Biological activity estimation results

Of **Chamomile**

Chamomile compounds:

α-bisabolol

CC1=CC[C@@H](CC1)[C@@](C)(CCC=C(C)C)O

bisabolol oxide A

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

bisabolene oxide

CC1CC(OC12CCC(=CC2)C)C=C(C)C

Chamazulene

CCC1=CC2=C(C=CC2=C(C=C1)C)C

Matricin

C[C@H]1[C@@H]2[C@H](CC(=C3C=C[C@@]([C@@H]3[C@H]2OC1=O)(C)O)C)OC(=O)C

Farnesene

CC(=CCC/C(=C/C/C=C(\C)/C=C)/C)C

Apigenin

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

Luteolin

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

Quercetin

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

Rutin

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=C(OC4=CC(=CC(=C4C3=O)O)O)C5=CC(=C(C=C5)O)O)O)O)O)O)O)O

Herniarin

COC1=CC2=C(C=C1)C=CC(=O)O2

Umbelliferone

C1=CC(=CC2=C1C=CC(=O)O2)O

chlorogenic acid

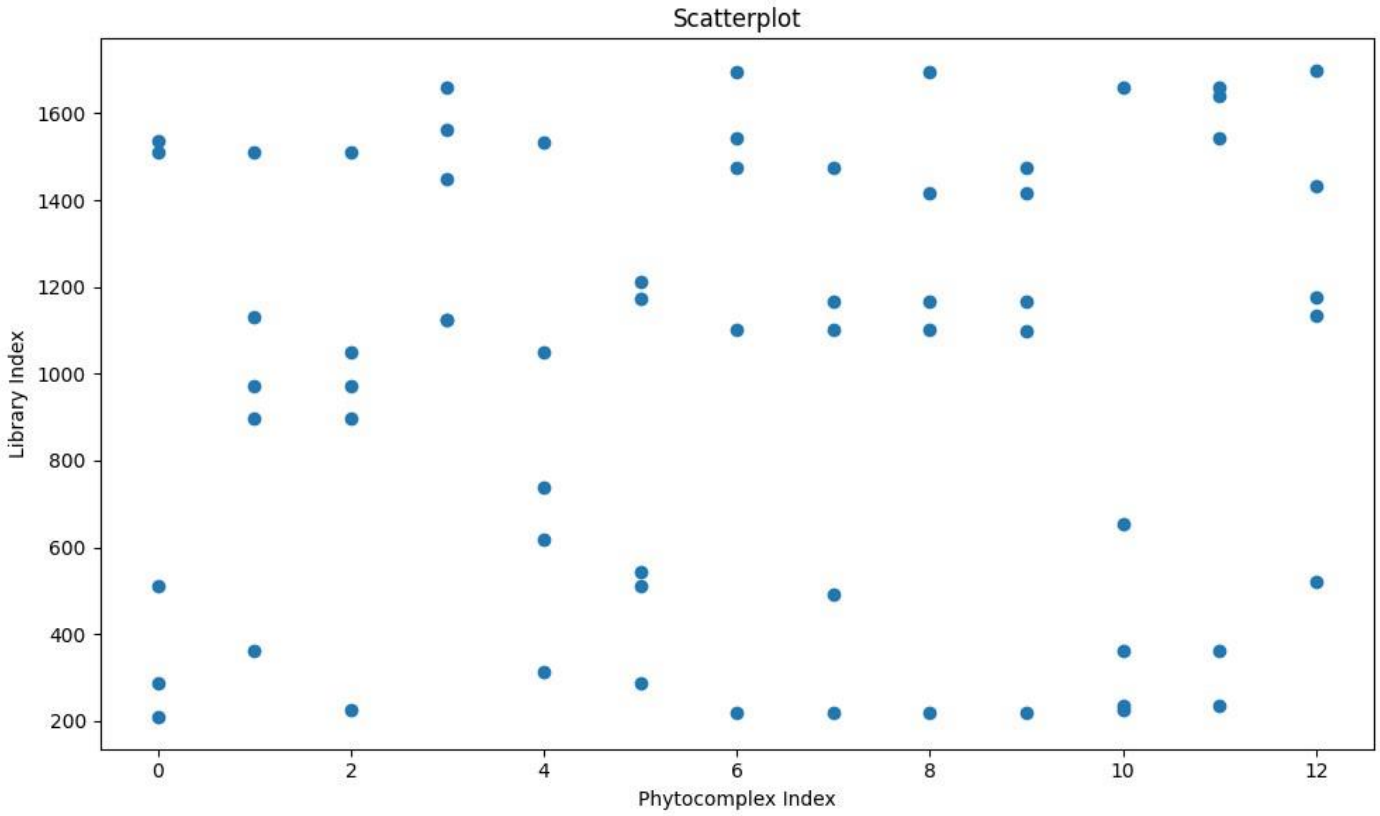
C1[C@H]([C@H]([C@@H](C[C@@]1(C(=O)O)O)OC(=O)/C=C/C2=CC(=C(C=C2)O)O)O)O

Reference:

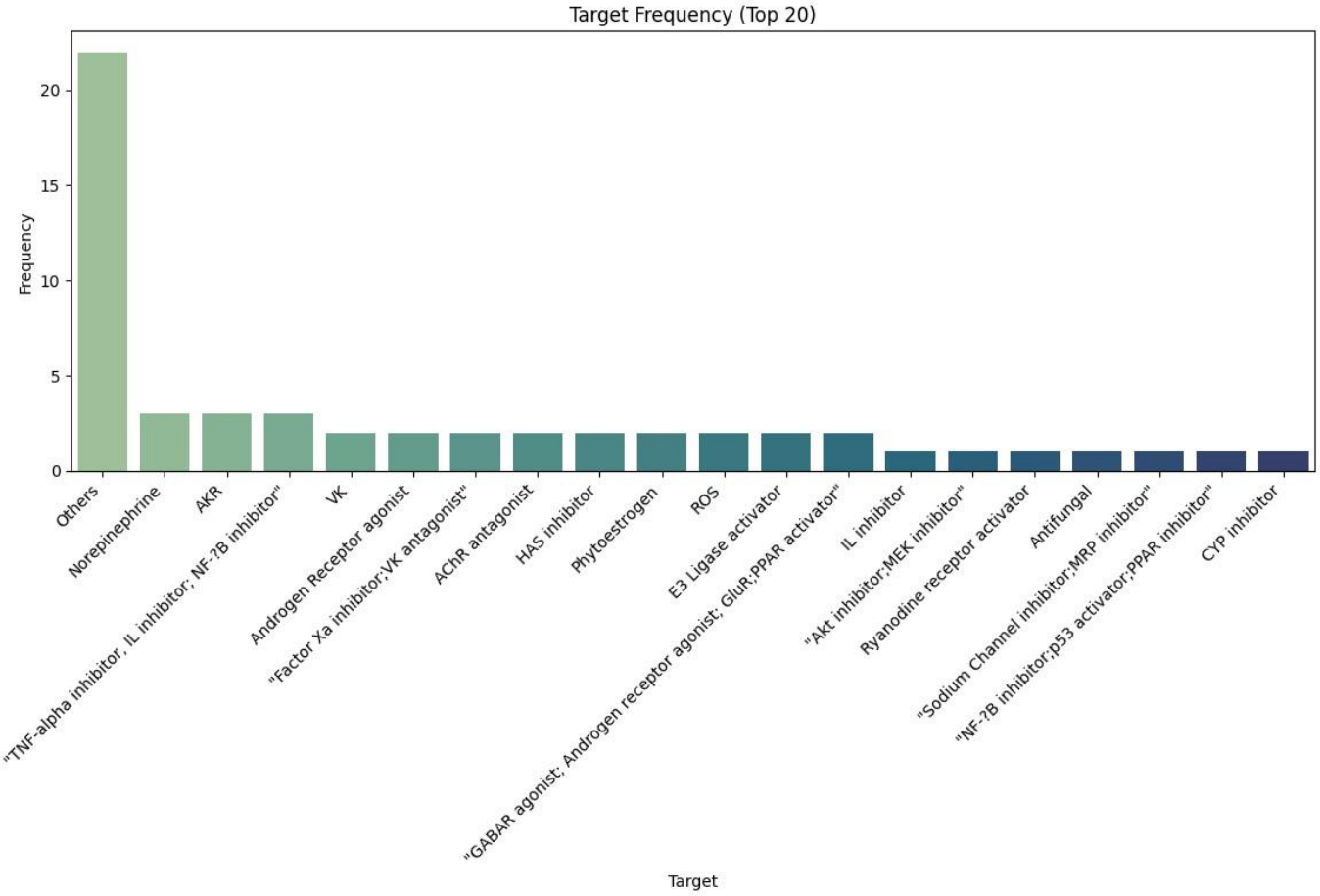
Dai YL, Li Y, Wang Q, Niu FJ, Li KW, Wang YY, Wang J, Zhou CZ, Gao LN. Chamomile: A Review of Its Traditional Uses, Chemical Constituents, Pharmacological Activities and Quality Control Studies. Molecules. 2022 Dec 23;28(1):133. doi: 10.3390/molecules28010133. PMID: 36615326; PMCID: PMC9822300.

Graph:

Scatterplot



Barplot



Let's analyze the chamomile compound fingerprint comparison barplot and relate the findings to its traditional uses.

Understanding the Barplot

The barplot shows the frequency of predicted targets for chamomile compounds when compared against a library of 1700 compounds. Each bar's height corresponds to how often a specific target is predicted to interact with chamomile's compounds.

Analysis of the Barplot

1. **"Others"**: This category usually represents a diverse set of targets not specifically listed. The high frequency here suggests chamomile compounds interact with a wide range of biological pathways, aligning with its traditional diverse applications.
2. **Norepinephrine**: This neurotransmitter is involved in the "fight-or-flight" response and stress regulation. The high frequency suggests chamomile compounds might interact with the adrenergic system, potentially explaining its calming and anti-anxiety effects.

3. **AKR**: This likely refers to Aldo-keto reductases, enzymes involved in various metabolic processes. The moderate frequency suggests chamomile compounds could interact with these enzymes, though the specific implications need further investigation.
4. **"TNF-alpha inhibitor; IL inhibitor; NF-?B inhibitor"**: This target relates to inflammation pathways. The moderate frequency suggests chamomile compounds might have some anti-inflammatory potential, supporting its traditional use for soothing inflammation.
5. **AChR antagonist**: This target relates to the cholinergic system, involved in muscle contraction and nerve signaling. The moderate frequency suggests chamomile compounds could interact with this system, potentially explaining its traditional use for digestive issues.
6. **Other Targets**: The remaining targets (VK, Androgen Receptor agonist, "Factor Xa inhibitor; VK antagonist", HAS inhibitor, Phytoestrogen) show lower frequencies, suggesting weaker interactions with chamomile compounds.

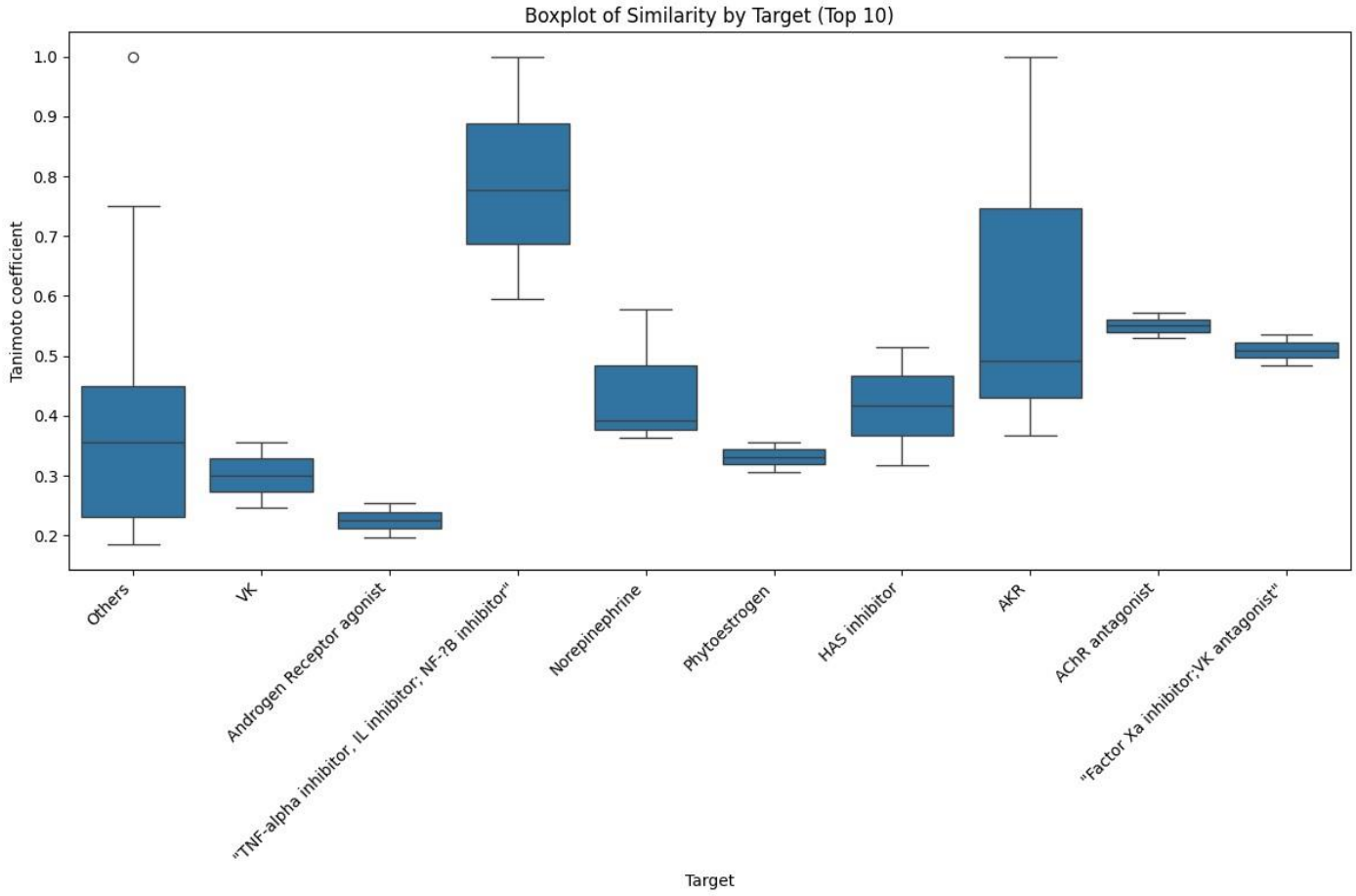
Comparison with Traditional Uses

- **Diverse Applications**: The high frequency in the "Others" category supports chamomile's traditional use for a wide range of ailments.
- **Calming Effects**: The strong interaction with the norepinephrine system could explain its use for relaxation and anxiety relief.
- **Anti-inflammatory**: The moderate interaction with inflammation-related targets supports its traditional use for soothing inflammation.
- **Digestive Aid**: The moderate interaction with the cholinergic system could relate to its use for digestive issues.

Important Considerations

- **Frequency vs. Activity**: High frequency in predicted targets doesn't automatically mean the compound has that biological activity. Further research is needed to validate these predictions.
- **Traditional Use**: Traditional uses are based on historical observations and may not have undergone rigorous scientific validation.

Boxplot



Let's analyze the chamomile compound fingerprint comparison boxplot and relate the findings to its traditional uses.

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 indicates a wider range of similarity.
- **Line in the Box**: The line inside represents the median similarity score for that target.
- **Whiskers**: They extend to the highest and lowest values within 1.5 times the IQR from the box. Outliers are plotted as individual points.

Analysis of the Boxplot

1. **"Others"**: This category usually encompasses a wide array of targets not specifically listed. The broad distribution here suggests chamomile compounds might interact with diverse biological pathways, fitting its traditional uses for various ailments.
2. **VK**: This likely refers to Vitamin K or a related target. The low similarity scores suggest chamomile compounds don't strongly resemble known Vitamin K-interacting molecules.
3. **Androgen Receptor agonist**: The low similarity scores here indicate that chamomile compounds do not exhibit strong similarity to known Androgen Receptor agonists.
4. **"TNF-alpha inhibitor; IL inhibitor; NF-7B inhibitor"**: This target relates to inflammation pathways. The moderate similarity scores suggest chamomile compounds might have some anti-inflammatory potential, aligning with its traditional use for soothing inflammation.

5. **Norepinephrine**: This neurotransmitter is involved in the "fight-or-flight" response. The moderate similarity scores suggest chamomile compounds could interact with the adrenergic system, potentially relating to its calming effects.
6. **Phytoestrogen**: These are plant-derived compounds with estrogen-like effects. The low similarity scores suggest that chamomile compounds do not exhibit strong similarity to known Phytoestrogens.
7. **HAS inhibitor**: This target relates to the histamine pathway, often involved in allergic reactions. The low similarity scores suggest that chamomile compounds do not exhibit strong similarity to known HAS inhibitors.
8. **AKR**: This likely refers to Aldo-keto reductases, enzymes involved in various metabolic processes. The high similarity scores suggest chamomile compounds might interact with these enzymes, though the specific implications need further investigation.
9. **AChR antagonist**: This target relates to the cholinergic system, involved in muscle contraction and nerve signaling. The moderate similarity scores suggest chamomile compounds could interact with this system, potentially explaining its traditional use for digestive issues.
10. **"Factor Xa inhibitor; VK antagonist"**: This target relates to blood clotting. The low similarity scores suggest that chamomile compounds do not exhibit strong similarity to known "Factor Xa inhibitor; VK antagonist".

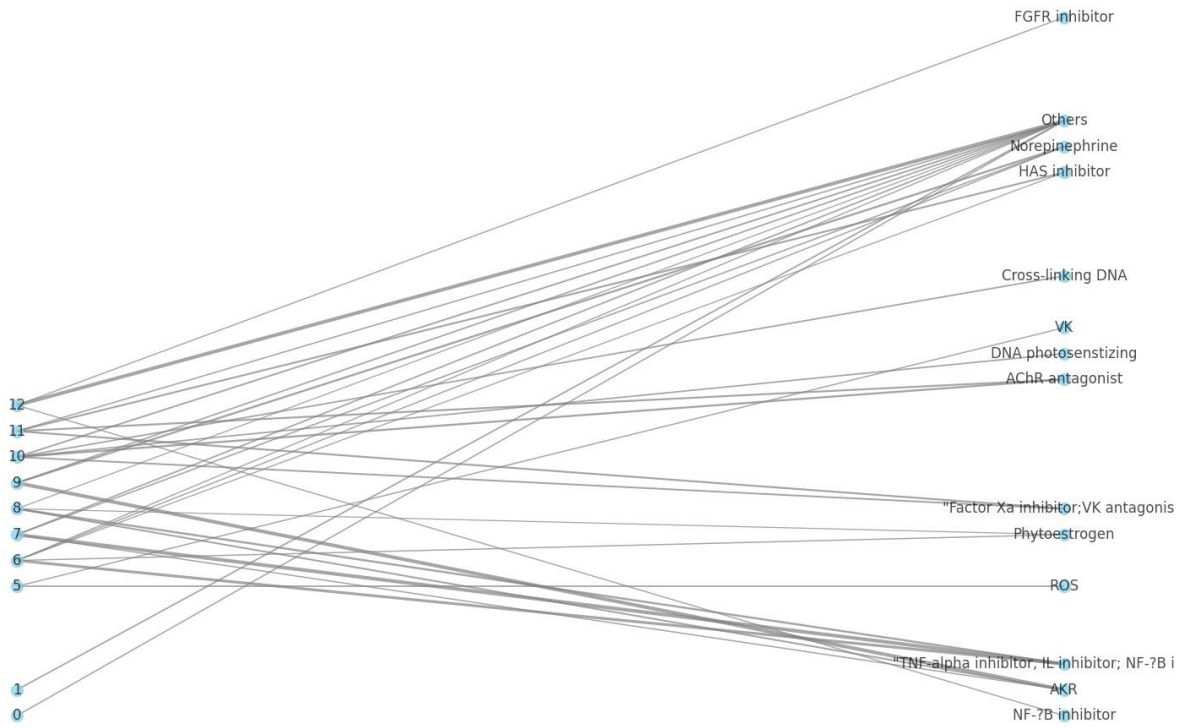
Comparison with Traditional Uses

- **Anti-inflammatory**: The moderate similarity to inflammation-related targets supports chamomile's traditional use for calming inflammation.
- **Calming effects**: The potential interaction with the norepinephrine system could explain its use for relaxation and anxiety relief.
- **Digestive aid**: The potential interaction with the cholinergic system could relate to its use for digestive issues.

Important Considerations

- **Similarity vs. Activity**: High similarity doesn't automatically mean the compound has that biological activity. Further research is needed to confirm these predictions.
- **Traditional Use**: Traditional uses are based on historical observations and may not have undergone rigorous scientific validation.

Network Graph:



Comparison Results (Tanimoto coefficient):

Query Index	Library Index	Tanimoto Similarity	Target	Bioactivity
0	1512	0.372	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
0	512	0.246	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
0	286	0.224	ROS	Extracted?from?Papaya fruit, marigold flower petals;Store?the?product?in?sealed,?cool?and?dry?condition
0	1538	0.217	Others	Terpin hydrate is an expectorant, commonly used to loosen mucus in patients presenting with acute or chronic bronchitis, and related conditions. It is derived from sources such as oil of turpentine, oregano, thyme and eucalyptus. Though it
0	210	0.209	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
1	1512	0.425	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

Query Library Tanimoto

	Target		Bioactivity
Index	**Index**	**Similarity**	

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