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Original Research Article

Revealing the Potential of New Immunomodulatory Agents from Katokkon Pepper as a Native Toraja Plant

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ABSTRACT

Plant bioprospecting aims to find bioactive chemicals that can be employed in various aspects of human life, including food, and medicine. The chili plant has great economic value because it is not only useful as a food ingredient but also as a medicine. Indonesia has many native chilies such as Katokkon pepper with great potential for food, and with high economic value. Katokkon pepper from Toraja have not been widely researched. This study aimed to identify the bioactive compounds in Katokkon pepper with potential immunomodulatory and anti-inflammatory activities through *in-silico* studies. The methods used were bioactive compounds data mining, Quantitative Structure-Activity Relationship (QSAR), drug similarity analysis, target protein prediction, gene ontology annotation, and network pharmacology. The results revealed that rutin, ascorbic acid, linoleic acid, alpha-linolenic acid, cryptoxanthin, zeaxanthin, oleic acid, palmitoleic acid, beta-carotene, and capsanthin were among the ten bioactive compounds found in Katokkon pepper that were predicted to have immunomodulatory and anti-inflammatory properties. These chemicals can modulate the expression and activities of various proteins involved in immunomodulation, inflammation, and apoptosis, including BAX, BCL2, CASP3, CAT, IKBKB, IL1B, IL6, MAPK1, MAPK3, NFE2L2, NFKBIA, PPARA, PPARB/PPARD, PPARG, PTGS2, RELA, RUNX2, SOD1, TNF, and TP53. These findings serve as critical preliminary data for further exploration of bioactive compounds from chili peppers to support human health and the food industry.

Keywords: Katokkon pepper, Immunomodulator, Bioactive compounds, *In-silico*.

Introduction

As a mega-biodiversity country, Indonesia has abundant natural resources, including various plant species. Plants are very useful organisms for other organisms, especially as primary producers in the ecosystem, as essential ingredients for food, and even as ingredients that are used as medicines. Plants contain many active compounds (secondary metabolites) that can be utilized in various fields of human life, especially as food, and medicines. Secondary metabolites are small compounds or chemicals produced from primary metabolites during the growth and development of plants which are necessary for adaption of plants to their natural environment.[1,2] Based on the biosynthetic pathway, there are three major types of plant metabolites, namely phenolic groups (consisting of simple sugars and benzene rings), terpenes and steroids (made primarily of carbon and hydrogen), and nitrogen-containing chemicals.[3,4]

Various kinds of plants in Indonesia contain many vitamins and minerals, which are believed to boost the immune system. The use of natural ingredients from plants around us, which are inherited from generations of traditional recipes, such as herbs or other concoctions, is believed to be healthier and safer because they do not contain synthetic ingredients. This encourages scientific research in identifying bioactive compounds in plants that are beneficial to health, and could be developed as medicines. Therefore, the implementation of research based on bioprospecting of plants has increased in recent time. Bioprospecting is a systematic and organized exploration or search for new resources or useful products from biodiversity to be developed and improved further for the economic, social, and health benefits of the society.[5] The advantages of bioprospecting include obtaining information on various chemicals, genes, metabolic pathways, structures, materials, and behavior that can serve as a physical blueprint or inspiration for the design and development of new product that are beneficial to various industries such as the pharmaceutical, environmental bioremediation, bioengineering, and nanotechnology industries.[6,7] Bioprospecting is a science that is aimed at bringing prosperity to humanity and supporting environmental sustainability in a responsible way to glorify God.[8]

One group of plants widely cultivated in Indonesia is the Solanaceae family or the eggplant tribe. This plant family consists of chilies, tomatoes, potatoes, tamarillos, etc. Chilli or pepper is a plant species from the genus *Capsicum*, Solanaceae family, originating from the Americas.[9] One type of chili or pepper widely found and cultivated in the Toraja region and several districts in South Sulawesi, Indonesia, is the Katokkon pepper. It has a unique fruit shape resembling small bell peppers, it has a spicy taste, and is rich in important nutrients like ascorbic acid, carotenoids, and capsaicin.[10] In 2014, Katokkon pepper was registered with the Center for Plant Variety Protection and Agricultural Licensing with publication number 055/BR/PVL/02/2014 as a local pepper from North Toraja Regency, which belongs to the red pepper (*Capsicum annuum* L.) variety.[11] In 2017, the Katokkon "Sayang" pepper variety from South Sulawesi Province was registered with publication number 96/BR/PVL/08/2017 as a species of cayenne pepper (*Capsicum frutescens* L.).[12] This pepper contains 85.40% water, 9.20% sugar, and 16.84 mg/100 g vitamin C.[11] The results showed that the capsaicin level in Katokkon pepper powder was 2665.493 to 3029.7 ppm or on a scale of 30,000 – 50,000 Scoville Heat Unit (SHU), a very

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spicy criterion.[13] The presence of vitamins, minerals, and active compounds or secondary metabolites in chilies causes this plant to have the potential to be developed not only as a good food source but also in the medical and health fields, especially as an immunomodulator.[14] Immunomodulators are substances that can modulate the immune response, decreasing or increasing it.[15] In clinical practice, immunomodulators are categorized as immunosuppressants, immunostimulants, and immunoadjuvants.[16] Currently, most clinically used immunostimulants and immunosuppressants tend to have adverse side effects, hence the therapeutic use of natural products such as plant extracts have been suggested due to their diverse immunomodulatory effects and favorable influence on the human immune system.[17]

The benefits of chili, including its potential to act as an immunomodulator, are generally known, but in-depth research needs to be carried out to identify the compounds responsible for this effect, and could be developed further in order to increase the value and quality of these plants. So far, few studies have reported the content of active compounds or secondary metabolites in Katokkon pepper as potential immunomodulators. *In-silico* studies are a popular choice because they require relatively low cost and save time, and the results obtained can later become important information to be maximized for direct testing in the laboratory. *In silico* studies regarding the immunomodulatory potential of several plants have been reported, for example, *Lindolefia stylosa,*[18] *Withania somnifera,*[19] *Curcuma longa,*[20] etc. An *in-silico* study has been carried out on chili plants regarding the potential of capsaicinoid from *Capsicum annuum* as an antibacterial agent.[21] In addition, *in-silico* analysis through molecular docking showed that capsaicin attaches to the Main protease (Mpro) enzyme, an important enzyme that regulates the replication and transcription of the SARS-CoV-2 virus.[22] Thus, the potential of bioactive compounds in chili plants can be studied using an *in-silico* approach, and their potential as immunomodulators need to be studied in more depth. Therefore, the purpose of this study was to identify the potential of the bioactive compound in Katokkon pepper as an immunomodulator through *in silico* studies.

Materials and Methods

The method used in this study is an in silico-based qualitative descriptive method which consists of the following stages; identification of active compounds (data mining bioactive compounds), analysis of active compounds (QSAR and Drug-Likeness), prediction of target proteins and gene ontology annotations, pharmacology networks. The tool used include hardware; ASUS laptop with an Intel Core i5 processor. The softwares used are; Dr. Duke, Pubchem, Swiss Target Prediction, Swiss ADMET, String DB, Cytoscape 3.8.2, DAVID, and STITCH.

Datamining of Bioactive Compounds

The bioactive compounds used were obtained from two closely related species of chili: *Capsicum annuum* and *Capsicum frutescens.* This is because there were two pieces of information regarding the identity of the Katokkon pepper species based on government agency references (PVTPP): *Capsicum annum* and *Capsicum frutescens*. The search for bioactive compounds was carried out using the Kanaya Knapsack KNApSAcK Core System database (Kyoto Encyclopedia of Genes and Genomes Natural Products Structural Analysis and Classification System) (http://www.knapsackfamily.com/KNApSAcK/) and Dr. Duke's Phytochemical and Ethnobotanical Databases USDA (https://phytochem.nal.usda.gov/). Compounds obtained from the data mining between the two species were compiled to obtain fingerprint compounds identified as contained in both species. Furthermore, the PubChem database (https://pubchem.ncbi.nlm.nih.gov/) was used to obtain SMILES for each bioactive compound found in the two chili species.

QSAR and Drug-Likeness analysis

Quantitative Structure-Activity Relationship (QSAR) analysis was performed using the Pass Online server from Way2Drug to predict the potential bioactivity of each ligand.[23] The drug-likeness character was determined for each ligand based on the Lipinski rule of five, which was analysed using the Protox II database and the ADMETLab 2.0 database.[24-27] The input for both databases was SMILES from each ligand.

Target Protein Prediction and Gene Ontology Annotation

Target proteins were analyzed using the Comparative Toxicogenomics Database (CTD) (http://ctdbase.org/voc.go?type=chem).[28] Target protein annotation was performed using DAVID (Database for Integrated Annotation, Visualization and Discovery) (https://david.ncifcrf.gov/home.jsp).[29]

Network Pharmacology

The interaction of bioactive compounds with target proteins was also analyzed using the STITCH database (http://stitch.embl.de/).[30] STITCH analysis was performed by entering the list of proteins in the multiple-name menu from STITCH. Then additional arrangements were made by selecting the type of organism that becomes *Homo sapiens* and a minimum interaction score of 0.400. The visualisation results were downloaded in a table/export with the file type TSV (tab-separated values). The file (.tsv) was imported into the Cytoscape v.3.8.2 software to obtain a visualization of the types of interactions, gene ontology (GO), and pathways of the network formed based on data from STITCH, which has been combined with data on types and interaction mechanisms from Comparative Toxicogenomics Database (CTD).

Results and Discussion

Bioactive Compounds of Chili

Data mining results of chilli bioactive compounds with *Capsicum annuum* species (Tables 1 and 2) and *Capsicum frutescens* (Tables 3 and 4) were obtained from two different databases to achieve more valid and complete data. The list of compounds obtained from the Knapsack database for *Capsicum annuum* species was 508 (Table 1). The list of compounds obtained from Dr. Duke's database for *Capsicum annuum* species was 416 compounds found in chili fruits and seeds (Table 2). The list of compounds obtained from the Knapsack database for the species *Capsicum frutescens* was nine compounds (Table 3). The list of compounds obtained from Dr. Duke's database for the species Capsicum frutescens was 244 found in chili fruits and seeds (Table 4).

On compilation of the compounds, it was found out that 121 compounds were common to both species. These compounds include 1-hexanol, 2-hexanol, 2-methoxy-3-isobutyl-pyrazine, 2-methyl-butanal, 2-methyl-butyric-acid, 2-pentyl-furan, 3-hydroxy-alpha-carotene, 3-isobutyl-2-methoxypyrazine, 3-methyl-butanal, 4-methyl-3-penten-2-one, 4-methyl-heptadecane, 4-methyl-hexadecane, 4-methylpentadecane, 4-methyl-pentanoic-acid, 4-methyltetradecane, 4-methyltridecane, 5-methyl-2-furfural, Alpha-carotene, Alpha-linolenic-acid, Alpha-phellandrene, Alpha-terpineol, Antheraxanthin, Apiin, Arachidic-acid, Ascorbic-acid, Behenic-acid, Benzaldehyde, Beta-carotene, Beta-carotene-epoxide, beta-Ionone, Beta-pinene, Beta-sitosterol, Caffeic-acid, Campesterol, Capsaicin, Capsanthin, Capsanthin-3,6-epoxide, Capsanthin-5,6-epoxide, Capsanthone, Capsiamide, Capsidiol, Capsolutein, Capsorubin, Carnaubic-acid, Caryophyllene, Chlorogenic-acid, Cinnamic-acid, cis-3-Hexenyl hexanoate, Citric-acid, Citroxanthin, Citrullin, Cryptocapsin, Cryptoxanthin, Cucurbitaxanthin-a, Cucurbitaxanthin-b, Cycloviolaxanthin, Decanoic-acid-vanillylamide, Delta-3-carene, Dihydrocapsaicin, Eriodictin, Ferulic-acid, Folacin, Foliaxanthin, Glutamic-acid, Heneicosane, Heptanoic-acid, Hesperidin, Hexadecane, Hexanoic-acid, Homocapsaicin, Homodihydrocapsaicin, Hydroxy -alpha-carotene, Isohexyl-isocaproate, Latoxanthin, Limonene, Linoleic-acid, Lutein, Margaric-acid, Myrcene, Myristic-acid, N-(13-methyltetradecyl)acetamide, Neoxanthin, N-hexanal, Niacin, Nigroxanthin, Nonadecane, Nonanoic-acid-vanillylamide, Nordihydrocapsaicin, Octanoic-acid, Oleic-acid, Oxalic-acid, Palmitic-acid, Palmitoleic-acid, Pantothenic-acid, P-coumaric-acid, Pentadecane, Pentadecanoic-acid, Phylloquinone, Phytosterols, Proline, Pulegone, P-xylene, Quercetin, Riboflavin, Rutin, Salicylates, Scopoletin, Solanidine, Solanine, Solasodine, Stearic-acid, Stigmasterol, Terpinen-4-ol, Tetradecane, Tocopherol, Toluene, Vanillyl-amine, Violaxanthin, Vit-b- 6, Xanthophyll-epoxide, and Zeaxanthin.

Table 1: List of compounds of *Capsicum annuum* obtained from the Knapsack database

S/N	Metabolite	Molecular Formula	Molecular Weight	Organism or InChIKey
1	Abscisic acid	$C_{15}H_{20}O_4$	264.1361591	*Capsicum annuum*
2	p-Coumaric acid	$C_9H_8O_3$	164.0473441	*Capsicum annuum*
3	Ethylene	C_2H_4	28.03130013	*Capsicum annuum*
4	Salicylic acid	$C_7H_6O_3$	138.0316941	*Capsicum annuum*
5	(-)-Jasmonic acid	$C_{12}H_{18}O_3$	210.1255944	*Capsicum annuum*
6	Dihydroactinidiolide	$C_{11}H_{16}O_2$	180.1150298	*Capsicum annuum*
7	trans-3-Hexenol	$C_6H_{12}O$	100.088815	*Capsicum annuum*
8	Hexanal	$C_6H_{12}O$	100.088815	*Capsicum annuum*
9	13(S)-Hydroperoxylinolenic acid	$C_{18}H_{30}O_4$	310.2144095	*Capsicum annuum*
10	(+)-Lariciresinol	$C_{20}H_{24}O_6$	360.1572885	*Capsicum annuum*
11	Caffeic acid	$C_9H_8O_4$	180.0422587	*Capsicum annuum*
12	(+-)-Grossamide	$C_{36}H_{36}N_2O_8$	624.2471661	*Capsicum annuum* var.grossum
13	Luteolin	$C_{15}H_{10}O_6$	286.0477381	*Capsicum annuum*
14	Dihydroquercetin	$C_{15}H_{12}O_7$	304.0583027	*Capsicum annuum*
15	Chorismate	$C_{10}H_{10}O_6$	226.0477381	*Capsicum annuum*
16	Citronellol	$C_{10}H_{20}O$	156.1514153	*Capsicum annuum*
17	4-hydroxybenzoic acid	$C_7H_6O_3$	138.0316941	*Capsicum annuum*
18	trans-beta-Ocimene	$C_{10}H_{16}$	136.1252005	*Capsicum annuum*
19	beta-Citraurin	$C_{30}H_{40}O_2$	432.3028305	*Capsicum annuum*
20	15,15'-cis-Phytoene	$C_{40}H_{64}$	544.500802	*Capsicum annuum*
21	Geranylgeranyl diphosphate	$C_{20}H_{36}O_7P_2$	450.1936265	*Capsicum annuum*
22	Lycopene	$C_{40}H_{56}$	536.4382018	*Capsicum annuum*
23	Neurosporene	$C_{40}H_{58}$	538.4538519	*Capsicum annuum*
24	15-cis-Phytofluene	$C_{40}H_{62}$	542.485152	*Capsicum annuum* L.
25	beta-Carotene	$C_{40}H_{56}$	536.4382018	*Capsicum annuum*
26	beta-Cryptoxanthin	$C_{40}H_{56}O$	552.4331164	*Capsicum annuum*
27	Canthaxanthin	$C_{40}H_{52}O_2$	564.3967309	*Capsicum annuum*
28	gamma-Carotene	$C_{40}H_{56}$	536.4382018	*Capsicum annuum*
29	Zeaxanthin	$C_{40}H_{56}O_2$	568.428031	*Capsicum annuum*
30	zehta-carotene	$C_{40}H_{60}$	540.4695019	*Capsicum annuum*

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31	Ampelopsin	$C_{15}H_{12}O_8$	320.0532174	*Capsicum annuum*
32	Butin	$C_{15}H_{12}O_5$	272.0684735	*Capsicum annuum*
33	(+)-Catechin	$C_{15}H_{14}O_6$	290.0790382	*Capsicum annuum*
34	Eriodictyol	$C_{15}H_{12}O_6$	288.0633881	*Capsicum annuum*
35	Fustin	$C_{15}H_{12}O_6$	288.0633881	*Capsicum annuum*
36	Hesperetin	$C_{16}H_{14}O_6$	302.0790382	*Capsicum annuum*
37	Homoeriodictyol	$C_{16}H_{14}O_6$	302.0790382	*Capsicum annuum*
38	Hesperidin	$C_{28}H_{34}O_{15}$	610.1897704	*Capsicum annuum*
39	Liquiritigenin	$C_{15}H_{12}O_4$	256.0735589	*Capsicum annuum*
40	Naringenin	$C_{15}H_{12}O_5$	272.0684735	*Capsicum annuum*
41	Naringin	$C_{27}H_{32}O_{14}$	580.1792057	*Capsicum annuum*
42	Neohesperidin	$C_{28}H_{34}O_{15}$	610.1897704	*Capsicum annuum*
43	Naringenin 7-*O*-beta-D-glucoside	$C_{21}H_{22}O_{10}$	434.1212969	*Capsicum annuum*
44	Sakuranetin	$C_{16}H_{14}O_5$	286.0841236	*Capsicum annuum*
45	Apigenin 7-*O*-beta-D-glucopyranoside	$C_{21}H_{20}O_{10}$	432.1056469	*Capsicum annuum*
46	Chrysoeriol	$C_{16}H_{12}O_6$	300.0633881	*Capsicum annuum*
47	Isoorientin	$C_{21}H_{20}O_{11}$	448.1005615	*Capsicum annuum*
48	Isovitexin	$C_{21}H_{20}O_{10}$	432.1056469	*Capsicum annuum*
49	Kaempferide	$C_{16}H_{12}O_6$	300.0633881	*Capsicum annuum*
50	Myricetin	$C_{15}H_{10}O_8$	318.0375673	*Capsicum annuum*
51	Nobiletin	$C_{21}H_{22}O_8$	402.1314677	*Capsicum annuum*
52	Tangeretin	$C_{20}H_{20}O_7$	372.120903	*Capsicum annuum*
53	alpha-D-Glucose	$C_6H_{12}O_6$	180.0633881	*Capsicum annuum*
54	Maltose	$C_{12}H_{22}O_{11}$	342.1162116	*Capsicum annuum*
55	Raffinose	$C_{18}H_{32}O_{16}$	504.169035	*Capsicum annuum*
56	D-Sucrose	$C_{12}H_{22}O_{11}$	342.1162116	*Capsicum annuum*
57	Trehalose	$C_{12}H_{22}O_{11}$	342.1162116	*Capsicum annuum*
58	Galactinol	$C_{12}H_{22}O_{11}$	342.1162116	*Capsicum annuum*
59	Glycerol	$C_3H_8O_3$	92.04734412	*Capsicum annuum*
60	Inositol	$C_6H_{12}O_6$	180.0633881	*Capsicum annuum*
61	Acetic acid	$C_2H_4O_2$	60.02112937	*Capsicum annuum*
62	(+)-Ascorbic acid	$C_6H_8O_6$	176.032088	*Capsicum annuum*

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63	Formic acid	CH_2O_2	46.00547931	*Capsicum annuum*
64	Fumaric acid	$C_4H_4O_4$	116.0109586	*Capsicum annuum*
65	D-Glyceric acid	$C_3H_6O_4$	106.0266087	*Capsicum annuum*
66	L-(-)-Malic acid	$C_4H_6O_5$	134.0215233	*Capsicum annuum*
67	Malonic acid	$C_3H_4O_4$	104.0109586	*Capsicum annuum*
68	Oxalic acid	$C_2H_2O_4$	89.99530855	*Capsicum annuum*
69	Pyruvic acid	$C_3H_4O_3$	88.01604399	*Capsicum annuum*
70	Shikimic acid	$C_7H_{10}O_5$	174.0528234	*Capsicum annuum*
71	Succinic acid	$C_4H_6O_4$	118.0266087	*Capsicum annuum*
72	Linoleic acid	$C_{18}H_{32}O_2$	280.2402303	*Capsicum annuum*
73	Palmitic acid	$C_{16}H_{32}O_2$	256.2402303	*Capsicum annuum*
74	Palmitoleic acid	$C_{16}H_{30}O_2$	254.2245802	*Capsicum annuum*
75	Octadecanoic acid	$C_{18}H_{36}O_2$	284.2715304	*Capsicum annuum*
76	n-Pentadecane	$C_{15}H_{32}$	212.250401	*Capsicum annuum*
77	gamma-Undecalactone	$C_{11}H_{20}O_2$	184.1463299	*Capsicum annuum*
78	L-Alanine	$C_3H_7NO_2$	89.04767848	*Capsicum annuum*
79	beta-Alanine	$C_3H_7NO_2$	89.04767848	*Capsicum annuum*
80	GABA	$C_4H_9NO_2$	103.0633285	*Capsicum annuum*
81	L-Asparagine	$C_4H_8N_2O_3$	132.0534921	*Capsicum annuum*
82	L-Aspartic acid	$C_4H_7NO_4$	133.0375077	*Capsicum annuum*
83	L-Citrulline	$C_6H_{13}N_3O_3$	175.0956913	*Capsicum annuum*
84	L-Cysteine	$C_3H_7NO_2S$	121.0197492	*Capsicum annuum*
85	L-Glutamic acid	$C_5H_9NO_4$	147.0531578	*Capsicum annuum*
86	L-Glutamine	$C_5H_{10}N_2O_3$	146.0691422	*Capsicum annuum*
87	Glycine	$C_2H_5NO_2$	75.03202841	*Capsicum annuum*
88	L-Histidine	$C_6H_9N_3O_2$	155.0694766	*Capsicum annuum*
89	L-Homoserine	$C_4H_9NO_3$	119.0582432	*Capsicum annuum*
90	trans-4-Hydroxy-L-proline	$C_5H_9NO_3$	131.0582432	*Capsicum annuum*
91	L-isoleucine	$C_6H_{13}NO_2$	131.0946287	*Capsicum annuum*
92	L-Leucine	$C_6H_{13}NO_2$	131.0946287	*Capsicum annuum*
93	L-Methionine	$C_5H_{11}NO_2S$	149.0510493	*Capsicum annuum*
94	L-Ornithine	$C_5H_{12}N_2O_2$	132.0898776	*Capsicum annuum*

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95	L-Phenylalanine	$C_9H_{11}NO_2$	165.0789786	*Capsicum annuum*
96	L-Proline	$C_5H_9NO_2$	115.0633285	*Capsicum annuum*
97	L-Serine	$C_3H_7NO_3$	105.0425931	*Capsicum annuum*
98	L-Threonine	$C_4H_9NO_3$	119.0582432	*Capsicum annuum*
99	L-Tryptophan	$C_{11}H_{12}N_2O_2$	204.0898776	*Capsicum annuum*
100	L-Tyrosine	$C_9H_{11}NO_3$	181.0738932	*Capsicum annuum*
101	L-Valine	$C_5H_{11}NO_2$	117.0789786	*Capsicum annuum*
102	Agmatine	$C_5H_{14}N_4$	130.1218465	*Capsicum annuum*
103	Cadaverine	$C_5H_{14}N_2$	102.1156985	*Capsicum annuum*
104	1,4-Butanediamine	$C_4H_{12}N_2$	88.1000484	*Capsicum annuum*
105	5-Hydroxytryptamine	$C_{10}H_{12}N_2O$	176.094963	*Capsicum annuum*
106	Spermidine	$C_7H_{19}N_3$	145.1578976	*Capsicum annuum*
107	Tryptamine	$C_{10}H_{12}N_2$	160.1000484	*Capsicum annuum*
108	Chlorophyll a	$C_{55}H_{72}MgN_4O_5$	892.5353133	*Capsicum annuum*
109	Cyanidin 3-*O*-glucoside	$C_{21}H_{21}O_{11}.Cl$	449.1083865	*Capsicum annuum*
110	Pelargonin	$C_{27}H_{31}O_{15}$	595.1662953	*Capsicum annuum*
111	Biochanin A	$C_{16}H_{12}O_5$	284.0684735	*Capsicum annuum*
112	Daidzin	$C_{21}H_{20}O_9$	416.1107322	*Capsicum annuum*
113	Genistein	$C_{15}H_{10}O_5$	270.0528234	*Capsicum annuum*
114	Genistein 7-*O*-glucoside	$C_{21}H_{20}O_{10}$	432.1056469	*Capsicum annuum*
115	Prunetin	$C_{16}H_{12}O_5$	284.0684735	*Capsicum annuum*
116	Gallic acid	$C_7H_6O_5$	170.0215233	*Capsicum annuum*
117	3,4-Dihydroxybenzoic acid	$C_7H_6O_4$	154.0266087	*Capsicum annuum*
118	Vanillic acid	$C_8H_8O_4$	168.0422587	*Capsicum annuum*
119	Vanillin	$C_8H_8O_3$	152.0473441	*Capsicum annuum*
120	N-Caffeoylputrescine	$C_{13}H_{18}N_2O_3$	250.1317425	*Capsicum annuum*
121	5-*O*-Caffeoylshikimic acid	$C_{16}H_{16}O_8$	336.0845175	*Capsicum annuum*
122	3-*O*-Caffeoylquinic acid	$C_{16}H_{18}O_9$	354.0950822	*Capsicum annuum*
123	Ferulic acid	$C_{10}H_{10}O_4$	194.0579088	*Capsicum annuum*
124	Sinapic acid	$C_{11}H_{12}O_5$	224.0684735	*Capsicum annuum*
125	linalool	$C_{10}H_{18}O$	154.1357652	*Capsicum annuum*
126	Botrydial	$C_{17}H_{26}O_5$	310.1780239	*Capsicum annuum*

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127	Capsidiol	$C_{15}H_{24}O_2$	236.17763	*Capsicum annuum*
128	alpha-Copaene	$C_{15}H_{24}$	204.1878008	*Capsicum annuum*
129	alpha-Farnesene	$C_{15}H_{24}$	204.1878008	*Capsicum annuum*
130	Longifolene	$C_{15}H_{24}$	204.1878008	*Capsicum annuum*
131	alpha-Ylangene	$C_{15}H_{24}$	204.1878008	*Capsicum annuum*
132	Capsicoside A	$C_{63}H_{106}O_{35}$	1422.651465	*Capsicum annuum*
133	Lanosterol	$C_{30}H_{50}O$	426.3861662	*Capsicum annuum* L.
134	(-)-beta-Sitosterol	$C_{29}H_{50}O$	414.3861662	*Capsicum annuum*
135	Antheraxanthin	$C_{40}H_{56}O_3$	584.4229457	*Capsicum annuum*
136	Capsanthin	$C_{40}H_{56}O_3$	584.4229457	*Capsicum annuum*
137	Capsorubin	$C_{40}H_{56}O_4$	600.4178603	*Capsicum annuum*
138	alpha-Carotene	$C_{40}H_{56}$	536.4382018	*Capsicum annuum*
139	beta-Carotene 5,6-epoxide	$C_{40}H_{56}O$	552.4331164	*Capsicum annuum*
140	alpha-Cryptoxanthin	C40H56O	552.4331164	*Capsicum annuum* L.
141	Lutein	$C_{40}H_{56}O_2$	568.428031	*Capsicum annuum* L.
142	Lutein 5,6-epoxide	$C_{40}H_{56}O_3$	584.4229457	*Capsicum annuum*
143	Mutatochrome	$C_{40}H_{56}O$	552.4331164	*Capsicum annuum*
144	Neoxanthin	$C_{40}H^{56}O_4$	600.4178603	*Capsicum annuum*
145	Violaxanthin	$C_{40}H_{56}O_4$	600.4178603	*Capsicum annuum*
146	Acacetin	$C_{16}H_{12}O_5$	284.0684735	*Capsicum annuum*
147	Velutin	$C_{17}H_{14}O_6$	314.0790382	*Capsicum annuum*
148	Toringin	$C_{21}H_{20}O_9$	416.1107322	*Capsicum annuum*
149	Apigenin 5-glucoside	$C_{21}H_{20}O_{10}$	432.1056469	*Capsicum annuum*
150	Apigenin 7-*O*-rutinoside	$C_{27}H_{30}O_{14}$	578.1635557	*Capsicum annuum*
151	Rhoifolin	$C_{27}H_{30}O_{14}$	578.1635557	*Capsicum annuum*
152	Cinaroside	$C_{21}H_{20}O_{11}$	448.1005615	*Capsicum annuum*
153	Luteolin 7-apiosyl-(1->2)-glucoside	$C_{26}H_{28}O_{15}$	580.1428202	*Capsicum annuum*
154	Luteolin 3',7-di-*O*-beta-glucoside	$C_{27}H_{30}O_{16}$	610.1533849	*Capsicum annuum*
155	Luteolin 3'-methyl ether 7-rutinoside	$C_{28}H_{32}O_{15}$	608.1741204	*Capsicum annuum*
156	Kaempferol	$C_{15}H_{10}O_6$	286.0477381	*Capsicum annuum*
157	Kumatakenin	$C_{17}H_{14}O_6$	314.0790382	*Capsicum annuum*
158	Fisetin	$C_{15}H_{10}O_6$	286.0477381	*Capsicum annuum*

159	Morin	$C_{15}H_{10}O_7$	302.0426527	*Capsicum annuum*
160	Quercetin	$C_{15}H_{10}O_7$	302.0426527	*Capsicum annuum*
161	Isorhamnetin	$C_{16}H_{12}O_7$	316.0583027	*Capsicum annuum*
162	Spinacetin	$C_{17}H_{14}O_8$	346.0688674	*Capsicum annuum*
163	Syringetin	$C_{17}H_{14}O_8$	346.0688674	*Capsicum annuum*
164	Trifolin	$C_{21}H_{20}O_{11}$	448.1005615	*Capsicum annuum*
165	Astragalin	$C_{21}H_{20}O_{11}$	448.1005615	*Capsicum annuum*
166	Afzelin	$C_{21}H_{20}O_{10}$	432.1056469	*Capsicum annuum*
167	Kaempferol 7-*O*-rhamnoside	$C_{21}H_{20}O_{10}$	432.1056469	*Capsicum annuum*
168	kaempferol 3-*O*-robinobioside	$C_{27}H_{30}O_{15}$	594.1584703	*Capsicum annuum*
169	Nicotiflorin	$C_{27}H_{30}O_{15}$	594.1584703	*Capsicum annuum*
170	Hirsutrin	$C_{21}H_{20}O_{12}$	464.0954761	*Capsicum annuum*
171	Quercetin 3-*O*-L-rhamnoside	$C_{21}H_{20}O_{11}$	448.1005615	*Capsicum annuum*
172	Quercetin 7-glucuronide	$C_{21}H_{18}O_{13}$	478.0747407	*Capsicum annuum*
173	Spiraeoside	$C_{21}H_{20}O_{12}$	464.0954761	*Capsicum annuum*
174	Rutin	$C_{27}H_{30}O_{16}$	610.1533849	*Capsicum annuum*
175	Quercetin-3-*O*-rhamnoside-7-*O*-glucoside	$C_{27}H_{30}O_{16}$	610.1533849	*Capsicum annuum*
176	Quercetin 7-*O*-rutinoside	$C_{27}H_{30}O_{16}$	610.1533849	*Capsicum annuum*
177	Myricetin 3-*O*-galactoside	$C_{21}H_{20}O_{13}$	480.0903907	*Capsicum annuum*
178	Myricitrin	$C_{21}H_{20}O_{12}$	464.0954761	*Capsicum annuum*
179	Quercetin 3-(6"-malonylglucoside)	$C_{24}H_{22}O_{15}$	550.09587	*Capsicum annuum*
180	Isohemiphloin	$C_{21}H_{22}O_{10}$	434.1212969	*Capsicum annuum*
181	Schaftoside	$C_{26}H_{28}O_{14}$	564.1479056	*Capsicum annuum*
182	Carlinoside	$C_{26}H_{28}O_{15}$	580.1428202	*Capsicum annuum*
183	Vitexin 2"-*O*-rhamnoside	$C_{27}H_{30}O_{14}$	578.1635557	*Capsicum annuum*
184	Isoschaftoside	$C_{26}H_{28}O_{14}$	564.1479056	*Capsicum annuum*
185	Cyanidin	$C_{15}H_{11}O_6^+$	287.0555631	*Capsicum annuum*
186	Peonidin 3-sophoroside-5-glucoside	$C_{34}H_{43}O_{21}$	787.2296834	*Capsicum annuum*
187	Myrtillin	$C_{21}H_{21}O_{12}.Cl$	465.1033011	*Capsicum annuum*
188	Petunidin 3-glucoside	$C_{22}H_{23}O_{12}$	479.1189512	*Capsicum annuum*
189	Primulin	$C_{23}H^{25}O_{12}$	493.1346013	*Capsicum annuum*
190	Oenin	$C_{23}H_{25}O_{12}$	493.1346013	*Capsicum annuum*

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191	Butein	$C_{15}H_{12}O_5$	272.0684735	*Capsicum annuum*
192	Xanthohumol	$C_{21}H_{22}O_5$	354.1467238	*Capsicum annuum*
193	Pelargonidin	$C_{15}H_{11}O_5$	271.0606485	*Capsicum annuum*
194	Naringenin chalcone	$C_{15}H_{12}O_5$	272.0684735	*Capsicum annuum*
195	(+)-Dihydrokaempferol	$C_{15}H_{12}O_6$	288.0633881	*Capsicum annuum*
196	Leucocyanidin	$C_{15}H_{14}O_7$	306.0739528	*Capsicum annuum*
197	4-Coumaroyl CoA	$C_{21}H_{36}N_7O_{16}P_3S$	767.1152084	*Capsicum annuum*
198	Malonyl-CoA	$C_{24}H_{38}N_7O_{19}P_3S$	853.1156023	*Capsicum annuum*
199	Feruloyl-CoA	$C_{31}H_{44}N_7O_{19}P_3S$	943.1625525	*Capsicum annuum*
200	2-Aminoethanol	C_2H_7NO	61.05276385	*Capsicum annuum*
201	p-Coumaroyl CoA	$C_{30}H_{42}N_7O_{18}P_3S$	913.1519878	*Capsicum annuum*
202	caffeoyl-CoA	$C_{30}H_{42}N_7O_{19}P_3S$	929.1469024	*Capsicum annuum*
203	3-Phosphoglycerate	$C_3H_7O_7P$	185.9929391	*Capsicum annuum*
204	D-Xylose	$C_5H_{10}O_5$	150.0528234	*Capsicum annuum*
205	Betaine	$C_5H_{11}NO_2$	117.0789786	*Capsicum annuum*
206	Choline	$C_5H_{14}NO$	104.1075391	*Capsicum annuum*
207	Phosphorylcholine	$C_5H_{15}NO_4P$	184.0738695	*Capsicum annuum*
208	D-Gluconate	$C_6H_{12}O_7$	196.0583027	*Capsicum annuum*
209	D-Fructose 6-phosphate	$C_6H_{13}O_9P$	260.0297185	*Capsicum annuum*
210	D-Glucose 6-phosphate	$C_6H_{13}O_9P$	260.0297185	*Capsicum annuum*
211	S-Adenosyl-L-methionine	$C_{15}H_{22}N_6O_5S$	398.1372386	*Capsicum annuum*
212	alpha-Tocopherol	$C_{29}H_{50}O_2$	430.3810808	*Capsicum annuum*
213	Obtusifoliol	$C_{30}H_{50}O$	426.3861662	*Capsicum annuum*
214	Chlorophyll b	$C_{55}H_{70}MgN_4O_6$	906.5145779	*Capsicum annuum*
215	5-Oxoproline	$C_5H_7NO_3$	129.0425931	*Capsicum annuum*
216	Adenosine	$C_{10}H_{13}N_5O_4$	267.0967539	*Capsicum annuum*
217	Benzeneacetaldehyde	C_8H_8O	120.0575149	*Capsicum annuum*
218	Citric acid	$C_6H_8O_7$	192.0270026	*Capsicum annuum*
219	Ketovaline	$C_5H_8O_3$	116.0473441	*Capsicum annuum*
220	delta-Cadinene	$C_{15}H_{24}$	204.1878008	*Capsicum annuum*
221	Phloretin	$C_{15}H_{14}O_5$	274.0841236	*Capsicum annuum*
222	Hesperetin 5-*O*-glucoside	$C_{22}H_{24}O_{11}$	464.1318616	*Capsicum annuum*

223	Sternbin	$C_{16}H_{14}O^{6}$	302.0790382	*Capsicum annuum*
224	(+)-Gallocatechin	$C_{15}H_{14}O_7$	306.0739528	*Capsicum annuum*
225	(-)-Epigallocatechin	$C_{15}H_{14}O_7$	306.0739528	*Capsicum annuum*
226	Daidzein	$C_{15}H_{10}O_4$	254.0579088	*Capsicum annuum*
227	2'-Hydroxydaidzein	$C_{15}H_{10}O_5$	270.0528234	*Capsicum annuum*
228	4',6,7-Trihydroxyisoflavone	$C_{15}H_{10}O_5$	270.0528234	*Capsicum annuum*
229	2'-Hydroxygenistein	$C_{15}H_{10}O_6$	286.0477381	*Capsicum annuum*
230	Biochanin A 7-O-glucoside	$C_{22}H_{22}O_{10}$	446.1212969	*Capsicum annuum*
231	Ellagic acid	$C_{14}H_6O_8$	302.0062672	*Capsicum annuum*
232	trans-p-Feruloyl-beta-D-glucopyranoside	$C_{16}H_{20}O_9$	356.1107322	*Capsicum annuum*
233	trans-p-Sinapoyl beta-D-glucopyranoside	$C_{17}H_{22}O_{10}$	386.1212969	*Capsicum annuum*
234	trans-p-Ferulyl alcohol 4-*O*-[6-(2-methyl-3-hydroxypropionyl)] glucopyranoside	$C_{20}H_{28}O_{10}$	428.1682471	*Capsicum annuum*
235	Luteolin 7-*O*-(2-apiofuranosyl-4-glucopyranosyl-6-malonyl)glucopyranoside	$C_{35}H_{40}O_{23}$	828.1960376	*Capsicum annuum*
236	Tricin	$C_{17}H_{14}O_7$	330.0739528	*Capsicum annuum*
237	Dihydrocapsenone	$C_{15}H_{24}O_2$	236.17763	*Capsicum annuum*
238	3,4-Dihydroxybenzaldehyde	$C_7H_6O_3$	138.0316941	*Capsicum annuum*
239	Ethanol	C_2H_6O	46.04186481	*Capsicum annuum*
240	Uridine	$C_9H_{12}N_2O_6$	244.0695361	*Capsicum annuum*
241	Guanosine	$C_{10}H_{13}N_5O_5$	283.0916686	*Capsicum annuum*
242	D-Galactose	$C_6H_{12}O_6$	180.0633881	*Capsicum annuum*
243	Leucopelargonidin	$C_{15}H_{14}O_6$	290.0790382	*Capsicum annuum*
244	Malvidin	$C_{17}H_{15}O_7$	331.0817778	*Capsicum annuum*
245	(+)-Aromadendrene	$C_{15}H_{24}$	204.1878008	*Capsicum annuum*
246	(3E,7E)-4,8,12-Trimethyl-1,3,7,11-tridecatetraene	$C_{16}H_{26}$	218.2034508	*Capsicum annuum*
247	(3R)-3-Hydroxyretinal	$C_{20}H_{28}O_2$	300.2089301	*Capsicum annuum*
248	Apo-10'-zeaxanthinal	$C_{27}H_{36}O_2$	392.2715304	*Capsicum annuum*
249	Apo-12'-zeaxanthinal	$C_{25}H_{34}O_2$	366.2558803	*Capsicum annuum*
250	Apo-14'-zeaxanthinal	$C_{22}H_{30}O_2$	326.2245802	*Capsicum annuum*
251	Apo-13-zeaxanthinone	$C_{18}H_{26}O_2$	274.1932801	*Capsicum annuum*
252	Apo-11-zeaxanthinal	$C_{15}H_{22}O_2$	234.16198	*Capsicum annuum*
253	Apo-9-zeaxanthinone	$C_{13}H_{20}O_2$	208.1463299	*Capsicum annuum*
254	Apo-12'-capsorubinal	$C_{25}H_{34}O_3$	382.250795	*Capsicum annuum*

255	Apo-8'-capsorubinal	$C_{30}H_{40}O_3$	448.2977451	*Capsicum annuum*
256	9,9'-Diapo-10,9'-retro-carotene-9,9'-dione	$C_{18}H_{22}O_2$	270.16198	*Capsicum annuum*
257	Nigroxanthin	$C_{40}H_{54}O_2$	566.412381	*Capsicum annuum* var. longum nigrum
258	Karpoxanthin	$C_{40}H_{58}O_4$	602.4335103	*Capsicum annuum*
259	6-Epiheteroxanthin	$C_{40}H_{58}O_4$	602.4335103	*Capsicum annuum*
260	(3S,3'R,5S,6S)-5,6-Dihydro-3,3',5,6-tetrahydroxy-beta,beta-carotene	$C_{40}H_{58}O_4$	602.4335103	*Capsicum annuum* var. longum
261	Latoxanthin	$C_{40}H_{58}O_5$	618.428425	*Capsicum annuum*
262	5,6-Diepilatoxanthin	$C_{40}H_{58}O_5$	618.428425	*Capsicum annuum* var. longum
263	Cucurbitaxanthin A	$C_{40}H_{56}O_3$	584.4229457	*Capsicum annuum* var. longum
264	Mutatoxanthin	$C_{40}H_{56}O_3$	584.4229457	*Capsicum annuum*
265	Cucurbitaxanthin B	$C_{40}H_{56}O_4$	600.4178603	*Capsicum annuum* var. longum
266	Cycloviolaxanthin	$C_{40}H_{56}O_4$	600.4178603	*Capsicum annuum* var. longum nigrum
267	Curcurbitachrome 1	$C_{40}H_{56}O_4$	600.4178603	*Capsicum annuum* var. longum
268	Cryptocapsin	$C_{40}H_{56}O_2$	568.428031	*Capsicum annuum*
269	5,6-Diepicapsokarpoxanthin	$C_{40}H_{58}O_5$	618.428425	*Capsicum annuum* var. longum
270	Capsanthin 5,6-epoxide	$C_{40}H_{56}O_4$	600.4178603	*Capsicum annuum*
271	Capsanthin 3,6-epoxide	$C_{40}H_{56}O_4$	600.4178603	*Capsicum annuum* var. longum
272	Capsanthone	$C_{40}H_{54}O_3$	582.4072956	*Capsicum annuum*
273	N-cis-Feruloyltyramine	$C_{18}H_{19}NO_4$	313.1314081	*Capsicum annuum*
274	N-trans-Feruloyltyramine	$C_{18}H_{19}NO_4$	313.1314081	*Capsicum annuum*
275	N-cis-Coumaroyltyramine	$C_{17}H_{17}NO_3$	283.1208434	*Capsicum annuum*
276	N-trans-Coumaroyltyramine	$C_{17}H_{17}NO_3$	283.1208434	*Capsicum annuum*
277	2-Decanol	$C_{10}H_{22}O$	158.1670653	*Capsicum annuum*
278	beta-Ionone	$C_{13}H_{20}O$	192.1514153	*Capsicum annuum*
279	Capsianoside C	$C_{82}H_{132}O_{38}$	1724.83966	*Capsicum annuum*
280	Capsianoside D	$C_{82}H_{134}O_{38}$	1726.85531	*Capsicum annuum* L.
281	Capsianoside E	$C_{82}H_{134}O_{37}$	1710.860395	*Capsicum annuum* L.
282	Capsianoside F	$C_{82}H_{134}O_{37}$	1710.860395	*Capsicum annuum* L.
283	Capsianoside II	$C_{50}H_{84}O_{25}$	1084.530168	*Capsicum annuum* L.
284	Capsianoside III	$C_{50}H_{84}O_{26}$	1100.525083	*Capsicum annuum* L.
285	Cinnamic acid	$C_9H_8O_2$	148.0524295	*Capsicum annuum*

286	Heptadecane	$C_{17}H_{36}$	240.2817012	*Capsicum annuum*
287	Hexyl 3-methyl butyrate	$C_{11}H_{22}O_2$	186.16198	*Capsicum annuum*
288	Methyl salicylate	$C_8H_8O_3$	152.0473441	*Capsicum annuum*
289	5-Caffeoylquinic acid	$C_{16}H_{18}O_9$	354.0950822	*Capsicum annuum*
290	Nonadecane	$C_{19}H_{40}$	268.3130013	*Capsicum annuum*
291	Octadecane	$C_{18}H_{38}$	254.2973512	*Capsicum annuum*
292	Retinol	$C_{20}H_{30}O$	286.2296656	*Capsicum annuum*
293	D-Fructose	$C_6H_{12}O_6$	180.0633881	*Capsicum annuum*
294	2-Pentylfuran	$C_9H_{14}O$	138.1044651	*Capsicum annuum*
295	trans-4-Hydroxy-N-methyl-L-proline	$C_6H_{11}NO_3$	145.0738932	*Capsicum annuum*
296	N-cis-Feruloyloctopamine	$C_{18}H^{19}NO_5$	329.1263227	*Capsicum annuum* var.grossum
297	alpha-Amorphene	$C_{15}H_{24}$	204.1878008	*Capsicum annuum*
298	Cetene	$C_{16}H_{32}$	224.250401	*Capsicum annuum*
299	Hexadecane	$C_{16}H_{34}$	226.2660511	*Capsicum annuum*
300	Hexyl 2-methylbutanoate	$C_{11}H_{22}O_2$	186.16198	*Capsicum annuum*
301	Hexyl caprylate	$C_{14}H_{28}O_2$	228.2089301	*Capsicum annuum*
302	Hexyl butanoate	$C_{10}H_{20}O_2$	172.1463299	*Capsicum annuum*
303	9-cis-Lutein	$C_{40}H_{56}O_2$	568.428031	*Capsicum annuum*
304	9'-cis-Lutein	$C_{40}H_{56}O_2$	568.428031	*Capsicum annuum*
305	n-Tetradecane	$C_{14}H_{30}$	198.234751	*Capsicum annuum*
306	alpha-Longipinene	$C_{15}H_{24}$	204.1878008	*Capsicum annuum*
307	Delphinidin-3,5-*O*-diglucoside	$C_{27}H_{31}O_{17}$	627.1561246	*Capsicum annuum*
308	Cytidine	$C_9H_{13}N_3O_5$	243.0855206	*Capsicum annuum*
309	13-Hydroxycapsidiol	$C_{15}H_{24}O_3$	252.1725446	*Capsicum annuum*
310	Canusesnol A	$C_{15}H_{22}O_3$	250.1568946	*Capsicum annuum*
311	Canusesnol B	$C_{15}H_{24}O_4$	268.1674593	*Capsicum annuum*
312	Canusesnol C	$C_{15}H_{24}O_4$	268.1674593	*Capsicum annuum*
313	Canusesnol D	$C_{15}H_{26}O_3$	254.1881947	*Capsicum annuum*
314	Canusesnol E	$C_{15}H_{24}O_3$	252.1725446	*Capsicum annuum*
315	Canusesnol F	$C_{15}H_{22}O_4$	266.1518092	*Capsicum annuum*
316	Canusesnol G	$C_{15}H_{26}O_3$	254.1881947	*Capsicum annuum*
317	Canusesnol H	$C_{14}H_{22}O_3$	238.1568946	*Capsicum annuum*

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318	Canusesnol I	$C_{15}H^{26}O_2$	238.1932801	*Capsicum annuum*
319	Canusesnol J	$C_{15}H_{22}O_3$	250.1568946	*Capsicum annuum*
320	Drummondol	$C_{13}H_{20}O_4$	240.1361591	*Capsicum annuum*
321	Lubiminol	$C_{15}H_{26}O_2$	238.1932801	*Capsicum annuum*
322	Prenigroxanthin	$C_{40}H_{56}O_3$	584.4229457	*Capsicum annuum*
323	omega-Hydroxycapsaicin	$C_{18}H_{27}NO_4$	321.1940084	*Capsicum annuum*
324	13-cis-Capsanthin	$C_{40}H_{56}O_3$	584.4229457	*Capsicum annuum*
325	9-cis-Capsanthin	$C_{40}H_{56}O_3$	584.4229457	*Capsicum annuum*
326	(9Z)-Violaxanthin	$C_{40}H_{56}O_4$	600.4178603	*Capsicum annuum*
327	Phytone	$C_{18}H_{36}O$	268.2766158	*Capsicum annuum*
328	Taurine	$C_2H_7NO_3S$	125.0146638	*Capsicum annuum*
329	Nordihydrocapsiate	$C_{17}H_{26}O_4$	294.1831093	*Capsicum annuum*
330	Lactic acid	$C_3H_6O_3$	90.03169406	*Capsicum annuum*
331	Methanol	CH_4O	32.02621475	*Capsicum annuum*
332	Malic acid	$C_4H_6O_5$	134.0215233	*Capsicum annuum*
333	Malvidin-3,5-diglucoside	$C_{29}H_{35}O_{17}$	655.1874247	*Capsicum annuum*
334	2-Hydroxybutanoic acid	$C_4H_8O_3$	104.0473441	*Capsicum annuum*
335	Capsaicin	$C_{18}H_{27}NO_3$	305.1990937	*Capsicum annuum*
336	2-Methoxy-3-isobutylpyrazine	$C_9H_{14}N_2O$	166.1106131	*Capsicum annuum*
337	3-Hydroxyflavone	$C_{15}H_{10}O_3$	238.0629942	*Capsicum annuum*
338	3-Methyl-5-propylnonane	$C_{13}H_{28}$	184.2191009	*Capsicum annuum*
339	8-Methyl-6-nonenoic acid	$C_{10}H_{18}O_2$	170.1306798	*Capsicum annuum*
340	8-Methyl-6-nonenoyl-CoA	$C_{31}H_{52}N_7O_{17}P_3S$	919.2353235	*Capsicum annuum*
341	Delphinidin	$C_{15}H_{11}O_7$	303.0504777	*Capsicum annuum*
342	Erythronic acid gamma-lactone	$C_4H_6O_4$	118.0266087	*Capsicum annuum*
343	Dihydrocapsaicin	$C_{18}H_{29}NO_3$	307.2147438	*Capsicum annuum*
344	Coumaric acid	$C_9H_8O_3$	164.0473441	*Capsicum annuum*
345	Dehydroascorbate	$C_6H_6O_6$	174.0164379	*Capsicum annuum*
346	Dibutyl phthalate	$C_{16}H_{22}O_4$	278.1518092	*Capsicum annuum*
347	Gentiobiose	$C_{12}H_{22}O_{11}$	342.1162116	*Capsicum annuum*
348	Heptanoic acid	$C_7H_{14}O_2$	130.0993797	*Capsicum annuum*
349	Hexyl hexanoate	$C_{12}H_{24}O_2$	200.17763	*Capsicum annuum*

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350	Isobutyryl CoA	$C_{25}H_{42}N_7O_{17}P_3S$	837.1570732	*Capsicum annuum*
351	L-Threonic acid	$C_4H_8O_5$	136.0371734	*Capsicum annuum*
352	Phytane	$C_{20}H_{42}$	282.3286513	*Capsicum annuum*
353	Quinate	$C_{26}H_{36}N_2O_9$	520.2420808	*Capsicum annuum*
354	Vanillylamine	$C_8H_{11}NO_2$	153.0789786	*Capsicum annuum*
355	Capsicoside C2	$C_{44}H_{72}O_{17}$	872.4769509	*Capsicum annuum*
356	Capsicoside A2	$C_{33}H_{54}O_8$	578.3818687	*Capsicum annuum*
357	Capsicoside B2	$C_{39}H_{64}O_{13}$	740.4346921	*Capsicum annuum*
358	Capsiate	$C_{18}H_{26}O_4$	306.1831093	*Capsicum annuum*
359	Dihydrocapsiate	$C_{18}H_{28}O_4$	308.1987594	*Capsicum annuum*
360	Capsoside B	$C_{18}H_{34}O_{11}$	426.2101119	*Capsicum annuum* var. acuminatum
361	N-cis-p-Coumaroyloctopamine	$C_{17}H_{17}NO_4$	299.115758	*Capsicum annuum* var. grossum
362	N-trans-p-Coumaroyloctopamine	$C_{17}H_{17}NO_4$	299.115758	*Capsicum annuum* var. grossum
363	N-trans-Caffeoyldopamine	$C_{17}H_{17}NO_5$	315.1106727	*Capsicum annuum*
364	Capsiamide	$C_{17}H_{35}NO$	269.2718648	*Capsicum annuum*
365	Capsoside A	$C_{33}H_{58}O_{15}$	694.3775712	*Capsicum annuum* var. acuminatum
366	Capsianoside IX	$C_{44}H_{74}O_{21}$	938.4722594	*Capsicum annuum*
367	Capsianoside L	$C_{76}H_{124}O_{34}$	1580.797401	*Capsicum annuum*
368	Cucurbitachrome 2	$C_{40}H_{56}O_4$	600.4178603	*Capsicum annuum* var. longum
369	Corticrocin	$C_{14}H_{14}O_4$	246.0892089	*Capsicum annuum*
370	Ceracyanin	$C_{27}H_{31}O_{15}$	595.1662953	*Capsicum annuum*
371	Capsianoside I	$C_{32}H_{52}O_{14}$	660.3357064	*Capsicum annuum* var. fascuilatum
372	Capsianoside A	$C_{76}H_{124}O_{33}$	1564.802486	*Capsicum annuum*
373	Capsianoside B	$C_{76}H_{124}O_{33}$	1564.802486	*Capsicum annuum*
374	5,8:5',8'-Diepoxy-5,5',8,8'-tetrahydro-beta,beta-carotene-3,3'-diol	$C_{40}H_{56}O_4$	600.4178603	*Capsicum annuum*
375	Capsochrome	$C_{40}H_{56}O_4$	600.4178603	*Capsicum annuum*
376	Cryptoxanthin epoxide	$C_{40}H_{56}O_2$	568.428031	*Capsicum annuum* var. lycopersiforme
377	Capsianoside XIV	$C_{38}H_{64}O_{16}$	776.419436	*Capsicum annuum* var. grossum
378	Capsianoside XV	$C_{50}H_{84}O_{26}$	1100.525083	*Capsicum annuum*

379	Capsianoside V methyl ester	$C_{27}H_{44}O_{10}$	528.2934476	*Capsicum annuum* var. grossum
380	Capsianoside XVII	$C_{44}H_{74}O_{21}$	938.4722594	*Capsicum annuum* var. grossum
381	8'-Apo-beta-carotene-3,8'-diol	$C_{30}H_{42}O_2$	434.3184806	*Capsicum annuum*
382	3'-Deoxycapsanthin	$C_{40}H_{56}O_2$	568.428031	*Capsicum annuum*
383	Capsicoside E1	$C_{56}H_{92}O_{28}$	1212.577512	*Capsicum annuum*
384	Capsicosin	$C_{57}H_{94}O_{29}$	1242.588077	*Capsicum annuum*
385	Capsicoside A3	$C_{33}H_{52}O_8$	576.3662186	*Capsicum annuum*
386	Capsicoside C3	$C_{44}H_{70}O_{17}$	870.4613008	*Capsicum annuum*
387	2,3-Dihydro-5-(3-hydroxy-1-propenyl)-2,7-dimethoxy-3-benzofuranmethanol	$C_{14}H_{18}O_5$	266.1154237	*Capsicum annuum* var. acuminatum
388	Capsicoside D	$C_{62}H_{104}O_{33}$	1376.645986	*Capsicum annuum*
389	Capsicoside B	$C_{58}H_{98}O_{30}$	1274.614292	*Capsicum annuum* var. fasciculatum
390	Capsicoside C	$C_{52}H_{88}O_{25}$	1112.561468	*Capsicum annuum* var. conides
391	Capsianoside IX	$C_{56}H_{94}O_{30}$	1246.582992	*Capsicum annuum*
392	Capsianoside VIII	$C_{50}H_{84}O_{25}$	1084.530168	*Capsicum annuum*
393	Capsianoside X	$C_{56}H_{94}O_{31}$	1262.577906	*Capsicum annuum*
394	Capsianoside XVI	$C_{62}H_{104}O_{35}$	1408.635815	*Capsicum annuum*
395	Capsianside III	$C_{32}H_{52}O_{14}$	660.3357064	*Capsicum annuum*
396	Apo-3-zeaxanthinal	$C_{27}H_{36}O_2$	392.2715304	*Capsicum annuum*
397	cis-3-Hexenyl hexanoate	$C_{12}H_{22}O_2$	198.16198	*Capsicum annuum*
398	2-Methyltetradecane	$C_{15}H_{32}$	212.250401	*Capsicum annuum*
399	cis-beta-Carotene	$C_{40}H_{56}$	536.4382018	*Capsicum annuum*
400	Diisobutyl phthalate	$C_{16}H_{22}O_4$	278.1518092	*Capsicum annuum*
401	Hexyl valerate	$C_{11}H_{22}O_2$	186.16198	*Capsicum annuum*
402	Peonidin	$C_{16}H_{13}O_6$	301.0712132	*Capsicum annuum*
403	Farnesyl cyanide	$C_{16}H_{25}N$	231.1986998	*Capsicum annuum*
404	3-Methyl-5-propyl-1,2-dithiolane	$C_7H_{14}S_2$	162.0536919	*Capsicum annuum*
405	2-Mercapto-4-heptanol	$C_7H_{16}OS$	148.0921859	*Capsicum annuum*
406	2,4-Dimercaptononane	$C_9H_{20}S_2$	192.1006421	*Capsicum annuum*
407	3-Methyl-5-pentyl-1,2-dithiolane	$C_9H_{18}S_2$	190.084992	*Capsicum annuum*
408	S-(1-Methylhexyl)cysteine	$C_{10}H_{21}NO_2S$	219.1292997	*Capsicum annuum*
409	Icariside E5	$C_{26}H_{34}O_{11}$	522.2101119	*Capsicum annuum* var. acuminatum

410	2-(Methylthio)-4-heptanethiol	$C_8H_{18}S_2$	178.084992	*Capsicum annuum*
411	Salicylic acid beta-D-glucoside	$C_{13}H_{16}O_8$	300.0845175	*Capsicum annuum*
412	Protodegalactotigonin	$C_{56}H_{94}O_{28}$	1214.593162	*Capsicum annuum*
413	Nordihydrocapsaicin	$C_{17}H_{27}NO_3$	293.1990937	*Capsicum annuum*
414	9-Methyl-N-vanillyl-7-decenamide	$C_{19}H_{29}NO_3$	319.2147438	*Capsicum annuum*
415	1-Nonen-4-one	$C_9H_{16}O$	140.1201151	*Capsicum annuum*
416	7-Methyl-N-vanillyl-5-octenamide	$C_{17}H_{25}NO_3$	291.1834437	*Capsicum annuum*
417	Nornorcapsaicin	$C_{16}H_{23}NO_3$	277.1677936	*Capsicum annuum*
418	6"-*O*-Vanilloylicariside E5	$C_{34}H_{40}O_{14}$	672.241806	*Capsicum annuum*
419	3-Glycerophosphate	$C_3H_9O_6P$	172.0136745	*Capsicum annuum*
420	Hexyl isobutanoate	$C_{10}H_{20}O_2$	172.1463299	*Capsicum annuum*
421	n-Nonylcyclohexane	$C_{15}H_{30}$	210.234751	*Capsicum annuum*
422	Benzyl pentanoate	$C_{12}H_{16}O_2$	192.1150298	*Capsicum annuum*
423	Hexyl decanoate	$C_{16}H_{32}O_2$	256.2402303	*Capsicum annuum*
424	Propenyl ether	$C_6H_{10}O$	98.07316494	*Capsicum annuum*
425	Tridecyl acetate	$C_{15}H_{30}O_2$	242.2245802	*Capsicum annuum*
426	3-Methylbutyl heptanoate	$C_{12}H_{24}O_2$	200.17763	*Capsicum annuum*
427	Normelatonin	$C_{12}H_{14}N_2O_2$	218.1055277	*Capsicum annuum*
428	2-Octanol	$C_8H_{18}O$	130.1357652	*Capsicum annuum*
429	beta-D-Glucopyranose 1-(3,4-dihydroxybenzoate)	$C_{13}H_{16}O_9$	316.0794321	*Capsicum annuum*
430	Auroxanthin 2	$C_{40}H_{56}O_4$	600.4178603	*Capsicum annuum*
431	Apigenin 4'-*O*-rhamnoside	$C_{21}H_{20}O_9$	416.1107322	*Capsicum annuum*
432	Peonidin chloride	$C_{16}H_{13}ClO_6$	336.0400659	*Capsicum annuum*
433	2-(4-Chlorophenylthio)triethylamine hydrochloride	$C_{12}H_{19}Cl_2NS$	279.0615258	*Capsicum annuum*
434	2,6,10-Trimethylundec-9-enal	$C_{14}H_{26}O$	210.1983655	*Capsicum annuum*
435	(7Z)-2-Methyl-7-hexadecene	$C_{17}H_{34}$	238.2660511	*Capsicum annuum*
436	Hexadecanoate	$C_{16}H_{31}O_2$	255.2324052	*Capsicum annuum*
437	cis-Capsanthin	$C_{40}H_{56}O_3$	584.4229457	*Capsicum annuum*
438	2-Methylheptadecane	$C_{18}H_{38}$	254.2973512	*Capsicum annuum*
439	2-Methylhexadecane	$C_{17}H_{36}$	240.2817012	*Capsicum annuum*
440	2-Methylpentadecane	$C_{16}H_{34}$	226.2660511	*Capsicum annuum*
441	2-Methyltridecane	$C_{14}H_{30}$	198.234751	*Capsicum annuum*

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442	3-Deoxy-L-arabino-hexaric acid	$C_6H_{10}O_7$	194.0426527	*Capsicum annuum*
443	D-Glycerol 1-beta-D-galactoside	$C_9H_{18}O_8$	254.1001676	*Capsicum annuum*
444	Cucurbitachrome	$C_{40}H_{56}O_4$	600.4178603	*Capsicum annuum*
445	Trihydroxy-kappa-pigment	$C_{40}H_{58}O_5$	618.428425	*Capsicum annuum*
446	beta-Cryptoxanthin 5,6-epoxide	$C_{40}H_{56}O_2$	568.428031	*Capsicum annuum*
447	1,1-Diphenyl-2-picrylhydrazyl	$C_{18}H_{12}N_5O_6$	394.0787582	*Capsicum annuum*
448	Luteoxanthin	$C_{40}H_{56}O_4$	600.4178603	*Capsicum annuum*
449	1-(4-Bromobutyl)-2-piperidinone	$C_9H_{16}BrNO$	233.041527	*Capsicum annuum*
450	(2S,3R)-2,3,4-Trihydroxybutanoic acid	$C_4H_8O_5$	136.0371734	*Capsicum annuum*
451	(Z)-11-Tetradecenyl acetate	$C_{16}H_{30}O_2$	254.2245802	*Capsicum annuum*
452	Tricin 5-*O*-rutinoside	$C_{29}H_{34}O_{16}$	638.184685	*Capsicum annuum*
453	Heptyl isobutanoate	$C_{11}H_{22}O_2$	186.16198	*Capsicum annuum*
454	Pentyl 3-methylbutanoate	$C_{10}H_{20}O_2$	172.1463299	*Capsicum annuum*
455	5,7-Dimethoxy-4'-hydroxyflavanone	$C_{17}H_{16}O_5$	300.0997736	*Capsicum annuum*
456	3-Methylbutyl-2-methylbutyrate	$C_{10}H_{20}O_2$	172.1463299	*Capsicum annuum*
457	2,2'-Azinobis (3-ethylbenzthiazoline-6-sulfonic acid)	$C_{18}H_{18}N_4O_6S_4$	514.0109173	*Capsicum annuum*
458	3-Methyl pentadecane	$C_{16}H_{34}$	226.2660511	*Capsicum annuum*
459	2-Methyl-1-pentadecene	$C_{16}H_{32}$	224.250401	*Capsicum annuum*
460	trans-Neoxanthin	$C_{40}H_{56}O_4$	600.4178603	*Capsicum annuum*
461	13-cis-Lutein	$C_{40}H_{56}O_2$	568.428031	*Capsicum annuum*
462	(3R,3'R-cis)-beta,beta-Carotene-3,3'-diol	$C_{40}H_{56}O_2$	568.428031	*Capsicum annuum*
463	Nonanoate	$C_9H_{17}O_2$	157.1228548	*Capsicum annuum*
464	(2E,4Z,6E,8E,10E)-11-[(4R)-4-Hydroxy-2,6,6-trimethyl-1-cyclohexen-1-yl]-5,9-dimethyl-2,4,6,8,10-undecapentaenal	$C_{22}H_{30}O_2$	326.2245802	*Capsicum annuum*
465	(3E,5Z,7E)-8-[(4R)-4-Hydroxy-2,6,6-trimethyl-1-cyclohexen-1-yl]-6-methyl-3,5,7-octatrien-2-one	$C_{18}H_{26}O_2$	274.1932801	*Capsicum annuum*
466	(2E,4E,6Z,8E,10E,12E)-13-[(4R)-4-Hydroxy-2,6,6-trimethyl-1-cyclohexen-1-yl]-2,7,11-trimethyl-2,4,6,8,10,12-tridecahexaenal	$C_{25}H_{34}O_2$	366.2558803	*Capsicum annuum*
467	cis-beta-Cryptoxanthin	$C_{40}H_{56}O$	552.4331164	*Capsicum annuum*
468	3-Tetradecene	$C_{14}H_{28}$	196.2191009	*Capsicum annuum*

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469	cis-Lutein	$C_{40}H_{56}O_2$	568.428031	*Capsicum annuum*
470	2-Isopropyl-5-methylhexyl acetate	$C_{12}H_{24}O_2$	200.17763	*Capsicum annuum*
471	D-Erythronic acid	$C_4H_8O_5$	136.0371734	*Capsicum annuum*
472	Heptyl 2-methylbutyrate	$C_{12}H_{24}O_2$	200.17763	*Capsicum annuum*
473	4,8-Dimethyl-1,3,7-nonatriene	$C_{11}H_{18}$	150.1408506	*Capsicum annuum*
474	Malonaldehyde	$C_3H_4O_2$	72.02112937	*Capsicum annuum*
475	Heptyl pentanoate	$C_{12}H_{24}O_2$	200.17763	*Capsicum annuum*
476	Butyl heptanoate	$C_{11}H_{22}O_2$	186.16198	*Capsicum annuum*
477	2-Butyl-1,1,3-trimethylcyclohexane	$C_{13}H_{26}$	182.2034508	*Capsicum annuum*
478	D-Galactonic acid	$C_6H_{12}O_7$	196.0583027	*Capsicum annuum*
479	2-[6-[2-(3-Ethyl-4-hydroxyphenyl)-5,7-dihydroxychromenylium-3-yl]oxy-3,4,5-trihydroxyoxan-2-yl]oxy-6-methyloxane-3,4,5-triol	$C_{27}H_{31}O_{16}$	611.16121	*Capsicum annuum*
480	2-Hydroxyisobutyric acid	$C_4H_8O_3$	104.0473441	*Capsicum annuum*
481	15-cis-Zeaxanthin	$C_{40}H_{56}O_2$	568.428031	*Capsicum annuum*
482	9-cis-Zeaxanthin	$C_{40}H_{56}O_2$	568.428031	*Capsicum annuum*
483	13-cis-Zeaxanthin	$C_{40}H_{56}O_2$	568.428031	*Capsicum annuum*
484	2-Ethenylbicyclo[2.2.1]hept-5-en-2-ol	$C_9H_{12}O$	136.088815	*Capsicum annuum*
485	1,1-Dimethyl-3-hexylcyclopentane	$C_{13}H_{26}$	182.2034508	*Capsicum annuum*
486	4alpha-Methyl-5alpha-cholest-8(14)-en-3beta-ol	$C_{28}H_{48}O$	400.3705162	*Capsicum annuum*
487	1,1,2-Trimethyl-cycloundecane	$C_{14}H_{28}$	196.2191009	*Capsicum annuum*
488	4-Methyl-1-pentanol	$C_6H_{14}O$	102.1044651	*Capsicum annuum*
489	D-Ribonic acid	$C_5H_{10}O_6$	166.0477381	*Capsicum annuum*
490	Octadecanoate	$C_{18}H_{35}O_2$	283.2637054	*Capsicum annuum*
491	Hexyl nonanoate	$C_{15}H_{30}O_2$	242.2245802	*Capsicum annuum*
492	(2E,4E,6E,8E,10E,12E,14E,16E,18E)-4,8,13,17-Tetramethyl-19-(2,6,6-trimethyl-1,3-cyclohexadien-1-yl)-1-[(1R)-1,2,2-trimethylcyclopentyl]-2,4,6,8,10,12,14,16,18-nonadecanonaen-1-one	$C_{40}H_{54}O$	550.4174663	*Capsicum annuum*
493	Pentyl 2-methylbutyrate	$C_{10}H_{20}O_2$	172.1463299	*Capsicum annuum*

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494	7-[(6-*O*-Acetyl-2-*O*-D-apio-beta-D-furanosyl-beta-D-glucopyranosyl)oxy]-2-(3,4-dihydroxyphenyl)-5-hydroxy-4H-1-benzopyran-4-one	$C_{28}H_{30}O_{16}$	622.1533849	*Capsicum annuum*
495	Luteolin 7-*O*-(2-apiosyl-6-malonylglucoside)	$C_{29}H_{30}O_{18}$	666.1432142	*Capsicum annuum*
496	7-[(6-*O*-Acetyl-2-*O*-D-apio-beta-D-furanosyl-beta-D-glucopyranosyl)oxy]-5-hydroxy-2-(4-hydroxy-3-methoxyphenyl)-4H-1-benzopyran-4-one	$C_{29}H_{32}O_{16}$	636.169035	*Capsicum annuum*
497	7-[6-*O*-Acetyl-(5-*O*-acetyl-2-*O*-D-apio-beta-D-furanosyl-beta-D-glucopyranosyl)oxy]-2-(3,4-dihydroxyphenyl)-5-hydroxy-4H-1-benzopyran-4-one	$C_{30}H3_2O_{17}$	664.1639496	*Capsicum annuum*
498	Inositol-2-phosphate	$C_6H_{13}O_9P$	260.0297185	*Capsicum annuum*
499	2,4a,5,6,9,9a-Hexahydro-3,5,5,9-tetramethyl-1H-benzocycloheptene	$C_{15}H_{24}$	204.1878008	*Capsicum annuum*
500	1-(Hexyloxy)-3-methylhexane	$C_{13}H_{28}O$	200.2140155	*Capsicum annuum*
501	1-(Hexyloxy)-4-methylhexane	$C_{13}H_{28}O$	200.2140155	*Capsicum annuum*
502	13-cis-Violaxanthin	$C_{40}H_{56}O_4$	600.4178603	*Capsicum annuum*
503	13'-cis-Lutein	$C_{40}H_{56}O_2$	568.428031	*Capsicum annuum*
504	trans-alpha-Himachalene	$C_{15}H_{24}$	204.1878008	*Capsicum annuum*
505	Hexanoic acid 3-hexenyl ester	$C_{12}H_{22}O_2$	198.16198	*Capsicum annuum*
506	Hexyl cyclobutanecarboxylate	$C_{11}H_{20}O_2$	184.1463299	*Capsicum annuum*
507	5,7-Dihydroxy-2-[4-[2-hydroxy-2-(4-hydroxy-3-methoxyphenyl)-1-(hydroxymethyl)ethoxy]-3,5-dimethoxyphenyl]-4H-1-benzopyran-4-one	$C_{27}H_{26}O_{11}$	526.1475117	*Capsicum annuum*
508	Cyclopentanecarboxylic acid, hexyl ester	$C_{12}H_{22}O_2$	198.16198	*Capsicum annuum*

Table 2: List of compounds of *Capsicum annuum* obtained from Dr Duke's database

Activity Count	Compound Name	Plant Part
112	Ascorbic-acid	Fruit
102	Caffeic-acid	Fruit
93	Tocopherol	Fruit
87	Rutin	Fruit
78	Luteolin	Fruit
77	Chlorogenic-acid	Fruit
77	Zinc	Fruit
76	Eugenol	Fruit
65	Magnesium	Fruit
60	Limonene	Fruit
60	Selenium	Fruit
53	Beta-carotene	Fruit
53	Linalool	Fruit
47	Beta-sitosterol	Fruit
44	Capsaicin	Fruit
44	Scopoletin	Fruit
39	Niacin	Fruit
34	Myricetin	Fruit
32	Alpha-tocopherol	Fruit
31	Caryophyllene	Fruit
31	Hesperidin	Fruit
31	Thiamin	Fruit
29	Tryptophan	Fruit
28	Alpha-pinene	Fruit
28	Calcium	Fruit
28	Pulegone	Fruit
27	Linoleic-acid	Fruit
26	Phenol	Fruit
26	Solanine	Fruit
25	P-coumaric-acid	Fruit
24	Benzaldehyde	Fruit
24	Chromium	Fruit
23	Alpha-terpineol	Fruit
23	Citric-acid	Fruit
23	Terpinen-4-ol	Fruit
22	Myrcene	Fruit
22	Tetramethyl-pyrazine	Fruit
21	Chlorophyll	Fruit
21	Lupeol	Seed
20	Choline	Seed
20	Choline	Pericarp
19	Acetyl-choline	Seed
19	Acetyl-choline	Pericarp
18	Guaiacol	Fruit

18	Oleic-acid	Seed
18	Oleic-acid	Fruit
18	Solasodine	Fruit
16	Acetic-acid	Fruit
16	P-cymene	Fruit
15	Alpha-linolenic-acid	Fruit
15	Fiber	Fruit
15	Folacin	Fruit
15	Lutein	Fruit
15	Methionine	Fruit
15	Riboflavin	Fruit
15	Trigonelline	Seed
14	Arginine	Fruit
14	Betaine	Fruit
14	Manganese	Fruit
14	Potassium	Fruit
14	Sulfur	Fruit
13	Beta-pinene	Fruit
13	Palmitic-acid	Seed
13	Palmitic-acid	Fruit
12	Copper	Fruit
12	Glycine	Fruit
12	Stigmasterol	Fruit
11	Alpha-phellandrene	Fruit
11	Gamma-terpinene	Fruit
11	Lithium	Fruit
11	Maltol	Fruit
11	Pantothenic-acid	Fruit
10	Piperidine	Fruit
9	Beta-amyrin	Seed
9	Camphene	Fruit
9	Oxalic-acid	Fruit
9	Terpinolene	Fruit
8	Delta-3-carene	Fruit
8	Glutamic-acid	Fruit
8	P-cresol	Fruit
8	Stearic-acid	Seed
8	Stearic-acid	Fruit
8	Tyrosine	Fruit
7	Alpha-carotene	Fruit
7	Cycloartenol	Seed
7	Glucose	Fruit
7	Histidine	Fruit
7	Phenylalanine	Fruit
7	Salicylates	Fruit
6	Ethyl-acetate	Fruit
6	Iron	Fruit

6	Myristic-acid	Fruit
6	O-cresol	Fruit
6	Propionic-acid	Fruit
5	24-methylene-cycloartanol	Seed
5	Aluminum	Fruit
5	Hexanal	Fruit
5	Octanoic-acid	Fruit
5	Phylloquinone	Fruit
5	Sabinene	Fruit
5	Solanidine	Fruit
5	Zeaxanthin	Fruit
4	Apiin	Fruit
4	Boron	Fruit
4	L-asparaginase	Fruit
4	Lysine	Fruit
4	Phosphorus	Fruit
4	Silicon	Fruit
4	Threonine	Fruit
4	Tin	Fruit
3	Alanine	Fruit
3	Aspartic-acid	Fruit
3	Cadmium	Fruit
3	Capsidiol	Fruit
3	Cycloeucalenol	Seed
3	Isoleucine	Fruit
3	Ligustrazine	Fruit
3	Nickel	Fruit
3	Pyridine	Fruit
3	Silver	Fruit
3	Valine	Fruit
3	Xylose	Fruit
2	Alpha-cryptoxanthin	Fruit
2	Arsenic	Fruit
2	Asparagine	Fruit
2	Beta-cryptoxanthin	Fruit
2	Campesterol	Fruit
2	Capsanthin	Fruit
2	Cobalt	Fruit
2	Cryptoxanthin	Fruit
2	Cystine	Fruit
2	Hexanoic-acid	Fruit
2	Leucine	Fruit
2	Molybdenum	Fruit
2	Neoxanthin	Fruit
2	Palmitoleic-acid	Fruit
2	Phytosterols	Fruit
2	Violaxanthin	Fruit

1	Antheraxanthin	Fruit
1	Behenic-acid	Fruit
1	Capsianoside-a	Fruit
1	Capsianoside-c	Fruit
1	Capsianoside-d	Fruit
1	Capsianoside-i	Fruit
1	Capsorubin	Fruit
1	Citrostadienol	Seed
1	Dihydrocapsaicin	Fruit
1	Epsilon-carotene	Fruit
1	Galactose	Fruit
1	Glucosamine	Fruit
1	Lanosterol	Seed
1	Malonic-acid	Fruit
1	Mercury	Fruit
1	Naphthalene	Fruit
1	Pentadecanoic-acid	Fruit
1	Pyrrolidine	Fruit
1	Rubixanthin	Fruit
1	Serine	Fruit
1	Sodium	Fruit
1	Toluene	Fruit
0	1,1-diethoxy-2-methylpropane	Fruit
0	1,1-diethoxy-3-methylbutane	Fruit
0	1-hexanol	Fruit
0	1-hydroxy-propan-2-one	Fruit
0	1-methylpyrrole-ketone	Fruit
0	1-*O*-caffeoyl-beta-d-glucose	Fruit
0	1-*O*-ferruloyl-beta-d-glucose	Fruit
0	13-cis-capsanthin	Fruit
0	13-cis-zeaxanthin	Fruit
0	15-cis-zeaxanthin	Fruit
0	2,3,5-trimethylpyrazine	Fruit
0	2,3-butanediol	Fruit
0	2,3-dimethyl-5-ethylpyrazine	Fruit
0	2,3-dimethyl-pyrazine	Fruit
0	2-butanone	Fruit
0	2-hexanol	Fruit
0	2-hexanone	Fruit
0	2-hydroxy-3-methyl-cyclopent-2-en-1-one	Fruit
0	2-methoxy-3-isobutyl-pyrazine	Fruit
0	2-methyl-5-ethylpyrazine	Fruit
0	2-methyl-butan-1-ol	Fruit
0	2-methyl-butan-2-ol	Fruit
0	2-methyl-butanal	Fruit
0	2-methyl-butyric-acid	Fruit
0	2-methyl-pentan-2-ol	Fruit

0	2-methyl-propanal	Fruit
0	2-methyl-propionic-acid	Fruit
0	2-pentyl-furan	Fruit
0	2-pentylpyridine	Fruit
0	24-(r)-ethyl-lophenol	Seed
0	24-dihydrolanosterol	Seed
0	24-methyl-lanost-9(11)-en-3-beta-ol	Seed
0	24-methyl-lophenol	Seed
0	3'-*O*-myristoylcapsanthin	Fruit
0	3,6-epoxide-5-hydroxy-5,6-dihydro-zeaxanthin	Fruit
0	3-(sec-butyl)-2-methoxypyrazine	Fruit
0	3-hexanol	Fruit
0	3-hydroxy-alpha-carotene	Fruit
0	3-isobutyl-2-methoxypyrazine	Fruit
0	3-isopropyl-2-methoxypyrazine	Fruit
0	3-methyl-1-pentyl-3-methyl-butyrate	Fruit
0	3-methyl-butanal	Fruit
0	3-methyl-butyric-acid	Fruit
0	3-methyl-cyclopent-2-en-1-one	Fruit
0	3-methyl-pentan-3-ol	Fruit
0	31-nor-lanost-8-en-3-beta-ol	Seed
0	31-nor-lanost-9(11)-en-3-beta-ol	Seed
0	31-nor-lanosterol	Seed
0	31-norcycloartanol	Seed
0	4-alpha-14-alpha-24-trimethyl-cholesta-8(24)-dien-3-beta-ol	Seed
0	4-alpha-24-dimethyl-cholesta-7,24-dien-3-beta-ol	Seed
0	4-alpha-methyl-24-ethyl-cholesta-7,24-dien-3-beta-ol	Seed
0	4-alpha-methyl-5-alpha-cholest-8(14)-en-3-beta-ol	Seed
0	4-ethyl-guaiacol	Fruit
0	4-methyl-1-pentyl-2-methyl-butyrate	Fruit
0	4-methyl-3-penten-2-one	Fruit
0	4-methyl-guaiacol	Fruit
0	4-methyl-heptadecane	Fruit
0	4-methyl-hexadecane	Fruit
0	4-methyl-pentanoic-acid	Fruit
0	4-methylpentadecane	Fruit
0	4-methyltetradecane	Fruit
0	4-methyltridecane	Fruit
0	5,6-dihydroxy-5,6-dihydro-zeaxanthin	Fruit
0	5-alpha-cholest-8(14)-en-3-beta-ol	Seed
0	5-hydroxy-capsanthin-3,6-epoxide	Fruit
0	5-hydroxy-capsanthin-5,6-epoxide	Fruit
0	5-hydroxycapsanthin	Fruit
0	5-methyl-2-furfural	Fruit

0	5-methyl-furfural	Fruit
0	9-cis-capsanthin	Fruit
0	9-cis-zeaxanthin	Fruit
0	Acetoin	Fruit
0	Acetylfuran	Fruit
0	Alpha-copaene	Fruit
0	Alpha-thujene	Fruit
0	Ammonia	Fruit
0	Ammonia(nh3)	Fruit
0	Arachidic-acid	Fruit
0	Ash	Fruit
0	Aurochrome	Fruit
0	Auroxanthin-1	Fruit
0	Auroxanthin-2	Fruit
0	Barium	Fruit
0	Beta-apo-8'-carotenal	Fruit
0	Beta-carotene-epoxide	Fruit
0	Bromine	Fruit
0	Butanal-2-methyl	Fruit
0	Butanal-3-methyl	Fruit
0	Butane-1,3-diol	Fruit
0	Butane-2,3-diol	Fruit
0	Capsanthin-3,6-epoxide	Fruit
0	Capsanthin-5,6-epoxide	Fruit
0	Capsanthone	Fruit
0	Capsiamide	Fruit
0	Capsianoside-b	Fruit
0	Capsianoside-e	Fruit
0	Capsianoside-f	Fruit
0	Capsianoside-ii	Fruit
0	Capsianoside-iii	Fruit
0	Capsianoside-iv	Fruit
0	Capsianoside-v	Fruit
0	Capsianside-a	Fruit
0	Capsicoside	Seed
0	Capsochrome	Fruit
0	Capsolutein	Fruit
0	Carbohydrates	Fruit
0	Carnaubic-acid	Seed
0	Carotenoids	Fruit
0	Cis-13'-capsanthin	Fruit
0	Cis-9'-capsanthin	Fruit
0	Cis-beta-carotene	Fruit
0	Cis-cryptoxanthin	Fruit
0	Citroxanthin	Fruit
0	Citrullin	Fruit
0	Cryptocapsin	Fruit

0	Cucurbitachrome	Fruit
0	Cucurbitaxanthin-a	Fruit
0	Cucurbitaxanthin-b	Fruit
0	Cycloartanol	Seed
0	Cyclohexanone	Fruit
0	Cyclopentanol	Fruit
0	Cycloviolaxanthin	Fruit
0	Decanoic-acid-vanillylamide	Fruit
0	Dehydroascorbic-acid	Fruit
0	Di-n-propyl-amine	Fruit
0	Din-n-propyl-amine	Fruit
0	Eo	Fruit
0	Eriodictin	Fruit
0	Ethyl-3-methylbutyrate	Fruit
0	Fat	Seed
0	Fat	Fruit
0	Fiber(crude)	Fruit
0	Fiber(dietary)	Fruit
0	Fluorine	Fruit
0	Foliaxanthin	Fruit
0	Galactosamine	Fruit
0	Gamma-butyrolactone	Fruit
0	Glutaminase	Fruit
0	Gramisterol	Seed
0	Heneicosane	Fruit
0	Heptadecane	Fruit
0	Hexadecane	Fruit
0	Hexan-1-al	Fruit
0	Homocapsaicin	Fruit
0	Homodihydrocapsaicin	Fruit
0	Hydroxy-alpha-carotene	Fruit
0	Hydroxy-benzoic-acid-4-beta-d-glucoside	Fruit
0	Isohexyl-isocaproate	Fruit
0	Karpoxanthin	Fruit
0	L-aspariginase	Fruit
0	Lanost-8-en-3-beta-ol	Seed
0	Latoxanthin	Fruit
0	Lead	Fruit
0	Linalol	Fruit
0	Linolenic-acid	Fruit
0	Lophenol	Seed
0	Luteoxanthin-1	Fruit
0	Luteoxanthin-2	Fruit
0	Margaric-acid	Fruit
0	Mutatoxanthin-1	Fruit
0	Mutatoxanthin-2	Fruit
0	N-(13-methyltetradecyl)acetamide	Fruit

0	N-hexanal	Fruit
0	N-methyl-aniline	Fruit
0	N-nitroso-dimethylamine	Fruit
0	N-nitroso-pyrrolidine	Fruit
0	N-pentyl-amine	Fruit
0	N-propyl-amine	Fruit
0	Nh3	Fruit
0	Nitrogen	Fruit
0	Nonadecane	Fruit
0	Nonanoic-acid-vanillylamide	Fruit
0	Norcapsaicine	Fruit
0	Nordihydrocapsaicin	Fruit
0	Obtusifoliol	Seed
0	Octane	Fruit
0	P-xylene	Fruit
0	Pentadecane	Fruit
0	Phosphatidyl-glycerol	Fruit
0	Phytoene	Fruit
0	Phytofluene	Fruit
0	Proline	Fruit
0	Protein	Fruit
0	Rubidium	Fruit
0	Strontium	Fruit
0	Sugars	Fruit
0	Sulfoquinovosyl-diacyl-glycerol	Fruit
0	Tetradecane	Fruit
0	Thiamine	Fruit
0	Titanium	Fruit
0	Vanillic-acid-4-beta-d-glucoside	Fruit
0	Vanilloyl-glucose	Fruit
0	Vanillyl-caproylamide	Fruit
0	Vanillyl-decanamide	Fruit
0	Vanillyl-octanamide	Fruit
0	Vit-b-6	Fruit
0	Water	Fruit
0	Xanthophyll-epoxide	Fruit
0	Zeta-carotene	Fruit
0	Zirconium	Fruit

Table 3: List of compounds of *Capsicum frutescens* obtained from the Knapsack database

Metabolite	Molecular Formula	Molecular Weight	Organism or InChIKey
Octopamine	$C_8H_{11}NO_2$	153.0789786	*Capsicum frutescens*
Solanidine	$C_{27}H_{43}NO$	397.334465	*Capsicum frutescens*
Solasodine	$C_{27}H_{43}NO_2$	413.3293796	*Capsicum frutescens*
Solasonine	$C_{45}H_{73}NO_{16}$	883.4929353	*Capsicum frutescens*
Capsidiol	$C_{15}H_{24}O_2$	236.17763	*Capsicum frutescens*
Methyl laurate	$C_{13}H_{26}O_2$	214.1932801	*Capsicum frutescens*
CAY-1	$C_{57}H_{94}O_{29}$	1242.588077	*Capsicum frutescens*
FEMA 2752	$C_6H_{12}O_2$	116.0837296	*Capsicum frutescens*
cis-3-Hexenyl hexanoate	$C_{12}H_{22}O_2$	198.16198	*Capsicum frutescens*

Table 4: List of compounds of *Capsicum frutescens* obtained from the Dr. Duke database

Activity Count	Compound Name	Plant Part
176	Quercetin	Fruit
112	Ascorbic-acid	Fruit
102	Caffeic-acid	Fruit
93	Tocopherol	Fruit
87	Rutin	Fruit
77	Chlorogenic-acid	Fruit
77	Zinc	Fruit
67	1,8-cineole	Fruit
65	Magnesium	Fruit
61	Ferulic-acid	Fruit
60	Limonene	Fruit
53	Beta-carotene	Fruit
47	Beta-sitosterol	Fruit
44	Capsaicin	Fruit
44	Capsaicin	Pericarp
44	Capsaicin	Seed
44	Scopoletin	Fruit
41	Camphor	Fruit
39	Niacin	Fruit
31	Caryophyllene	Fruit
31	Hesperidin	Fruit
31	Thiamin	Fruit
29	Tryptophan	Fruit
28	Calcium	Fruit
28	Pulegone	Fruit
27	Linoleic-acid	Fruit
26	Solanine	Fruit
25	P-coumaric-acid	Fruit
24	Benzaldehyde	Fruit
24	Chromium	Fruit
23	Alpha-terpineol	Fruit

23	Citric-acid	Fruit
23	Terpinen-4-ol	Fruit
22	Myrcene	Fruit
19	Carvone	Fruit
18	Cinnamic-acid	Fruit
18	Oleic-acid	Seed
18	Oleic-acid	Fruit
18	Solasodine	Fruit
17	Thujone	Fruit
15	Alpha-linolenic-acid	Fruit
15	Fiber	Fruit
15	Folacin	Fruit
15	Lutein	Fruit
15	Methionine	Fruit
15	Riboflavin	Fruit
14	Arginine	Fruit
14	Betaine	Fruit
14	Manganese	Fruit
14	Potassium	Fruit
13	Beta-ionone	Fruit
13	Beta-pinene	Fruit
13	Palmitic-acid	Seed
13	Palmitic-acid	Fruit
12	Copper	Fruit
12	Glycine	Fruit
12	Stigmasterol	Fruit
11	Alpha-phellandrene	Fruit
11	Lithium	Fruit
11	Pantothenic-acid	Fruit
9	Oxalic-acid	Fruit
8	Delta-3-carene	Fruit
8	Glutamic-acid	Fruit
8	Stearic-acid	Seed
8	Stearic-acid	Fruit
8	Tyrosine	Fruit
7	Alpha-carotene	Fruit
7	Glucose	Fruit
7	Histidine	Fruit
7	Phenylalanine	Fruit
7	Salicylates	Fruit
6	Iron	Fruit
6	Myristic-acid	Seed
6	Myristic-acid	Fruit
5	Aluminum	Fruit
5	Octanoic-acid	Fruit
5	Phylloquinone	Fruit
5	Solanidine	Fruit

5	Zeaxanthin	Fruit
4	2-undecanone	Fruit
4	Apiin	Fruit
4	Boron	Fruit
4	Lysine	Fruit
4	Phosphorus	Fruit
4	Silicon	Fruit
4	Threonine	Fruit
3	Alanine	Fruit
3	Aspartic-acid	Fruit
3	Isoleucine	Fruit
3	Nickel	Fruit
3	Valine	Fruit
3	Xylose	Fruit
2	Asparagine	Fruit
2	Campesterol	Fruit
2	Capsanthin	Fruit
2	Cobalt	Fruit
2	Cryptoxanthin	Fruit
2	Cystine	Fruit
2	Geranyl-acetone	Fruit
2	Hexanoic-acid	Fruit
2	Leucine	Fruit
2	Methyl-nonanoate	Fruit
2	Methyl-phenylacetate	Fruit
2	Neoxanthin	Fruit
2	Nonanoic-acid	Fruit
2	P-methyl-acetophenone	Fruit
2	Palmitoleic-acid	Fruit
2	Phytosterols	Fruit
2	Violaxanthin	Fruit
1	Antheraxanthin	Fruit
1	Behenic-acid	Fruit
1	Capsorubin	Fruit
1	Dihydrocapsaicin	Fruit
1	Dihydrocapsaicin	Pericarp
1	Galactose	Fruit
1	Pentadecanoic-acid	Fruit
1	Serine	Fruit
1	Sodium	Fruit
1	Toluene	Fruit
1	Vanillyl-amine	Fruit
0	1-hexanol	Fruit
0	1-pentanol	Fruit
0	2-decenoic-acid	Fruit
0	2-heptanone	Fruit
0	2-hexanol	Fruit

0	2-iso-butyl-3-methoxy-pyrazine	Fruit
0	2-methoxy-3-isobutyl-pyrazine	Fruit
0	2-methyl-butanal	Fruit
0	2-methyl-butyric-acid	Fruit
0	2-octanone	Fruit
0	2-octenoic-acid	Fruit
0	2-pentyl-furan	Fruit
0	3-acetamido-2-methyl-pentadecane	Fruit
0	3-acetamido-2-methyl-tetradecane	Fruit
0	3-hydroxy-alpha-carotene	Fruit
0	3-isobutyl-2-methoxypyrazine	Fruit
0	3-methyl-butan-1-ol	Fruit
0	3-methyl-butanal	Fruit
0	4-methyl-3-penten-2-one	Fruit
0	4-methyl-heptadecane	Fruit
0	4-methyl-hexadecane	Fruit
0	4-methyl-pentan-1-ol	Fruit
0	4-methyl-pentanoic-acid	Fruit
0	4-methylpentadecane	Fruit
0	4-methylpentyl-2-methyl-butyrate	Fruit
0	4-methylpentyl-3-methyl-butyrate	Fruit
0	4-methyltetradecane	Fruit
0	4-methyltridecane	Fruit
0	5-methyl-2-furfural	Fruit
0	7-methyl-octanoic-acid	Fruit
0	8-methyl-nonanoate	Fruit
0	8-methyl-nonanoic-acid	Fruit
0	Arachidic-acid	Fruit
0	Ash	Fruit
0	Aurochrome	Fruit
0	Barium	Fruit
0	Beta-carotene-epoxide	Fruit
0	Beta-phenethylacetate	Fruit
0	Capsanthin-3,6-epoxide	Fruit
0	Capsanthin-5,6-epoxide	Fruit
0	Capsanthone	Fruit
0	Capsiamide	Fruit
0	Capsolutein	Fruit
0	Carbohydrates	Fruit
0	Carnaubic-acid	Seed
0	Cis-3-hexen-1-ol	Fruit
0	Citroxanthin	Fruit
0	Citrullin	Fruit
0	Cryptocapsin	Fruit
0	Cucurbitaxanthin-a	Fruit
0	Cucurbitaxanthin-b	Fruit
0	Cycloviolaxanthin	Fruit

0	Decanoic-acid-vanillylamide	Fruit
0	Eo	Fruit
0	Eriodictin	Fruit
0	Ethyl-dodecanoate	Fruit
0	Ethyl-octanoate	Fruit
0	Ethyl-tetradecanoate	Fruit
0	Fat	Seed
0	Fat	Fruit
0	Foliaxanthin	Fruit
0	Heneicosane	Fruit
0	Heptadecane	Fruit
0	Heptanoic-acid	Fruit
0	Hexadecane	Fruit
0	Homocapsaicin	Fruit
0	Homodihydrocapsaicin	Fruit
0	Homodihydrocapsaicin-i	Fruit
0	Hydroxy-alpha-carotene	Fruit
0	Isohexyl-isocaproate	Fruit
0	Isothujone	Fruit
0	Latoxanthin	Fruit
0	Luteolin-7-monoglucoside	Fruit
0	Margaric-acid	Fruit
0	Methyl-8-methyl-6-nonanoate	Fruit
0	Methyl-beta-phenylpropionate	Fruit
0	Methyl-decanoate	Fruit
0	Methyl-dodecanoate	Fruit
0	Methyl-heptanoate	Fruit
0	Methyl-hexadecanoate	Fruit
0	Methyl-hexanoate	Fruit
0	Methyl-octadecanoate	Fruit
0	Methyl-octanoate	Fruit
0	Methyl-pentanoate	Fruit
0	Methyl-tetradecanoate	Fruit
0	Mevalonic-acid	Fruit
0	N-(13-methyltetradecyl)acetamide	Fruit
0	N-hexanal	Fruit
0	Nigroxanthin	Fruit
0	Nonadecane	Fruit
0	Nonanoic-acid-vanillylamide	Fruit
0	Norcapsaicin	Fruit
0	Nordihydrocapsaicin	Fruit
0	Novivamide	Fruit
0	P-xylene	Fruit
0	Pentadecane	Fruit
0	Pentanoic-acid	Fruit
0	Proline	Fruit
0	Protein	Fruit

0	Tetradecane	Fruit
0	Titanium	Fruit
0	Trans-2-hexen-1-ol	Fruit
0	Vanillyl-amide	Fruit
0	Vit-b-6	Fruit
0	Water	Fruit
0	Xanthophyll-epoxide	Fruit
0	Zucapsaicin	Fruit

QSAR and Drug-Likeness of the Compounds

The results of the analysis of the bioactivity of the compounds as immunomodulators and anti-inflammatory agents based on the QSAR prediction showed that 37 out of 121 compounds had an average PA (Probability to be Active) value above 0.4 (Table 5). Furthermore, these 37 compounds were again analyzed for their potency based on their bioactivity, which supports immunomodulatory and anti-inflammatory roles such as antioxidant, wound healing, free radical scavenging, apoptotic, TNF expression inhibitory, and MMP9 expression inhibitory activities (Figure 1). The results of the second QSAR analysis succeeded in selecting 12 potential compounds, namely Rutin, Ascorbic-acid, Linoleic-acid, Alpha-linolenic-acid, Cryptoxanthin, Zeaxanthin, Oleic-acid, Palmitoleic-acid, Beta-carotene, Capsanthin, Cryptocapsin, and Capsanthone. Only 10 of the potential compounds proceeded to the next stage. This was due to the lack of data regarding the potential protein targets of Cryptocapsin and Capsanthone.

In addition to carrying out bioactivity analysis based on QSAR predictions, each of the ten selected compounds were also analyzed for drug-likeness and ADMET characteristics (Tables 6 and 7). The analysis showed that only five compounds met the Lipinski rule of 5. The Lipinski rule of 5 includes molecular masses of less than 500 Daltons, high lipophilicity (expressed as LogP less than 5), having less than five hydrogen bond donors, having less than ten hydrogen bond acceptors, and molar refraction should be between 40-130. However, this drug-likeness does not mean that the other five compounds have no potential as drugs but instead require more energy or require an active transport mechanism to be localized within cells. Meanwhile, the ADMET (absorption, distribution, metabolism, excretion, and toxicity) analysis showed that the ten compounds had good pharmacodynamics and pharmacokinetics properties. In addition, almost all the compounds do not have the potential to cause toxicity except for a few compounds, which show the potential to cause immunotoxicity and mutagenicity. These compounds are Rutin, Cryptocapsin (immunotoxicity), and Beta-carotene (mutagenicity).

Target Protein Prediction and Gene Ontology Annotation

The target prediction results obtained from the CTD database indicate that each of the predicted potentially bioactive compounds can interact and affect several target proteins (Table 8). The number of targets for each identified compound were as follows; Ascorbic acid (46), Alpha-linolenic acid (4), Linoleic acid (6), Oleic acid (13), Palmitoleic acid (7), Cryptoxanthin (22), Zeaxanthin (5), Beta carotene (12), Rutin (12), and Capsanthin (3). In addition to analyzing the protein targets of each compound, proteins targeted by more than one red chili bioactive compound were also identified (Table 9).

Furthermore, the list of target proteins, especially cross-targets, was further analyzed using fold enrichment DAVID with a p-value < 0.05 to obtain high validity and reliability. Fold enrichment analysis was carried out for biological processes (BP) from gene ontology (GO) (Table 10 and Figure 2) and pathways from KEGG (Table 11 and Figure 3). Based on the analysis results, it was found that ten compounds were related to proteins associated with immunomodulation and inflammation, namely; BAX, BCL2, CASP3, CAT, IKBKB, IL1B, IL6, MAPK1, MAPK3, NFE2L2, NFKBIA, PPARA, PPARB/PPARD, PPARG, PTGS2, RELA, RUNX2, SOD1, TNF, and TP53.

Pharmacology Network

Visualization of the results of the type of analysis and interaction mechanism of the Katokkon pepper bioactive compounds with target proteins involved in immunomodulatory and inflammatory processes was carried out using Cytoscape software (Figure 4). The results of the analysis showed that ascorbic acid could inhibit the activity and result in decreased expression of BCL2,[31] CASP3,[32] IKBKB,[33] IL1B,[34] IL6,[35] MAPK1,[36] MAPK3,[37] NFKBIA,[38] PTGS2,[39] RELA,[40] TNF,[41] and TP53.[42] This compound can also indirectly reduce PPARG expression.[43] As listed in Table 11, several genes such as IL6, CASP3, BCL2, TNF, TP53, and PPARG are involved in apoptosis. Other genes whose expression was suppressed by ascorbic acid were IKBKB, IL6, MAPK1, MAPK3, NFKBIA, PTGS2, RELA, and TNF, which are involved in tumor necrosis factor-mediated signaling pathways. Meanwhile, several proteins whose expression was increased by ascorbic acid were BAX,[44] CAT,[45] NFE2L2,[46] RUNX2,[47] and SOD1.[48] As shown in Table 11, BAX is a gene involved in apoptosis-positive regulation, while CAT is involved in negative regulation. The NFE2L2 is a transcription factor that regulates several antioxidant enzymes and plays an essential physiological role in controlling oxidative stress and inflammation.[49] RUNX2 serves as a transcription factor of osteoblast differentiation,[50] and SOD1 is an antioxidant enzyme that protects cells.[51] These results showed that ascorbic acid has a crucial role as an immunomodulator and can work in two opposing ways by decreasing or increasing the expression of genes involved in each specific functional pathway, such as apoptosis, inflammation, antioxidants, etc. Ascorbic acid is essential to stimulate the immune system by increasing the strength and protection of the organism through its immunostimulatory, anti-inflammatory, antiviral, and antibacterial activities.[52]

Capsanthin was predicted to inhibit and reduce the activity and phosphorylation of MAPK1 and MAPK3.[53] As shown in Table 11, MAPK1 and MAPK3 play a role in several signaling pathways such as tumor necrosis factor-mediated pathways, apoptosis, T & B cell receptors, and response to viral infections. A study reported that capsanthin from *Capsicum annum* fruits has antiglaucoma, antioxidant, and anti-inflammatory activities, and also increase the expression of proinflammatory cytokine gene in a rat model of dry eye disease.[54]

Beta-carotene inhibits the activity, and results in decreased expression of MAPK1 and MAPK3.[55] This compound can also indirectly reduce the expression of BCL2.[56] This suggests that beta-carotene has a similar effect as capsanthin

in reducing the expression of the MAPKs gene. Meanwhile, several proteins whose expression was increased by beta carotene were BAX,[56] CAT,[57] and TNF.[58] Studies have reported that beta-carotene could stimulate immune function in humans by increasing plasma levels of TNF-alpha, enhancing the population of specific lymphocyte subsets, and stimulate the production of various cytokines.[59]

Cryptoxanthin inhibits activity, and results in decreased expression of IL1B, IL6, MAPK1, MAPK3, RELA, and TNF.[60] This compound inhibits processes similar to ascorbic acid, resulting in lower IL1B, IL6, MAPK1, MAPK3, RELA, and TNF expression. A study reported that in mouse Sertoli cells, β-cryptoxanthin inhibited NF-B activation, and MAPK phosphorylation, resulting in anti-inflammatory actions.[61]

Table 5: List of compounds and the results of the bioactivity analysis of the compounds as immunomodulators

S/N	Bioactive Compound	CID	Immunostimulant	Immunosuppressant	Immunomodulator	Anti-inflammatory	Mean
1	Rutin	5280805	0.607	0.602	0.318	0.728	0.56375
2	Ascorbic-acid	54670067	0.557	0.43	0.422	0.779	0.547
3	Linoleic-acid	5280450	0.558	0.448	0.438	0.73	0.5435
4	Stigmasterol	5280794	0.36	0.782	0.46	0.542	0.536
5	Alpha-linolenic-acid	5280934	0.505	0.418	0.413	0.804	0.535
6	Campesterol	173183	0.526	0.761	0.341	0.502	0.5325
7	2-hexanol	12297	0.563	0.481	0.52	0.557	0.53025
8	Beta-sitosterol	222284	0.615	0.762	0.276	0.467	0.53
9	Phytosterols	12303662	0.615	0.762	0.276	0.467	0.53
10	Cryptoxanthin	5281235	0.432	0.76	0.219	0.698	0.52725
11	Zeaxanthin	5280899	0.441	0.745	0.217	0.675	0.5195
12	Oleic-acid	445639	0.54	0.505	0.416	0.614	0.51875
13	Palmitoleic-acid	445638	0.54	0.505	0.416	0.614	0.51875
14	cis-3-Hexenyl hexanoate	5352543	0.511	0.367	0.386	0.768	0.508
15	Apiin	5280746	0.768	0.44	0	0.743	0.48775
16	Beta-carotene	5280489	0.363	0.686	0.198	0.69	0.48425
17	Isohexyl-isocaproate	88168807	0.492	0.472	0.428	0.519	0.47775
18	Arachidic-acid	10467	0.504	0.451	0.419	0.515	0.47225
19	Carnaubic-acid	11197	0.504	0.451	0.419	0.515	0.47225

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20	Heptanoic-acid	8094	0.504	0.451	0.419	0.515	0.47225
21	Hexanoic-acid	8892	0.504	0.451	0.419	0.515	0.47225
22	Myristic-acid	11005	0.504	0.451	0.419	0.515	0.47225
23	Octanoic-acid	379	0.504	0.451	0.419	0.515	0.47225
24	Palmitic-acid	985	0.504	0.451	0.419	0.515	0.47225
25	Pentadecanoic-acid	13849	0.504	0.451	0.419	0.515	0.47225
26	Stearic-acid	5281	0.504	0.451	0.419	0.515	0.47225
27	1-hexanol	8103	0.472	0.43	0.469	0.498	0.46725
28	Capsanthin	5281228	0.287	0.633	0	0.901	0.45525
29	Cryptocapsin	14515709	0.284	0.628	0	0.894	0.4515
30	Hesperidin	10621	0.487	0.591	0	0.691	0.44225
31	Capsanthone	21764964	0.244	0.613	0	0.888	0.43625
32	Eriodictin	101789466	0.391	0.596	0	0.733	0.43
33	Caryophyllene	5281515	0	0.626	0.345	0.745	0.429
34	Solanine	262500	0.553	0.721	0	0.416	0.4225
35	Phylloquinone	5284607	0.467	0.625	0	0.579	0.41775
36	Cinnamic-acid	444539	0.241	0.443	0.287	0.656	0.40675
37	Capsorubin	5281229	0.255	0.435	0	0.92	0.4025

Meanwhile, this compound can indirectly increase the production of CASP3 and the expression of RUNX2.[62] In general, β-cryptoxanthin may increase humoral immunity in mammals and potentially have a major impact on human health.[61]

Linoleic acid inhibits the activity and decreases NFKBIA expression. Meanwhile, several activated proteins expressions, namely; PPARA, PPARD, PPARG, PTGS2, and TNF are increased by linoleic acid.[63] Linoleic acid has been identified as having the potential to bind to PPARA, PPARD, and PPARG in the activation process.[64] This compound also indirectly increases the expression of CASP3,[63] CAT,[65] and IL6.[66]

Linolenic acid inhibits the activity and results in decreased expression of PTGS2.[67] Meanwhile, the expression of several activated proteins such as PPARA, PPARD, and PPARG are increase by linolenic acid by binding to the active site of the protein during the activation process.[64]

Oleic acid indirectly reduces the expression of BCL2,[68] CAT,[69] and SOD1.[70] Meanwhile, several proteins like PPARA, PPARD, and PPARG are activated by oleic acid, by binding to the protein's active site during the activation process.[64] This compound can also indirectly increase the expression of CASP3,[68] IL6,[71] and TNF.[69] Like oleic acid, palmitoleic acid indirectly increases IL6 expression and influences PPARA expression.[72] Another study also showed that palmitoleic acid has more anti-inflammatory potential than other fatty acids in human endothelial cells.[73]

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Table 6: Results of drug-likeness and ADMET analysis of potential immunomodulatory compounds using AdmetLab2.0

Compd. Name	Mol Wt	Num. H-bond acceptors	Num. H-bond donors	TPSA	LogS (log mol/L)	AlogP	Pgp-inhibitor		Pgp-substrate		Human Intestinal Absorption		F (20% Bioavailability)		F (30% Bioavailability)		Blood Brain Barrier		H-HT (Human Hepatotoxicity)		DILI (Drug Induced Liver Injury)		FDAMDD (Maximum Recommended Daily Dose)		Drug likeness		
							Value	Prob	Value	Prob	Value	Prob	Value	Pro	Value	Prob	Value	Prob	Value	Prob	Value	Prob	Value	Prob	Lipinski	Pfizer	GSK
Ascorbic acid	176.03	6	5	114.29	-0.613	-1.42	---	0.001	---	0.089	---	0.069	+++	0.918	+++	0.978	---	0.073	--	0.168	+++	0.936	---	0.009	Accepted	Accepted	Accepted
Alpha linolenic acid	278.22	2	1	37.3	-4.973	6.156	---	0	---	0.002	---	0.007	---	0.003	++	0.849	--	0.295	---	0.006	---	0.007	---	0.017	Accepted	Rejected	Rejected
Linoleic acid	280.24	2	1	37.3	-5.23	6.652	---	0	---	0.002	---	0.01	---	0.009	+	0.549	--	0.196	---	0.013	---	0.009	---	0.017	Accepted	Rejected	Rejected
Oleic acid	282.26	2	1	37.3	-5.559	7.131	---	0	---	0	---	0.007	--	0.116	+	0.658	--	0.101	---	0.018	---	0.013	---	0.013	Accepted	Rejected	Rejected
Palmitoleic acid	254.22	2	1	37.3	-4.791	6.293	---	0.001	---	0.001	---	0.007	---	0.082	-	0.408	--	0.215	---	0.021	---	0.013	---	0.014	Accepted	Rejected	Rejected
Cryptoxanthin	552.43	1	1	20.23	-7.58	10.181	++	0.999	++	0.785	---	0.045	---	0.007	---	0.045	---	0.002	--	0.224	---	0.003	--	0.929	Rejected	Rejected	Rejected
Zeaxanthin	568.43	2	2	40.46	-7.119	9.238	++	0.999	++	0.906	--	0.118	---	0.005	---	0.011	---	0.011	--	0.189	---	0.001	+++	0.954	Rejected	Rejected	Rejected
Beta carotene	536.44	0	0	0	-7.973	11.15	++	1	-	0.437	--	0.117	---	0.011	-	0.318	---	0	--	0.281	---	0.009	++	0.874	Rejected	Rejected	Rejected
Rutin	610.15	16	10	269.43	-3.928	-0.763	---	0.002	++	0.978	+++	0.925	--	0.234	+++	0.999	--	0.111	+++	0.092	++	0.982	---	0.014	Rejected	Accepted	Rejected
Capsanthin	584.42	3	2	57.53	-6.578	8.455	++	0.999	++	0.903	--	0.19	---	0.004	---	0.001	---	0.016	-	0.352	---	0.001	+++	0.957	Rejected	Rejected	Rejected

Key: Red font: inappropriate or warning, Green font: Pa first stage (immunomodulator and anti-inflammatory) and second stage (supporting bioactivity) analysis above 0.5, Blue font: Pa analysis of first stage bioactivity (immunomodulator and anti-inflammatory) above 0.4 and second stage (supporting bioactivity) above 0.5.

Table 7: Results of analysis of drug-likeness and toxicity of potential immunomodulatory compounds using Protox II

CompdName	LD50 (mg/kg)	Toxicity Class	Average similarity	Prediction accuracy	MW	Number of hydrogen bond acceptors	Number of hydrogen bond donors	Number of rotable bonds	Molecular refractivity	Topological Polar Surface Area	octanol/water partition coefficient(logP)	Hepatotoxicity		Carcinogenicity		Immunotoxicity		Mutagenicity		Cytotoxicity	
												Prediction	Probability	Prediction	Probability	Prediction	Probability	Prediction	Probability	Prediction	Probability
Cryptoxanthin	**10**	**2**	**82.54**	**70.97**	**552.87**	**57**	**1**	**10**	**185.59**	**20.23**	**11.58**	**Inactive**	**0.81**	**Inactive**	**0.73**	**Inactive**	**0.84**	**Inactive**	**0.76**	**Inactive**	**0.9**
Zeaxanthin	10	2	82.54	70.97	568.87	58	2	10	186.76	40.46	10.55	Inactive	0.79	Inactive	0.67	Inactive	0.92	Inactive	0.81	Inactive	0.89
Beta-carotene	1510	4	83.45	70.97	536.87	56	0	10	184.43	0	12.61	Inactive	0.85	Inactive	0.86	Inactive	0.88	Active	0.71	Inactive	0.81
Rutin	5000	5	100	100	610.52	45	10	6	141.38	269.43	-1.69	Inactive	0.8	Inactive	0.91	Active	0.98	Inactive	0.88	Inactive	0.64
Capsanthin	650	4	70.65	69.26	584.87	59	2	11	187.17	57.53	9.81	Inactive	0.64	Inactive	0.51	Inactive	0.8	Inactive	0.67	Inactive	0.89
Cryptocapsin	4000	5	77.15	69.26	568.87	58	1	11	186.01	37.3	10.84	Inactive	0.58	Inactive	0.65	Active	0.56	Inactive	0.77	Inactive	0.91
Ascorbic-acid	3367	5	100	100	176.12	14	4	2	35.12	107.22	-1.41	Inactive	0.86	Inactive	0.92	Inactive	0.99	Inactive	0.87	Inactive	0.65
Alpha-linolenic-acid	10000	6	100	100	278.43	32	1	13	88.99	37.3	5.66	Inactive	0.54	Inactive	0.63	Inactive	0.99	Inactive	0.95	Inactive	0.71
Capsanthone	4600	5	69.9	68.07	582.86	57	1	11	186.21	54.37	10.01	Inactive	0.73	Inactive	0.54	Inactive	0.79	Inactive	0.64	Inactive	0.81
Linoleic-acid	10000	6	100	100	280.45	34	1	14	89.46	37.3	5.88	Inactive	0.55	Inactive	0.64	Inactive	0.96	Inactive	1	Inactive	0.71
Oleic-acid	48	2	100	100	282.46	36	1	15	89.94	37.3	6.11	Inactive	0.55	Inactive	0.64	Inactive	0.99	Inactive	1	Inactive	0.71
Palmitoleic-acid	48	2	100	100	254.41	32	1	13	80.32	37.3	5.33	Inactive	0.55	Inactive	0.64	Inactive	0.99	Inactive	1	Inactive	0.71

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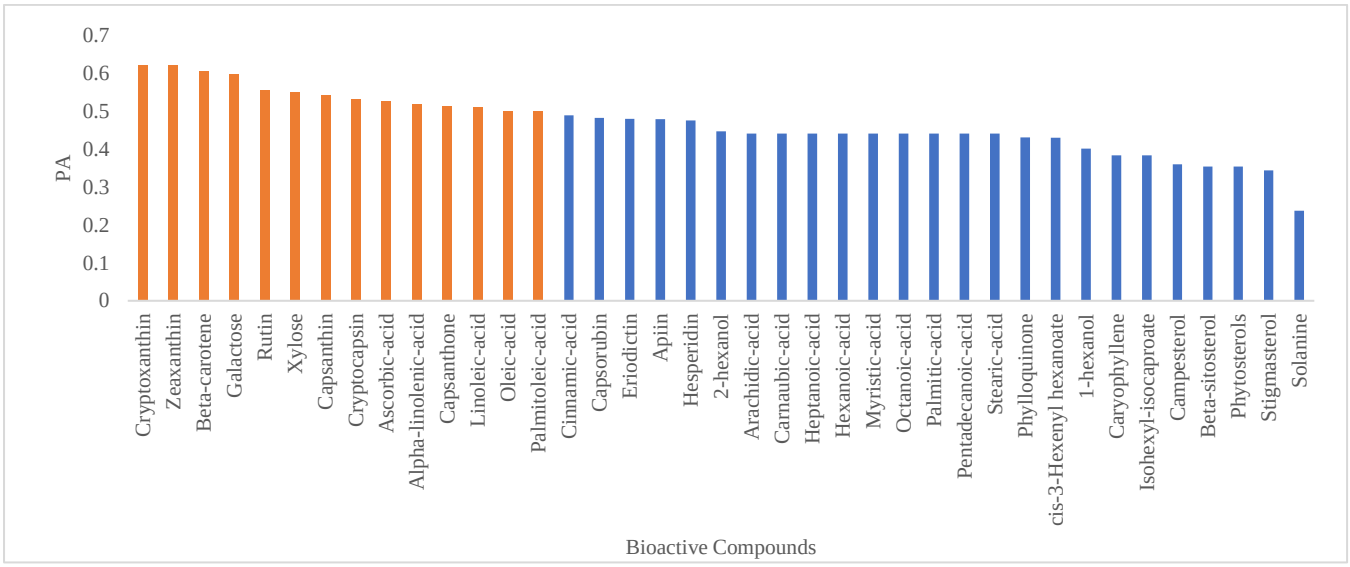

Figure 1: Results of QSAR analysis of compounds as immunomodulators, anti-inflammatory agents, and other supporting bioactivities. Note: Orange means the PA value is above 0.4 (predicted to have potential computationally and based on experiments).

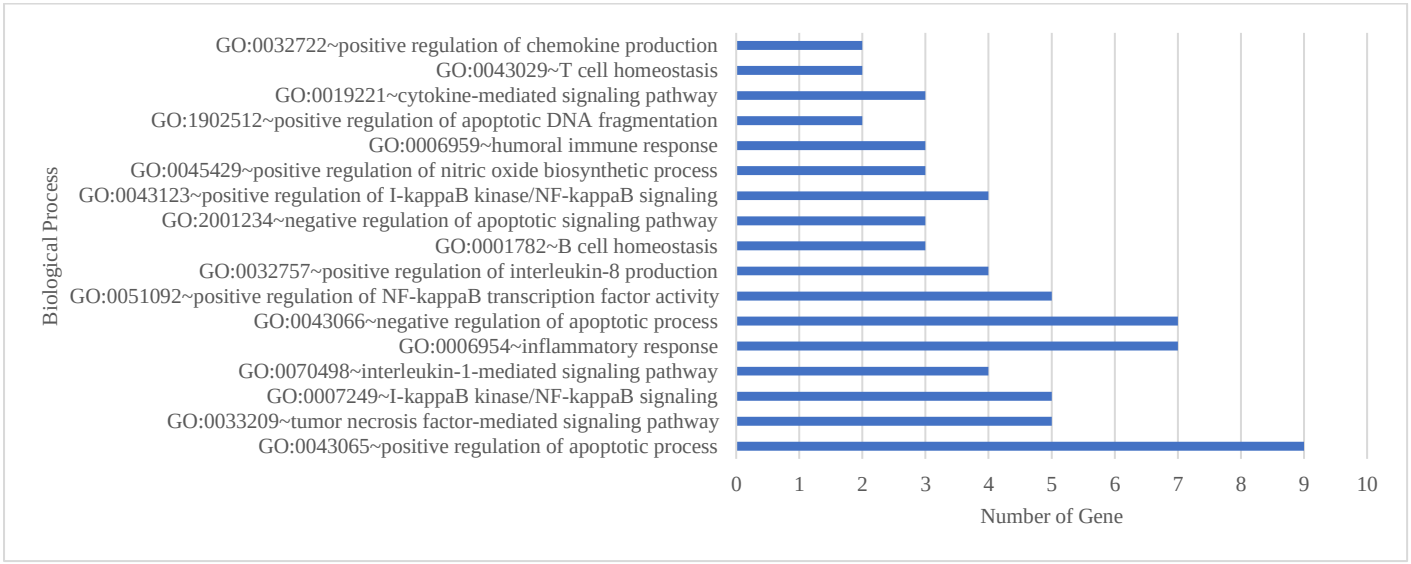

Figure 2: Results of the analysis of fold enrichment biological process (BP) from gene ontology (GO)

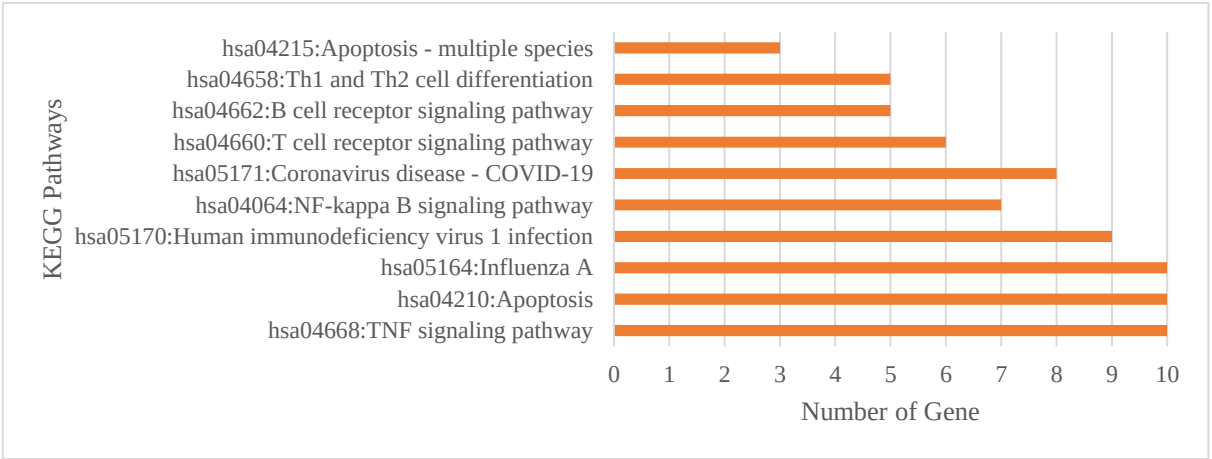

Figure 3: The results of the analysis of fold enrichment pathways from KEGG

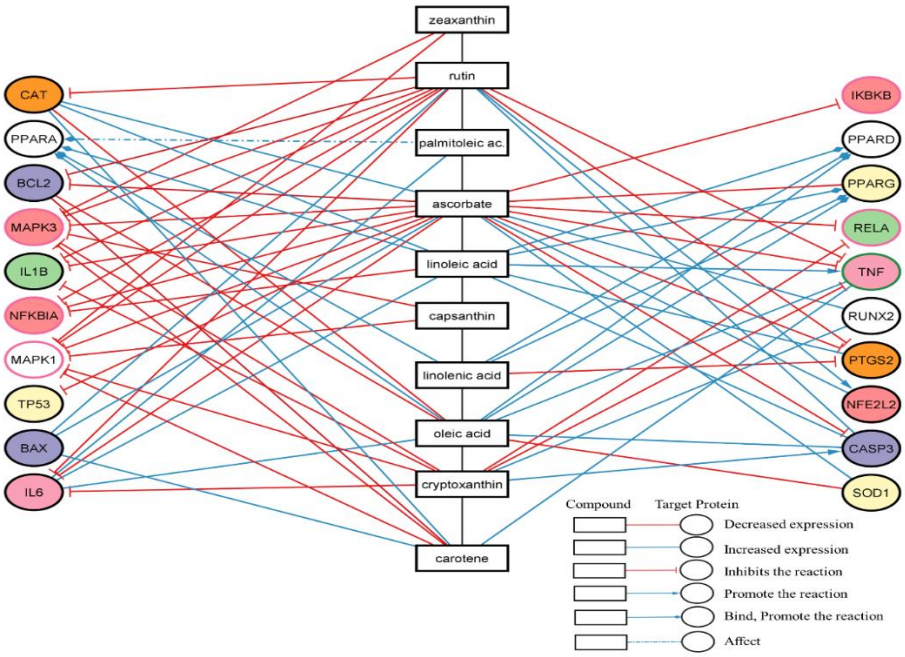

Figure 4: Types and mechanisms of interaction of potential bioactive compounds of Katokkon pepper with target proteins in immunomodulatory and anti-inflammatory processes.
Note: Blue node colour plays a role in the immunomodulatory mechanism; pink node colour plays a role in anti-inflammatory mechanism; yellow node colour plays a role in the mechanism of apoptosis; pink node colour plays a role in the mechanism of immunomodulator-anti-inflammatory-apoptosis; green node colour plays a role in the immunomodulator-anti-inflammatory mechanism; orange node colour plays a role in the anti-inflammatory-apoptotic mechanism; purple node colour plays a role in the mechanism of immunomodulator-apoptosis; pink node border colour plays a role in B cell pathways and helper T cells; and the green node border colour plays a role in the pathways of B cells, T cells, and helper T cells.

Table 8: List of targets for each bioactive compound based on the CTD database

S/N	Compound	Code	Target
1	Ascorbic acid	AA	CAT, TNF, HMOX1, RUNX2, CASP3, BGLAP, IL1B, NFE2L2, GSR, NOS2, TP53, BCL2, BMP2, COL1A1, PTGS2, SLC23A2, SOD1, PPARG, SLC23A1, BAX, FABP4, GPX1, ACHE, NQO1, PARP1, RELA, TGFB1, IGF1, SPP1, ALPL, CDKN1A, CTNNB1, IBSP, IL6, MAPK1, MAPK3, ACTA2, COL2A1, CYP2E1, NOS3, CCND1, CEBPA, HMGCR, PCNA, S100B, GFAP
2	Alpha linolenic acid	AL	PPARA, PTGS2, PPARG, PPARB
3	Linoleic acid	LA	PPARA, PPARG, TNF, PTGS2, IL6, PPARB
4	Oleic acid	OA	PPARA, CPT1A, SREBF1, IL6, PLIN2, PPARG, CD36, APOB, FASN, AKT1, PPARB, HSPA5, SOD2
5	Palmitoleic acid	PA	ABCA1, PON1, APOA1, IL6, INS, PCK1
6	Cryptoxanthin	CX	CASP3, CSF1, TNFSF11, COL1A1, RUNX2, ACP5, AR, BCO2, CREB1, CTSK, FSHR, HSF2, INHBB, NFATC1, SHBG, IL10, IL1B, IL6, MAPK1, MAPK3, RELA, TNF CASP3, CSF1, TNFSF11, COL1A1, RUNX2, ACP5, AR, BCO2, CREB1, CTSK, FSHR, HSF2, INHBB, NFATC1, SHBG, IL10, IL1B, IL6, MAPK1, MAPK3, RELA, TNF
7	Zeaxanthin	ZX	BCO2, GSTP1, HIF1A, MAPK1, MAPK3
8	Rutin	RT	BCO1, TNF, MAPK1, MAPK3
9	Beta carotene	BC	TNF, CASP3, IL6, BCL2, IL1B, PTGS2, BAX, CAT, MAPK1, MAPK3, CASP9, NFE2L2
10	Capsanthin	CS	GJA1, MAPK1, MAPK3

Table 9: List of cross-targets of potential Katokkon pepper bioactive compounds

Compound	Target
AA-RT	BAX, BCL2, CAT, NFE2L2
CX-ZX	BCO2
AA-OA	SOD1
AA-CX	COL1A1, RELA, RUNX2
AA-CX-RT	CASP3, IL1B
AL-LA-OA	PPARA, PPARB
AA-AL-LA-OA	PPARG
AA-AL-LA-RT	PTGS2
AA-LA-CX-BC-RT	TNF
AA-CX-ZX-BC-RT-CS	MAPK1, MAPK3
AA-LA-OA-PA-CX-RT	IL6

Furthermore, it serves as lipokine that regulates several metabolic processes, including increased cell proliferation, insulin sensitivity in muscle, endoplasmic reticulum stress mitigation, and lipogenic activity in white adipocytes.[74]

Rutin inhibits the activity, and results in decreased expression of BCL2,[75] CAT,[76] IL1B & IL6, TGS2[77] MAPK1 & MAPK3, TNF,[78] and NFKBIA.[79] Meanwhile, the expression of proteins like CASP3,[80] and NFE2L2[81] are increased by rutin. This compound can also indirectly increase the expression of BAX.[75] This is supported by a study which reported that rutin can boost immunological function through both cellular and humoral pathways.[82] Rutin inhibited TNF and IL6 production, as well as HMGB1 activation of nuclear factor-B and extracellular regulated kinases 1/2, so it could be a potential therapeutic drug for treating many severe vascular inflammatory disorders by suppressing the HMGB1 signaling pathway.[83]

Zeaxanthin inhibits the activity and decreases the expression and phosphorylation of MAPK1 and MAPK3.[84] Through modulation of the MAPK pathway, zeaxanthin dipalmitate enhanced hepatic functioning in an alcoholic fatty liver disease model.[85] It has also been reported that zeaxanthin alleviated allergic asthma in mice by modulating the p38 MAPK/-catenin signaling pathway.[86]

Finally, the Katokkon pepper, as a member of the *Capsicum* genus, has the potential as an immunomodulator. Our findings are consistent with and supported by an *in vitro* study which reported that capsicum extract increases immunoglobulin production in intestinal B cells.[87]

Table 10: Results of the analysis of fold enrichment biological process (BP) from gene ontology (GO)

Term	P Value	Genes
GO:0043065~positive regulation of apoptotic process	4.46E-10	IL6, CASP3, BCL2, BAX, PPARG, PTGS2, TNF, TP53, SOD1
GO:0033209~tumor necrosis factor-mediated signaling pathway	2.20E-07	NFKBIA, IKBKB, TNF, TP53, RELA
GO:0007249~I-kappaB kinase/NF-kappaB signaling	3.36E-07	NFKBIA, IKBKB, IL1B, TNF, RELA
GO:0070498~interleukin-1-mediated signaling pathway	1.06E-06	IKBKB, IL1B, RELA, MAPK3
GO:0006954~inflammatory response	1.96E-06	IKBKB, IL6, IL1B, PTGS2, TNF, RELA, NFE2L2
GO:0043066~negative regulation of apoptotic process	8.26E-06	IL6, CASP3, CAT, BCL2, TP53, RELA, PPARD
GO:0051092~positive regulation of NF-kappaB transcription factor activity	1.63E-05	IKBKB, IL1B, CAT, TNF, RELA
GO:0032757~positive regulation of interleukin-8 production	3.38E-05	IL6, IL1B, TNF, RELA
GO:0001782~B cell homeostasis	2.93E-04	CASP3, BCL2, BAX
GO:2001234~negative regulation of apoptotic signaling pathway	4.74E-04	BCL2, BAX, TNF
GO:0043123~positive regulation of I-kappaB kinase/NF-kappaB signaling	8.31E-04	IKBKB, IL1B, TNF, RELA
GO:0045429~positive regulation of nitric oxide biosynthetic process	0.001047	IL1B, PTGS2, TNF
GO:0006959~humoral immune response	0.001618	IL6, BCL2, TNF
GO:1902512~positive regulation of apoptotic DNA fragmentation	0.004905	IL6, BAX
GO:0019221~cytokine-mediated signaling pathway	0.01011	IL6, IL1B, RELA
GO:0043029~T cell homeostasis	0.031953	CASP3, BCL2
GO:0032722~positive regulation of chemokine production	0.04333	IL6, TNF

Table 11: Results of the analysis of fold enrichment pathways from KEGG

Term	P Value	Genes
hsa04668:TNF signaling pathway	9.80E-13	NFKBIA, IKBKB, IL6, IL1B, CASP3, MAPK1, PTGS2, TNF, RELA, MAPK3
hsa04210:Apoptosis	5.81E-12	NFKBIA, IKBKB, CASP3, BCL2, BAX, MAPK1, TNF, TP53, RELA, MAPK3
hsa05164:Influenza A	4.64E-11	NFKBIA, IKBKB, IL6, IL1B, CASP3, BAX, MAPK1, TNF, RELA, MAPK3
hsa05170:Human immunodeficiency virus 1 infection	1.03E-08	NFKBIA, IKBKB, CASP3, BCL2, BAX, MAPK1, TNF, RELA, MAPK3
hsa04064:NF-kappa B signaling pathway	8.51E-08	NFKBIA, IKBKB, IL1B, BCL2, PTGS2, TNF, RELA
hsa05171:Coronavirus disease - COVID-19	4.98E-07	NFKBIA, IKBKB, IL6, IL1B, MAPK1, TNF, RELA, MAPK3
hsa04660:T cell receptor signaling pathway	3.00E-06	NFKBIA, IKBKB, MAPK1, TNF, RELA, MAPK3
hsa04662:B cell receptor signaling pathway	3.20E-05	NFKBIA, IKBKB, MAPK1, RELA, MAPK3
hsa04658:Th1 and Th2 cell differentiation	5.04E-05	NFKBIA, IKBKB, MAPK1, RELA, MAPK3
hsa04215:Apoptosis - multiple species	0.002418	CASP3, BCL2, BAX

Conclusion

From the findings of the present sudy, it can be concluded that the Katokkon pepper, as well as all members of red pepper and cayenne pepper, have the potential to be used as immunomodulators. Bioactive compounds in these peppers that were predicted to have potential as immunomodulators and anti-inflammatory agents include rutin, ascorbic acid, linoleic-acid, alpha-linolenic acid, cryptoxanthin, zeaxanthin, oleic acid, palmitoleic acid, beta-carotene, and capsanthin. These compounds can affect the expression and activity of several proteins that play a role in immunomodulation, inflammation, and apoptosis, namely; BAX, BCL2, CASP3, CAT, IKBKB, IL1B, IL6, MAPK1, MAPK3, NFE2L2, NFKBIA, PPARA, PPARB/PPARD, PPARG, PTGS2, RELA, RUNX2, SOD1, TNF, and TP53. These findings are useful as important preliminary data for conducting further study on compounds from chili peppers for wider applications in human health and in the food industry.

Conflict of Interest

The authors declare no conflict of interest.

Authors' Declaration

The authors hereby declare that the work presented in this article is original and that any liability for claims relating to the content of this article will be borne by them.

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