

Biological activity estimation results

of valerian

Valerian compounds (from Capasso, Grandolini, Izzo **Fitoterapia**, Springer):

borneol,

CC1(C2CCC1(C(C2)O)C)C

actinidin,

C[C@H]1CCC2=C1C=NC=C2C

isovaleramide,

CC(C)CC(=O)N

GABA

C(CC(=O)O)CN

valeric acid

CCCCC(=O)O

isovaleric acid

CC(C)CC(=O)O

valerenic acid

C[C@@H]1CC[C@H](C2=C(CC[C@H]12)C)/C=C(\C)/C(=O)O

Valeranone

CC(C)[C@H]1CC[C@]2(CCCC(=O)[C@]2(C1)C)C

Hesperidin

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(=O)C[C@H](OC4=C3)C5=CC(=C(C=C5)OC)O)O)O)O)O)O)O

apigenin

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

protocatechuic acid

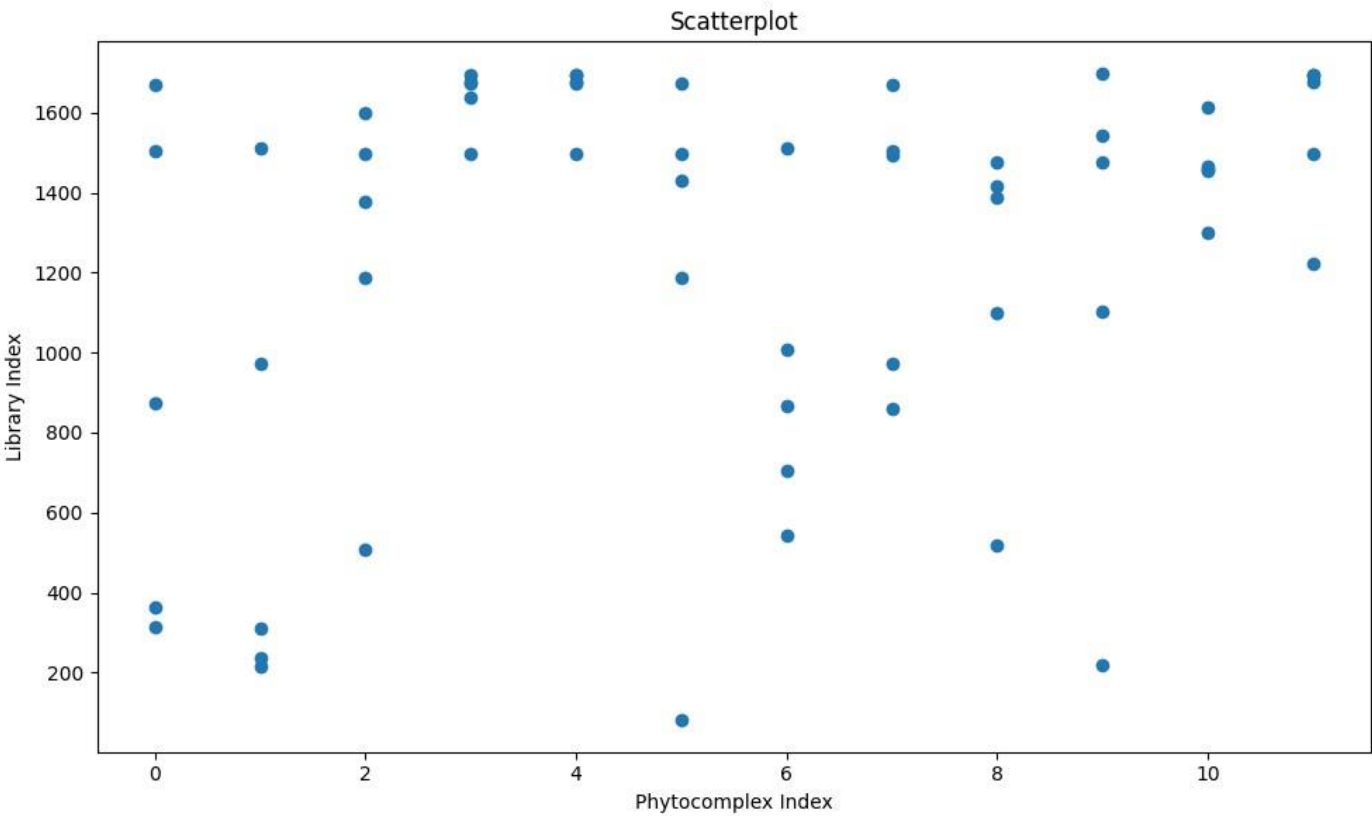
C1=CC(=C(C=C1C(=O)O)O)O

5-Acetylvaleric Acid

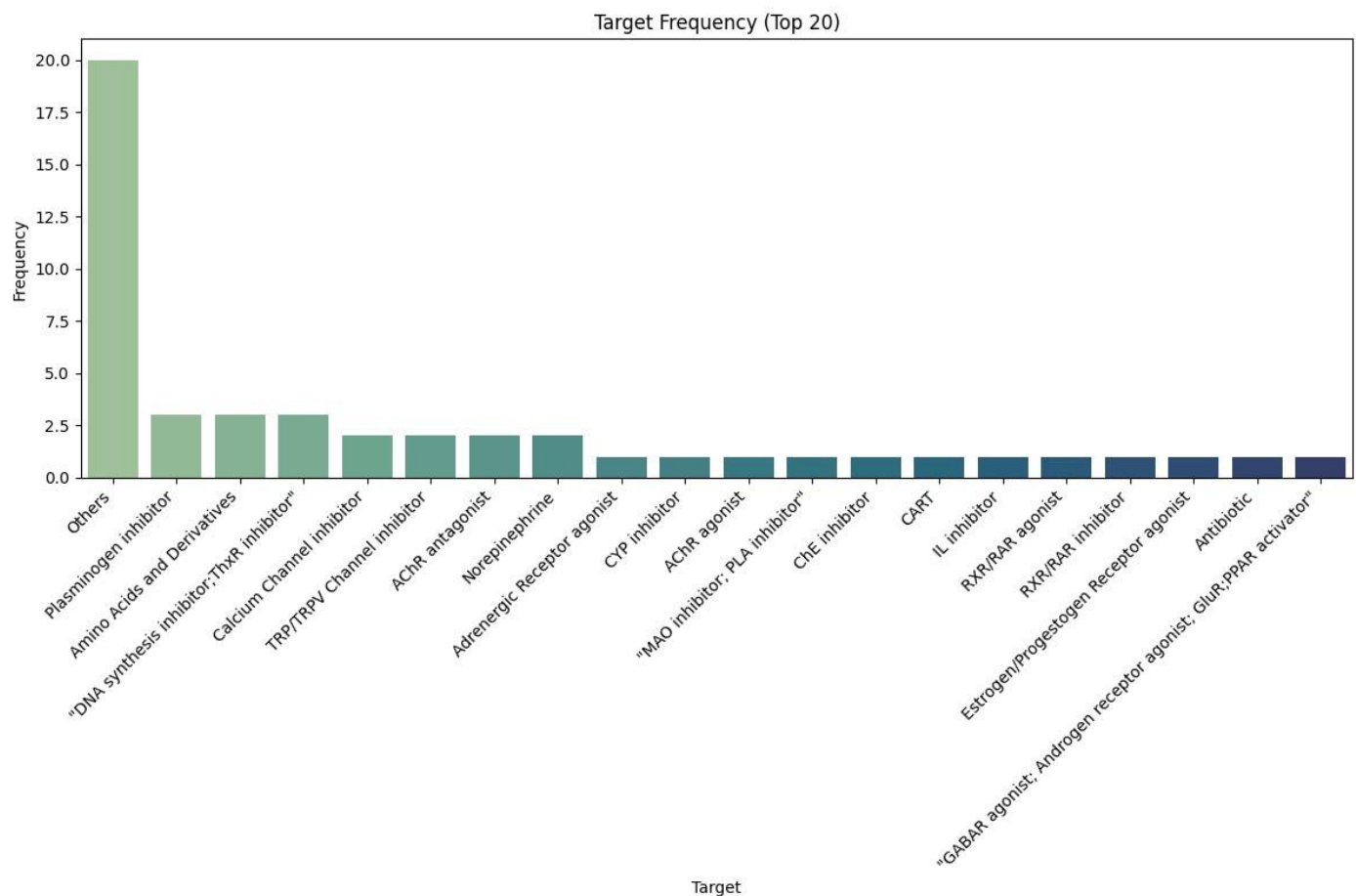
CC(=O)CCCCC(=O)O

Graph:

Scatterplot



Barplot



Let's analyze the target profile of Valerian compounds from your bar plot and compare it with the traditional uses of Valerian.

Analysis of the Bar Plot

Based on the information you've provided, the bar plot of target frequencies for Valerian compounds shows the top targets as:

- **Others:** This likely represents a diverse range of targets that didn't make the top 20 individually.
- **Plasminogen inhibitor:** This suggests potential effects on the fibrinolytic system, which could be relevant to cardiovascular health.
- **Amino Acids and Derivatives:** This could indicate interactions with neurotransmitter pathways or other metabolic processes.
- **DNA synthesis inhibitor; ThxR inhibitor:** This combination is interesting and could point to potential anti-cancer or immunomodulatory effects.
- **Calcium Channel inhibitor:** This is a well-known target for many neurological and cardiovascular drugs.
- **TRP/TRPV Channel inhibitor:** These channels are involved in pain perception and other sensory functions.
- **AChR antagonist:** This indicates potential interactions with the cholinergic system, which is relevant to Alzheimer's disease.
- **Norepinephrine:** This suggests potential effects on the adrenergic system, which is involved in stress response and mood regulation.
- **Adrenergic Receptor agonist:** This further supports the potential interaction with the adrenergic system.
- **CYP inhibitor:** This indicates potential effects on drug metabolism.

- **AChR agonist:** This is interesting considering the presence of AChR antagonist activity and could suggest complex interactions with the cholinergic system.
- **MAO inhibitor; PLA inhibitor:** This combination suggests potential antidepressant and anti-inflammatory effects.
- **ChE inhibitor:** This confirms the expected interaction with cholinesterase enzymes.
- **CART:** This neuropeptide is involved in appetite regulation and energy balance.
- **IL inhibitor:** This suggests potential anti-inflammatory effects.
- **RXR/RAR agonist and inhibitor:** These are nuclear receptors involved in various cellular processes, including inflammation and metabolism.
- **Estrogen/Progestogen Receptor agonist:** This suggests potential hormonal effects.
- **Antibiotic:** This is interesting and could point to potential antimicrobial properties.
- **GABAR agonist; Androgen receptor agonist; GluR:PPAR activator:** This combination is complex and suggests potential effects on multiple pathways, including the GABAergic, androgenic, and glutamatergic systems.

Traditional Uses of Valerian

Valerian has a long history of traditional use for various conditions, including:

- **Sleep disorders:** Valerian is commonly used as a natural remedy for insomnia and to improve sleep quality.
- **Anxiety:** Valerian has anxiolytic properties and is used to reduce anxiety and nervousness.
- **Stress:** Valerian is used to manage stress and promote relaxation.
- **Muscle spasms:** Valerian has muscle relaxant properties and is used to relieve muscle tension and spasms.
- **Menstrual cramps:** Valerian is used to alleviate menstrual cramps.

Comparison of Results with Traditional Uses

The target profile of Valerian compounds from your bar plot aligns with some of the traditional uses of Valerian:

- **Sleep and anxiety:** The interactions with the GABAergic, cholinergic, and adrenergic systems support the use of Valerian for sleep disorders and anxiety.
- **Muscle relaxation:** The interactions with calcium channels and other targets could contribute to the muscle relaxant properties of Valerian.
- **Anti-inflammatory effects:** The inhibition of PLA and IL suggests potential anti-inflammatory effects, which could be relevant to various conditions.

However, some of the targets identified in the bar plot, such as those related to cancer, metabolism, and hormonal activity, are not directly related to the traditional uses of Valerian. These findings could suggest potential new applications for Valerian or its compounds, but further research is needed to confirm these effects.

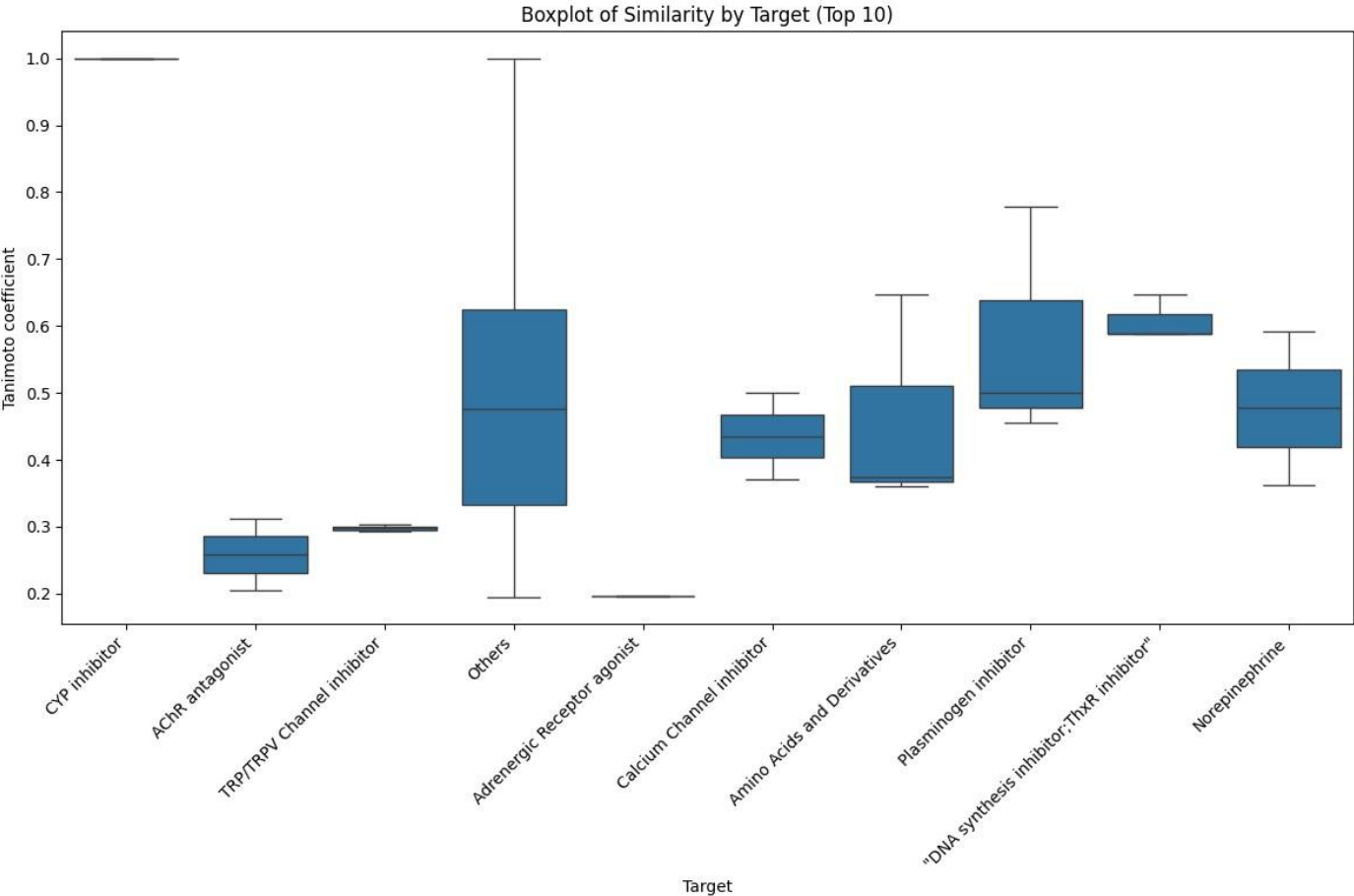
Additional Considerations

- **Complexity of Valerian:** Valerian contains a complex mixture of compounds, and their combined effects may be responsible for its therapeutic properties.
- **Variability in composition:** The composition of Valerian extracts can vary depending on the source and preparation methods, which could affect their target profile and therapeutic effects.
- **Need for further research:** While the target profile of Valerian compounds provides insights into their potential mechanisms of action, further research is needed to confirm these effects and explore their clinical applications.

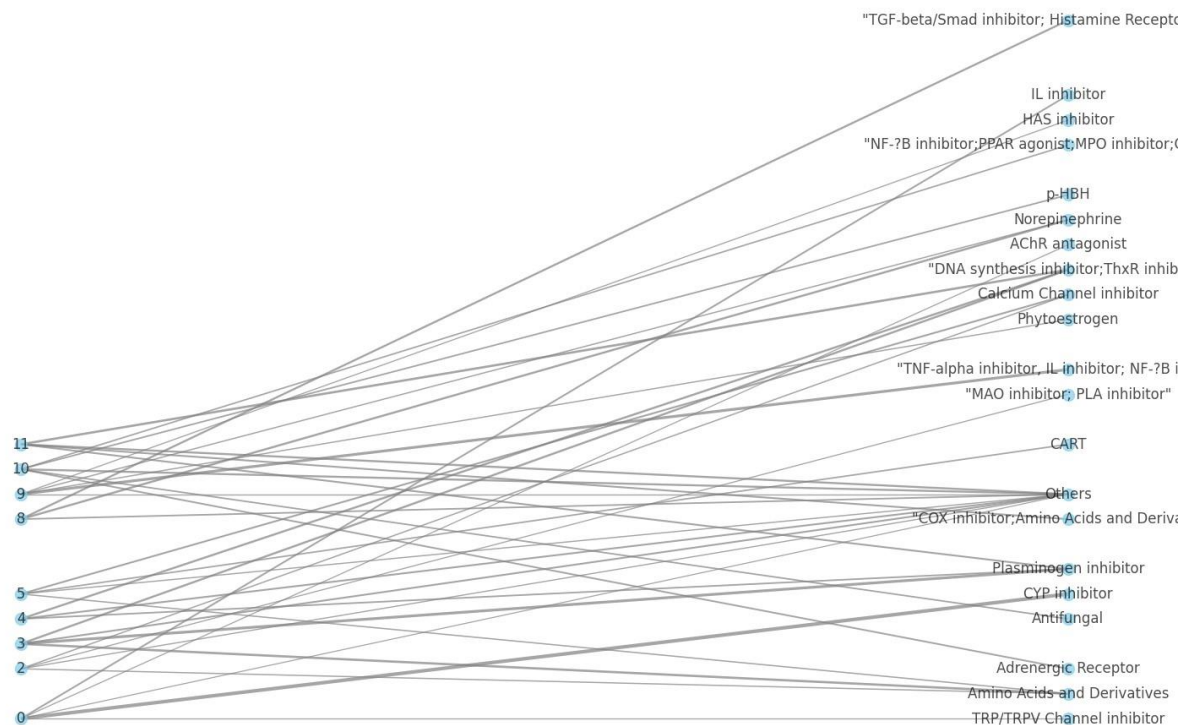
Overall, the comparison of the target profile of Valerian compounds with its traditional uses highlights the potential of this plant for various health conditions. However, it also emphasizes the need for further research to fully understand its complex mechanisms of action and explore its potential therapeutic applications.

The textual data analysis was performed with the aid of Gemini 2.0 Flash."

Boxplot



Network Graph:



Comparison Results (Tanimoto coefficient):

Query Index	Library Index	Tanimoto Similarity	Target	Bioactivity
0	362	1.000	CYP inhibitor	Extracted from Cinnamomum cassia; Suitability: Ethanol, ether, petroleum ether, benzene, toluene, acetone, decalin, tetralin; Store the product in sealed, cool and dry condition
0	314	0.485	IL inhibitor	Bornyl acetate is the main volatile constituent in numerous conifer oils and some Chinese traditional herbs, which has displayed an anti-inflammatory effect before.
0	874	0.313	AChR antagonist	A nicotinic antagonist that is well absorbed from the gastrointestinal tract and crosses the blood-brain barrier. Mecamylamine has been used as a ganglionic blocker in treating hypertension, but, like most ganglionic blockers, is more often
0	1504	0.303	TRP/TRPV Channel inhibitor	Camphor is readily absorbed through the skin producing either a coolness or warmth sensation by activating the ion channel TRPV3, and acts as slight local anesthetic and antimicrobial substance. There are anti-itch gels and cooling gels with
0	1671	0.303	Others	Camphor is a bicyclic monoterpene ketone found widely in plants, especially CINNAMOMUM CAMPHORA. It is used topically as a skin antipruritic and as an anti-infective agent.
1	309	0.204	AChR antagonist	Actions Daidzein is a phytoestrogen that is suggested to play a role in preventing hormone-induced cancers.

Query Library Tanimoto

			Target	Bioactivity
Index	Index	Similarity		
1	237	0.200	AChR agonist	Extracted?from?Nicotiana sanderae;Store?the?product? in?sealed,?cool?and?dry?condition
1	214	0.196	Adrenergic Receptor agonist	Dexmedetomidine is a sedative medication used by intensive care units and anesthetists.
1	974	0.196	ChE inhibitor	A cholinesterase inhibitor that crosses the blood-brain barrier. Tacrine has been used to counter the effects of muscle relaxants, as a respiratory stimulant, and in the treatment of Alzheimer's disease and other central nervous system diso Limonene is a colourless liquid hydrocarbon classified as a cyclic terpene. The more common d-isomer
1	1512	0.195	Others	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 Pregabalin is an anticonvulsant drug used for neuropathic pain, as an adjunct therapy for partial Calcium Channel
2	1188	0.370	seizures, and in generalized anxiety disorder. It was	inhibitor designed as a more potent successor to gabapentin. Pregabalin is marketed by Pfizer unde An essential branched-chain aliphatic amino acid found in many proteins. It is an isomer of LEUCINE. It is
2	1496	0.360	Amino Acids and Derivatives	important in hemoglobin synthesis and regulation of blood sugar and energy levels. Bromisoval is a sedative and mild hypnotic with
2	508	0.333	Others	potentially toxic effects.
2	1379	0.333	Others	Valpromide is a carboxamide derivative of valproic acid used in the treatment of epilepsy and some affective disorders. Ethyl carbamate (also known as urethan and urethane), formerly marketed as an inactive ingredient in Profenil "MAO inhibitor; PLA
2	1601	0.318	injection, was determined to be carcinogenic and was	inhibitor" removed from the Canadian, US, and UK markets in 1963. (6-)-?-Aminocaproic acid is a derivative and analogue of the amino acid lysine. Aminocaproic acid is an
3	1498	0.778	Plasminogen inhibitor Antifibrinolytic Agent. The physiologic effect of	aminocaproic acid is by means of Decreased Fibrinolysis. An amino acid formed in vivo by the degradation of dihydrouracil and carnosine. Since neuronal uptake and Amino Acids and neuronal receptor sensitivity to beta-alanine have been
3	1639	0.647	Derivatives	demonstrated, the compound may be a false transmitter replacing GAMMA-AMINOBUT
3	1694	0.625	Others	From an industrial perspective, it is the most important dicarboxylic acid, mainly as a precursor for the production of nylon. Azelaic acid is a saturated dicarboxylic acid found naturally in wheat, rye, and barley. It is a natural substance that is produced by Malassezia furfur (also known as Pityrosporum ovale), a yeast that lives on normal skin. It is effective
3	1678	0.588	"DNA synthesis inhibitor;ThxR inhibitor"	Extracted from Amber;Suitability:Water;Store the
3	1674	0.500	Others	product in sealed,cool and dry condition Extracted?from?Palm tree fruit;Store?the?product?in?
4	1696	0.778	Others	sealed,?cool?and?dry?condition
4	1694	0.625	Others	From an industrial perspective, it is the most important dicarboxylic acid, mainly as a precursor for the production of nylon.

Query Library Tanimoto

Index			Index Similarity	Target	Bioactivity
4	1678	0.588		"DNA synthesis inhibitor;ThxR inhibitor"	Azelaic acid is a saturated dicarboxylic acid found naturally in wheat, rye, and barley. It is a natural substance that is produced by Malassezia furfur (also known as Pityrosporum ovale), a yeast that lives on normal skin. It is effective
4	1674	0.500		Others	Extracted from Amber;Suitability:Water;Store the product in sealed,cool and dry condition
4	1498	0.455	Plasminogen inhibitor	Antifibrinolytic Agent.	The physiologic effect of aminocaproic acid is by means of Decreased Fibrinolysis.
5	1188	0.500		adjunct therapy for partial seizures, and in generalized anxiety disorder. It was inhibitor designed as a more potent successor to gabapentin.	Pregabalin is an anticonvulsant drug used for neuropathic pain, as an Constituent of striated muscle and liver. It is used therapeutically to stimulate gastric and pancreatic
5	1429	0.417		CART	secretions and in the treatment of hyperlipoproteinemias.
5	1496	0.375		Amino Acids and Derivatives	An essential branched-chain aliphatic amino acid found in many proteins. It is an isomer of LEUCINE. It is important in hemoglobin synthesis and regulation of blood sugar and energy levels.
5	1674	0.353		Others	Extracted from Amber;Suitability:Water;Store the product in sealed,cool and dry condition
5	82	0.346	Others	excretion in the disease cystinuria. Due to the rarity of the disorder, tioronin falls under the classification of an orphan dr	An important regulator of GENE EXPRESSION during growth and development, and in NEOPLASMS.
6	703	0.217		RXR/RAR agonist	Tretinoin, also known as retinoic acid and derived from
6					maternal VITAMIN A, is essential for normal GROWTH; and EMBRYONIC DEVELOPMENT. An excess of t
6					It was developed to be used as a chemotherapy
6	1512	0.208		Others	868 0.217 RXR/RAR inhibitor medication for the treatment of brain cancer, pancreatic cancer and more.
6	544	0.208		Antibiotic	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
6					chemical synthesis as a precursor to carvone and as a renewables-based solvent in clean
6					An antibiotic isolated from the fermentation broth of Fusidium coccineum. (From Merck Index, 11th ed) It acts by inhibiting translocation during protein synthesis.
6	1006	0.203		Estrogen/Progestogen	Altrenogest is a progestogen structurally related to
7				Receptor agonist	veterinary steroid trenbolone.
7	1504	0.293		ion channel TRPV3, and acts as slight local anesthetic inhibitor and antimicrobial substance. There are anti-itch gels and cooling gels with	Camphor is readily absorbed through the skin producing either a coolness or warmth sensation by activating the TRP/TRPV Channel
7	1671	0.293		Others	Camphor is a bicyclic monoterpene ketone found widely in plants, especially CINNAMOMUM CAMPHORA. It is used topically as a skin antipruritic and as an antiinfective agent.

Query Library Tanimoto

				Target	Bioactivity
Index	Index	Similarity			
7	973	0.236		"GABAR agonist; produced by the adrenal cortex. It is also produced in Androgen receptor agonist; GluR;PPAR	Dehydroepiandrosterone (DHEA) is a major C19 steroid used in the treatment of estrogen-receptor positive breast cancer in post-menopausal women. Formestane suppresses estrogen production from anabolic steroids or prohor
7	860	0.226		Aromatase Inhibitor	Dehydroepiandrosterone (DHEA) can be converted to Formestane was the first selective, type I, steroidal aromatase inhibitor used in the treatment of estrogen-receptor positive breast cancer in post-menopausal women. Formestane suppresses estrogen production from anabolic steroids or prohor
7	1492	0.224	Lipid		A semisynthetic bile acid made from cholic acid. It is used as a cholagogue, hydrocholeretic, diuretic, and as a diagnostic aid.
8	1100	1.000	Others		Hesperidin is a flavanone glycoside found abundantly in citrus fruits. Flavanone glycoside with antioxidant and neuroprotective properties. Unlike other citrus
8	517	0.776		Others	flavanones,it does not inhibit oral carcinogenesis in a rat model. Diosmin is a semisynthetic phlebotropic agent and a member of the flavonoid family. Extracted from
8	1476	0.593		Norepinephrine	hesperidin;Store the product in sealed, cool and dry condition
8	1388	0.565		"TGF-beta/Smad inhibitor; Histamine antagonist"	Hesperetin is a bioflavonoid and, to be more specific, a flavanone. Receptor
8	1415	0.451	Others	japonica., has been reported to have many benefits and medicinal properties.	Troxeutin, a natural bioflavonoid isolated from Sophora
9	1102	0.778	IL inhibitor; NF-?B inhibitor"		Luteolin is a flavone, a type of flavonoid. Like all flavonoids, it has a yellow crystalline appearance.
9	1476	0.362		Norepinephrine	Diosmin is a semisynthetic phlebotropic agent and a member of the flavonoid family. Extracted from
9	1697	0.356		Phytoestrogen	hesperidin;Store the product in sealed, cool and dry condition
9	218	0.339		Others	Daidzein is a natural isoflavone phytoestrogen found in Leguminosae, used as a component of foods and dietary supplements.
9	1543	0.318	HAS inhibitor		Extracted from CLUSIACEAE fruit;Suitability:Ethanol,methanol,acetone and pyridine;Store the product in sealed,cool and dry condition
10	1464	0.565	Others	for their high gallic acid content include	A coumarin derivative possessing properties as a spasmolytic, choleretic and light-protective agent. It is also used in ANALYTICAL CHEMISTRY TECHNIQUES for the determination of NITRIC ACID. Gallic acid is found in almost all plants. Plants known

Query Library Tanimoto

			Target	Bioactivity
Index	Index Similarity			
10				gallnuts,grapes,tea,hops and oak bark. Adrenalone is an adrenergic agonist used as a topical 1299 0.469 Adrenergic Receptor vasoconstrictor and hemostatic, mainly acts on alpha-1 adrenergic receptors. An aminobenzoic acid isomer that combines with pteridine and GLUTAMIC ACID to form FOLIC ACID.
10	1456	0.440	p-HBH	The fact that 4-aminobenzoic acid absorbs light throughout the UVB range has also resulted in its use as an ingredient in SUNSCREENS.
10	1458	0.435	Antifungal	Benzoic acid is a Nitrogen Binding Agent. The mechanism of action of benzoic acid is as an Ammonium Ion Binding Activity.
10	1613	0.414	"NF-?B agonist;MPO SULPHASALAZINE. (From Martindale, The inhibitor"	An anti-inflammatory agent, structurally related to the inhibitor;PPAR SALICYLATES, which is active in INFLAMMATORY BOWEL DISEASE. It is considered to be the active inhibitor;COX moiety of Extra Pharmacopoeia, 30th ed) From an industrial perspective, it is the most important
11	1694	0.688	Others dicarboxylic acid, mainly as a precursor for the production of nylon.	
11	1678	0.647	"DNA synthesis inhibitor;ThxR inhibitor"	Azelaic acid is a saturated dicarboxylic acid found naturally in wheat, rye, and barley. It is a natural substance that is produced by Malassezia furfur (also known as Pityrosporum ovale), a yeast that lives on normal skin. It is effective
11	1696	0.571	Others	Extracted?from?Palm tree fruit;Store?the?product?in? sealed,?cool?and?dry?condition
11	1223	0.500	"COX inhibitor;Amino Acids and Derivatives"	6-Acetamidohexanoic acid is a kind of amino acids derivate.
11	1498	0.500	Plasminogen inhibitor	(6-)-?-?Aminocaproic acid is a derivative and analogue of the amino acid lysine. Aminocaproic acid is an Antifibrinolytic Agent. The physiologic effect of aminocaproic acid is by means of Decreased Fibrinolysis.

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