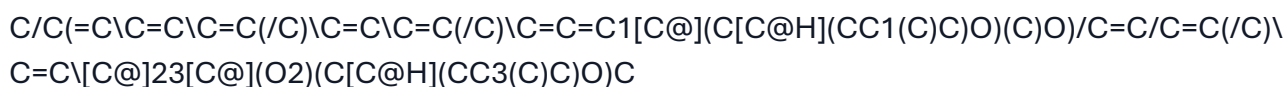
chlorophyll A



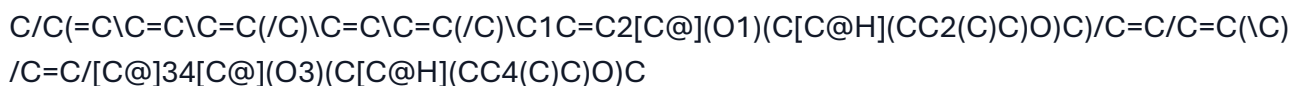
Violaxanthin



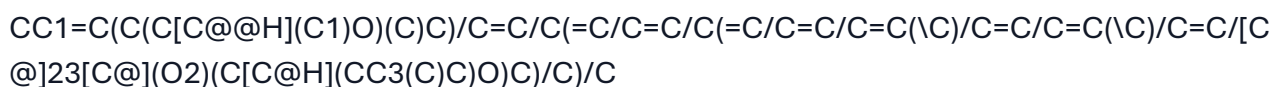
Neoxanthin



Luteoxanthin

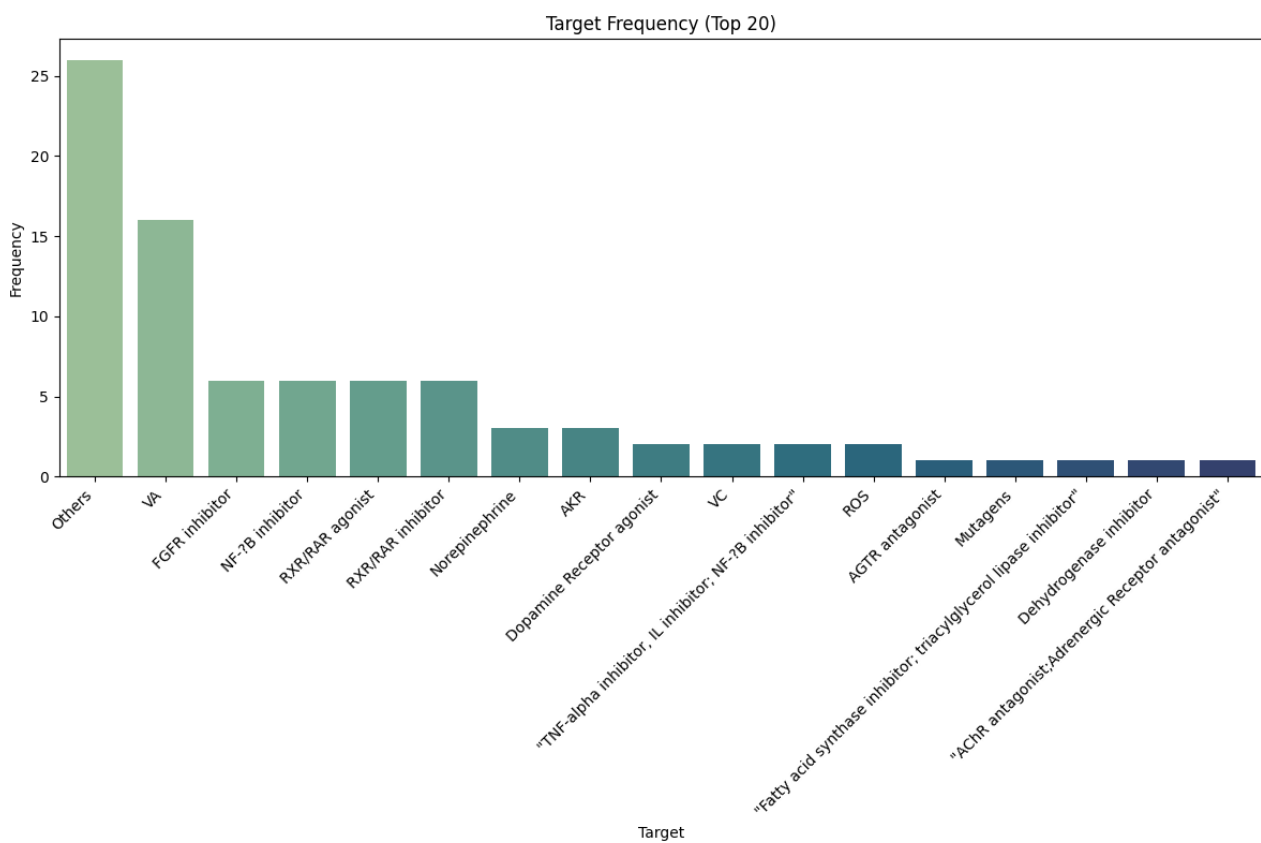
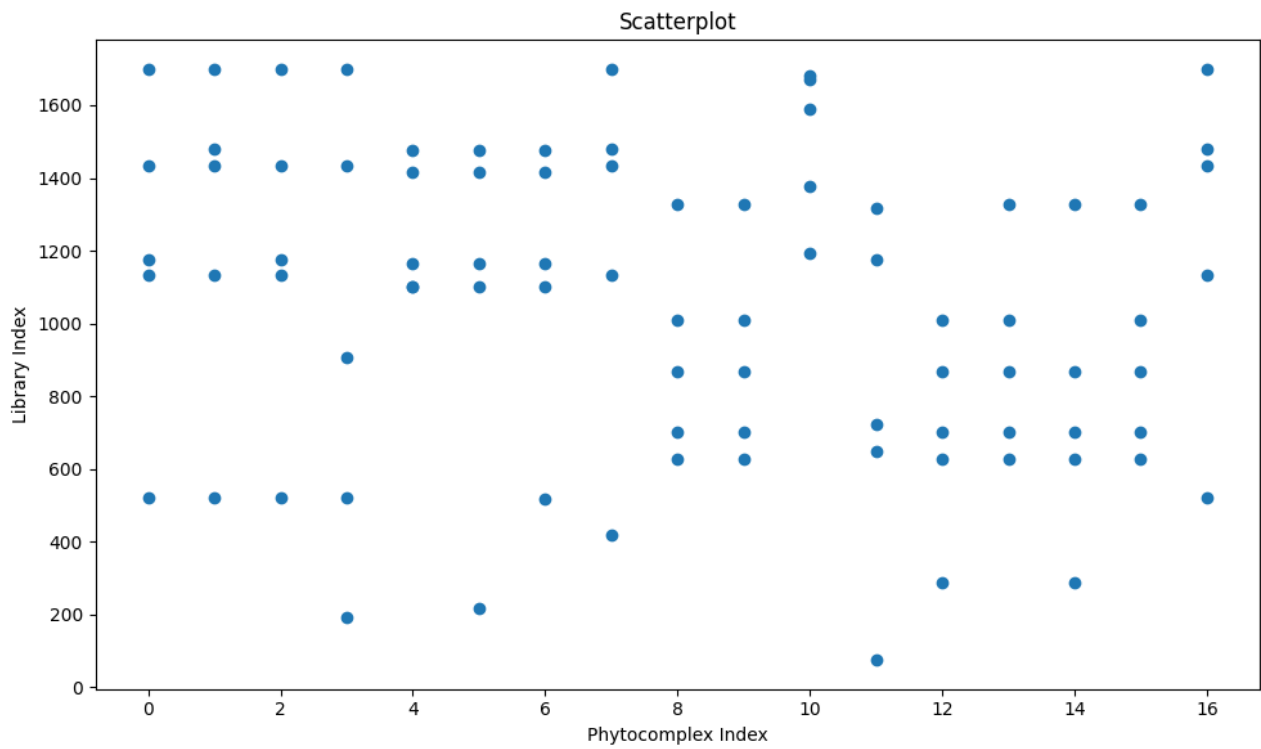


Anthraxanthin



Caffeic acid





Let's analyze with Gemini the TestBio results for Valerianella locusta and discuss the potential phytotherapeutic uses.

Analysis of Results:

"Others":

As for feverfew, this category is dominant, suggesting the presence of compounds with complex or not yet well defined mechanisms of action.

FGFR Inhibitor:

Fibroblast growth factor receptor (FGFR) inhibitors may have applications in oncology and inflammatory diseases.

This suggests a potential use of valerianella in inflammatory or proliferative conditions.

NF-κB is involved in inflammation.

This reinforces the idea of a potential anti-inflammatory use of valerianella.

Dopamine Receptor Agonist:

Dopamine receptor agonists may influence mood, motivation and motor function.

This suggests a potential use of valerianella in mood or neurological disorders.

Norepinephrine:

As you mentioned, norepinephrine increases arousal and alertness.

The high Tanimoto values and boxplot distribution suggest that valerianella may have stimulant effects.

This may support a potential use in narcolepsy or fatigue conditions.

AKR:

AKRs are involved in the metabolism of various compounds.

This suggests a potential detoxifying or metabolic modulating effect.

RXR/RAR Agonist:

RXR/RAR receptor agonists may affect cell differentiation and metabolism.

This suggests potential applications in dermatology or metabolic disorders.

RXR/RAR Inhibitor:

Inhibition of these receptors may have opposite effects to agonism.

Vitamin C:

VC may refer to various molecules or targets. Additional context is needed to interpret this result.

Potential Herbal Uses:

Narcolepsy and Fatigue:

Interaction with norepinephrine suggests potential use as a natural stimulant.

Mood Disorders:

Dopamine receptor agonism may indicate potential antidepressant or anxiolytic effects.

Inflammation:

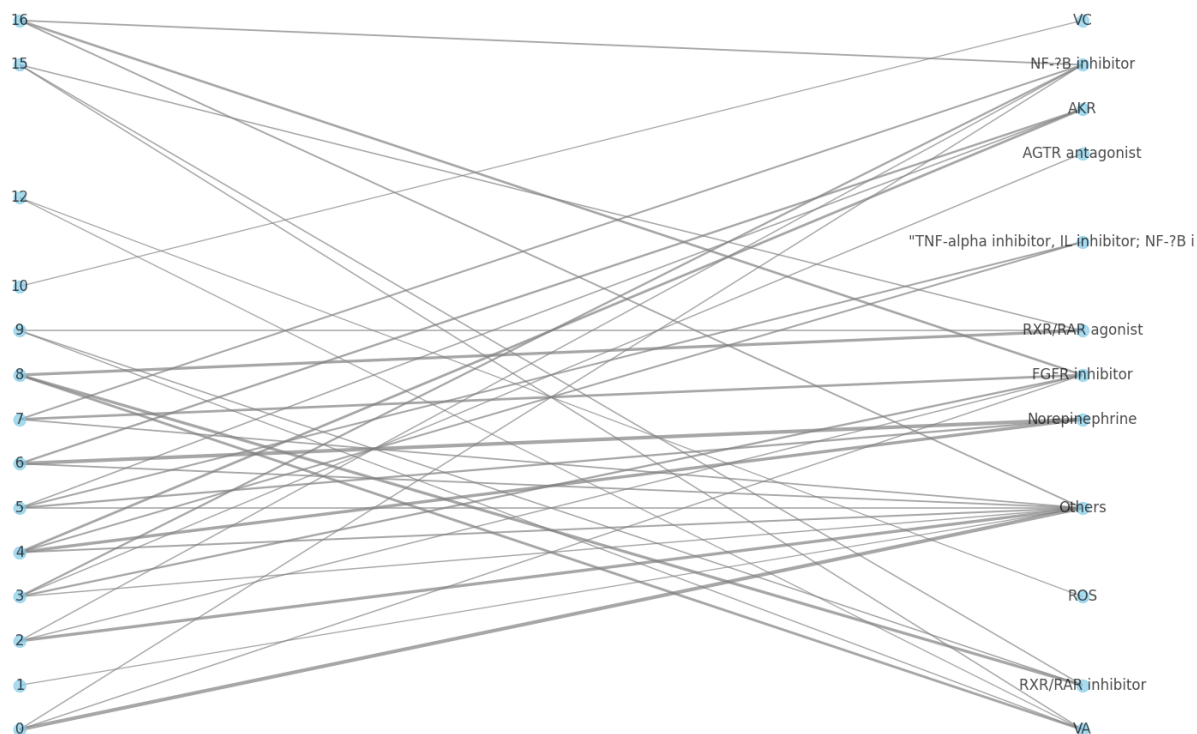
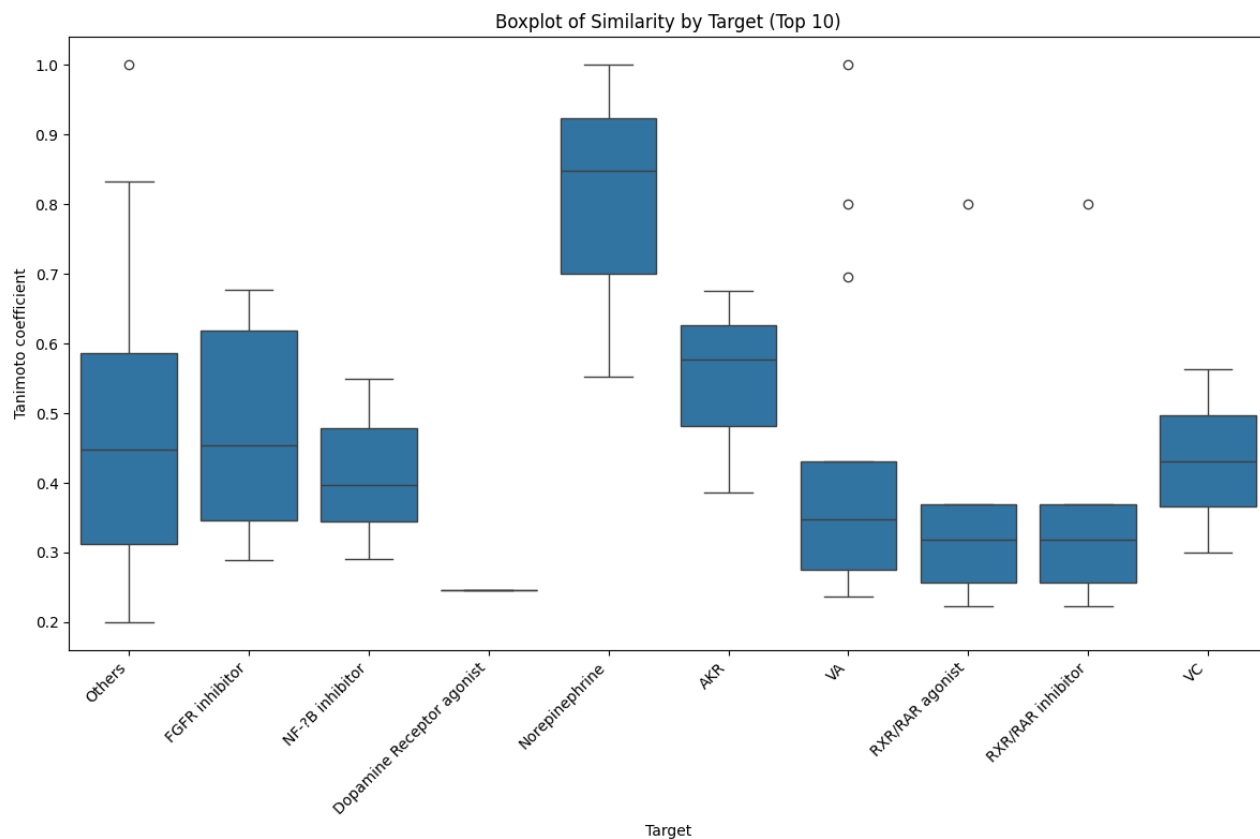
Inhibition of NF- κ B and FGFR suggests potential use in inflammatory conditions.

Skin Health:

Interaction with RXR/RAR may indicate potential applications in dermatology.

Disclaimer:

It is important to emphasize that these are only potential uses based on in silico analysis. Experimental and clinical studies are needed to confirm these findings and evaluate the safety and efficacy of valerianella for these uses.



Comparison Results (Tanimoto coefficient):

Query Index	Library Index	Tanimoto Similarity	Target	Bioactivity
0	520	1.000	Others	Extracted from <i>Lonicera acuminata</i> .Wall.;Suitability:Ethanol and acetone;Store the product in sealed,cool and dry condition
0	1698	0.345	FGFR inhibitor	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> .
0	1432	0.345	NF- κ B inhibitor	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
0	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
0	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
1	520	0.588	Others	Extracted from <i>Lonicera acuminata</i> .Wall.;Suitability:Ethanol and acetone;Store the product in sealed,cool and dry condition
1	1134	0.450	Others	: Actions Hydroxycinnamic acid found in many fruits and vegetables. Other Notes :Predominantly trans isomer. Packaging: 1,5,10,25 g in poly bottle
1	1480	0.302	Others	Cinnamic acid exerts anti-diabetic activity by improving glucose tolerance in vivo and by stimulating insulin secretion in vitro.
1	1432	0.291	NF- κ B inhibitor	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
1	1698	0.288	FGFR inhibitor	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> .

Query Index	Library Index	Tanimoto Similarity	Target	Bioactivity
2	520	0.833	Others	Extracted from <i>Lonicera acuminata</i> .Wall.;Suitability:Ethanol and acetone;Store the product in sealed,cool and dry condition
2	1698	0.345	FGFR inhibitor	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> .
2	1432	0.345	NF- κ B inhibitor	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
2	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
2	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
3	520	0.618	Others	Extracted from <i>Lonicera acuminata</i> .Wall.;Suitability:Ethanol and acetone;Store the product in sealed,cool and dry condition
3	1698	0.563	FGFR inhibitor	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> .
3	1432	0.549	NF- κ B inhibitor	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
3	193	0.344	AGTR antagonist	Trans-Tranilast is an antiallergic drug, used to treat bronchial asthma, allergic rhinitis and atopic dermatitis.
3	907	0.344	Others	Tranilast is an antiallergic drug by inhibiting lipid mediator and cytokine release from inflammatory cells, used for the treatment of allergic disorders such as asthma, allergic rhinitis and atopic dermatitis.

Quer y Index	Librar y Index	Tanimoto Similarit y	Target	Bioactivity
4	1476	0.848	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
4	1166	0.676	AKR	Rutin, a flavonol glycoside found in many plants including buckwheat; tobacco; forsythia; hydrangea; viola, etc., which possesses healthy effects for human.
4	1415	0.582	Others	Troxeutin, a natural bioflavonoid isolated from Sophora japonica., has been reported to have many benefits and medicinal properties.
4	1100	0.488	Others	Hesperidin is a flavanone glycoside found abundantly in citrus fruits.
4	1102	0.484	"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.
5	1476	0.553	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
5	1102	0.492	"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.
5	218	0.427	Others	Extracted from CLUSIACEAE fruit;Suitability:Ethanol, methanol, acetone and pyridine;Store the product in sealed, cool and dry condition
5	1415	0.391	Others	Troxeutin, a natural bioflavonoid isolated from Sophora japonica., has been reported to have many benefits and medicinal properties.
5	1166	0.386	AKR	Rutin, a flavonol glycoside found in many plants including buckwheat; tobacco; forsythia; hydrangea; viola, etc., which possesses healthy effects for human.
6	1476	1.000	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
6	1100	0.593	Others	Hesperidin is a flavanone glycoside found abundantly in citrus fruits.

Quer y Index	Librar y Index	Tanimoto Similarit y	Target	Bioactivity
6	1415	0.593	Others	Troloxerutin, a natural bioflavonoid isolated from <i>Sophora japonica</i> ., has been reported to have many benefits and medicinal properties.
6	1166	0.577	AKR	Rutin, a flavonol glycoside found in many plants including buckwheat; tobacco; forsythia; hydrangea; viola, etc., which possesses healthy effects for human.
6	517	0.451	Others	Flavanone glycoside with antioxidant and neuroprotective properties. Unlike other citrus flavanones, it does not inhibit oral carcinogenesis in a rat model.
7	1698	0.676	FGFR inhibitor	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> .
7	1432	0.488	NF- κ B inhibitor	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
7	1134	0.455	Others	: Actions Hydroxycinnamic acid found in many fruits and vegetables. Other Notes :Predominantly trans isomer. Packaging: 1,5,10,25 g in poly bottle
7	1480	0.438	Others	Cinnamic acid exerts anti-diabetic activity by improving glucose tolerance in vivo and by stimulating insulin secretion in vitro.
7	420	0.423	Others	Cinepazide maleate is a maleate salt form of cinepazide which is a vasodilator.
8	626	1.000	VA	Beta Carotene is an organic compound and classified as a terpenoid. It is a precursor (inactive form) of vitamin A.
8	703	0.800	RXR/RAR agonist	An important regulator of GENE EXPRESSION during growth and development, and in NEOPLASMS. Tretinoin, also known as retinoic acid and derived from maternal VITAMIN A, is essential for normal GROWTH; and EMBRYONIC DEVELOPMENT. An excess of t
8	868	0.800	RXR/RAR inhibitor	It was developed to be used as a chemotherapy medication for the treatment of brain cancer, pancreatic cancer and more.
8	1010	0.800	VA	Retinol and derivatives of retinol that play an essential role in metabolic functioning of the retina, the growth of and

Query Index	Library Index	Tanimoto Similarity	Target	Bioactivity
				differentiation of epithelial tissue, the growth of bone, reproduction, and the immune response. Dietary vitamin A is d
8	1329	0.696	VA	Vitamin A is a group of unsaturated nutritional hydrocarbons, that includes retinol, retinal, retinoic acid, and several provitamin A carotenoids, among which beta-carotene is the most important.
9	626	0.431	VA	Beta Carotene is an organic compound and classified as a terpenoid. It is a precursor (inactive form) of vitamin A.
9	703	0.369	RXR/RAR agonist	An important regulator of GENE EXPRESSION during growth and development, and in NEOPLASMS. Tretinoin, also known as retinoic acid and derived from maternal VITAMIN A, is essential for normal GROWTH; and EMBRYONIC DEVELOPMENT. An excess of t
9	868	0.369	RXR/RAR inhibitor	It was developed to be used as a chemotherapy medication for the treatment of brain cancer, pancreatic cancer and more.
9	1010	0.369	VA	Retinol and derivatives of retinol that play an essential role in metabolic functioning of the retina, the growth of and differentiation of epithelial tissue, the growth of bone, reproduction, and the immune response. Dietary vitamin A is d
9	1329	0.338	VA	Vitamin A is a group of unsaturated nutritional hydrocarbons, that includes retinol, retinal, retinoic acid, and several provitamin A carotenoids, among which beta-carotene is the most important.
10	1672	0.563	VC	Vitamin C is a water-soluble vitamin indicated for the prevention and treatment of scurvy.
10	1590	0.300	VC	Ascorbyl palmitate is an ester formed from ascorbic acid and palmitic acid creating a fat-soluble form of vitamin C.
10	1682	0.237	Others	Gluconolactone is a naturally-occurring food additive used as a sequestrant, an acidifier, or a curing, pickling, or leavening agent. It is a cyclic ester of D-gluconic acid. Pure gluconolactone is a white odorless crystalline powder.
10	1376	0.220	Others	Glucuronolactone is a naturally occurring chemical that is an important structural component of nearly all connective tissues. Glucuronolactone is also found in many plant gums.
10	1194	0.200	Others	A polyhydric alcohol with about half the sweetness of sucrose. Sorbitol occurs naturally and is also produced synthetically

Query Index	Library Index	Tanimoto Similarity	Target	Bioactivity
				from glucose. It was formerly used as a diuretic and may still be used as a laxative and in irrigating solutions for
11	1174	0.274	Others	A family of phyloquinones that contains a ring of 2-methyl-1,4-naphthoquinone and an isoprenoid side chain. Members of this group of vitamin K 1 have only one double bond on the proximal isoprene unit. Rich sources of vitamin K 1 include g
11	649	0.225	Mutagens	Chlorophyllin refers to any one of a group of closely related water-soluble salts that are semi-synthetic derivatives of chlorophyll, differing in the identity of the cations associated with the anion. Its most common form is a sodium/coppe
11	1316	0.198	"Fatty acid synthase inhibitor; triacylglycerol lipase inhibitor"	Orlistat is a drug designed to treat obesity. Its primary function is preventing the absorption of fats from the human diet, thereby reducing caloric intake. Orlistat works by inhibiting pancreatic lipase, an enzyme that breaks down triglyc
11	721	0.195	Dehydrogenase inhibitor	Mycophenolate mofetil is the 2-morpholinoethyl ester of mycophenolic acid (MPA), an immunosuppressive agent, inosine monophosphate dehydrogenase (IMPDH) inhibitor.
11	76	0.192	"AChR antagonist;Adrenergic Receptor antagonist"	Cisatracurium Besylate is a nondepolarizing skeletal muscle relaxant for intravenous administration. Cisatracurium Besylate acts on cholinergic receptors, blocking neuromuscular transmission. This action is antagonized by acetylcholinestera
12	626	0.308	VA	Beta Carotene is an organic compound and classified as a terpenoid. It is a precursor (inactive form) of vitamin A.
12	286	0.304	ROS	Extracted?from?Papaya fruit, marigold flower petals;Store?the?product?in?sealed,?cool?and?dry?condition
12	703	0.254	RXR/RAR agonist	An important regulator of GENE EXPRESSION during growth and development, and in NEOPLASMS. Tretinoin, also known as retinoic acid and derived from maternal VITAMIN A, is essential for normal GROWTH; and EMBRYONIC DEVELOPMENT. An excess of t
12	868	0.254	RXR/RAR inhibitor	It was developed to be used as a chemotherapy medication for the treatment of brain cancer, pancreatic cancer and more.
12	1010	0.254	VA	Retinol and derivatives of retinol that play an essential role in metabolic functioning of the retina, the growth of and differentiation of epithelial tissue, the growth of bone, reproduction, and the immune response. Dietary vitamin A is d

Query Index	Library Index	Tanimoto Similarity	Target	Bioactivity
13	626	0.292	VA	Beta Carotene is an organic compound and classified as a terpenoid. It is a precursor (inactive form) of vitamin A.
13	1329	0.280	VA	Vitamin A is a group of unsaturated nutritional hydrocarbons, that includes retinol, retinal, retinoic acid, and several provitamin A carotenoids, among which beta-carotene is the most important.
13	703	0.268	RXR/RAR agonist	An important regulator of GENE EXPRESSION during growth and development, and in NEOPLASMS. Tretinoin, also known as retinoic acid and derived from maternal VITAMIN A, is essential for normal GROWTH; and EMBRYONIC DEVELOPMENT. An excess of t
13	868	0.268	RXR/RAR inhibitor	It was developed to be used as a chemotherapy medication for the treatment of brain cancer, pancreatic cancer and more.
13	1010	0.250	VA	Retinol and derivatives of retinol that play an essential role in metabolic functioning of the retina, the growth of and differentiation of epithelial tissue, the growth of bone, reproduction, and the immune response. Dietary vitamin A is d
14	626	0.261	VA	Beta Carotene is an organic compound and classified as a terpenoid. It is a precursor (inactive form) of vitamin A.
14	1329	0.238	VA	Vitamin A is a group of unsaturated nutritional hydrocarbons, that includes retinol, retinal, retinoic acid, and several provitamin A carotenoids, among which beta-carotene is the most important.
14	286	0.234	ROS	Extracted?from?Papaya fruit, marigold flower petals;Store?the?product?in?sealed,?cool?and?dry?condition
14	703	0.224	RXR/RAR agonist	An important regulator of GENE EXPRESSION during growth and development, and in NEOPLASMS. Tretinoin, also known as retinoic acid and derived from maternal VITAMIN A, is essential for normal GROWTH; and EMBRYONIC DEVELOPMENT. An excess of t
14	868	0.224	RXR/RAR inhibitor	It was developed to be used as a chemotherapy medication for the treatment of brain cancer, pancreatic cancer and more.
15	626	0.431	VA	Beta Carotene is an organic compound and classified as a terpenoid. It is a precursor (inactive form) of vitamin A.
15	703	0.369	RXR/RAR agonist	An important regulator of GENE EXPRESSION during growth and development, and in NEOPLASMS. Tretinoin, also known

Query Index	Library Index	Tanimoto Similarity	Target	Bioactivity
				as retinoic acid and derived from maternal VITAMIN A, is essential for normal GROWTH; and EMBRYONIC DEVELOPMENT. An excess of t
15	868	0.369	RXR/RAR inhibitor	It was developed to be used as a chemotherapy medication for the treatment of brain cancer, pancreatic cancer and more.
15	1010	0.369	VA	Retinol and derivatives of retinol that play an essential role in metabolic functioning of the retina, the growth of and differentiation of epithelial tissue, the growth of bone, reproduction, and the immune response. Dietary vitamin A is d
15	1329	0.357	VA	Vitamin A is a group of unsaturated nutritional hydrocarbons, that includes retinol, retinal, retinoic acid, and several provitamin A carotenoids, among which beta-carotene is the most important.
16	1698	0.636	FGFR inhibitor	Ferulic Acid is a hydroxycinnamic acid and a type of organic compound found in the Ferula assafoetida L. or Ligusticum chuanxiong.
16	1134	0.607	Others	: Actions Hydroxycinnamic acid found in many fruits and vegetables. Other Notes :Predominantly trans isomer. Packaging: 1,5,10,25 g in poly bottle
16	1480	0.536	Others	Cinnamic acid exerts anti-diabetic activity by improving glucose tolerance in vivo and by stimulating insulin secretion in vitro.
16	1432	0.450	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
16	520	0.447	Others	Extracted from Lonicera acuminata.Wall.;Suitability:Ethanol and acetone;Store the product in sealed,cool and dry condition

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