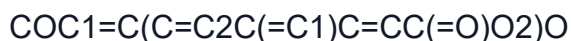


Biological Activity Estimation

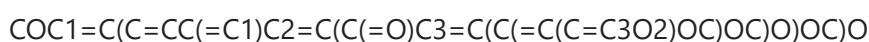
Results of *Artemisia annua*

Artemisia annua compounds:

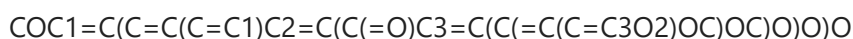
scopoletin



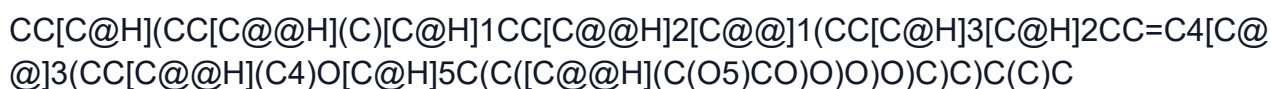
Chrysosplenetin



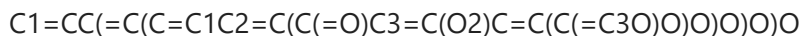
Eupatin



3-O-β-d-glucopyranoside of sitosterol



Quercetagetina



acido artemisico



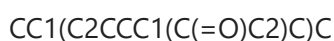
4,5-Epoxyartemisinic acid



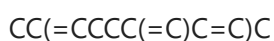
artemisia ketone



Canphor



Myrcene



α-pinene

CC1=CCC2CC1C2(C)C

canphene

CC1(C2CCC(C2)C1=C)C

β -canphene

CC1(C2CCC(C2)C1=C)C

1-8 cyneol

CC1(C2CCC(O1)(CC2)C)C

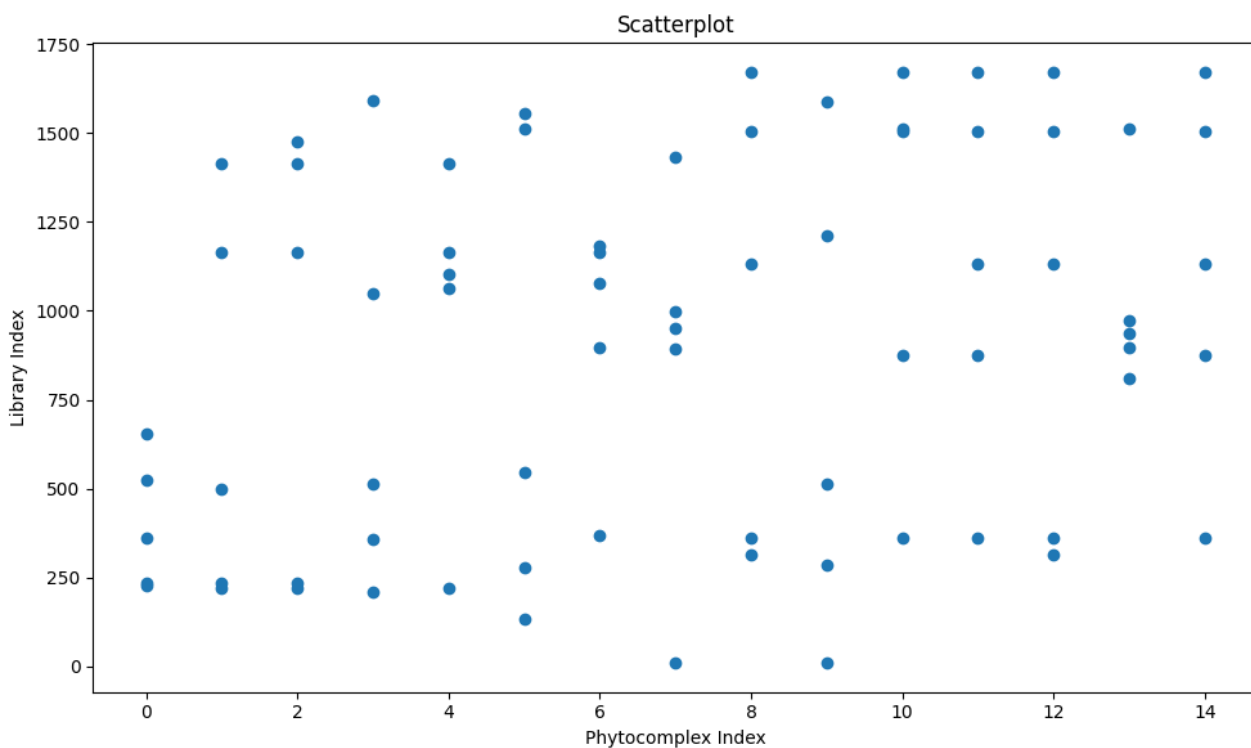
Beta-caryophyllene

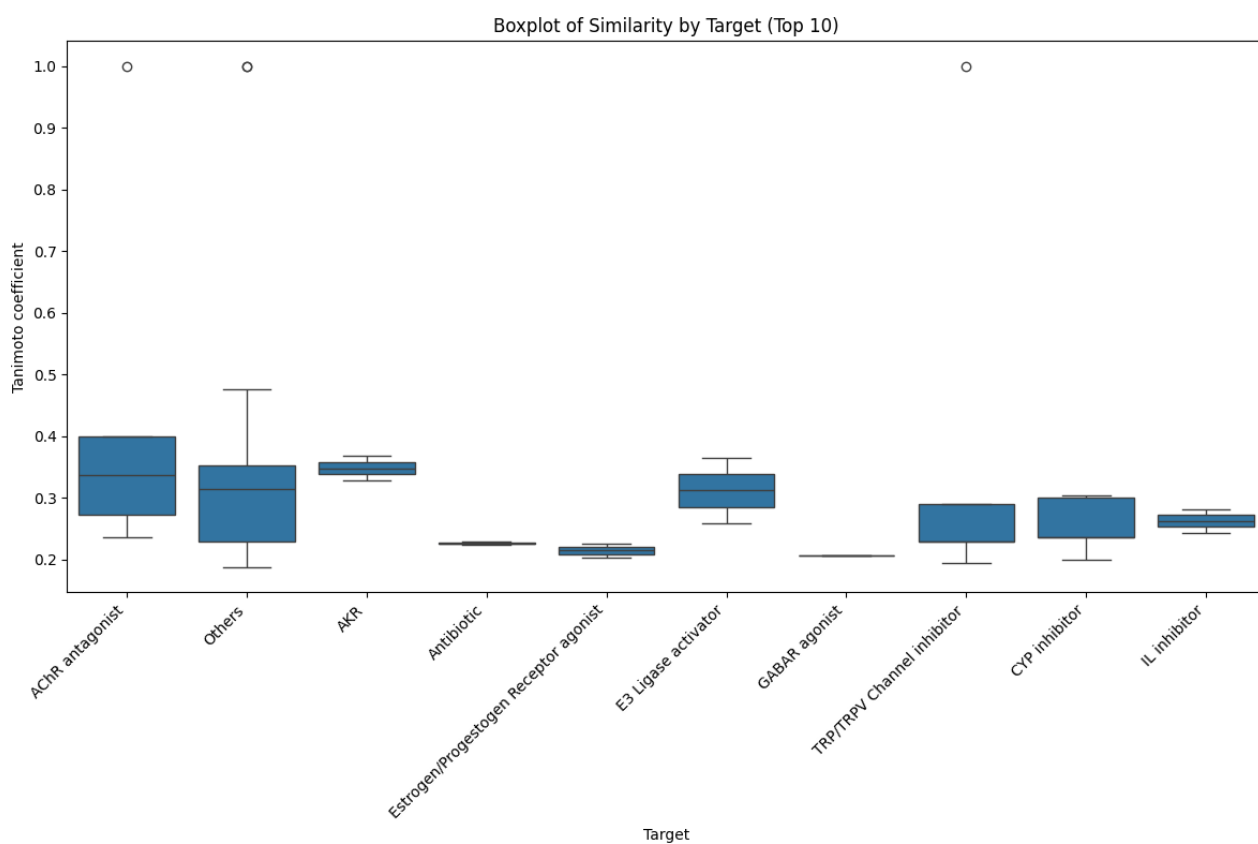
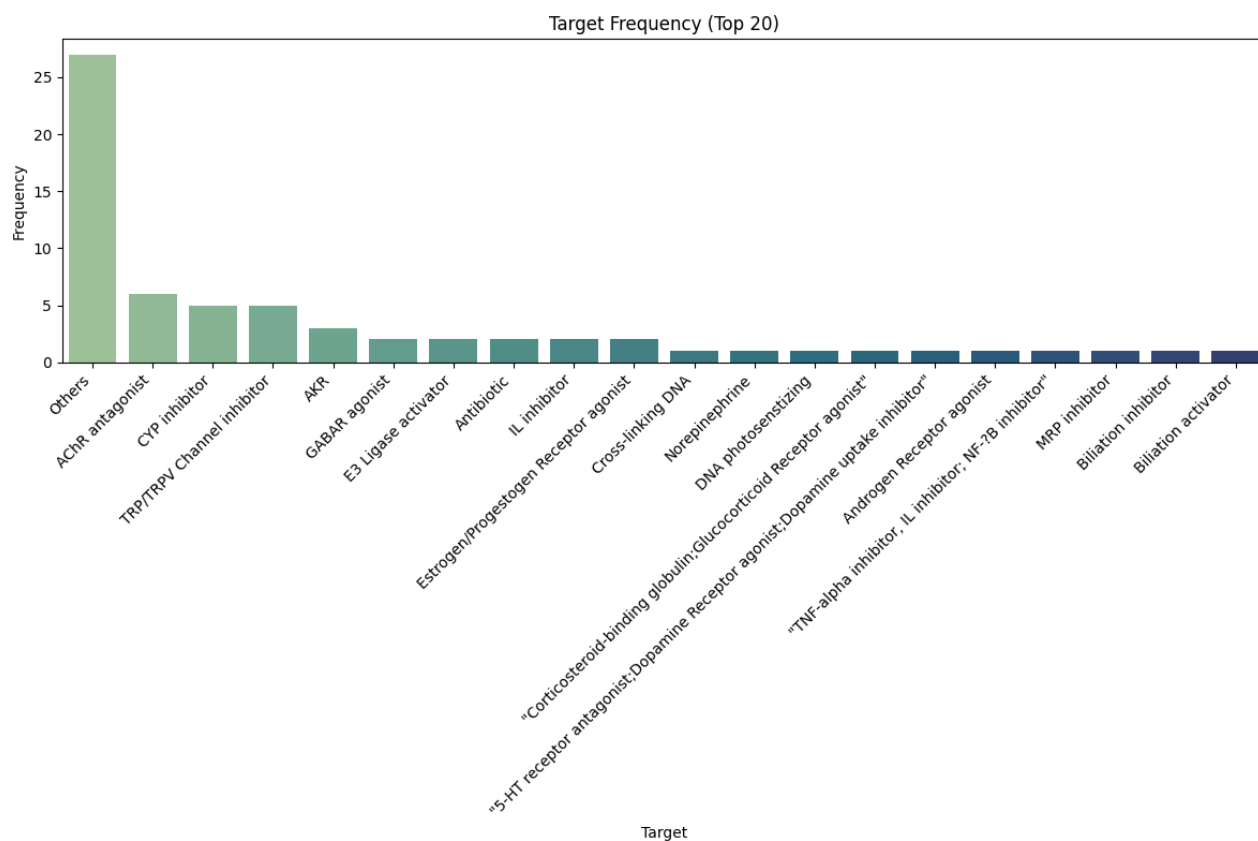
C/C/1=C\CCC(=C)[C@H]2CC([C@@H]2CC1)(C)C

β -pinene

CC1(C2CCC(=C)C1C2)C

Graph





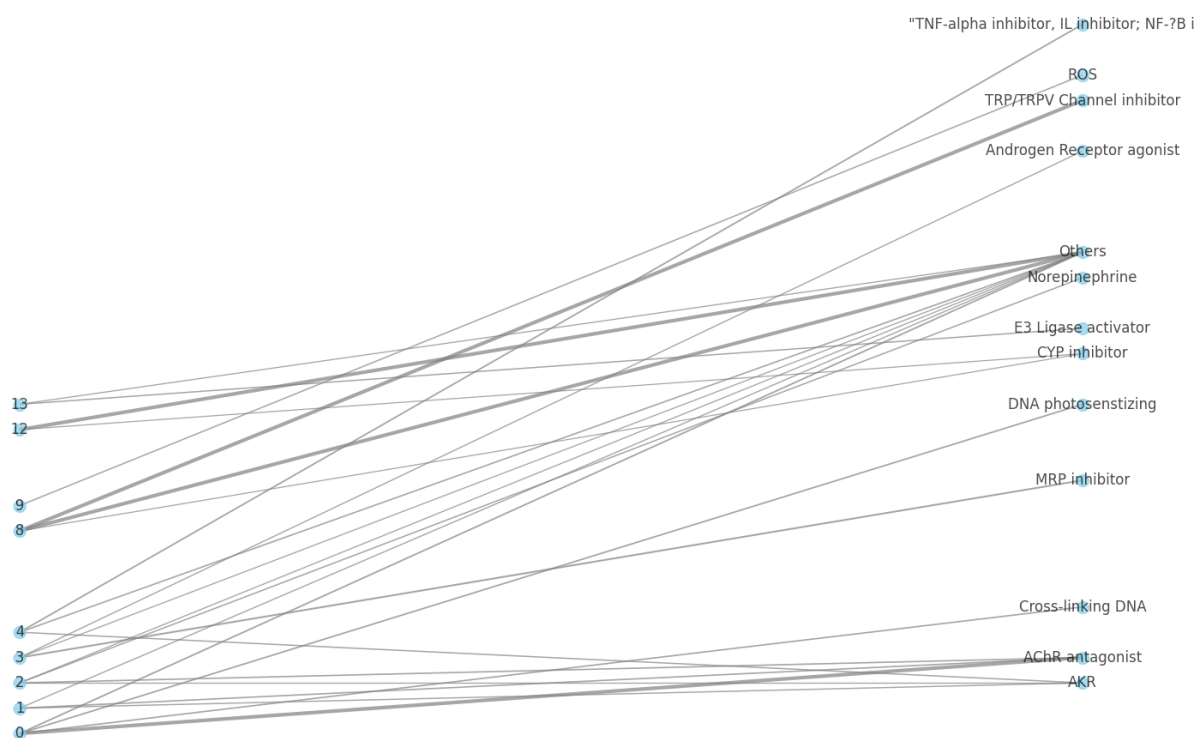
Certainly, let's break down the boxplot and the functions of the targets.

Boxplot Analysis

Target Functions

Here's a brief explanation of each target's function:

- **AChR antagonist:** Acetylcholine receptors (AChRs) are involved in muscle contraction, nerve transmission, and various brain functions. Antagonists block these receptors. Drugs with muscarinic antagonist activity are widely used in medicine, in the treatment of low heart rate, overactive bladder, respiratory problems such as asthma and chronic obstructive pulmonary disease (COPD), and neurological problems such as Parkinson's disease and Alzheimer's disease.
- **AKR:** Aldo-keto reductases (AKRs) are a family of enzymes involved in reducing aldehydes and ketones. They play roles in detoxification and metabolism.
- **Antibiotic:** Antibiotics are substances that kill or inhibit the growth of bacteria.
- **CYP inhibitor:** Cytochrome P450 (CYP) enzymes are involved in metabolizing many drugs and other compounds. Inhibitors can affect drug metabolism.
- **E3 Ligase activator:** E3 ubiquitin ligases are enzymes that tag proteins for degradation. Activators can enhance this process.
- **Estrogen/Progestogen Receptor agonist:** These receptors are involved in regulating sexual development and reproduction. Agonists activate these receptors.
- **GABAR agonist:** Gamma-aminobutyric acid (GABA) receptors are involved in inhibiting nerve transmission. Agonists enhance this inhibition.
- **IL inhibitor:** Interleukins (ILs) are a group of signaling molecules involved in immune responses. Inhibitors can suppress inflammation.
- **TRP/TRPV Channel inhibitor:** Transient receptor potential (TRP) and vanilloid receptor potential (TRPV) channels are involved in sensing temperature, pain, and other stimuli. Inhibitors can block these sensations.



Comparison Results (Tanimoto coefficient):

Que Index	Library Index	Tanimoto Similarity	Target	Bioactivity
0	234	1.000	AChR antagonist	Plant growth factor derived from the root of Scopolia carniolica or Scopolia japonica.
0	361	0.459	Others	Psoralen is used as photochemical probe in studies of DNA mutation and repair mechanisms. Causes photosensitization in human.
0	522	0.444	Others	Active constituent of Cnidium monnieri, a traditional Chinese medicine used for its anti-inflammatory, analgesic, and anti-lipedemic activities.
0	654	0.429	DNA photosensitizing	A naturally occurring furocoumarin compound found in several species of plants, including Psoralea corylifolia. It is a

Query Index	Library Index	Tanimoto Similarity	Target	Bioactivity
0	227	0.405	Cross-linking DNA	photoactive substance that forms DNA ADDUCTS in the presence of ultraviolet A irradiation. Bergapten is a psoralen that can be photoactivated and is capable of cross-linking DNA, covalently modifying proteins and lipids, and consequently inhibiting cell replication.
1	234	0.400	AChR antagonist	Plant growth factor derived from the root of <i>Scopolia carniolica</i> or <i>Scopolia japonica</i>.
1	218	0.368	Others	Extracted from CLUSIACEAE fruit; Suitability: Ethanol, methanol, acetone and pyridine; Store the product in sealed, cool and dry condition
1	1166	0.347	AKR	Rutin, a flavonol glycoside found in many plants including buckwheat; tobacco; forsythia; hydrangea; viola, etc., which possesses healthy effects for human.
1	1415	0.338	Others	Troloxerutin, a natural bioflavonoid isolated from <i>Sophora japonica</i>., has been reported to have many benefits and medicinal properties.
1	498	0.333	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.
2	234	0.400	AChR antagonist	Plant growth factor derived from the root of <i>Scopolia carniolica</i> or <i>Scopolia japonica</i>.
2	1476	0.368	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
2	1166	0.329	AKR	Rutin, a flavonol glycoside found in many plants including buckwheat; tobacco; forsythia; hydrangea; viola, etc., which possesses healthy effects for human.

Que ry Index	Libra ry Index	Tanim oto Similar ity	Target	Bioactivity
2	218	0.329	Others	Extracted from CLUSIACEAE fruit;Suitability:Ethanol,methanol,acetone and pyridine;Store the product in sealed,cool and dry condition
2	1415	0.321	Others	Troxeutin, a natural bioflavonoid isolated from Sophora japonica., has been reported to have many benefits and medicinal properties.
3	1592	0.494	MRP inhibitor	The principal sterol of all higher animals, distributed in body tissues, especially the brain and spinal cord, and in animal fats and oils.
3	514	0.476	Others	Extracted from Glycine max(L.)Merr.;Suitability:Chloroform,benzene, ethyl acetate,pyridine,ethanol,acetone;Store the product in sealed,cool and dry condition
3	1050	0.333	Androgen Receptor agonist	Dehydroepiandrosterone (DHEA) is a major C19 steroid produced by the adrenal cortex. It is also produced in small quantities in the testis and the ovary. Dehydroepiandrosterone (DHEA) can be converted to testosterone; androstenedione; estra
3	357	0.315	Others	Ginsenoside Re may have properties that inhibit or prevent the growth of tumors.
3	210	0.314	Others	Ginsenosides are a class of steroid glycosides, and triterpene saponins, found exclusively in the plant genus Panax (ginseng). Ginsenosides have been the target of research, as they are viewed as the active compounds behind the claims of gi
4	1102	0.435	"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.
4	218	0.393	Others	Extracted from CLUSIACEAE fruit;Suitability:Ethanol,methanol,acetone

Que ry Index	Libra ry Index	Tanim oto Similar ity	Target	Bioactivity
				and pyridine;Store the product in sealed,cool and dry condition
4	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.
4	1063	0.273	"5-HT receptor antagonist;Dopamine Receptor agonist;Dopamine uptake inhibitor"	One of the catecholamine NEUROTRANSMITTERS in the brain. Dopamine hydrochloride is derived from TYROSINE and is the precursor to NOREPINEPHRINE and EPINEPHRINE. Dopamine is a major transmitter in the extrapyramidal system of the brain, and
4	1415	0.269	Others	Troloxerutin, a natural bioflavonoid isolated from Sophora japonica., has been reported to have many benefits and medicinal properties. 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 cleani
5	1512	0.289	Others	An antibiotic isolated from the fermentation broth of Fusidium coccineum. (From Merck Index, 11th ed) It acts by inhibiting translocation during protein synthesis.
5	278	0.206	"Corticosteroid-binding globulin;Glucocorticoid Receptor agonist"	Medrysone is a corticosteroid used in ophthalmology.
5	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

Que ry Index	Libra ry Index	Tanim oto Similar ity	Target	Bioactivity
				used to treat breast and endometrial neoplasms.
5	1556	0.200	"Lipid; Calcium Channel inhibitor"	A direct-acting smooth muscle relaxant used to dilate blood vessels. It may cause gastrointestinal distress and tachycardia.
6	897	0.258	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.
6	369	0.228	Antibiotic	Sodium Monensin, isolated from <i>Streptomyces cinnamomensis</i> , is a well-known representative of naturally polyether ionophore antibiotics.
6	1078	0.225	Others	Artesunate is a part of the artemisinin group of agents with an IC ₅₀ of < 5 μ M for small cell lung carcinoma cell line H69. Artesunate is a semi-synthetic derivative of artemisinin that is water-soluble and may therefore be given by injecti
6	1165	0.221	Biliation activator	A bile acid, usually conjugated with either glycine or taurine. It acts as a detergent to solubilize fats for intestinal absorption and is reabsorbed by the small intestine. It is used as cholagogue, a choleretic laxative, and to prevent or
6	1183	0.221	Biliation inhibitor	An epimer of chenodeoxycholic acid. It is a mammalian bile acid found first in the bear and is apparently either a precursor or a product of chenodeoxycholate. Its administration changes the composition of bile and may dissolve gallstones.
7	10	0.206	GABAR agonist	An analogue of gamma-aminobutyric acid, vigabatrin is an irreversible inhibitor of 4-aminobutyrate transaminase, the enzyme responsible for the catabolism of gamma-

Que ry Index	Libra ry Index	Tanim oto Similar ity	Target	Bioactivity
7	894	0.200	MMP inhibitor	aminobutyric acid. (From Martindale The Extra Pharmacopoeia, 31st ed). Off-l Acetohydroxamic Acid, a synthetic drug derived from hydroxylamine and ethyl acetate, is similar in structure to urea. In the urine, it acts as an antagonist of the bacterial enzyme urease. Acetohydroxamic Acid has no direct antimicrobial ac
7	1432	0.200	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
7	951	0.188	Chelator	3-Mercapto-D-valine. The most characteristic degradation product of the penicillin antibiotics. It is used as an antirheumatic and as a chelating agent in Wilson's disease.
7	998	0.188	Others	The most characteristic degradation product of the penicillin antibiotics. It is used as an antirheumatic and as a chelating agent in Wilson's disease. .
8	1504	1.000	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
8	1671	1.000	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.
8	362	0.303	CYP inhibitor	Extracted from Cinnamomum cassia; Suitability: Ethanol, ether, petroleum ether, benzene, toluene, acetone, decalin, tetrali

Que ry Index	Libra ry Index	Tanim oto Similar ity	Target	Bioactivity
				n;Store the product in sealed,cool and dry condition
8	1132	0.290	Others	Eucalyptol is a natural organic compound which is a colorless liquid. It is a cyclic ether and a monoterpene. Eucalyptol is an ingredient in many brands of mouthwash and cough suppressant. It controls airway mucus hypersecretion and asthma
8	314	0.282	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.
9	286	0.364	ROS	Extracted from Papaya fruit, marigold flower petals;Store the product in sealed,cool and dry condition
9	512	0.273	VK	Menatetrenone is a menaquinone compound and form of vitamin K2 with potential antineoplastic activity. Menatetrenone may act by modulating the signalling of certain tyrosine kinases, thereby affecting several transcription factors including
9	1213	0.250	Others	Undecylenic acid is an organic unsaturated fatty acid pyrolysis product of ricinoleic acid from castor oil. It is used in the manufacture of pharmaceuticals, cosmetics and perfumery, including antidandruff shampoos, antimicrobial powders and
9	1588	0.235	Antifungal	A synthetic antifungal agent.
9	10	0.206	GABAR agonist	An analogue of gamma-aminobutyric acid, vigabatrin is an irreversible inhibitor of 4-aminobutyrate transaminase, the enzyme responsible for the catabolism of gamma-aminobutyric acid. (From Martindale The Extra Pharmacopoeia, 31st ed). Off-l
10	874	0.235	AChR antagonist	A nicotinic antagonist that is well absorbed from the gastrointestinal tract and crosses the

Que ry Index	Libra ry Index	Tanim oto Similar ity	Target	Bioactivity
10	1512	0.216	Others	blood-brain barrier. Mecamylamine has been used as a ganglionic blocker in treating hypertension, but, like most ganglionic blockers, is more often 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 cleani
10	362	0.200	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
10	1504	0.194	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
10	1671	0.194	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.
11	874	0.273	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
11	362	0.235	CYP inhibitor	Extracted from Cinnamomum cassia;Suitability:Ethanol,ether,petroleum ether,benzene,toluene,acetone,decalin,tetrali

Que ry Index	Libra ry Index	Tanim oto Similar ity	Target	Bioactivity
11	1504	0.229	TRP/TRPV Channel inhibitor	n;Store the product in sealed,cool and dry condition 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
11	1671	0.229	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.
11	1132	0.219	Others	Eucalyptol is a natural organic compound which is a colorless liquid. It is a cyclic ether and a monoterpene. Eucalyptol is an ingredient in many brands of mouthwash and cough suppressant. It controls airway mucus hypersecretion and asthm
12	1132	1.000	Others	Eucalyptol is a natural organic compound which is a colorless liquid. It is a cyclic ether and a monoterpene. Eucalyptol is an ingredient in many brands of mouthwash and cough suppressant. It controls airway mucus hypersecretion and asthm
12	362	0.300	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
12	1504	0.290	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

Que ry Index	Libra ry Index	Tanim oto Similar ity	Target	Bioactivity
12	1671	0.290	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.
12	314	0.243	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.
13	897	0.365	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.
13	1512	0.317	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 cleani
13	935	0.226	Estrogen/Progestogen Receptor agonist	Allylestrenol is a synthetic steroid with progestational activity.
13	808	0.224	Aromatase inhibitor	Exemestane is an oral steroidal aromatase inhibitor used in the adjuvant treatment of hormonally-responsive (also called hormone-receptor-positive, estrogen-responsive) breast cancer in postmenopausal women. It acts as a false substrate for
13	973	0.218	"GABAR agonist; Androgen receptor agonist; GluR;PPAR activator"	Dehydroepiandrosterone (DHEA) is a major C19 steroid produced by the adrenal cortex. It is also produced in small quantities in the testis and the ovary. Dehydroepiandrosterone (DHEA) can be converted to testosterone; androstenedione; estra

Que ry Inde x	Libra ry Inde x	Tanim oto Similar ity	Target	Bioactivity
14	874	0.273	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
14	362	0.235	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
14	1504	0.229	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
14	1671	0.229	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.
14	1132	0.219	Others	Eucalyptol is a natural organic compound which is a colorless liquid. It is a cyclic ether and a monoterpene. Eucalyptol is an ingredient in many brands of mouthwash and cough suppressant. It controls airway mucus hypersecretion and asthma

[Torna al form](#)

Reference:

Chougouo, R.D.K., Nguekeu, Y.M.M., Dzoyem, J.P. *et al.* Anti-inflammatory and acetylcholinesterase activity of extract, fractions and five compounds isolated from the leaves and twigs of *Artemisia annua* growing in Cameroon. *SpringerPlus* **5**, 1525 (2016).
<https://doi.org/10.1186/s40064-016-3199-9>

Essential oil:

Charles, DJ, Cebert, E., & Simon, JE (1991). Caratterizzazione dell'olio essenziale di *Artemisia annua* L. *Journal of Essential Oil Research* , 3 (1), 33–39.
<https://doi.org/10.1080/10412905.1991.9697903>