

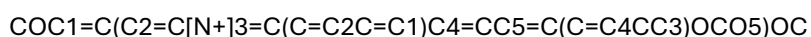
Biological activity estimation results Of

Pumpkin seeds

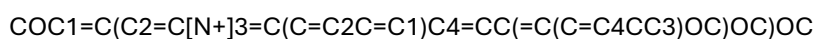
Pumpkin seeds compounds(Evaluation of Anthelmintic Activity and Composition of Pumpkin (Cucurbita pepo L.) Seed Extracts—In Vitro and in Vivo Studies)

by Maciej Grzybek ,Wirginia Kukula-Koch ,Aneta Strachecka ,Aleksandra Jaworska ,Andrew M. Phiri ,Jerzy Paleolog andKrzysztof Tomczuk)

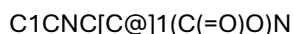
Berberine



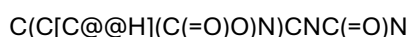
Palmatine



Cucurbitine



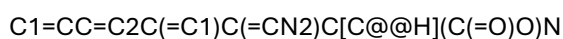
Citrulline



Valine



Tryptophan



Phenylalanine



Adenosine



Palmitic acid



Palmitoleic acid



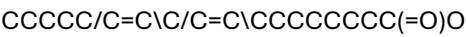
stearic acid



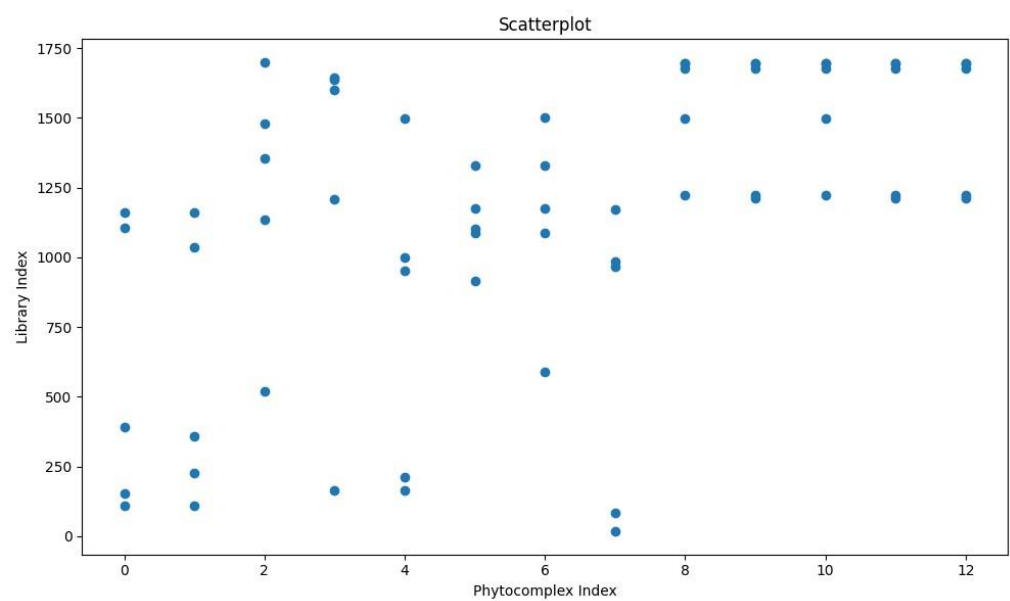
Oleic acid



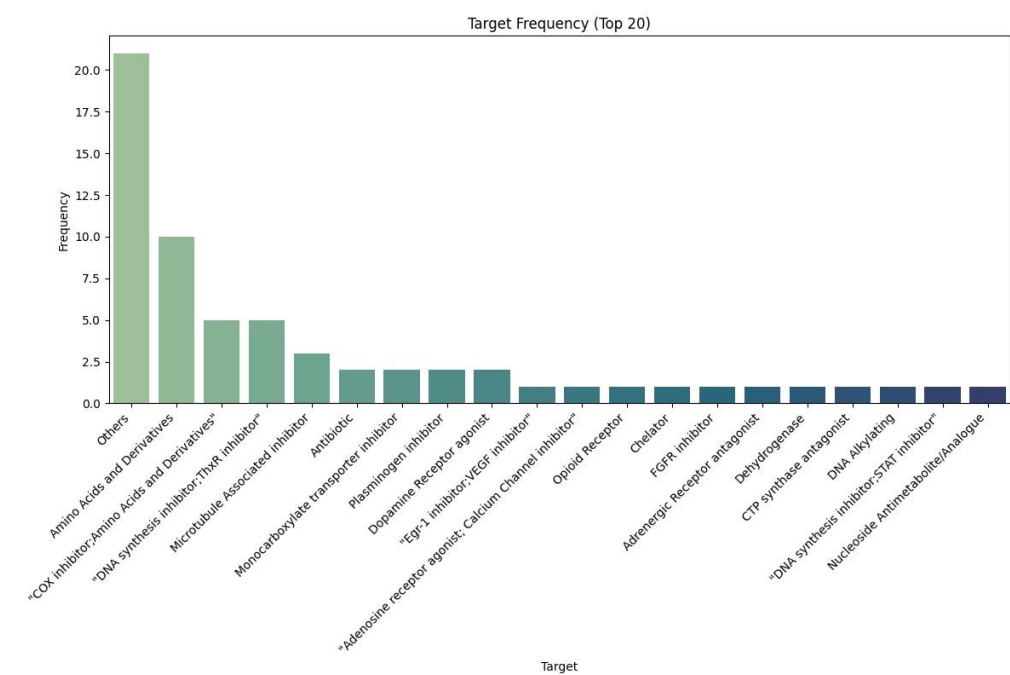
alpha linoleic acid



Scatterplot



Barplot



Let's analyze with Gemini (2.0) the TestBio graph of pumpkin seed compounds, compare the results with traditional uses, and explore their applications in supplements.

Analysis of TestBio Results

The graph reveals the top 20 targets (likely proteins or biological pathways) that pumpkin seed compounds interact with, based on TestBio's library comparison. Here's a breakdown:

- **Dominant Targets:** The most frequent targets suggest that pumpkin seeds have a strong affinity for compounds that influence:
 - Amino acid and derivative pathways
 - Cox inhibition (related to inflammation)
 - DNA synthesis and ThxR inhibition (potentially impacting cell growth)
 - Microtubule-associated inhibition (also related to cell growth)
- **Diverse Interactions:** The presence of various targets indicates that pumpkin seeds may exert a range of biological effects. These include potential:
 - Antibiotic activity
 - Effects on transporters and receptors (impacting signaling and cellular processes)
 - Modulation of enzymes (like dehydrogenase and CTP synthase)
 - Interactions with DNA alkylating agents and other compounds with potential therapeutic applications.

Comparison with Traditional Uses

Traditional medicine has utilized pumpkin seeds for centuries, particularly for:

- **Prostate Health:** Traditional uses for pumpkin seeds often include treating benign prostatic hyperplasia (BPH) and related urinary issues. This aligns with the graph's indication of interactions with receptors and pathways relevant to the prostate.
- **Parasite Elimination:** Pumpkin seeds have been used as a natural remedy for intestinal parasites. The graph's suggestion of potential antibiotic activity could provide a scientific basis for this use.
- **Diuretic Effects:** Traditional medicine also employed pumpkin seeds to increase urine flow. This may be linked to the compound's influence on transporters and kidney function.

Use in Supplements

The diverse potential bioactivities suggested by TestBio results are reflected in the growing popularity of pumpkin seed supplements. These supplements are marketed for:

- **Prostate Health:** Saw palmetto is a commonly used herbal remedy for BPH, but pumpkin seed extracts are gaining traction as a natural alternative.
- **Urinary Tract Health:** Pumpkin seed supplements are included in formulations aimed at supporting overall urinary function.
- **General Wellness:** Due to their nutritional profile and potential antioxidant effects, pumpkin seeds are sometimes included in general wellness supplements.

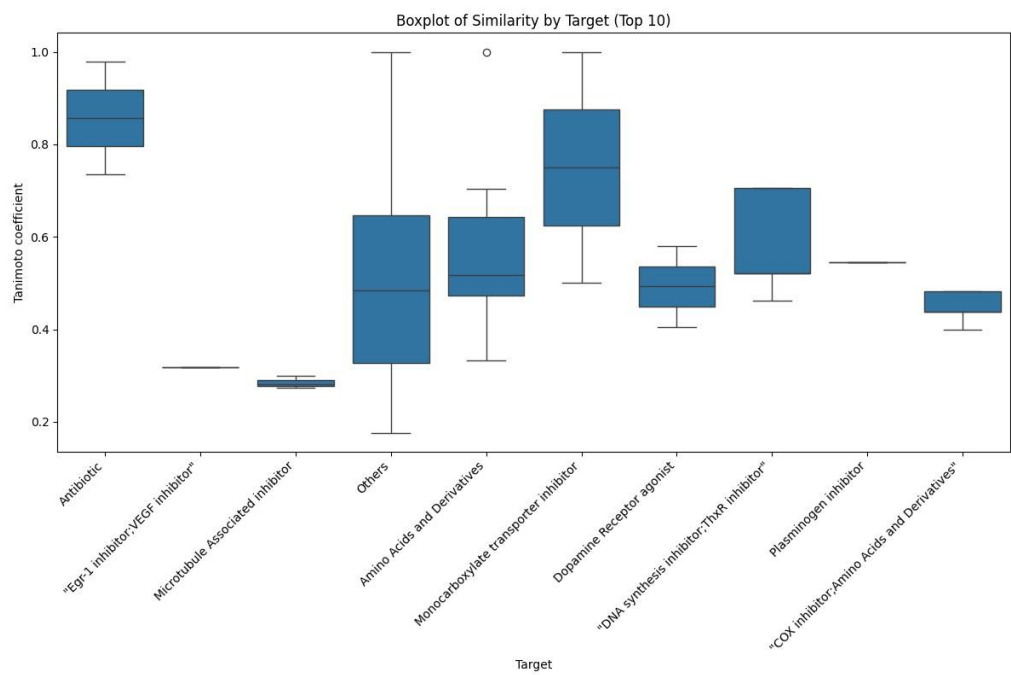
Important Considerations

- **TestBio's In Silico Analysis:** Remember that TestBio's analysis is based on computational predictions. Further research, including in vitro and in vivo studies, is needed to confirm these potential bioactivities.
- **Dosage and Standardization:** The efficacy of pumpkin seeds can vary depending on the preparation, dosage, and standardization of active compounds.
- **Individual Variability:** As with any natural remedy or supplement, individual responses to pumpkin seeds may differ.

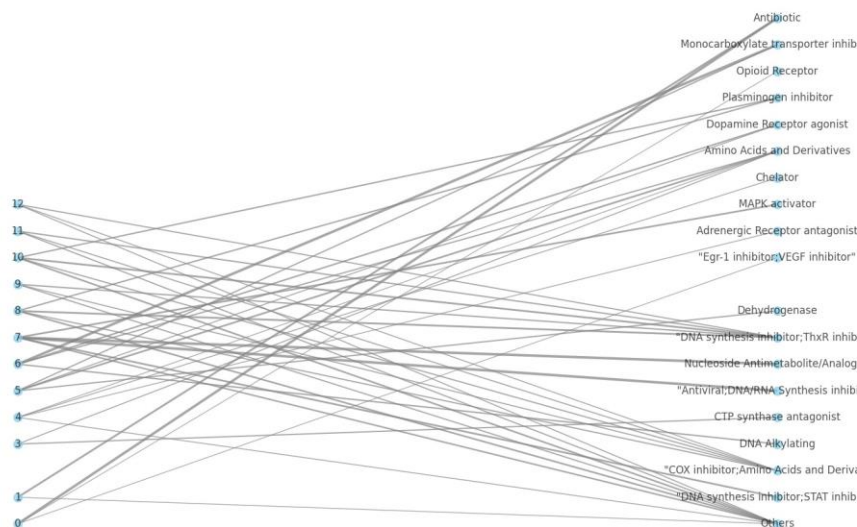
Conclusion

TestBio's analysis suggests that pumpkin seeds contain a variety of compounds with diverse potential bioactivities, particularly related to prostate health, inflammation, and cell regulation. These findings align with some traditional uses of pumpkin seeds and support their growing application in supplements. While further research is needed to validate these findings, pumpkin seeds hold promise as a natural source of health-promoting compounds.

Boxplot



Network graph



Comparison Results (Tanimoto coefficient):

Query Index	Library Index	Tanimoto Similarity	Target	Bioactivity
0	1159	0.978	Antibiotic	An alkaloid from Hydrastis canadensis L., Berberidaceae. It is also found in many other plants. It is relatively toxic parenterally, but has been used orally for various parasitic and fungal infections and as antidiarrheal.
0	154	0.317	"Egr-1 inhibitor;VEGF inhibitor"	Sanguinarine-containing mouthwashes are marketed as anti-plaque and anti-malodor.
0	1107	0.312	Opioid Receptor	A naturally occurring opium alkaloid that is a centrally acting antitussive agent.
0	391	0.282	Microtubule Associated inhibitor	Podophyllotoxin is a lignan (LIGNANS) found in PODOPHYLLIN resin from the roots of PODOPHYLLUM plants. It is a potent spindle poison, toxic if taken internally, and has been used as a cathartic. It is very irritating to skin and mucous memb
0	109	0.274	Microtubule Associated inhibitor	A major alkaloid from Colchicum autumnale L. and found also in other Colchicum species. Its primary therapeutic use is in the treatment of gout, but it has been used also in the therapy of familial Mediterranean fever (PERIODIC DISEASE).
1	1159	0.735	Antibiotic	An alkaloid from Hydrastis canadensis L., Berberidaceae. It is also found in many other plants. It is relatively toxic parenterally, but has been used orally for various parasitic and fungal infections and as antidiarrheal.
1	226	0.328	Others	Tetrahydropalmatine (THP) is an alkaloid found in several different plant species, mainly in the Corydalis genus (Yan Hu Suo), but also in other plants such as Stephania rotunda.
1	109	0.299	Microtubule Associated inhibitor	A major alkaloid from Colchicum autumnale L. and found also in other Colchicum species. Its primary therapeutic use is in the treatment of gout, but it has been used also in the therapy of familial Mediterranean fever (PERIODIC DISEASE).
1	359	0.276	Others	Extracted from Schisandra chinensis (Turcz.) Baill.;Suitability:DMSO;Store the product in sealed,cool and dry condition
1	1038	0.259	Others	A vasodilator used in angina of effort or ischemic heart disease.

Query Index	Library Index	Tanimoto Similarity	Target	Bioactivity
2	1354	0.265	"Adenosine receptor agonist; Calcium Channel inhibitor"	Gabapentin (brand name Neurontin) is a medication originally developed for the treatment of epilepsy. Presently, gabapentin is widely used to relieve pain, especially neuropathic pain. Gabapentin is well tolerated in most patients, has a re
2	1134	0.200	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	1698	0.186	FGFR inhibitor	Ferulic Acid is a hydroxycinnamic acid and a type of organic compound found in the Ferula assafoetida L. or Ligusticum chuanxiong.
2	520	0.182	Others	Extracted from Lonicera acuminata.Wall.;Suitability:Ethanol and acetone;Store the product in sealed,cool and dry condition
2	1480	0.176	Others	Cinnamic acid exerts anti-diabetic activity by improving glucose tolerance in vivo and by stimulating insulin secretion in vitro.
3	1600	0.536	Amino Acids and Derivatives	An amino acid produced in the urea cycle by the splitting off of urea from arginine.
3	1209	0.483	Amino Acids and Derivatives	A non-essential amino acid present abundantly throughout the body and is involved in many metabolic processes. It is synthesized from glutamic acid and ammonia. It is the principal carrier of nitrogen in the body and is an important energy
3	1637	0.483	CTP synthase antagonist	L-glutamine is a non-essential amino acid present abundantly throughout the body and is involved in many metabolic processes. It is synthesized from GLUTAMIC ACID and AMMONIA. It is the principal carrier of NITROGEN in the body and is an im
3	1644	0.471	Amino Acids and Derivatives	L-Arginine is the nitrogen donor for synthesis of nitric oxide, a potent vasodilator that is deficient during times of sickle cell crisis.
3	163	0.406	Amino Acids and Derivatives	Diagnostic aid in pancreas function determination.
4	1496	0.545	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.
4	951	0.375	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.
4	998	0.375	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. .
4	213	0.355	Adrenergic Receptor antagonist	Droxidopa is a psychoactive drug and acts as a prodrug to the neurotransmitters norepinephrine (noradrenaline) and epinephrine (adrenaline).
4	163	0.333	Amino Acids and Derivatives	Diagnostic aid in pancreas function determination.
5	1089	1.000	Amino Acids and Derivatives	An essential amino acid that is necessary for normal growth in infants and for NITROGEN balance in adults. It is a precursor of INDOLE ALKALOIDS in plants. It is a precursor of SEROTONIN (hence its use as an antidepressant and sleep aid). I
5	916	0.675	Amino Acids and Derivatives	The immediate precursor in the biosynthesis of SEROTONIN from tryptophan. It is used as an antiepileptic and antidepressant.

Query Index	Library Index	Tanimoto Similarity	Target	Bioactivity
5	1101	0.500	Dehydrogenase	Tryptamine is a monoamine alkaloid found in plants, fungi, and animals. It contains an indole ring structure, and is structurally similar to the amino acid tryptophan, from which it derives its name. Tryptamine is found in trace amounts in
5	1330	0.500	Monocarboxylate transporter inhibitor	An essential aromatic amino acid that is a precursor of melanin; dopamine; noradrenalin (norepinephrine), and thyroxine.
5	1175	0.405	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
6	1330	1.000	Monocarboxylate transporter inhibitor	An essential aromatic amino acid that is a precursor of melanin; dopamine; noradrenalin (norepinephrine), and thyroxine.
6	1501	0.704	Amino Acids and Derivatives	A non-essential amino acid. In animals it is synthesized from PHENYLALANINE. It is also the precursor of EPINEPHRINE; THYROID HORMONES; and melanin.
6	1175	0.581	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
6	588	0.543	DNA Alkylating	An alkylating nitrogen mustard that is used as an antineoplastic in the form of the levo isomer - MELPHALAN, the racemic mixture - MERPHALAN, and the dextro isomer - MEDPHALAN; toxic to bone marrow, but little vesicant action; potential car
6	1089	0.500	Amino Acids and Derivatives	An essential amino acid that is necessary for normal growth in infants and for NITROGEN balance in adults. It is a precursor of INDOLE ALKALOIDS in plants. It is a precursor of SEROTONIN (hence its use as an antidepressant and sleep aid). I
7	84	1.000	"Antiviral;DNA/RNA Synthesis inhibitor"	A nucleoside antibiotic isolated from Streptomyces antibioticus. It has some antineoplastic properties and has broad spectrum activity against DNA viruses in cell cultures and significant antiviral activity against infections caused by a va
7	1173	1.000	Nucleoside Antimetabolite/Analogue	Adenosine is a nucleoside composed of a molecule of adenine attached to a ribose sugar molecule (ribofuranose) moiety via a β -N9-glycosidic bond.
7	19	0.681	"DNA synthesis inhibitor;STAT inhibitor"	Purine analog that inhibits DNA synthesis. Exhibits antiproliferative activity and triggers apoptosis through increasing Bax and decreasing Bid, XIAP and survivin expression.
7	986	0.667	MAPK activator	Adenosine monophosphate (AMP), also known as 5'-adenylic acid, is a nucleotide that is used as a monomer in RNA. It is an ester of phosphoric acid and the nucleoside adenosine. AMP consists of a phosphate group, the sugar ribose, and the nu
7	968	0.596	Others	Adenosine triphosphate (ATP) is a nucleoside triphosphate used in cells as a coenzyme often called the ""molecular unit of currency"" of intracellular energy transfer.
8	1696	1.000	Others	Extracted?from?Palm tree fruit;Store?the?product?in?sealed,?cool?and?dry?condition

Query Index	Library Index	Tanimoto Similarity	Target	Bioactivity
8	1678	0.706	"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 <i>Malassezia furfur</i> (also known as <i>Pityrosporum ovale</i>), a yeast that lives on normal skin. It is effective
8	1694	0.647	Others	From an industrial perspective, it is the most important dicarboxylic acid, mainly as a precursor for the production of nylon.
8	1498	0.545	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.
8	1223	0.481	"COX inhibitor;Amino Acids and Derivatives"	6-Acetamidohexanoic acid is a kind of amino acids derivate.
9	1696	0.739	Others	Extracted?from?Palm tree fruit;Store?the?product?in?sealed,?cool?and?dry?condition
9	1213	0.536	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 a
9	1678	0.522	"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 <i>Malassezia furfur</i> (also known as <i>Pityrosporum ovale</i>), a yeast that lives on normal skin. It is effective
9	1694	0.478	Others	From an industrial perspective, it is the most important dicarboxylic acid, mainly as a precursor for the production of nylon.
9	1223	0.438	"COX inhibitor;Amino Acids and Derivatives"	6-Acetamidohexanoic acid is a kind of amino acids derivate.
10	1696	1.000	Others	Extracted?from?Palm tree fruit;Store?the?product?in?sealed,?cool?and?dry?condition
10	1678	0.706	"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 <i>Malassezia furfur</i> (also known as <i>Pityrosporum ovale</i>), a yeast that lives on normal skin. It is effective
10	1694	0.647	Others	From an industrial perspective, it is the most important dicarboxylic acid, mainly as a precursor for the production of nylon.
10	1498	0.545	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.
10	1223	0.481	"COX inhibitor;Amino Acids and Derivatives"	6-Acetamidohexanoic acid is a kind of amino acids derivate.
11	1696	0.739	Others	Extracted?from?Palm tree fruit;Store?the?product?in?sealed,?cool?and?dry?condition
11	1213	0.536	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 a

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11	1694	0.478	Others	From an industrial perspective, it is the most important dicarboxylic acid, mainly as a precursor for the production of nylon.
11	1223	0.438	"COX inhibitor;Amino Acids and Derivatives"	6-Acetamidohexanoic acid is a kind of amino acids derivate.
12	1696	0.654	Others	Extracted?from?Palm tree fruit;Store?the?product?in?sealed,?cool?and?dry?condition
12	1213	0.484	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 a
12	1678	0.462	"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
12	1694	0.423	Others	From an industrial perspective, it is the most important dicarboxylic acid, mainly as a precursor for the production of nylon.
12	1223	0.400	"COX inhibitor;Amino Acids and Derivatives"	6-Acetamidohexanoic acid is a kind of amino acids derivate.

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