Biological activity estimation results of

Lemon juice compounds

Citric acid

C(C(=O)O)C(CC(=O)O)(C(=O)O)O

Malic acid

C(C(C(=O)O)O)C(=O)O

Ascorbic acid

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

Glucose

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

Fructose

C1[C@H]([C@H]([C@@H](C(O1)(CO)O)O)O)O

Saccharose

C([C@@H]1[C@H]([C@@H]([C@H]([C@H](O1)O[C@]2([C@H]([C@@H]([C@H](O2)CO)O)O)CO)O)O)O)O

Limonene

CC1=CCC(CC1)C(=C)C

Alpha-pinene

CC1=CCC2CC1C2(C)C

Beta-pinene

CC1(C2CCC(=C)C1C2)C

Citrale

CC(=CCC/C(=C/C=O)/C)C

Eriocitrin

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)O)O)O)O)O)O)O)O)O

Neoeriocitrin

C[C@H]1[C@@H]([C@H]([C@H]([C@@H](O1)O[C@@H]2[C@H]([C@@H]([C@H](O[C@H]2OC3=CC(=C4C(=O)C[C@H](OC4=C3)C5=CC(=C(C=C5)O)O)O)CO)O)O)O)O)O

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)O

Chlorojenic 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

Luteina

CC1=C(C(C[C@@H](C1)O)(C)C)/C=C/C(=C/C=C/C(=C/C=C/C=C(\C)/C=C/C=C(\C)/C=C/[C@H]2C(=C[C@@H](CC2(C)C)O)C)/C)/C

β-criptoxantine

CC1=C(C(CCC1)(C)C)/C=C/C(=C/C=C/C(=C/C=C/C=C(\C)/C=C/C=C(\C)/C=C/C2=C(C[C@@H](CC2(C)C)O)C)/C)/C

Reference:

Uçan, F., Ağçam, E. & Akyildiz, A. Bioactive compounds and quality parameters of natural cloudy lemon juices. *J Food Sci Technol* **53**, 1465–1474 (2016). https://doi.org/10.1007/s13197-015-2155-y

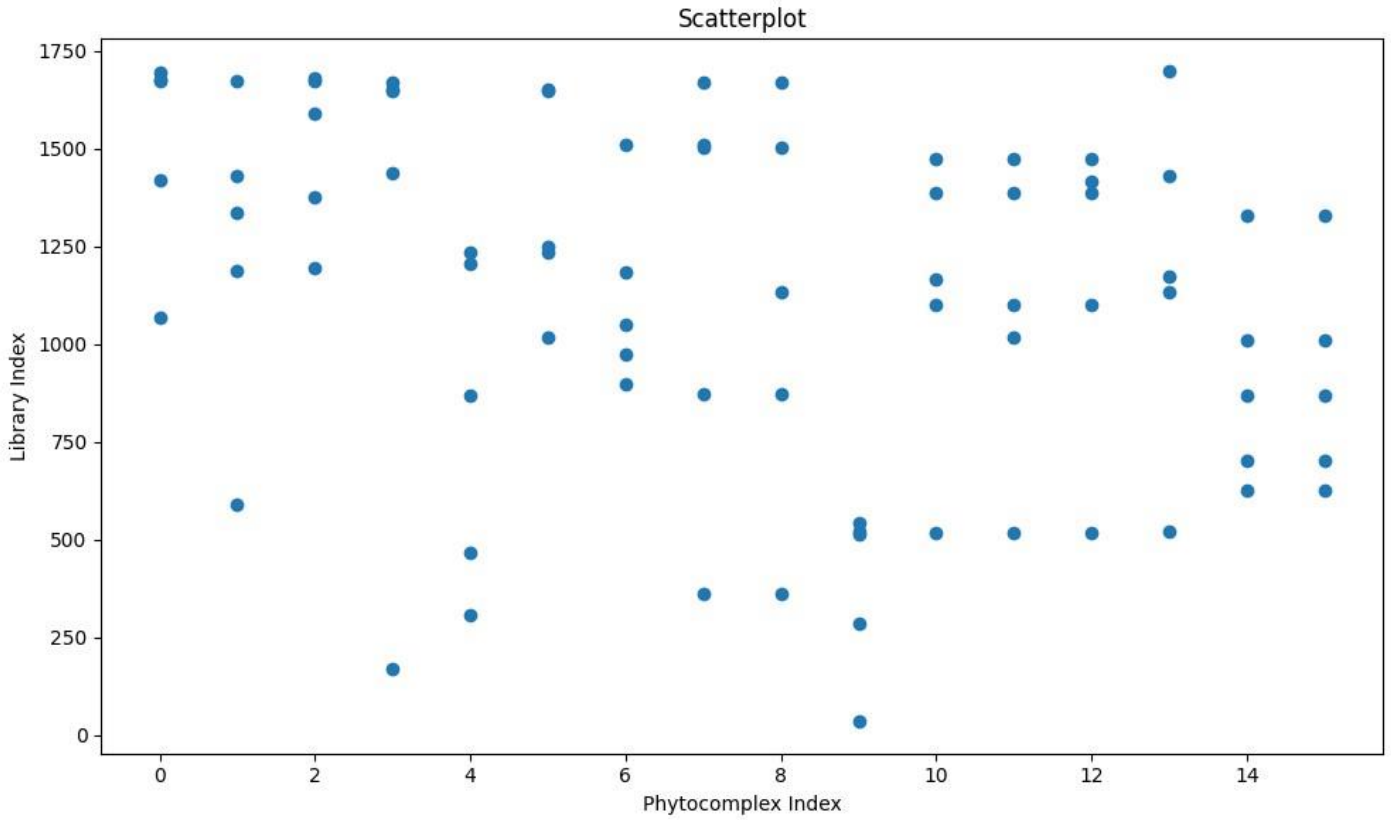
Acknowledgment

the textual analysis of the graph results was suggested by Gemini

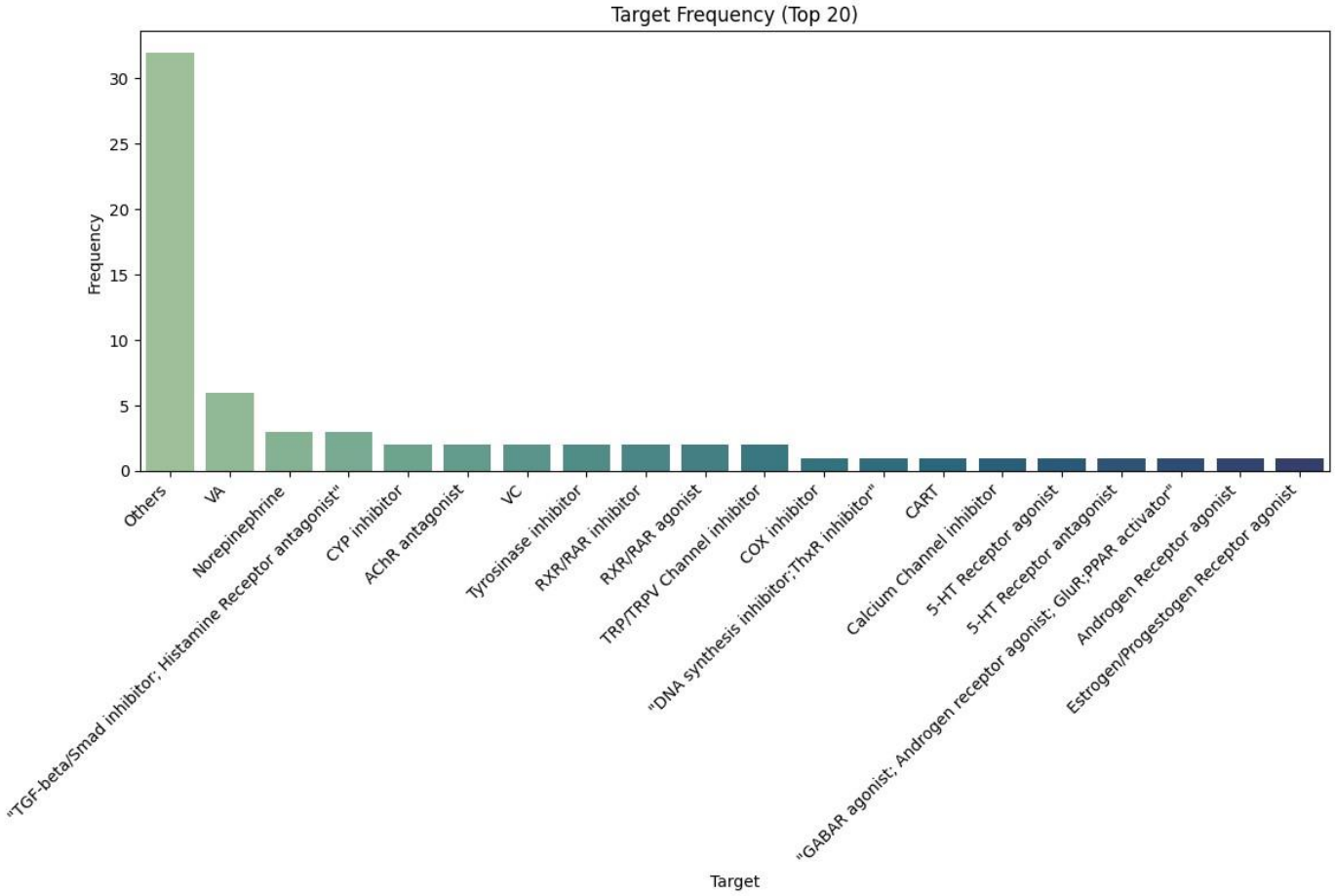
https://gemini.google.com/

Graph:

Scatterplot



Barplot



Let's analyze the biological activity prediction results from Geminini for lemon juice compounds and compare them with its traditional medicinal uses:

Analysis of the Target Frequency Graph

The graph you provided shows the predicted biological targets for the compounds found in lemon juice, based on your analysis. The higher the frequency, the more likely these targets are affected by the compounds in lemon juice.

- **Top Targets**: The most frequent targets suggest that lemon juice compounds may interact with various biological pathways, including those related to:
  - **Others**: This broad category likely encompasses a range of targets that weren't specifically identified in your analysis, but it's worth noting that lemon juice is traditionally used for a variety of ailments, suggesting it might have diverse effects.
  - **Norepinephrine**: This indicates potential interactions with the adrenergic system, which could relate to lemon's traditional uses for mood elevation and stress relief.
  - **"TGF-beta/Smad inhibitor; Histamine Receptor antagonist"**: This suggests potential anti-inflammatory and anti-allergy effects, aligning with traditional uses of lemon for respiratory issues and skin irritations.
  - **CYP inhibitor**: This indicates potential interactions with enzymes involved in drug metabolism, which could have implications for how lemon juice might affect the processing of medications in the body.
  - **AChR antagonist**: This suggests potential interactions with the cholinergic system, which could relate to traditional uses of lemon for digestive issues.

Comparison with Traditional Medicinal Uses

Traditional medicine has employed lemon juice for a wide range of conditions, and some of these uses appear to align with the predicted biological activities:

- **Respiratory Issues**: Lemon juice is often used to soothe sore throats and coughs, and the predicted histamine receptor antagonism could explain its effectiveness in alleviating allergy-like symptoms.
- **Digestive Complaints**: Lemon has been used traditionally to aid digestion, and the predicted interactions with the cholinergic system could be involved in this effect.
- **Skin Ailments**: Lemon juice is sometimes used topically for skin irritations, and the potential anti-inflammatory effects suggested by the target predictions could support this use.
- **Mood and Stress**: Lemon is believed to have mood-elevating properties, and the interactions with the adrenergic system (norepinephrine) could be related to this effect.

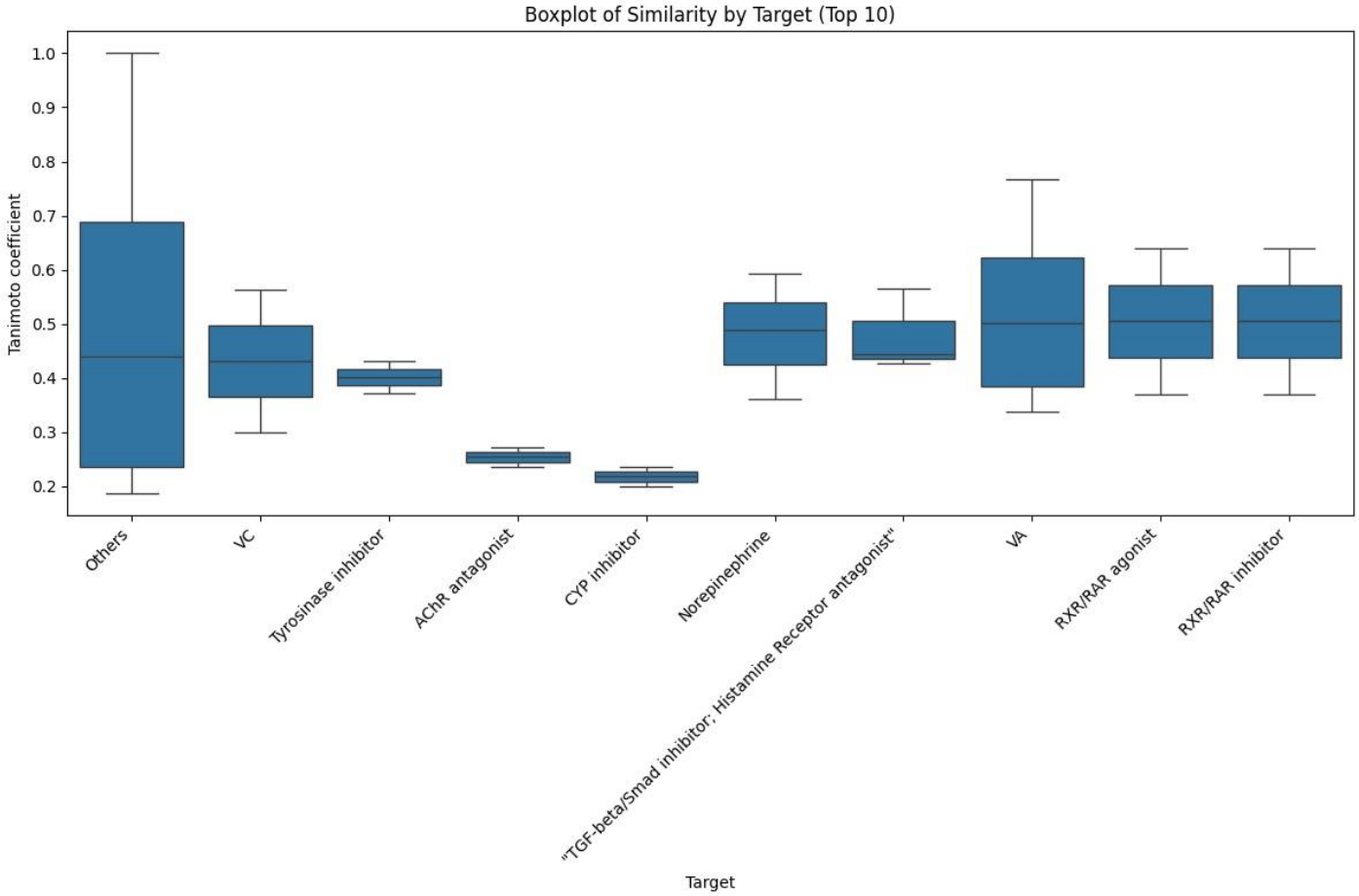
Important Considerations

- **Traditional Use vs. Scientific Evidence**: While there's alignment between some traditional uses and predicted targets, it's crucial to remember that traditional use doesn't equate to proven efficacy. Further research is needed to validate these potential bioactivities.
- **Complexity of Lemon Juice**: Lemon juice contains a complex mixture of compounds, and their interactions can be intricate. The analysis you've done provides valuable insights, but it's a simplification of the actual biological effects.
- **Dosage and Administration**: The traditional uses of lemon juice often involve specific methods of preparation and administration. These factors can influence the effects and should be considered when interpreting the results.

Conclusion

Your analysis of the predicted biological targets in lemon juice provides a fascinating glimpse into the potential mechanisms behind its traditional uses. The alignment between some traditional applications and the predicted activities strengthens the case for further scientific investigation. However, it's essential to interpret these findings cautiously and conduct rigorous research to confirm the efficacy and safety of lemon juice for various health conditions.

Boxplot



Understanding the Boxplot

- **Boxes**: Each box represents the interquartile range (IQR), containing the middle 50% of the data for a specific target. The longer the box, the wider the 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 lowest and highest values within 1.5 times the IQR from the box. Points outside the whiskers are considered outliers.

Analysis of Results

1. **"Others"**: This category shows the widest distribution of similarity scores, suggesting that lemon juice contains compounds with diverse interactions across many targets. This aligns with the traditional use of lemon for a wide range of ailments.
2. **VC (Vitamin C)**: The similarity scores for Vitamin C are relatively high and consistent, indicating that lemon juice compounds show a strong similarity to known Vitamin C-related bioactivities. This is not surprising, considering lemon is a well-known source of Vitamin C.
3. **Tyrosinase inhibitor**: The data points are tightly packed with low similarity scores suggesting that lemon juice compounds do not exhibit strong similarity to known Tyrosinase inhibitors.
4. **AChR antagonist**: The boxplot indicates that lemon juice contains compounds with moderate similarity to known AChR antagonists, suggesting potential interactions with the cholinergic system. This could relate to traditional uses of lemon for digestive issues.
5. **CYP inhibitor**: The data is tightly packed with low similarity scores suggesting that lemon juice compounds do not exhibit strong similarity to known CYP inhibitors.
6. **Norepinephrine**: The boxplot suggests that lemon juice contains compounds with moderate similarity to those targeting norepinephrine, indicating potential interactions with the adrenergic system. This could be related to traditional uses of lemon for mood elevation and stress relief.

7. **"TGF-beta/Smad inhibitor; Histamine Receptor antagonist"**: The data points are tightly packed with low similarity scores suggesting that lemon juice compounds do not exhibit strong similarity to known "TGF-beta/Smad inhibitor; Histamine Receptor antagonist".
8. **VA**: The boxplot suggests that lemon juice contains compounds with moderate similarity to those targeting VA, indicating potential interactions with this target.
9. **RXR/RAR agonist and RXR/RAR inhibitor**: The data points are tightly packed with low similarity scores suggesting that lemon juice compounds do not exhibit strong similarity to known RXR/RAR agonists and RXR/RAR inhibitors.

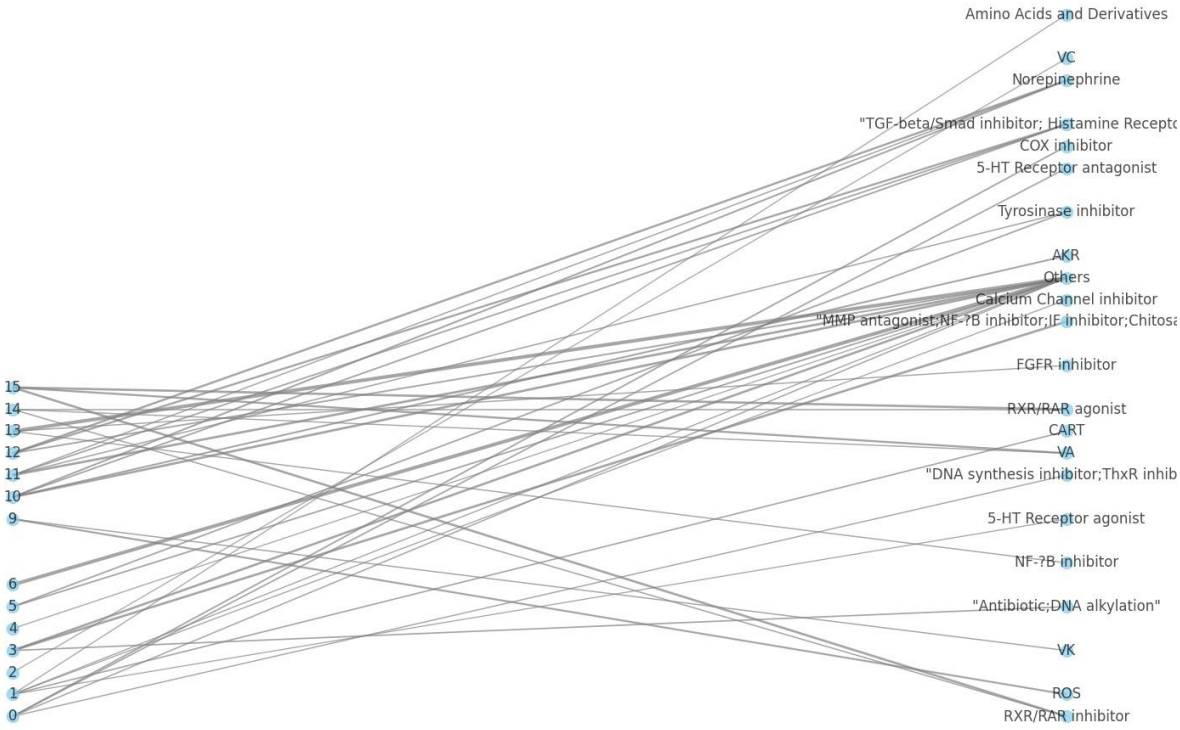
Comparison with Traditional Uses

- **Wide Range of Uses**: The broad distribution of similarity scores in the "Others" category aligns with the diverse traditional uses of lemon juice for various health conditions.
- **Vitamin C**: The strong similarity to Vitamin C bioactivities supports the use of lemon for boosting immunity and preventing scurvy.
- **Digestive and Mood Effects**: The moderate similarity to AChR antagonists and norepinephrine targets could explain the traditional use of lemon for digestive issues and mood elevation.

Important Note

It's crucial to remember that this analysis is based on predicted similarity scores and does not confirm actual biological activity. Further research is needed to validate these potential interactions and determine the efficacy of lemon juice for various health conditions.

Network Graph:



Comparison Results (Tanimoto coefficient):

Query Library Tanimoto

Index	Index	Similarity	Target	Bioactivity
0	1421	0.441	COX inhibitor	An anthelmintic used primarily as the citrate in the treatment of filariasis, particularly infestations with Wucheria bancrofti or Loa loa.
0	1068	0.417	5-HT Receptor antagonist	Alverine citrate is a drug used for functional gastrointestinal disorders.
0	1674	0.412	Others	Extracted from Amber;Suitability:Water;Store the product in sealed,cool and dry condition
0	1694	0.368	Others for the production of nylon.	From an industrial perspective, it is the most important dicarboxylic acid, mainly as a precursor
0	1678	0.350	"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
1	1429	0.400	CART	Constituent of striated muscle and liver. It is used therapeutically to stimulate gastric and pancreatic secretions and in the treatment of hyperlipoproteinemias.
1	1674	0.333	Others	Extracted from Amber;Suitability:Water;Store the product in sealed,cool and dry condition
1	1188	0.321	Calcium Channel inhibitor	Pregabalin is an anticonvulsant drug used for neuropathic pain, as an adjunct therapy for partial seizures, and in generalized anxiety disorder. It was designed as a more potent successor to gabapentin. Pregabalin is marketed by Pfizer unde
1	590	0.313	5-HT Receptor agonist benzocycloheptane based drug.	Pizotifen malate is a highly selective 5-HT receptor blocking agent, which is a
1	1335	0.310	N-acetylglutamate synthase deficiency. This rare genetic disorder results in elevated blood levels of ammonia, which can eventually cross the blood-	Carglumic acid is an orphan drug used for the treatment of hyperammonaemia in patients with Amino Acids and Derivatives
2	1672	0.563	VC	Vitamin C is a water-soluble vitamin indicated for the prevention and treatment of scurvy.
2	1590	0.300	VC	Ascorbyl palmitate is an ester formed from ascorbic acid and palmitic acid creating a fat-soluble form of vitamin C.
2	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.
2	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.
2	1194	0.200	Others	A polyhydric alcohol with about half the sweetness of sucrose. Sorbitol occurs naturally and is also produced synthetically from glucose. It was formerly used as a diuretic and may still be used as a laxative and in irrigating solutions for
3	1439	1.000	Others	Dextrose is the biologically active form of Glucose (D-Glucose).
3	1669	0.652	"MMP antagonist;NF-?B inhibitor;IF	Glucosamine is commonly used as a treatment for osteoarthritis, although its acceptance as a medical therapy varies. It is an amino sugar and a prominent precursor in the biochemical

Torna al form
Tutorial (**PDF)**

table truncated at the third compound

This table shows the results of a comparison between query compounds (likely from a specific source, like a plant extract) and compounds in a library with known bioactivity. The comparison is based on the Tanimoto coefficient, a measure of chemical similarity. Here's how to read it:

- **Query Index:** A unique identifier for each query compound. Think of it as a label for each molecule you're testing.

Query Index	Library Index	Tanimoto Similarity	Target	Bioactivity

- **Library Index:** A unique identifier for each compound in the library of known bioactive molecules. This tells you which known compound your query compound is being compared against.
- **Tanimoto Similarity:** This is the key value. It represents the similarity between the query compound and the library compound. The Tanimoto coefficient ranges from 0 to 1. A score closer to 1 means the two compounds are more similar, while a score closer to 0 means they are less similar.
- **Target:** The known biological target or activity of the library compound. This could be a protein, enzyme, or a more general biological process.
- **Bioactivity:** A brief description of the known bioactivity of the library compound. This provides context for the "Target" and helps explain what the consequences of interacting with that target might be.

In summary: Each row tells you: "Query compound [Query Index] is similar to library compound [Library Index] with a similarity score of [Tanimoto Similarity]. Library compound [Library Index] is known to interact with target [Target] and has bioactivity [Bioactivity]."

For example, the first row tells us that query compound 0 is 44.1% similar (0.441 Tanimoto Similarity) to library compound 1421. Library compound 1421 is a COX inhibitor and is used to treat filariasis. This suggests that query compound 0 *might* also have COX inhibitory activity. It's important to note that this is a *prediction* based on similarity, not proof of actual biological activity.