Biological activity estimation results of ivy

Reference:

Pharmacological and therapeutic activities of Hederahelix- A review IOSR Journal Of Pharmacy
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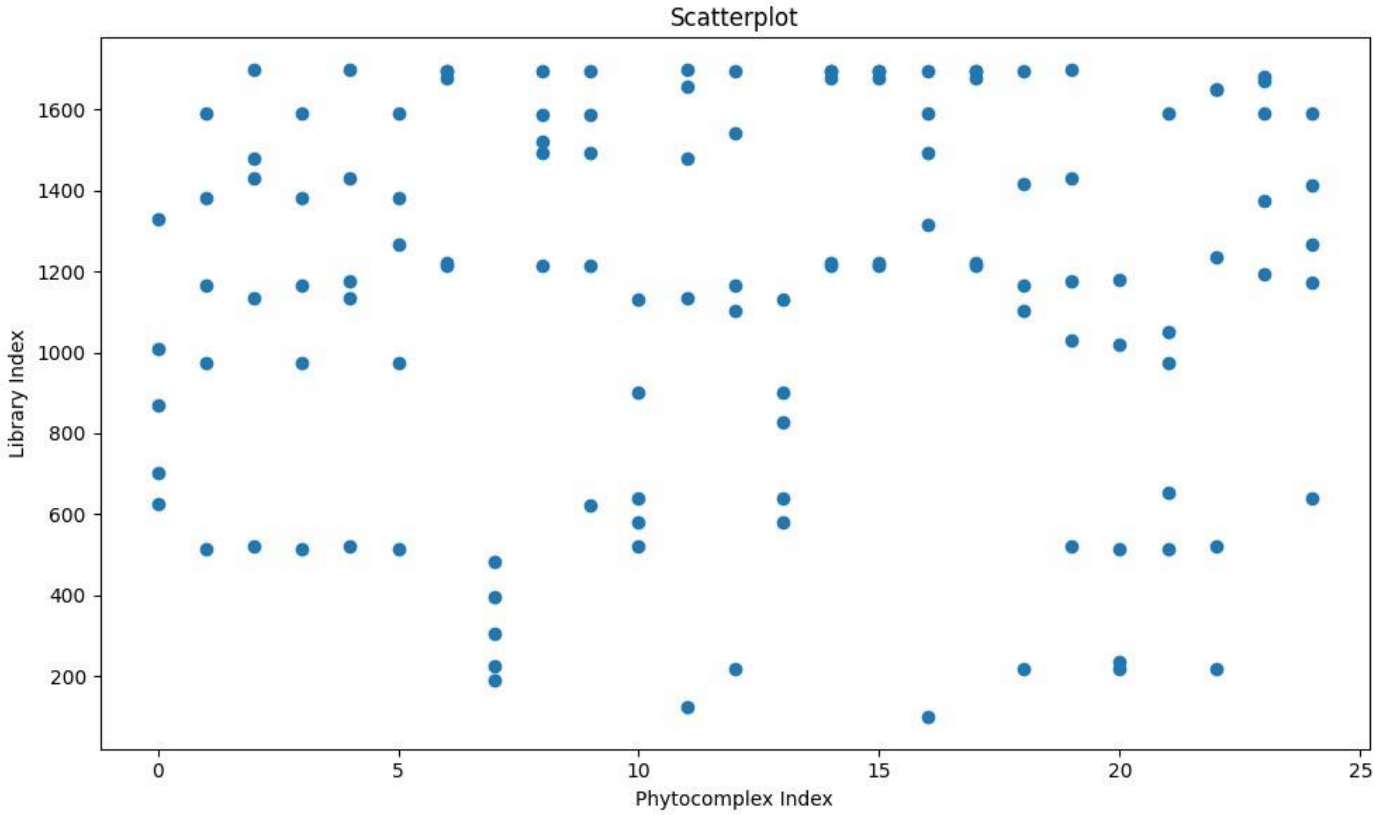
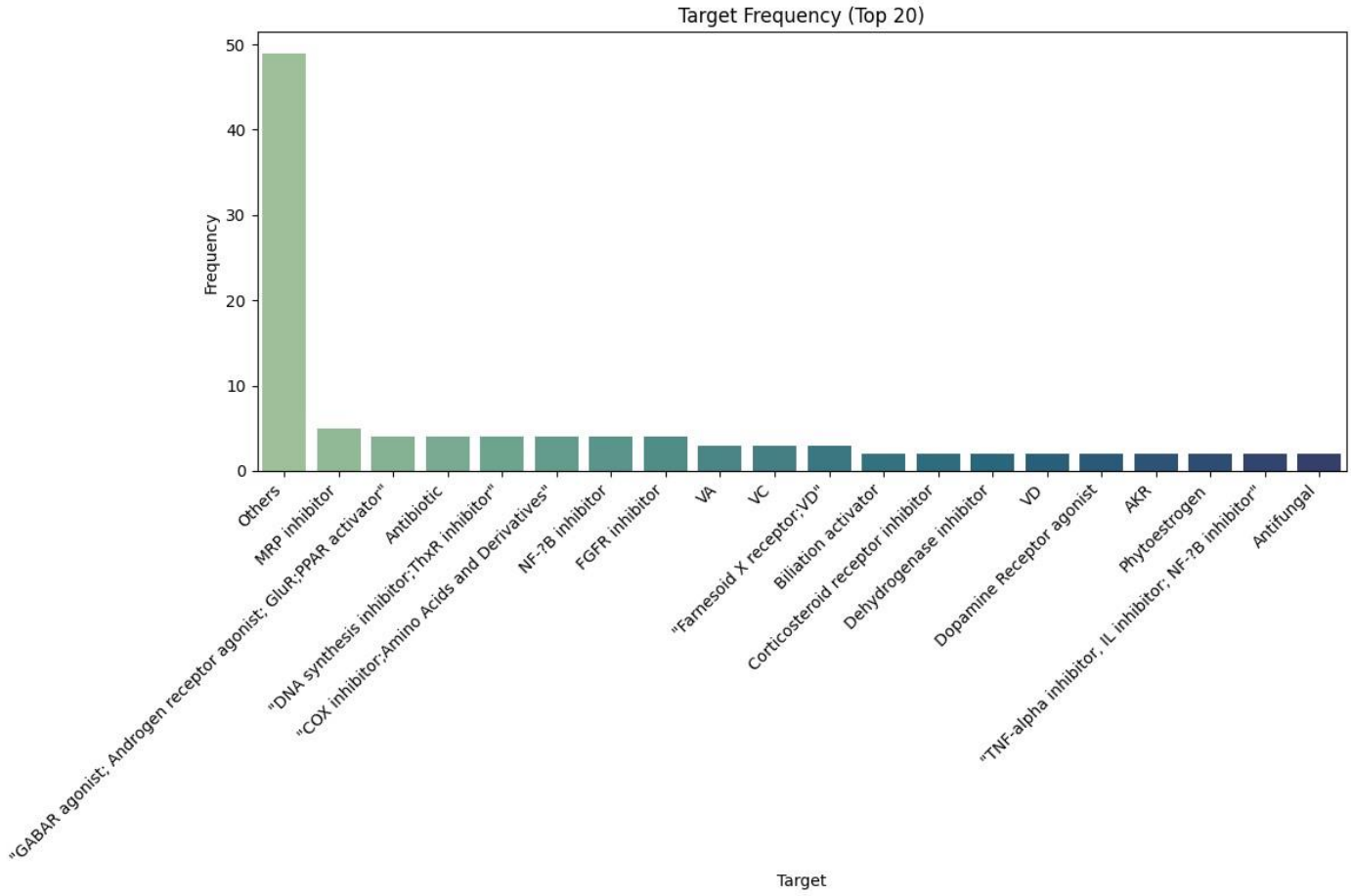
Graph:

Scatterplot



Barplot



Let's compare the pharmacological effects of ivy (Hedera helix) described in your provided text with the target frequency barplot you shared.

Summary of Ivy's Pharmacological Effects:

The text details a wide range of pharmacological effects for ivy, primarily attributed to its various compounds, including α-hederin, hederacoside C, and others. Here's a breakdown by category:

- **Respiratory Effects:** Bronchodilatory, anti-asthmatic, reduces inflammation in airways, decreases mucus production.
- **Anti-inflammatory and Analgesic Effects:** Reduces inflammation in various models (paw edema, arthritis), exhibits pain-reducing activity.
- **Anticancer Effects:** Cytotoxic activity against various cancer cell lines, potential to enhance the effects of chemotherapy drugs, induces apoptosis in cancer cells.
- **Antimicrobial Effects:** Antibacterial activity against both Gram-positive and Gram-negative bacteria, antifungal activity, some antiviral effects (influenza, EV71).
- **Anti-parasitic Effects:** Activity against Leishmania, some anthelmintic activity (against certain worms).
- **Antioxidant Effects:** Scavenges free radicals, inhibits lipid peroxidation.
- **Digestive System Effects:** Prevents ulcers, affects gut motility (both contraction and antispasmodic activity).
- **Antimutagenic Effect:** Protects against DNA damage.
- **Immunological Effect:** Reduces IL-6 release, suggesting potential immune modulation.
- **Anti-thrombin Effect:** Inhibits blood clotting.

Comparison with the Target Frequency Barplot:

The barplot you provided shows the frequency of predicted targets for ivy compounds when compared against a library of 1700 compounds. Let's see how it aligns with the known pharmacology:

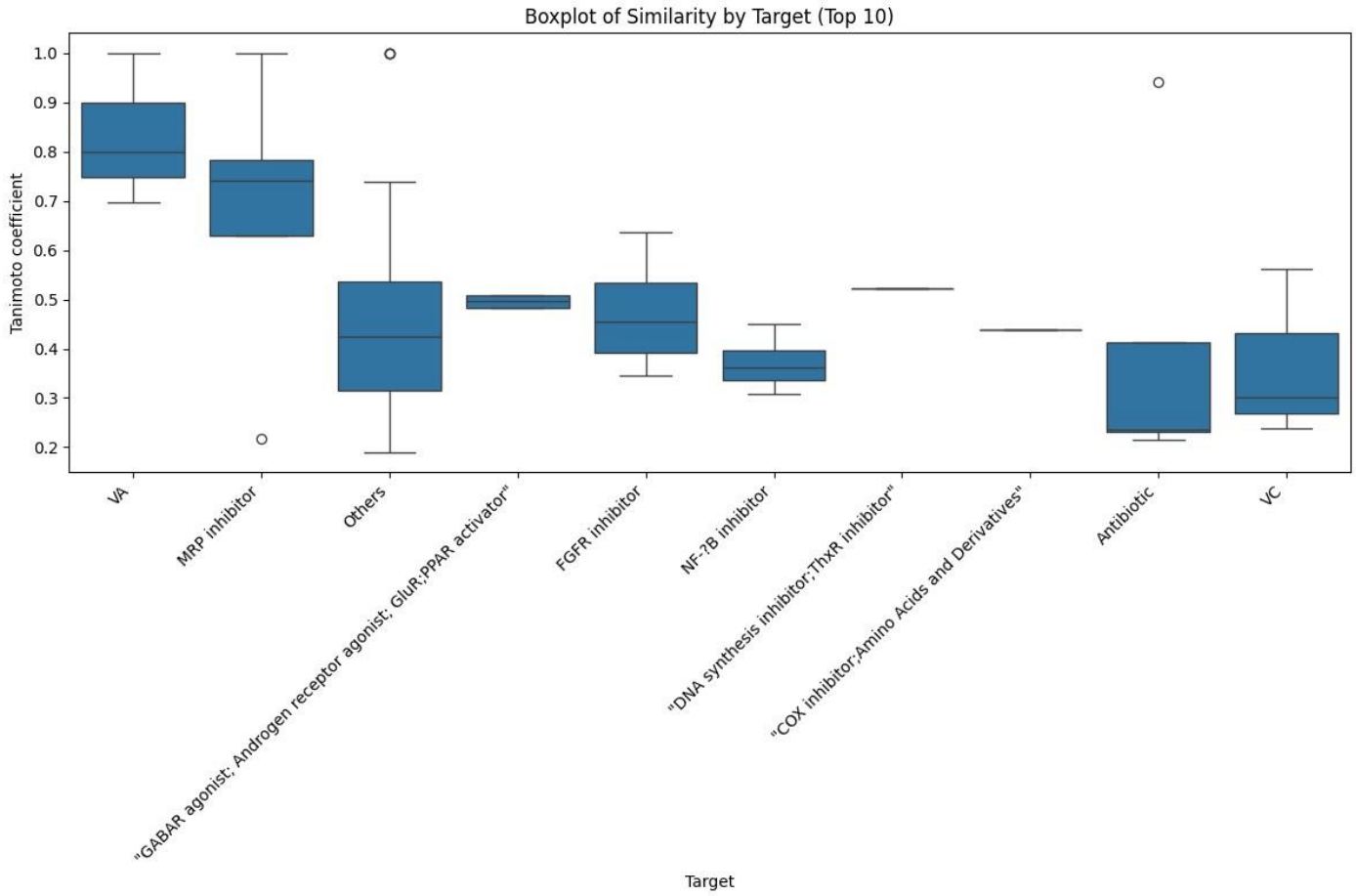
- **"Others":** The high frequency in "Others" suggests a broad range of interactions, which is consistent with the diverse pharmacological effects described. Ivy interacts with many systems.
- **Norepinephrine:** The relatively high frequency for norepinephrine targets could relate to some of the observed effects, though the connection isn't immediately clear from the pharmacology text. Further investigation would be needed.
- **AKR:** The moderate frequency for AKR (Aldo-keto reductases) is interesting. While the pharmacology text doesn't explicitly mention AKR, these enzymes are involved in various metabolic processes. This could be an area for further research to see if AKR plays a role in any of ivy's observed effects.
- **"TNF-alpha inhibitor; IL inhibitor; NF-?B inhibitor":** The presence of this target aligns strongly with the reported anti-inflammatory effects. TNF-alpha, IL (interleukins), and NF-?B are all key players in inflammation.
- **GABA Receptor agonist; Androgen receptor agonist; GluR; PPAR activator:** The presence of these targets, while not directly corresponding to the provided pharmacology, suggests potential interactions with neurological and endocrine systems. This warrants further investigation, as it could reveal additional mechanisms of action.
- **Other Targets:** The remaining targets in the barplot (MRP inhibitor, Antibiotic, DNA synthesis inhibitor, COX inhibitor, etc.) have varying degrees of correspondence to the pharmacology. Some, like "DNA synthesis inhibitor," might relate to the anticancer effects, while others are less clear and would require more in-depth analysis.

Key Observations and Next Steps:

- **Overall Alignment:** There's a reasonable degree of alignment between the reported pharmacology and the predicted targets, especially regarding anti-inflammatory effects.
- **Further Research:** The barplot suggests potential mechanisms of action that aren't explicitly covered in the pharmacology text. For example, the interaction with AKR, GABA receptors, and other targets could reveal new aspects of ivy's activity.
- **Specificity:** The pharmacology text often refers to specific compounds (like α-hederin) being responsible for certain effects. The barplot, however, looks at the overall fingerprint of ivy compounds. More detailed analysis focusing on individual compounds might provide a clearer picture.
- **Validation:** Computational predictions need experimental validation. Just because a target is predicted doesn't mean the interaction actually occurs in vivo.

In summary, the barplot provides a valuable starting point for understanding the potential mechanisms of action of ivy. Combining this information with the detailed pharmacological studies allows for a more comprehensive understanding of this plant's properties and can guide future research.

Boxplot



Understanding the Boxplot

- **Boxes**: Each box represents the interquartile range (IQR), containing the middle 50% of the data (similarity scores) for a specific target. A longer box means a wider range of similarity scores for that target.
- **Line in the Box**: The line inside the box represents the median similarity score.
- **Whiskers**: The "whiskers" extend to the highest and lowest values within 1.5 times the IQR from the box. Points outside the whiskers are considered outliers.

Comparison with Ivy Uses

Here's how the targets in the boxplot relate to the uses of ivy mentioned in your text:

- **VA**: This likely refers to "Vanillic Acid" or a related target. The moderate similarity scores suggest that ivy compounds might interact with this target, but the connection to the listed uses isn't clear from the information provided.
- **MRP inhibitor**: Multidrug resistance-associated protein inhibitors. This target relates to the ability of cells to pump out toxins, including some drugs. The moderate similarity scores here could be related to the potential of ivy compounds to modulate drug resistance in cancer cells, as mentioned in the text.
- **Others**: This category usually encompasses a wide range of targets not specifically listed. The broad distribution here suggests ivy compounds might interact with diverse biological pathways, fitting its traditional uses for various ailments.
- **"GABAR agonist; Androgen receptor agonist; GluR; PPAR activator"**: This combination of targets suggests potential interactions with neurological and endocrine

systems. While the provided text doesn't explicitly mention these systems, it does discuss ivy's potential anti-anxiety and anti-inflammatory effects, which could be related to these targets.

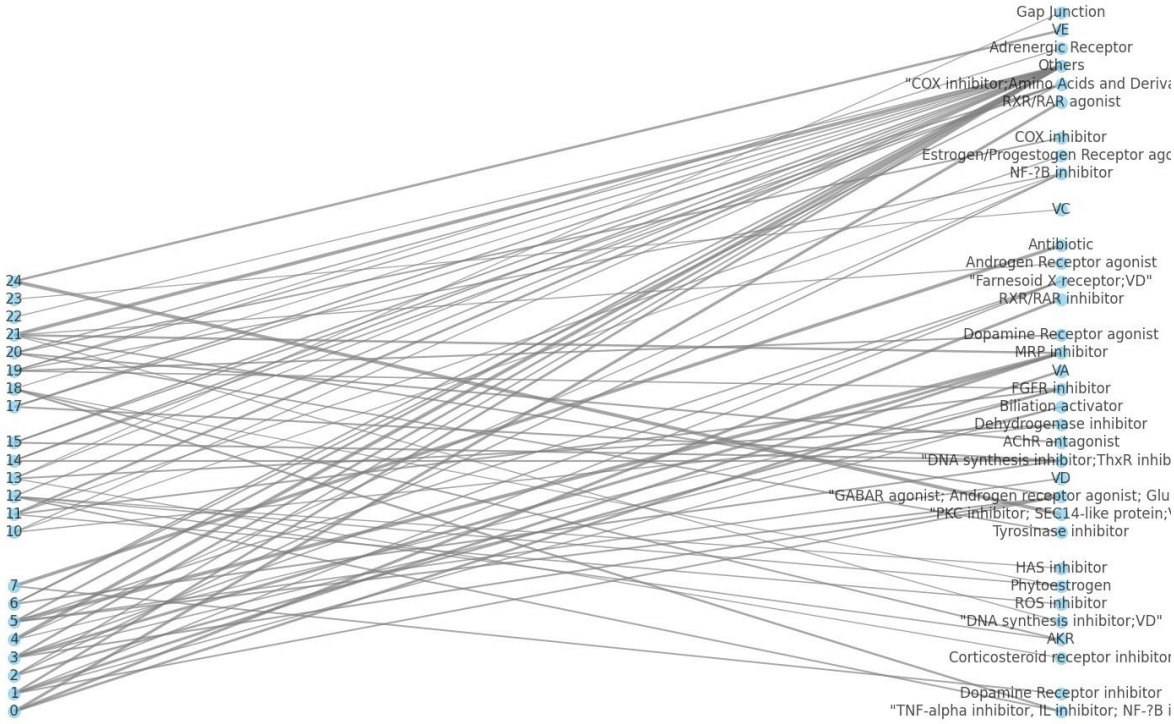
- **FGFR inhibitor**: Fibroblast growth factor receptor inhibitors. This target is often associated with cancer research. The moderate similarity scores here could be related to the anticancer effects of ivy mentioned in the text.
- **NF-?B inhibitor**: Nuclear factor kappa B inhibitors. NF-?B is a key player in inflammation. This target aligns with the reported anti-inflammatory effects of ivy.
- **"DNA synthesis inhibitor; ThxR inhibitor"**: This target relates to the ability to inhibit DNA synthesis, which is relevant to cancer treatment. This aligns with the anticancer effects of ivy mentioned in the text.
- **"COX inhibitor; Amino Acids and Derivatives"**: Cyclooxygenase inhibitors, which are commonly used as anti-inflammatories. This target aligns with the anti-inflammatory effects of ivy.
- **Antibiotic**: This target suggests potential antibacterial activity. The text mentions that ivy has antibacterial activity against various bacteria, supporting this finding.
- **VC**: This likely refers to "Vitamin C" or a related target. The low similarity scores suggest that ivy compounds don't strongly resemble known Vitamin C-interacting molecules.

Key Observations

- **Anti-inflammatory Effects**: The boxplot shows several targets related to inflammation (NF-?B inhibitor, COX inhibitor), which aligns with the reported anti-inflammatory uses of ivy.
- **Anticancer Potential**: The presence of targets like "DNA synthesis inhibitor" and FGFR inhibitor suggests potential anticancer activity, which is consistent with the text.
- **Antibacterial Activity**: The "Antibiotic" target aligns with the reported antibacterial effects of ivy.
- **Diverse Activities**: The broad distribution in the "Others" category suggests that ivy interacts with a variety of targets, which is consistent with its diverse traditional uses.

Important Note: This boxplot shows predicted targets based on similarity scores. It's crucial to remember that these are predictions, and further research is needed to confirm these interactions and determine their actual biological relevance.

Network Graph:



Comparison Results (Tanimoto coefficient):

Query Index	Library Index	Tanimoto Similarity	Target	Bioactivity
0	626	1.000	VA	Beta Carotene is an organic compound and classified as a terpenoid. It is a precursor (inactive form) of vitamin A.
0	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
0	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.
0	1010	0.800	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
0	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.

1	1592	0.741	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.

1	514	0.677	Others	Extracted from Glycine max(L.)Merr.;Suitability:Chloroform,benzene,ethyl acetate,pyridine,ethanol,acetone;Store the product in sealed,cool and dry condition
1	973	0.483	"GABAR agonist; GluR;PPAR agonist; androstenedione; estra	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;
1	1381	0.406	"Farnesoid X receptor;VD"	A bile acid formed from chenodeoxycholate by bacterial action, usually conjugated with glycine or taurine. It acts as a detergent to solubilize fats for absorption and is itself absorbed. It is used as cholagogue and choleretic.
1	1165	0.380	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
2	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.
2	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
2	1480	0.536	Others	Cinnamic acid exerts anti-diabetic activity by improving glucose tolerance in vivo and by stimulating insulin secretion in vitro.
2	1432	0.450	NF-?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
2	520	0.447	Others	Extracted from Lonicera acuminata.Wall.;Suitability:Ethanol and acetone;Store the product in sealed,cool and dry condition
3	1592	0.782	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	0.656	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	973	0.509	"GABAR agonist; GluR;PPAR agonist; androstenedione; estra	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;
3	1381	0.424	"Farnesoid X receptor;VD"	A bile acid formed from chenodeoxycholate by bacterial action, usually conjugated with glycine or taurine. It acts as a detergent to solubilize fats for absorption and is
3	1165	0.397	Biliation activator	itself absorbed. It is used as cholagogue and choleretic.
4	520	1.000	Others	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 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-?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

4	1134	0.275	Others	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
4	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
5	1592	1.000	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.
5	514	0.629	Others	Extracted from Glycine max(L.)Merr.;Suitability:Chloroform,benzene,ethyl

Torna al form
| Tutorial (PDF) | | lemon (PDF) | | chamomile (PDF) |

Ivy compounds:

Ederacoside

C[C@H]1[C@@H]([C@H]([C@H]([C@@H](O1)O[C@@H]2[C@H](O[C@H]([C@@H]([C@H]2O)O)OC[C@@H]3[C@H]([C@@H]([C@H]([C@@H](O3)OC(=O)[C@@]45CC[C@@]6(C(=CC[C@H]7[C@]6(CC[C@@H]8[C@@]7(CC[C@@H]([C@@]8(C)CO)O[C@H]9[C@@H]([C@H]([C@H](CO9)O)O)O)O[C@H]1[C@@H]([C@@H]([C@H]([C@@H](O1)C)O)O)O)C)C)[C@@H]4CC(CC5)(C)C)C)O)O)CO)O)O)O

Alfa hederin

C[C@H]1[C@@H]([C@H]([C@H]([C@@H](O1)O[C@@H]2[C@H]([C@H](CO[C@H]2O[C@H]3CC[C@]4([C@H]([C@]3(C)CO)CC[C@@]5([C@@H]4CC=C6[C@]5(CC[C@@]7([C@H]6CC(CC7)(C)C)C(=O)O)C)C)C)O)O)O)O

Beta carotene

CC1=C(C(CCC1)(C)C)/C=C/C(=C/C=C/C(=C/C=C/C=C(/C=C/C=C(/C=C/C2=C(CCCC2(C)C)C)\C)\C)/C)/C

Beta sitosterol

CC[C@H](CC[C@@H](C)[C@H]1CC[C@@H]2[C@@]1(CC[C@H]3[C@H]2CC=C4[C@@]3(CC[C@@H](C4)O)C)C)C(C)C

Caffeic acid

C1=CC(=C(C=C1/C=C/C(=O)O)O)O

Campesterol

C[C@H](CC[C@@H](C)C(C)C)[C@H]1CC[C@@H]2[C@@]1(CC[C@H]3[C@H]2CC=C4[C@@]3(CC[C@@H](C4)O)C)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

Cholesterol

C[C@H](CCCC(C)C)[C@H]1CC[C@@H]2[C@@]1(CC[C@H]3[C@H]2CC=C4[C@@]3(CC[C@@H](C4)O)C)C

Cis vaccenic acid

CCCCCC/C=C\CCCCCCCCCC(=O)O

Emetin

CC[C@H]1CN2CCC3=CC(=C(C=C3[C@@H]2C[C@@H]1C[C@@H]4C5=CC(=C(C=C5CCN4)OC)OC)OC)OC

Falcarinol

CCCCCCC/C=C\CC#CC#C[C@@H](C=C)O

Falcarinone

CCCCCCC/C=C\CC#CC#CC(=O)C=C

Ederagenin

C[C@]12CC[C@@H]([C@@]([C@@H]1CC[C@@]3([C@@H]2CC=C4[C@]3(CC[C@@]5([C@H]4CC(CC5)(C)C)C(=O)O)C)C)(C)CO)O

Hidroxy cinnamic acid

C1=CC(=CC=C1/C=C/C(=O)O)O

Kaempferol

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

Oleanolic acid

C[C@]12CC[C@@H](C([C@@H]1CC[C@@]3([C@@H]2CC=C4[C@]3(CC[C@@]5([C@H]4CC(CC5)(C)C)C(=O)O)C)C)(C)C)O

Oleic acid

CCCCCCCC/C=C\CCCCCCCC(=O)O

Palmitoleic acid

CCCCCC/C=C\CCCCCCCC(=O)O

Panaxidol

CCCCCCC[C@H]1[C@H](O1)CC#CC#C[C@@H](C=C)O

Petroselinic acid

CCCCCCCCCCC/C=C\CCCCC(=O)O

Quercetin

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

Rosmarinic acid

C1=CC(=C(C=C1C[C@H](C(=O)O)OC(=O)/C=C/C2=CC(=C(C=C2)O)O)O)O

Scopolin

COC1=C(C=C2C(=C1)C=CC(=O)O2)O[C@H]3[C@@H]([C@H]([C@@H]([C@H](O3)CO)O)O)O

Stigmasterol

CC[C@H](/C=C/[C@@H](C)[C@H]1CC[C@@H]2[C@@]1(CC[C@H]3[C@H]2CC=C4[C@@]3(CC[C@@H](C4)O)C)C)C(C)C

Hellicoside

C1=CC(=C(C=C1/C=C/C(=O)O[C@@H]2[C@H](O[C@H]([C@@H]([C@H]2O[C@H]3[C@@H]([C@H]([C@@H]([C@H](O3)CO)O)O)O)O)OC[C@H](C4=CC(=C(C=C4)O)O)O)CO)O)O

Vitamin C

C([C@@H]([C@@H]1C(=C(C(=O)O1)O)O)O)O

Vitamin E

CC1=C(C2=C(CC[C@@](O2)(C)CCC[C@H](C)CCC[C@H](C)CCCC(C)C)C(=C1O)C)C