

Integrated *In-Silico* Prioritization of Anti-Diabetic Candidates from *Helianthus Tuberosus* Using Bibliometrics, Target Prediction, Docking, MD, and ADMET Profiling



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Table S1. Queries for the bibliometric analysis of the medicinal potential of *Helianthus tuberosus* (H. tuberosus) in Web of Science and Scopus databases.

Code	Search Within	Query
#1	Title	"Jerusalem Artichoke" OR "Artichoke, Jerusalem" OR "Helianthus tuberosus"
#2	Title, abstract and keywords	"Alkaloids" OR "Alkaloid" OR "Plant Alkaloids" OR "Alkaloids" OR "Plant" OR "Plant Alkaloid" OR "Alkaloid, Plant" OR "Flavonoids" OR "2-Phenyl-Chromene" OR "2 Phenyl Chromene" OR "Flavonoid" OR "2-Phenyl-Benzopyran" OR "2 Phenyl Benzopyran" OR "2-Phenyl-Benzopyrans" OR "2 Phenyl Benzopyrans" OR "2-Phenyl-Chromenes" OR "2 Phenyl Chromenes" OR "Bioflavonoids" OR "Bioflavonoid" OR "Caffeic Acids" OR "Acids, Caffeic" OR "Terpenes" OR "Terpenoid" OR "Terpene" OR "Terpenoids" OR "Isoprenoids" OR "Isoprenoid" OR "Saponins" OR "Saponin" OR "Tannins" OR "Tannin" OR "Carotenoids" OR "Carotenoid" OR "Carotenes" OR "Carotene" OR "Tetraterpenes" OR "Tetraterpene derivatives" OR "Derivatives" OR "Tetraterpene" OR "Glucosinolates" OR "Glucosinolate" OR "Phytoestrogens" OR "Phytoestrogens" OR "Plant Estrogens" OR "Estrogens, Plant" OR "Plant Estrogen" OR "Estrogen, Plant" OR "Phyto-Estrogen" OR "Phyto Estrogen" OR "Phytoestrogen" OR "Estrogen-Like" OR "Plant Extracts" OR "Estrogen Like" OR "Plant Extracts" OR "Extracts, Estrogen-Like Plant" OR "Plant Extracts, Estrogen-Like" OR "Lignans" OR "Lignan" OR "Neolignans" OR "Neolignan" OR "Chlorophyll" OR "Chlorophyll 740" OR "Phyllobilins" OR "Cucurbitacins" OR "Cucurbitacin" OR "Sulfur Compounds" OR "Compounds, Sulfur" OR "Sulfur Compound" OR "Compound, Sulfur" OR "Fatty Acids" OR "Fatty Acid" OR "Aliphatic Acids" OR "Aliphatic Acid" OR "Acid, Aliphatic" OR "Fatty Acids, Esterified" OR "Esterified Fatty Acids" OR "Esterified Fatty Acid" OR "Acid, Esterified Fatty" OR "Fatty Acid, Esterified" OR "Fatty Acids, Saturated" OR "Saturated Fatty Acids" OR "Saturated Fatty Acid" OR "Acid, Saturated Fatty" OR "Fatty Acid, Saturated" OR "Phytosterols" OR "Plant Sterol" OR "Sterol, Plant" OR "Plant Steroid" OR "Steroid, Plant" OR "Phytosteroids" OR "Phytosteroid" OR "Plant Sterols" OR "Sterols, Plant" OR "Phytosterol" OR "Plant Steroids" OR "Steroids, Plant" OR "Sulfides" OR "Sulfide" OR "Thioethers" OR "Thioether" OR "Sulfur Ethers" OR "Ethers, Sulfur" OR "Anthraquinones" OR "Anthracenedione" OR "Anthranoid" OR "Anthraquinone Compound" OR "Compound, Anthraquinone" OR "Anthraquinone Derivative" OR "Derivative, Anthraquinone" OR "Anthraquinone" OR "Anthracenediones" OR "Anthranoids" OR "Anthraquinone Compounds" OR "Anthraquinone Derivatives" OR "Dianthrones" OR "Dianthraquinones" OR "Flavonols" OR "2-Phenyl-3-Hydroxy-Benzopyran-4-Ones" OR "2 Phenyl 3 Hydroxy Benzopyran 4 Ones" OR "3-hydroxy-4-keto-Flavonoids" OR "3 hydroxy 4 keto Flavonoids" OR "Pueraria" OR "Puerarias" OR "Puerariae" OR "Kudzu" OR "Kudzu" OR "Pueraria lobata" OR "lobatas, Pueraria" OR "Pueraria lobatas" OR "Pueraria tuberosa" OR "Pueraria tuberosas" OR "tuberosa, Pueraria" OR "Pueraria montana" OR "montana, Pueraria" OR "Pueraria montanas" OR "Pachyrhizus thunbergianus" OR "Coumarins" OR "Coumarine" OR "Coumarin Derivative" OR "Derivative, Coumarin" OR "1,2-Benzopyrones" OR "1,2 Benzopyrones" OR "1,2-Benzopyrone Derivatives" OR "1,2 Benzopyrone Derivatives" OR "Derivatives, 1,2-Benzopyrone" OR "Coumarines" OR "1,2-Benzo-Pyrones" OR "1,2 Benzo Pyrones" OR "Benzopyran-2-ones" OR "Benzopyran 2 ones" OR "Coumarin Derivatives" OR "Derivatives, Coumarin" OR "Lignans" OR "Lignan" OR "Neolignans" OR "Neolignan" OR "Lectins" OR "Lectin" OR "Isolectins" OR "Isolectin" OR "Animal Lectins" OR "Lectins, Animal" OR "Animal Lectin" OR "Lectin, Animal" OR "Betalains" OR "Betalain" OR "Betalain Pigments" OR "Triterpenes" OR "Triterpenoid" OR "Triterpene" OR "Triterpenoids" OR "Glutathione" OR "gamma-L-Glu-L-Cys-Gly" OR "gamma L Glu L Cys Gly" OR "gamma-L-Glutamyl-L-Cysteinylglycine" OR "gamma L Glutamyl L Cysteinylglycine" OR "Reduced Glutathione" OR "Glutathione, Reduced" OR "Proanthocyanidins" OR "Anthocyanidin Polymers" OR "Polymers, Anthocyanidin" OR "Tannin, Condensed" OR "Condensed Tannins" OR "Tannins, Condensed" OR "Condensed Tannin" OR "Procyranidins" OR "Plant Mucilage" OR "Mucilage, Plant" OR

(Table S1) contd.....

Code	Search Within	Query
#2	Title, abstract and keywords	"Plant Mucilages" OR "Mucilages, Plant" OR "Resveratrol" OR "3,4',5-Stilbenetriol" OR "3,5,4'-Trihydroxystilbene" OR "3,4',5-Trihydroxystilbene" OR "trans-Resveratrol" OR "trans Resveratrol" OR "Resveratrol-3-sulfate" OR "Resveratrol 3 sulfate" OR "SRT 501" OR "SRT-501" OR "SRT501" OR "cis-Resveratrol" OR "cis Resveratrol" OR "Resveratrol" OR "trans-Resveratrol-3-O-sulfate" OR "trans Resveratrol 3 O sulfate" OR "Silymarin" OR "Silimarín" OR "Carsil" OR "Karsil" OR "Legalon" OR "cyanogenic glycosides" OR "Phenolic Lipids" OR "Catechin" OR "Cyanidinol" OR "Catechin" OR "3,3',4',5,7-Flavanepentol" OR "Catechic Acid" OR "Catechuic Acid" OR "Cyanidanol" OR "Catergen" OR "Cyanidanol-3" OR "Cyanidanol 3" OR "Epicatechin" OR "(-)Epicatechin" OR "Zyma" OR "Z 7300" OR "Cyanidanol-3" OR "KB-53" OR "KB53" OR "KB 53" OR "hydroxycinnamoyl-CoA hydroxyanthranilate N-hydroxycinnamoyltranseferase" OR "Furocoumarins" OR "Furocumarin" OR "Furanocoumarin" OR "Furanocoumarins" OR "Psoralens" OR "Angelicans" OR "Peganum" OR "Terpenes" OR "Terpenoid" OR "Terpene" OR "Terpenoids" OR "Isoprenoids" OR "Isoprenoid" OR "Phenylalanine Derivatives" OR "Amino Acids" OR "Acids, Amino" OR "Amino Acid" OR "Acid, Amino" OR "Flavones" OR "2-Phenyl-2-Ene-Benzopyran-4-One Compounds" OR "Probiotics" OR "Prebiotics" OR "Choline" OR "Choline Bitartrate" OR "Bitartrate, Choline" OR "Choline Chloride" OR "Chloride, Choline" OR "Choline Citrate" OR "Citrate, Choline" OR "Choline O-Sulfate" OR "Choline O Sulfate" OR "O-Sulfate, Choline" OR "Bursine" OR "Fagine" OR "Vidine" OR "Choline Hydroxide" OR "Hydroxide, Choline" OR "Allium" OR "Allicaeae" OR "Folic Acid" OR "Pteroylglytamic Acid" OR "Vitamin M9" OR "Vitamin B9" OR "B9, Vitamin" OR "Folacin" OR "Folvite" OR "Folic Acid, Potassium Salt" OR "Folic Acid, Monopotassium Salt" OR "Folic Acid, Sodium Salt" OR "Folic Acid, Monosodium Salt" OR "Folic Acid, (D)-Isomer" OR "Folic Acid, (DL)-Isomer" OR "Folic Acid, Calcium Salt" OR "Folate" OR "Xanthoness" OR "Xanthoness" OR "Xanthone Derivatives" OR "Derivatives, Xanthone" OR "Coumaric Acids" OR "Acids, Coumaric" OR "Coumaric Acid" OR "Acid, Coumaric" OR "Hydroxycinnamic Acid" OR "Acid, Hydroxycinnamic" OR "Hydroxycinnamic Acids" OR "Acids, Hydroxycinnamic" OR "Triterpenoid Saponins" OR "Eugenol" OR "Eugenol" OR "Phenol, 2-methoxy-4-(2-propenyl)" OR "Solanine" OR "Furocoumarins" OR "Furocumarin" OR "Furanocoumarin" OR "Furanocoumarins" OR "Psoralens" OR "Angelicans" OR "Glycine Betaine" OR "Betaine, Glycine" OR "Lycine" OR "Oxynurine" OR "Betaine Hydrochloride" OR "Hydrochloride, Betaine" OR "ystadane" OR "Scorbobétaine" OR "Scorbobétaine" OR "Scorbobétaine" OR "Hepastyl" OR "C.B.B." OR "Citrate de Bétaine Beaufour" OR "Citrate de Bétaine UPSA" OR "Steal-16" OR "Steal16" OR "Steal 16" OR "Acidin-Pepsin" OR "AcidinPepsin" OR "Acidin Pepsin" OR "Novobetaine" OR "Betaine" OR "Glycosides" OR "Lactones" OR "Lactones" OR "Lactone" OR "Glycoside" OR "Peptides" OR "Peptide" OR "Polypeptides" OR "Polypeptide" OR "Protease Inhibitors" OR "Inhibitors, Protease" OR "Peptide Peptidohydrolase Inhibitor" OR "Inhibitor, Peptide Peptidohydrolase" OR "Peptidohydrolase Inhibitor, Peptide" OR "Antiprotease" OR "Endopeptidase Inhibitor" OR "Inhibitor, Endopeptidase" OR "Peptidase Inhibitor" OR "Inhibitor, Peptidase" OR "Peptide Hydrolase Inhibitor" OR "Hydrolase Inhibitor, Peptide" OR "Inhibitor, Peptide Hydrolase" OR "Protease Antagonist" OR "Antagonist, Protease" OR "Endopeptidase Inhibitors" OR "Inhibitors, Endopeptidase" OR "Peptidase Inhibitors" OR "Inhibitors, Peptidase" OR "Peptide Hydrolase Inhibitors" OR "Hydrolase Inhibitors, Peptide" OR "Inhibitors, Peptide Hydrolase" OR "Peptide Peptidohydrolase Inhibitors" OR "Inhibitors, Peptide" OR "eptidohydrolase" OR "Peptidohydrolase Inhibitors, Peptide" OR "Protease Antagonists" OR "Antagonists, Protease" OR "Antiproteases" OR "Protease Inhibitor" OR "Inhibitor, Protease" OR "Phenolic Alcohols" OR "Lactones" OR "Isoflavonoid Glycosides" OR "Flavonolignans" OR "inulin" OR "Alkyne" OR "Acetylenes" OR "Acetylenic" OR "Compounds" OR "Pterocarpanes" OR "Isoflavones" OR "Isoflavone" OR "Isoflavone Derivatives" OR "Derivatives, Isoflavone" OR "Isoflavone Derivative" OR "Derivative, Isoflavone" OR "Homoisoflavones" OR "cyanidin-3-O-beta-glucopyranoside" OR "Acids" OR "Catecholamines" OR "Catecholamine" OR "Sympathin" OR "Sympathins" OR "geraniol" OR "Phytocannabinoids" OR "Diarylheptanoids" OR "Diarylheptanoid Diarylheptanoid Derivative" OR "Derivative, Diarylheptanoid" OR "Vitamins" OR "Vitamin" OR "Caffeic Acids" OR "Acids, Caffeic" OR "dibutyltin 3-hydroxyflavone" OR "Flavonoids" OR "Ascorbic Acid" OR "Bisphenol Compounds" OR "Tannins" OR "Coumarins" OR "Lignans" OR "Lignan" OR "Neolignans" OR "Neolignan" OR "Phytosterols" OR "Plant Sterol" OR "Sterol, Plant" OR "Plant Steroid" OR "Steroid, Plant" OR "Phytosteroids" OR "Phytosteroïd" OR "Plant Sterols" OR "Sterols, Plant" OR "Phytosterol" OR "Plant Steroids" OR "Steroids, Plant" OR "Oils, Volatile" OR "Volatile Oils" OR "Volatile Oil" OR "Oil, Volatile" OR "Essential Oil" OR "Oils, Essential" OR "Essential Oils" OR "Oil, Essential" OR "Sulfanilic Acids" OR "Cold Shock Proteins" OR "Peptides" OR "Pueraria" OR "Carotenoids" OR "Lignin" OR "Lignins" OR "Catechin" OR "Proanthocyanidins" OR "Quinones" OR "Furocoumarins" OR "Furocumarin" OR "Furanocoumarin" OR "Furanocoumarins" OR "Psoralens" OR "Angelicans" OR "Iridoids" OR "Iridoid" OR "Iridoid Derivatives" OR "Derivatives, Iridoid" OR "Secoiridoids" OR "Iridoid Aglycones" OR "Aglycones, Iridoid" OR "Sesquiterpenes" OR "Sesquiterpene" OR "Sesquiterpenoid" OR "Sesquiterpene Derivatives" OR "Derivatives, Sesquiterpene" OR "Sesquiterpenoids" OR "Farnesanes" OR "Farnesenes" OR "Farnesene" OR "Hydrolyzable Tannins" OR "Tannins, Hydrolyzable" OR "Galotannins" OR "Gallo-Tannins" OR "Gallo Tannins" OR "Ellagitannins" OR "Ellagi-Tannins" OR "Ellaggi Tannins" OR "Pyrogallol Tannins" OR "Tannins, Pyrogallol" OR "Gallic Acid" OR "Ferulic acid" OR "caffeic acid" OR "Chlorogenic Acid" OR "Rutin" OR "Rutoside" OR "Quercetin-3-Rutinoside" OR "Hesperidin" OR "Hesperidin 2S" OR "2S, Hesperidin" OR "Quercetin" OR "Luteolin" OR "3',4',5,7-Tetrahydroxyflavone Luteoline" OR "3',4',5,7-Tetrahydroxy-Flavone" OR "Apigenin" OR "Zeaxanthins" OR "Zeaxanthin" OR "Lycopene" OR "Polycopene" OR "Pro-Lycopene" OR "astaxanthine" OR "Betalains" OR "Betalain" OR "Betalain" OR "Pigments" OR "Chlorophyll Binding Proteins" OR "Chlorophyll Protein Complexes" OR "Chlorophyll a-c Binding Proteins" OR "Chlorophyll a c Binding Proteins" OR "Chlorophyll ab-Proteins" OR "Chlorophyll a-c Proteins" OR "Chlorophyll a-Binding Proteins" OR "Chlorophyll a Binding Proteins" OR "Chlorophyll a-Proteins" OR "Chlorophyll a Proteins" OR "Fucoxanthin Chlorophyll a-c Binding Proteins" OR "Fucoxanthin Chlorophyll a c Binding Proteins" OR "Fucoxanthin Chlorophyll Binding Proteins" OR "Xanthophylls" OR "alpha-carotene" OR "beta Carotene" OR "Carotene, beta" OR "beta-Carotene" OR "Betacarotene" OR "Vetoron" OR "BellaCarotin" OR "Carotaban" OR "MaxCaro" OR "MaxCaro" OR "Max Caro" OR "Provatenene" OR "Solatene" OR "Glycyrrhizic Acid" OR "Acid, Glycyrrhizic" OR "Glycyrrhizin" OR "Glycyrrhizic Acid" OR "Acid, Glycyrrhizic" OR "Dipotassium Glycyrrhizinate" OR "Glycyrrhizinate, Dipotassium" OR "Zinc Glycyrrhizate" OR "Glycyrrhizate, Zinc" OR "Diammonium Glycyrrhizinate" OR "Glycyrrhizinate, Diammonium" OR "Humic Substances" OR "Ursolic Acid" OR "Oleanolic Acid" OR "Oleanol" OR "Oleanane Triterpenes" OR "Triterpenes, Oleanane" OR "Hederins" OR "Betulinic Acid" OR "Phytoncides" OR "Xanthoness" OR "Flavanones" OR "2-Phenyl-Benzopyran-4-Ones" OR "2 Phenyl Benzopyran 4 Ones" OR "Vaccinium myrtillus extract" OR "Flavones" OR "Flavonols" OR "2-Phenyl-3-Hydroxy-Benzopyran-4-Ones" OR "2 Phenyl 3 Hydroxy Benzopyran 4 Ones" OR "3-hydroxy-4-keto-Flavonoids" OR "3 hydroxy 4 keto Flavonoids" OR "Flavanols" OR "Pyrocatechins" OR "Leptoclascins" OR "Catechins" OR "Neoflavonoids" OR "sulforaphane" OR "Glucosinolates" OR "Glucosinolate" OR "Indazoles" OR "IndazoleIndazole" OR "Furocoumarins" OR "Furocumarin" OR "Furanocoumarin" OR "Furanocoumarins" OR "Psoralens" OR "Angelicans" OR "Phenylpropanoids" OR "Hematopoietic Cell Growth Factors" OR "Hematopoietic Cell Growth Factor" OR "Hematopoietins" OR "Hematopoietic-CGF" OR "Hematopoietic CGF" OR "Hematopoietic Stem Cell Stimulators" OR "Hematopoietic Stem Cell-Activating Factors" OR "Melatonin" OR "Adenosine" OR "Adenocard" OR "Adenoscan" OR "Phenylalanine" OR "L-Phenylalanine" OR "Phenylalanine, L-isomer" OR "L-Isomer Phenylalanine" OR "Phenylalanine, L Isomer" OR "Endorpheny" OR "Liganes" OR "Lipophilic vitamins" OR "Hydrophilic vitamins" OR "Fructans" OR "Fructan" OR "Levans" OR "Oligosaccharides" OR "Oligosaccharide" OR "protopectinase-F" OR "protopectinase-C" OR "protopectinase-F" OR "PPase-F" OR "protopectinase-L" OR "PPase-L" OR "protopectinase-S" OR "PPase-S" OR "protopectinase-T" OR "PPase-T" OR "Dietary Fiber" OR "Dietary Fibers" OR "Fibers, Dietary" OR "Fiber, Dietary" OR "Wheat Bran" OR "Brans, Wheat" OR "Bran, Wheat" OR "Wheat Brans" OR "Roughage" OR "Roughages" OR "Oils, Volatile" OR "Volatile Oils" OR "Volatile Oil" OR "Oil, Volatile" OR "Essential Oil" OR "Oils, Essential" OR "Essential Oils" OR "Oil, Essential" OR "Amino Acids, Peptides, Proteins" OR "Phytosterols" OR "Plant Sterol" OR "Sterol, Plant" OR "Plant Steroid" OR "Steroid, Plant" OR "Phytosteroids" OR "Phytosteroïd" OR "Plant Sterols" OR "Sterols, Plant" OR "Phytosterol" OR "Plant Steroids" OR "Steroids, Plant" OR "Microelements" OR "Pharmacological action" OR "Terpenes" OR "Terpenoid" OR "Terpene" OR "Terpenoids" OR "Isoprenoids" OR "Isoprenoid" OR "Phenolic acids" OR "Lipids, Fatty acids" OR "Mucilages, Gums" OR "Scavenger Receptors, Class E" OR "SR-E Proteins" OR "Scavenger Receptors, Class E, Type I" OR "Oxidized Low-Density Lipoprotein Receptor 1" OR "Oxidized Low Density Lipoprotein Receptor 1" OR "ORLI Protein" OR "Lectin-Like Oxidized Low-Density Lipoprotein Receptor-1" OR "Lectin Like Oxidized Low Density Lipoprotein Receptor 1" OR "SR-EI Proteins" OR "SR EI Proteins" OR "arabinogalactan proteins" OR "arabinogalactan-peptide" OR "arabinogalactan-protein" OR "AtFLA11 protein, Arabidopsis" OR "Gl

Table S2. Comprehensive list of compounds screened in the data-driven pipeline and their progression through computational analyses.

Compound Name	Category	Literature Source(s)	Bibliometric Frequency*	Included in Docking	Included in MD Simulation	Reason for Exclusion (if applicable)
Acetate	Fermentation-derived metabolite	(1, 2)	High	No	No	Low specificity in SwissTargetPrediction; no high-confidence human protein target
Butyrate	Fermentation-derived metabolite	(1, 2, 3)	Very high	Yes	Yes	-
Ethyl acetate	Fermentation-derived metabolite	(4)	Moderate	No	No	No relevant diabetes-related human target predicted
Lactate	Fermentation-derived metabolite	(1)	Moderate	No	No	Ubiquitous metabolite; low target specificity
Propionate	Fermentation-derived metabolite	(1, 2)	High	No	No	Weak docking affinity and low target relevance
Succinate	Fermentation-derived metabolite	(1, 5)	Moderate	Yes	Yes	High RMSD instability during MD simulation
Faradiol	Phytochemical	(4)	Moderate	Yes	Yes	Moderate RMSD variability; not advanced to ADMET
5-Feruloylquinic acid	Phytochemical	(4)	Low	No	No	No high-confidence predicted diabetes-related target
Ferulic acid	Phytochemical	(4, 6)	High	Yes	Yes	-
Sulferein glycoside	Phytochemical	(4)	Low	No	No	Insufficient target prediction confidence
Vanillin	Phytochemical	(4)	Moderate	No	No	Weak docking affinity and poor target relevance

Footnote: * Bibliometric frequency refers to the relative occurrence of each compound in the retrieved Web of Science and Scopus dataset (February 2025), based on keyword co-occurrence and compound mentions in titles, abstracts, and keywords.

Table S3. The results of the analysis of Butyrate with the Way2Drug online tool and possible side effects of Butyrate as an anti-diabetic drug.

Pa	Pi	Activity
Butyrate		
0.974	0.006	Toxic, respiration
0.951	0.004	Acidosis, metabolic
0.945	0.003	Shivering
0.937	0.002	Skin irritation. corrosive
0.938	0.004	Pure red cell aplasia
0.936	0.005	Euphoria
0.918	0.002	Fibrosis, interstitial
0.891	0.004	Hematemesis
0.882	0.005	Ulcer, aphthous

(Table S3) contd.....

Pa	Pi	Activity
0.879	0.004	Gastrointestinal hemorrhage
0.876	0.003	Hypomagnesemia
0.872	0.004	Occult bleeding
0.861	0.007	Edema
0.858	0.005	Apnea
0.853	0.003	Pseudoporphyria
0.861	0.013	Twitching
0.857	0.011	Weakness
0.847	0.004	Weight gain
0.850	0.010	Muscle weakness
0.833	0.003	Anemia, sideroblastic
0.830	0.012	Anemia
0.820	0.004	Hypercholesterolemic
0.831	0.015	Acidosis
0.817	0.004	Hematuria
0.832	0.019	Conjunctivitis
0.810	0.003	Acneiform eruption
0.816	0.016	Sweating
0.812	0.012	Fibrillation, atrial
0.803	0.007	Splenomegaly
0.806	0.012	Weight loss
0.801	0.006	Pulmonary edema
0.795	0.003	Bullous pemphigoid
0.797	0.006	Hyperuricemia
0.798	0.006	Allergic contact dermatitis
0.813	0.023	Diarrhea
0.801	0.016	Respiratory failure
0.788	0.005	Psychoses
0.792	0.019	Reproductive dysfunction
0.791	0.019	Toxic, vascular
0.776	0.010	Hyperthermic
0.761	0.009	Withdrawal
0.762	0.015	Dyspnea
0.754	0.009	Demyelination
0.749	0.005	Eye irritation, high
0.761	0.020	Excitability
0.749	0.008	Respiratory impairment
0.758	0.020	Necrosis
0.746	0.011	Optic neuropathy

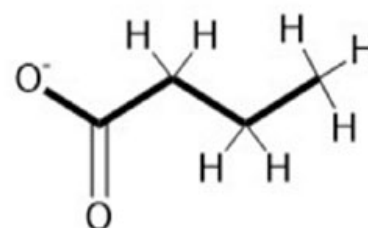
A. Butyrate

A

SwissTargetPrediction

Target	Common name	Uniprot ID	ChEMBL ID	Target Class	Probability*	Known actives (3D/2D)
Histone deacetylase 3	HDAC3	O15379	CHEMBL1829	Eraser	1.0	1 / 1
Egl nine homolog 1	EGLN1	Q9GZT9	CHEMBL5697	Oxidoreductase	0.0743164735672	0 / 2
GABA transporter 1	SLC6A1	P30531	CHEMBL1903	Electrochemical transporter	0.0238327432783	0 / 1
GABA-A receptor, alpha-1/beta-2/gamma-2	GABRA1 GABRB2 GABRG2	P14867 P47870 P18507	CHEMBL2095172	Ligand-gated ion channel	0.0238327432783	0 / 1
GABA A receptor alpha-3/beta-2/gamma-2	GABRA3 GABRB2 GABRG2	P34903 P47870 P18507	CHEMBL2111339	Ligand-gated ion channel	0.0238327432783	0 / 1
GABA A receptor alpha-2/beta-2/gamma-2	GABRA2 GABRB2 GABRG2	P47869 P47870 P18507	CHEMBL2111413	Ligand-gated ion channel	0.0238327432783	0 / 2
GABA-B receptor	GABBR2 GABBR1	O75899 Q9UBS5	CHEMBL2111463	Family C G protein-coupled receptor	0.0238327432783	0 / 1
GABA receptor rho-1 subunit	GABRR1	P24046	CHEMBL3561	Ligand-gated ion channel	0.0238327432783	0 / 1
GABA transporter 3	SLC6A11	P48066	CHEMBL5208	Electrochemical transporter	0.0238327432783	0 / 1
Solute carrier family 22 member 6 (by homology)	SLC22A6	Q4U2R8	CHEMBL1641347	Electrochemical transporter	0.0238327432783	0 / 2
GABA transporter 2 (by homology)	SLC6A13	Q9NSD5	CHEMBL4535	Electrochemical transporter	0.0238327432783	0 / 1
Fatty acid binding protein adipocyte	FABP4	P15090	CHEMBL2083	Fatty acid binding protein family	0.0	0 / 1
Peroxisome proliferator-activated receptor alpha	PPARA	Q07869	CHEMBL239	Nuclear receptor	0.0	0 / 3
Fatty acid binding protein muscle	FABP3	P05413	CHEMBL3344	Fatty acid binding protein family	0.0	0 / 1
Fatty acid binding protein epidermal	FABP5	Q01469	CHEMBL3674	Fatty acid binding protein family	0.0	0 / 1
Peroxisome proliferator-activated receptor delta	PPARD	Q03181	CHEMBL3979	Nuclear receptor	0.0	0 / 2
Free fatty acid receptor 1	FFAR1	O14842	CHEMBL4422	Family A G protein-coupled receptor	0.0	0 / 1
Fatty acid binding protein intestinal	FABP2	P12104	CHEMBL4879	Fatty acid binding protein family	0.0	0 / 1
HMG-CoA reductase	HMGCR	P04035	CHEMBL402	Oxidoreductase	0.0	0 / 1
11-beta-hydroxysteroid dehydrogenase 1	HSD11B1	P28845	CHEMBL4235	Enzyme	0.0	0 / 3
Androgen Receptor	AR	P10275	CHEMBL1871	Nuclear receptor	0.0	0 / 4
Vitamin D receptor	VDR	P11473	CHEMBL1977	Nuclear receptor	0.0	0 / 1

B



C

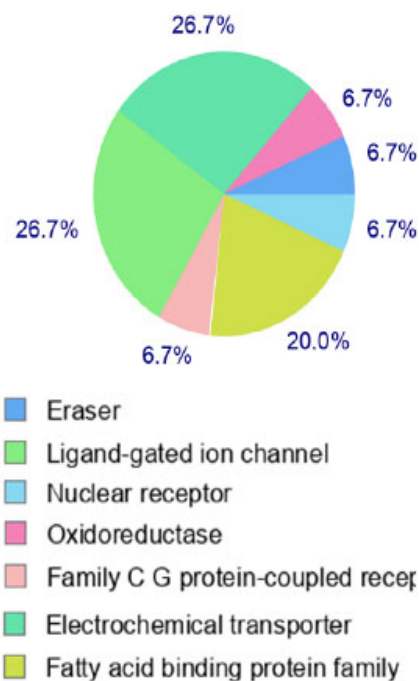


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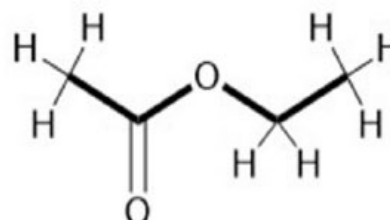
B. Ethyl acetate

A

SwissTargetPrediction

Target	Common name	Uniprot ID	ChEMBL ID	Target Class	Probability*	Known actives (3D/2D)
Carbonic anhydrase I	CA1	P00915	CHEMBL261	Lyase	0.0544879468076	4 / 0
Transient receptor potential cation channel subfamily A member 1	TRPA1	O75762	CHEMBL6007	Voltage-gated ion channel	0.033970689612	1 / 1
Carbonic anhydrase IX	CA9	Q16790	CHEMBL3594	Lyase	0.0238327432783	6 / 1
Nischarin	NISCH	Q9Y211	CHEMBL3923	Other cytosolic protein	0.0	2 / 0
Epidermal growth factor receptor erbB1	EGFR	P00533	CHEMBL203	Kinase	0.0	1 / 0
Cyclin-dependent kinase 2/cyclin E1	CCNE1 CDK2	P24864 P24941	CHEMBL1907605	Kinase	0.0	1 / 0
Tyrosine-protein kinase FYN	FYN	P06241	CHEMBL1841	Kinase	0.0	0 / 1
Tyrosine-protein kinase LCK	LCK	P06239	CHEMBL258	Kinase	0.0	0 / 1
Cytochrome P450 19A1	CYP19A1	P11511	CHEMBL1978	Cytochrome P450	0.0	3 / 0
Induced myeloid leukemia cell differentiation protein Mcl-1	MCL1	Q07820	CHEMBL4361	Other cytosolic protein	0.0	2 / 0
Glycogen synthase kinase-3 beta	GSK3B	P49841	CHEMBL262	Kinase	0.0	13 / 0
Cytochrome P450 2A6	CYP2A6	P11509	CHEMBL5282	Cytochrome P450	0.0	2 / 0
Monoglyceride lipase	MGLL	Q99685	CHEMBL4191	Enzyme	0.0	7 / 0
Thymidylate synthase	TYMS	P04818	CHEMBL1952	Transferase	0.0	3 / 0
Carbonic anhydrase II	CA2	P00918	CHEMBL205	Lyase	0.0	2 / 0
Carbonic anhydrase VII	CA7	P43166	CHEMBL2326	Lyase	0.0	2 / 0
Carbonic anhydrase XII	CA12	O43570	CHEMBL3242	Lyase	0.0	3 / 0
Carbonic anhydrase XIV	CA14	Q9ULX7	CHEMBL3510	Lyase	0.0	2 / 0
Macrophage migration inhibitory factor	MIF	P14174	CHEMBL2085	Enzyme	0.0	1 / 0
Cytochrome P450 11B1	CYP11B1	P15538	CHEMBL1908	Cytochrome P450	0.0	3 / 0
Cytochrome P450 11B2	CYP11B2	P19099	CHEMBL2722	Cytochrome P450	0.0	1 / 0
Plasma kallikrein	KLKB1	P03952	CHEMBL2000	Protease	0.0	2 / 0
Thrombin	F2	P00734	CHEMBL204	Protease	0.0	3 / 0
Leukocyte elastase	ELANE	P08246	CHEMBL248	Protease	0.0	6 / 0
Urokinase-type plasminogen activator	PLAU	P00749	CHEMBL3286	Protease	0.0	3 / 0
Beta-chymotrypsin	CTRB1	P17538	CHEMBL4796	Protease	0.0	1 / 0
DNA (cytosine-5)-methyltransferase 1	DNMT1	P26358	CHEMBL1993	Writer	0.0	1 / 0
Vascular endothelial growth factor receptor 2	KDR	P35968	CHEMBL279	Kinase	0.0	1 / 0

B



C

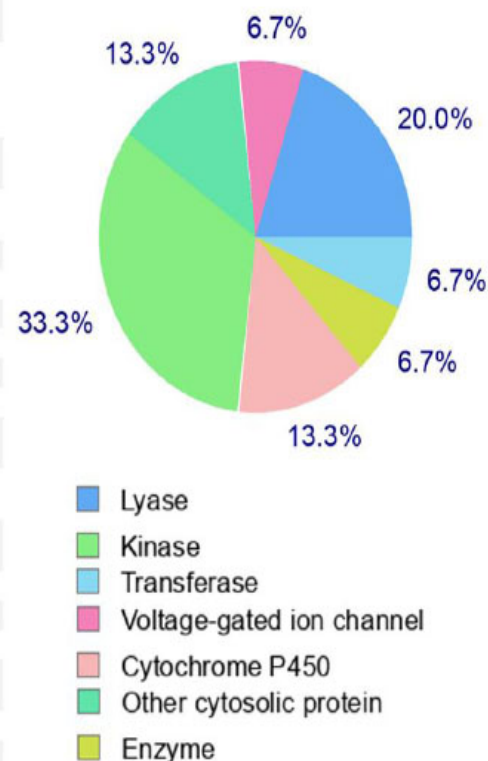


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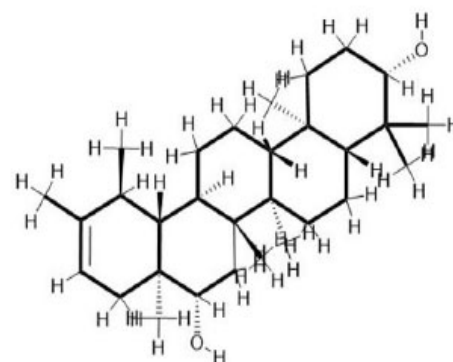
C. Faradiol

A

SwissTargetPrediction

Target	Common name	Uniprot ID	ChEMBL ID	Target Class	Probability*	Known actives (3D/2D)
Protein-tyrosine phosphatase 1B	PTPN1	P18031	CHEMBL335	Phosphatase	0.887071370227	11 / 56
Butyrylcholinesterase	BCHE	P06276	CHEMBL1914	Hydrolase	0.471694253895	5 / 2
Cytochrome P450 19A1	CYP19A1	P11511	CHEMBL1978	Cytochrome P450	0.181232775887	9 / 152
LXR-alpha	NR1H3	Q13133	CHEMBL2808	Nuclear receptor	0.139714053544	16 / 20
Cytochrome P450 2C19	CYP2C19	P33261	CHEMBL3622	Cytochrome P450	0.12313842565	0 / 2
Androgen Receptor	AR	P10275	CHEMBL1871	Nuclear receptor	0.12313842565	27 / 84
Niemann-Pick C1-like protein 1	NPC1L1	Q9UHC9	CHEMBL2027	Other membrane protein	0.114839422585	8 / 11
Nuclear receptor subfamily 1 group I member 3 (by homology)	NR1I3	Q14994	CHEMBL5503	Nuclear receptor	0.114839422585	0 / 2
Cytochrome P450 17A1	CYP17A1	P05093	CHEMBL3522	Cytochrome P450	0.114839422585	57 / 43
Norepinephrine transporter	SLC6A2	P23975	CHEMBL222	Electrochemical transporter	0.106542925976	3 / 2
Nuclear receptor ROR-gamma	RORC	P51449	CHEMBL1741186	Nuclear receptor	0.106542925976	9 / 9
11-beta-hydroxysteroid dehydrogenase 1	HSD11B1	P28845	CHEMBL4235	Enzyme	0.106542925976	33 / 28
Muscarinic acetylcholine receptor M2	CHRM2	P08172	CHEMBL211	Family A G protein-coupled receptor	0.106542925976	11 / 2
Acetylcholinesterase	ACHE	P22303	CHEMBL220	Hydrolase	0.106542925976	6 / 1
Serotonin transporter	SLC6A4	P31645	CHEMBL228	Electrochemical transporter	0.106542925976	15 / 5
Estrogen receptor alpha	ESR1	P03372	CHEMBL206	Nuclear receptor	0.106542925976	16 / 39
HMG-CoA reductase	HMGCR	P04035	CHEMBL402	Oxidoreductase	0.106542925976	26 / 24
Cytochrome P450 51 (by homology)	CYP51A1	Q16850	CHEMBL3849	Cytochrome P450	0.106542925976	2 / 2
Sterol regulatory element-binding protein 2	SREBF2	Q12772	CHEMBL1795166	Unclassified protein	0.106542925976	1 / 1
Estrogen receptor beta	ESR2	Q92731	CHEMBL242	Nuclear receptor	0.106542925976	15 / 47
Squalene monooxygenase	SQLE	Q14534	CHEMBL3592	Enzyme	0.106542925976	0 / 4
Testis-specific androgen-binding protein	SHBG	P04278	CHEMBL3305	Secreted protein	0.106542925976	9 / 42
DNA polymerase beta	POLB	P06746	CHEMBL2392	Enzyme	0.106542925976	0 / 7
Phosphodiesterase 4D	PDE4D	Q08499	CHEMBL288	Phosphodiesterase	0.106542925976	0 / 1
Receptor-type tyrosine-protein phosphatase F (LAR)	PTPRF	P10586	CHEMBL3521	Membrane receptor	0.106542925976	0 / 1
T-cell protein-tyrosine phosphatase	PTPN2	P17706	CHEMBL3807	Phosphatase	0.106542925976	0 / 19
Phospholipase A2 group 1B	PLA2G1B	P04054	CHEMBL4426	Enzyme	0.106542925976	0 / 1
Low molecular weight	ACP1	P24666	CHEMBL4903	Phosphatase	0.106542925976	0 / 1

B



C

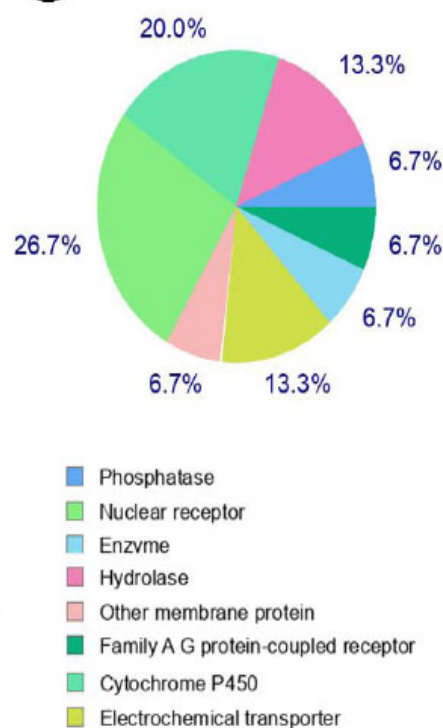


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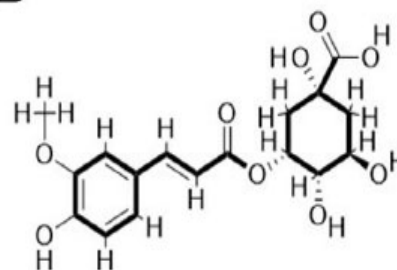
D. 5-Feruloylquinic acid

A

SwissTargetPrediction

Target	Common name	Uniprot ID	ChEMBL ID	Target Class	Probability*	Known actives (3D/2D)
Aldose reductase	AKR1B1	P15121	CHEMBL1900	Enzyme	0.296003135521	6 / 25
Matrix metalloproteinase 13	MMP13	P45452	CHEMBL280	Protease	0.166154076087	0 / 3
Matrix metalloproteinase 2	MMP2	P08253	CHEMBL333	Protease	0.166154076087	0 / 8
Aldo-keto reductase family 1 member B10	AKR1B10	O60218	CHEMBL5983	Enzyme	0.117454607039	2 / 18
Beta amyloid A4 protein	APP	P05067	CHEMBL2487	Membrane receptor	0.117454607039	2 / 29
Matrix metalloproteinase 12	MMP12	P39900	CHEMBL4393	Protease	0.109339753231	1 / 7
Glucose-6-phosphate translocase	SLC37A4	O43826	CHEMBL3217398	Electrochemical transporter	0.109339753231	0 / 2
Leukocyte elastase	ELANE	P08246	CHEMBL248	Protease	0.109339753231	0 / 2
Protein kinase C alpha	PRKCA	P17252	CHEMBL299	Kinase	0.109339753231	0 / 212
Carbonic anhydrase II	CA2	P00918	CHEMBL205	Lyase	0.109339753231	31 / 23
Carbonic anhydrase I	CA1	P00915	CHEMBL261	Lyase	0.109339753231	21 / 31
Carbonic anhydrase XII	CA12	O43570	CHEMBL3242	Lyase	0.109339753231	7 / 34
Carbonic anhydrase IX	CA9	Q16790	CHEMBL3594	Lyase	0.109339753231	6 / 36
Liver glycogen phosphorylase	PYGL	P06737	CHEMBL2568	Enzyme	0.109339753231	3 / 1
Protein kinase C delta (by homology)	PRKCD	Q05655	CHEMBL2996	Kinase	0.109339753231	0 / 36
Arachidonate 5-lipoxygenase	ALOX5	P09917	CHEMBL215	Oxidoreductase	0.109339753231	0 / 26
Carbonic anhydrase VI	CA6	P23280	CHEMBL3025	Lyase	0.109339753231	0 / 16
Carbonic anhydrase XIII	CA13	Q8N1Q1	CHEMBL3912	Lyase	0.109339753231	0 / 15
Carbonic anhydrase VB	CA5B	Q9Y2D0	CHEMBL3969	Lyase	0.109339753231	0 / 14
Carbonic anhydrase VA	CA5A	P35218	CHEMBL4789	Lyase	0.109339753231	0 / 18
Transthyretin	TTR	P02766	CHEMBL3194	Secreted protein	0.109339753231	0 / 3
P-glycoprotein 1	ABCB1	P08183	CHEMBL4302	Primary active transporter	0.0	0 / 72
Beta-secretase 1	BACE1	P56817	CHEMBL4822	Protease	0.0	0 / 23
Phosphodiesterase 4D	PDE4D	Q08499	CHEMBL288	Phosphodiesterase	0.0	0 / 3
Phosphodiesterase 9A	PDE9A	O76083	CHEMBL3535	Phosphodiesterase	0.0	0 / 1
Phosphodiesterase 1B	PDE1B	Q01064	CHEMBL4425	Phosphodiesterase	0.0	0 / 1
Monoamine oxidase B	MAOB	P27338	CHEMBL2039	Oxidoreductase	0.0	0 / 5

B



C

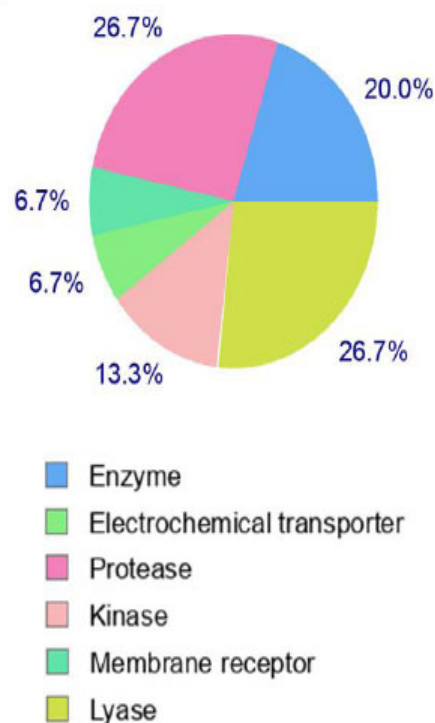


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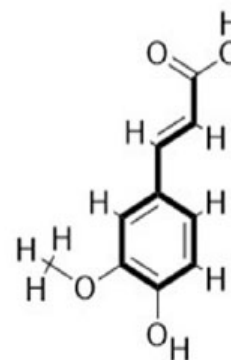
E. Ferulic acid

A

SwissTargetPrediction

Target	Common name	Uniprot ID	ChEMBL ID	Target Class	Probability*	Known actives (3D/2D)
Carbonic anhydrase II	CA2	P00918	CHEMBL205	Lyase	0.937741277923	41 / 20
Carbonic anhydrase VII	CA7	P43166	CHEMBL2326	Lyase	0.937741277923	7 / 19
Carbonic anhydrase I	CA1	P00915	CHEMBL261	Lyase	0.937741277923	36 / 24
Carbonic anhydrase VI	CA6	P23280	CHEMBL3025	Lyase	0.937741277923	5 / 15
Carbonic anhydrase XII	CA12	O43570	CHEMBL3242	Lyase	0.937741277923	19 / 21
Carbonic anhydrase XIV	CA14	Q9ULX7	CHEMBL3510	Lyase	0.937741277923	7 / 19
Carbonic anhydrase IX	CA9	Q16790	CHEMBL3594	Lyase	0.937741277923	15 / 26
Carbonic anhydrase VA	CA5A	P35218	CHEMBL4789	Lyase	0.937741277923	6 / 15
Carbonic anhydrase VB	CA5B	Q9Y2D0	CHEMBL3969	Lyase	0.133586596823	5 / 13
Arachidonate 5-lipoxygenase	ALOX5	P09917	CHEMBL215	Oxidoreductase	0.0721804396226	1 / 44
Matrix metalloproteinase 9	MMP9	P14780	CHEMBL321	Protease	0.0721804396226	1 / 24
Matrix metalloproteinase 1	MMP1	P03956	CHEMBL332	Protease	0.0721804396226	1 / 24
Matrix metalloproteinase 2	MMP2	P08253	CHEMBL333	Protease	0.0721804396226	1 / 23
Protein-tyrosine phosphatase 1B	PTPN1	P18031	CHEMBL335	Phosphatase	0.0721804396226	27 / 2
Monoamine oxidase B	MAOB	P27338	CHEMBL2039	Oxidoreductase	0.0721804396226	2 / 38
Carbonic anhydrase XIII (by homology)	CA13	Q8N1Q1	CHEMBL3912	Lyase	0.0619149311119	4 / 10
Aldose reductase	AKR1B1	P15121	CHEMBL1900	Enzyme	0.0619149311119	64 / 34
Carbonic anhydrase III	CA3	P07451	CHEMBL2885	Lyase	0.0619149311119	4 / 4
Beta amyloid A4 protein	APP	P05067	CHEMBL2487	Membrane receptor	0.0517133123472	0 / 55
Nuclear factor erythroid 2-related factor 2	NFE2L2	Q16236	CHEMBL1075094	Unclassified protein	0.0414702990123	0 / 4
Signal transducer and activator of transcription 3	STAT3	P40763	CHEMBL4026	Transcription factor	0.0414702990123	0 / 1
11-beta-hydroxysteroid dehydrogenase 1	HSD11B1	P28845	CHEMBL4235	Enzyme	0.0414702990123	0 / 4
Estrogen receptor beta	ESR2	Q92731	CHEMBL242	Nuclear receptor	0.0414702990123	4 / 17
Carbonic anhydrase IV	CA4	P22748	CHEMBL3729	Lyase	0.0414702990123	1 / 7
Toll-like receptor 4	TLR4	O00206	CHEMBL5255	Toll-like and IL-1	0.0414702990123	0 / 13

B



C

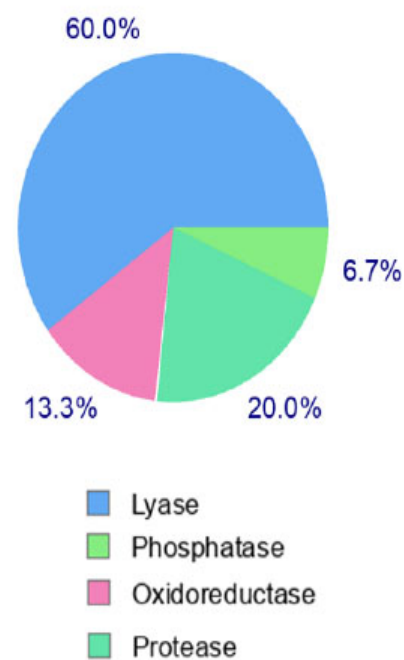


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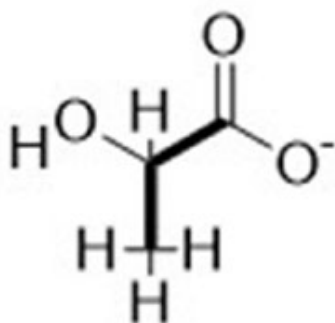
F. Lactate

A

SwissTargetPrediction

Target	Common name	Uniprot ID	ChEMBL ID	Target Class	Probability*	Known actives (3D/2D)
Aldose reductase	AKR1B1	P15121	CHEMBL1900	Enzyme	0.0849737018175	0 / 1
Histone deacetylase 3	HDAC3	O15379	CHEMBL1829	Eraser	0.0	0 / 1
HMG-CoA reductase	HMGCR	P04035	CHEMBL402	Oxidoreductase	0.0	1 / 0
Estrogen receptor beta	ESR2	Q92731	CHEMBL242	Nuclear receptor	0.0	1 / 0
Tyrosine-protein kinase FYN	FYN	P06241	CHEMBL1841	Kinase	0.0	0 / 1
Tyrosine-protein kinase LCK	LCK	P06239	CHEMBL258	Kinase	0.0	0 / 1
Adenylosuccinate synthetase 2	ADSS	P30520	CHEMBL4875	Enzyme	0.0	1 / 0
Egl nine homolog 1	EGLN1	Q9GZT9	CHEMBL5697	Oxidoreductase	0.0	0 / 1
Matrix metalloproteinase 9	MMP9	P14780	CHEMBL321	Protease	0.0	1 / 0
Matrix metalloproteinase 2	MMP2	P08253	CHEMBL333	Protease	0.0	1 / 0

B



C

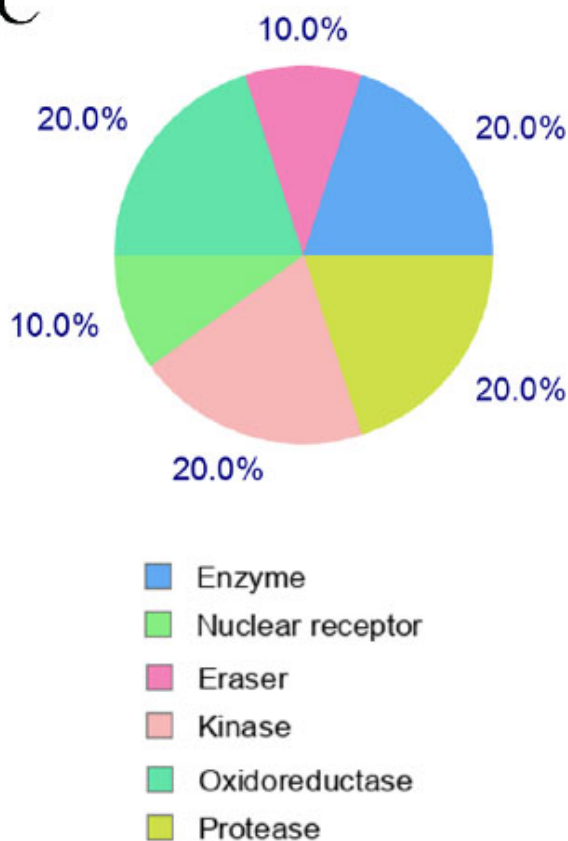


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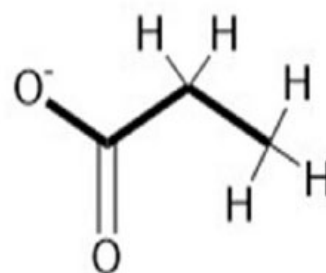
G. Propionate

A

SwissTargetPrediction

Target	Common name	Uniprot ID	ChEMBL ID	Target Class	Probability*	Known actives (3D/2D)
Aldose reductase	AKR1B1	P15121	CHEMBL1900	Enzyme	0.0238327432783	0 / 1
Histone deacetylase 3	HDAC3	Q15379	CHEMBL1829	Eraser	0.0	1 / 1
Egl nine homolog 1	EGLN1	Q9GZT9	CHEMBL5697	Oxidoreductase	0.0	0 / 1
GABA transporter 1	SLC6A1	P30531	CHEMBL1903	Electrochemical transporter	0.0	0 / 1
GABA-A receptor; alpha-1/beta-2/gamma-2	GABRA1 GABRB2 GABRG2	P14867 P47870 P18507	CHEMBL2095172	Ligand-gated ion channel	0.0	0 / 1
GABA A receptor alpha-3/beta-2/gamma-2	GABRA3 GABRB2 GABRG2	P34903 P47870 P18507	CHEMBL2111339	Ligand-gated ion channel	0.0	0 / 1
GABA A receptor alpha-2/beta-2/gamma-2	GABRA2 GABRB2 GABRG2	P47869 P47870 P18507	CHEMBL2111413	Ligand-gated ion channel	0.0	0 / 1
GABA-B receptor	GABBR2 GABBR1	Q75899 Q9UBS5	CHEMBL2111463	Family C G protein-coupled receptor	0.0	0 / 1
GABA receptor rho-1 subunit	GABRR1	P24046	CHEMBL3561	Ligand-gated ion channel	0.0	0 / 1
GABA transporter 3	SLC6A11	P48066	CHEMBL5208	Electrochemical transporter	0.0	0 / 1
GABA transporter 2 (by homology)	SLC6A13	Q9NSD5	CHEMBL4535	Electrochemical transporter	0.0	0 / 1
Tyrosine-protein kinase FYN	FYN	P06241	CHEMBL1841	Kinase	0.0	1 / 1
Tyrosine-protein kinase LCK	LCK	P06239	CHEMBL258	Kinase	0.0	1 / 1
D-amino-acid oxidase	DAO	P14920	CHEMBL5485	Enzyme	0.0	1 / 0
Fatty acid binding protein adipocyte	FABP4	P15090	CHEMBL2083	Fatty acid binding protein family	0.0	0 / 1
Peroxisome proliferator-activated receptor alpha	PPARA	Q07869	CHEMBL239	Nuclear receptor	0.0	0 / 3
Fatty acid binding protein muscle	FABP3	P05413	CHEMBL3344	Fatty acid binding protein family	0.0	0 / 1
Fatty acid binding protein epidermal	FABP5	Q01469	CHEMBL3674	Fatty acid binding protein family	0.0	0 / 1
Peroxisome proliferator-activated receptor delta	PPARD	Q03181	CHEMBL3979	Nuclear receptor	0.0	0 / 2
Free fatty acid	FFAR1	Q14842	CHEMBL4422	Family A G	0.0	0 / 1

B



C

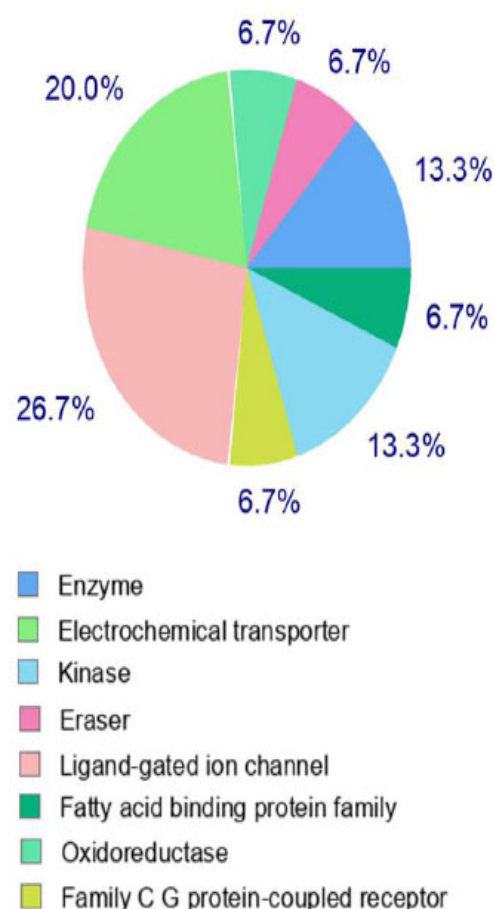


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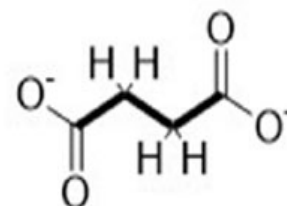
H. Succinate

A

SwissTargetPrediction

Target	Common name	Uniprot ID	ChEMBL ID	Target Class	Probability*	Known actives (3D/2D)
Egl nine homolog 1	EGLN1	Q9GZT9	CHEMBL5697	Oxidoreductase	1.0	3 / 3
Histone deacetylase 3	HDAC3	O15379	CHEMBL1829	Eraser	0.0743164735672	0 / 1
Histone lysine demethylase PHF8	PHF8	Q9UPP1	CHEMBL1938212	Eraser	0.0	0 / 4
ATP-citrate synthase	ACLY	P53396	CHEMBL3720	Enzyme	0.0	0 / 1
Protein farnesyltransferase	FNTA FNTB	P49354 P49356	CHEMBL2094108	Enzyme	0.0	0 / 5
GABA transporter 1	SLC6A1	P30531	CHEMBL1903	Electrochemical transporter	0.0	0 / 1
GABA-A receptor, alpha-1/beta-2/gamma-2	GABRA1 GABRB2 GABRG2	P14867 P47870 P18507	CHEMBL2095172	Ligand-gated ion channel	0.0	0 / 1
GABA A receptor alpha-3/beta-2/gamma-2	GABRA3 GABRB2 GABRG2	P34903 P47870 P18507	CHEMBL2111339	Ligand-gated ion channel	0.0	0 / 1
GABA A receptor alpha-2/beta-2/gamma-2	GABRA2 GABRB2 GABRG2	P47869 P47870 P18507	CHEMBL2111413	Ligand-gated ion channel	0.0	0 / 1
GABA-B receptor	GABBR2 GABBR1	O75899 Q9UBS5	CHEMBL2111463	Family C G protein-coupled receptor	0.0	0 / 1
GABA receptor rho-1 subunit	GABRR1	P24046	CHEMBL3561	Ligand-gated ion channel	0.0	0 / 1
GABA transporter 3	SLC6A11	P48066	CHEMBL5208	Electrochemical transporter	0.0	0 / 1
Solute carrier family 22 member 6 (by homology)	SLC22A6	Q4U2R8	CHEMBL1641347	Electrochemical transporter	0.0	0 / 2
GABA transporter 2 (by homology)	SLC6A13	Q9NSD5	CHEMBL4535	Electrochemical transporter	0.0	0 / 1
Hydroxyacid oxidase 1	HAO1	Q9UJM8	CHEMBL4229	Enzyme	0.0	0 / 1
Fatty acid binding protein adipocyte	FABP4	P15090	CHEMBL2083	Fatty acid binding protein family	0.0	0 / 1
Peroxisome proliferator-activated receptor alpha	PPARA	Q07869	CHEMBL239	Nuclear receptor	0.0	0 / 3
Fatty acid binding protein muscle	FABP3	P05413	CHEMBL3344	Fatty acid binding protein family	0.0	0 / 1
Fatty acid binding protein epidermal	FABP5	Q01469	CHEMBL3674	Fatty acid binding protein family	0.0	0 / 1
Peroxisome proliferator-activated receptor delta	PPARD	Q03181	CHEMBL3979	Nuclear receptor	0.0	0 / 2
Free fatty acid receptor 1	FFAR1	O14842	CHEMBL4422	Family A G protein-coupled receptor	0.0	0 / 1
Fatty acid binding protein intestinal	FABP2	P12104	CHEMBL4879	Fatty acid binding protein family	0.0	0 / 1

B



C

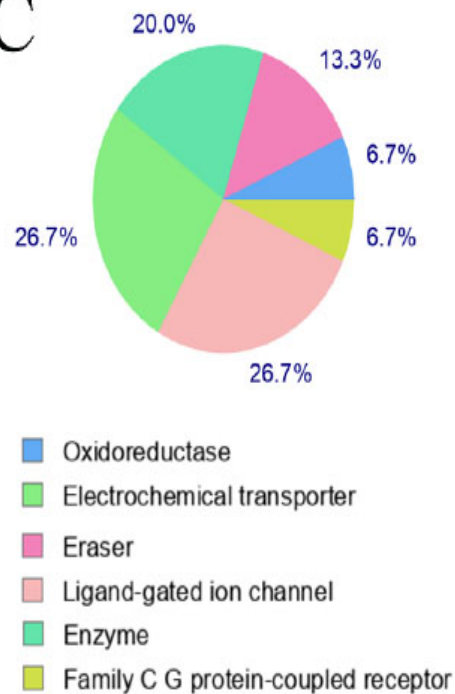


Fig. S1 contd.....

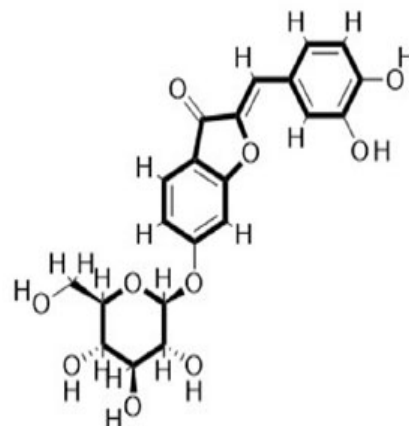
I. Sulferein glycoside

A

SwissTargetPrediction

Target	Common name	Uniprot ID	ChEMBL ID	Target Class	Probability*	Known actives (3D/2D)
Aldose reductase	AKR1B1	P15121	CHEMBL1900	Enzyme	0.134971891997	12 / 10
TNF-alpha	TNF	P01375	CHEMBL1825	Secreted protein	0.118883306718	3 / 0
Adenosine A2a receptor (by homology)	ADORA2A	P29274	CHEMBL251	Family A G protein-coupled receptor	0.118883306718	214 / 0
Interleukin-2	IL2	P60568	CHEMBL5880	Secreted protein	0.118883306718	5 / 0
Cyclin-dependent kinase 5/CDK5 activator 1	CDK5R1 CDK5	Q15078 Q00535	CHEMBL1907600	Kinase	0.118883306718	0 / 1
Acetylcholinesterase (by homology)	ACHE	P22303	CHEMBL220	Hydrolase	0.118883306718	0 / 40
Aldehyde dehydrogenase	ALDH2	P05091	CHEMBL1935	Oxidoreductase	0.118883306718	2 / 0
Carbonic anhydrase II	CA2	P00918	CHEMBL205	Lyase	0.118883306718	104 / 0
Carbonic anhydrase I	CA1	P00915	CHEMBL261	Lyase	0.118883306718	102 / 0
Carbonic anhydrase XII	CA12	O43570	CHEMBL3242	Lyase	0.118883306718	69 / 0
Carbonic anhydrase IX	CA9	Q16790	CHEMBL3594	Lyase	0.118883306718	78 / 0
Vascular endothelial growth factor receptor 1	FLT1	P17948	CHEMBL1868	Kinase	0.118883306718	0 / 1
Histone deacetylase 2	HDAC2	Q92769	CHEMBL1937	Eraser	0.118883306718	0 / 1
Vascular endothelial growth factor receptor 3	FLT4	P35916	CHEMBL1955	Kinase	0.118883306718	0 / 1
Platelet-derived growth factor receptor alpha	PDGFRA	P16234	CHEMBL2007	Kinase	0.118883306718	0 / 1
Serine/threonine-protein kinase Aurora-B	AURKB	Q96GD4	CHEMBL2185	Kinase	0.118883306718	0 / 1
Glycogen synthase kinase-3 beta	GSK3B	P49841	CHEMBL262	Kinase	0.118883306718	0 / 2
Serine/threonine-protein kinase Aurora-C	AURKC	Q9UQB9	CHEMBL3935	Kinase	0.118883306718	0 / 1
Serine/threonine-protein kinase Aurora-A	AURKA	O14965	CHEMBL4722	Kinase	0.118883306718	0 / 1
Equilibrative nucleoside transporter 1	SLC29A1	Q99808	CHEMBL1997	Electrochemical transporter	0.118883306718	93 / 0
Matrix metalloproteinase 13	MMP13	P45452	CHEMBL280	Protease	0.118883306718	5 / 0
Matrix metalloproteinase 1	MMP1	P03956	CHEMBL332	Protease	0.118883306718	10 / 0
Matrix metalloproteinase 7	MMP7	P09237	CHEMBL4073	Protease	0.118883306718	1 / 0
Matrix metalloproteinase 8	MMP8	P22894	CHEMBL4588	Protease	0.118883306718	6 / 0
Adenosine A1 receptor	ADORA1	P30542	CHEMBL226	Family A G protein-coupled	0.118883306718	363 / 0

B



C

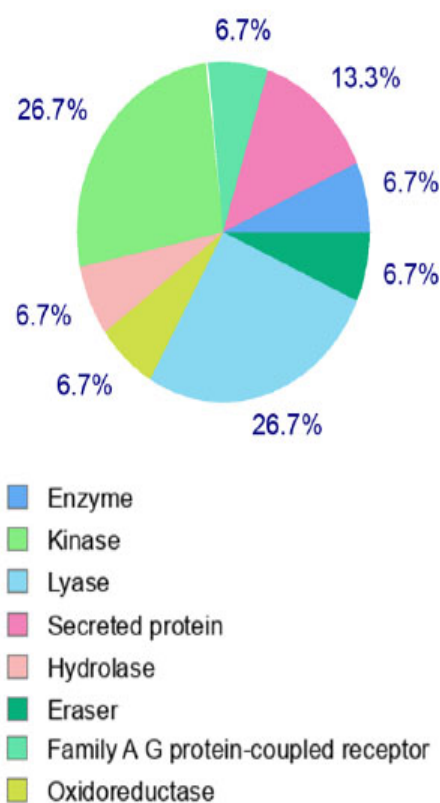


Fig. S1 contd.....

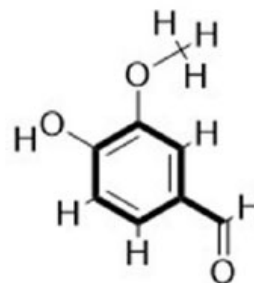
J. Vanillin

A

SwissTargetPrediction

Target	Common name	Uniprot ID	ChEMBL ID	Target Class	Probability*	Known actives (3D/2D)
Serine/threonine-protein kinase/endoribonuclease IRE1	ERN1	O75460	CHEMBL1163101	Enzyme	0.261667695979	32 / 77
Carbonic anhydrase II	CA2	P00918	CHEMBL205	Lyase	0.168421357392	36 / 39
Carbonic anhydrase VII	CA7	P43166	CHEMBL2326	Lyase	0.0630257148888	17 / 25
Carbonic anhydrase I	CA1	P00915	CHEMBL261	Lyase	0.0630257148888	24 / 35
Carbonic anhydrase XII	CA12	O43570	CHEMBL3242	Lyase	0.0630257148888	24 / 29
Carbonic anhydrase XIV	CA14	Q9ULX7	CHEMBL3510	Lyase	0.0630257148888	13 / 25
Carbonic anhydrase IX	CA9	Q16790	CHEMBL3594	Lyase	0.0630257148888	32 / 27
Carbonic anhydrase IV	CA4	P22748	CHEMBL3729	Lyase	0.0630257148888	0 / 4
Carbonic anhydrase III	CA3	P07451	CHEMBL2885	Lyase	0.053517944289	0 / 3
Carbonic anhydrase VI	CA6	P23280	CHEMBL3025	Lyase	0.053517944289	0 / 6
Carbonic anhydrase VA	CA5A	P35218	CHEMBL4789	Lyase	0.053517944289	0 / 4
Dual specificity phosphatase Cdc25B	CDC25B	P30305	CHEMBL4804	Phosphatase	0.053517944289	3 / 0
Leukocyte common antigen	PTPRC	P08575	CHEMBL3243	Enzyme	0.0439186325197	5 / 0
Histone acetyltransferase p300	EP300	Q09472	CHEMBL3784	Writer	0.0439186325197	1 / 0
Transthyretin	TTR	P02766	CHEMBL3194	Secreted protein	0.0439186325197	2 / 9
Arylamine N-acetyltransferase 1	NAT1	P18440	CHEMBL5101	Enzyme	0.0439186325197	2 / 0
Alkaline phosphatase placental-like	ALPG	P10696	CHEMBL3402	Enzyme	0.0439186325197	2 / 0
Phospholipase A-2-activating protein	PLAA	Q9Y263	CHEMBL6114	Unclassified protein	0.0439186325197	5 / 0
Aldo-keto-reductase family 1 member C3	AKR1C3	P42330	CHEMBL4681	Enzyme	0.0439186325197	0 / 2
Matrix metalloproteinase 1	MMP1	P03956	CHEMBL332	Protease	0.0	15 / 0
Myoglobin	MB	P02144	CHEMBL2406892	Unclassified protein	0.0	3 / 0
Serine/threonine-protein kinase PIM1	PIM1	P11309	CHEMBL2147	Kinase	0.0	11 / 0
Histone deacetylase 3	HDAC3	O15379	CHEMBL1829	Eraser	0.0	2 / 0
Angiotensin-converting enzyme (by homology)	ACE	P12821	CHEMBL1808	Protease	0.0	2 / 0
Acetylcholinesterase	ACHE	P22303	CHEMBL220	Hydrolase	0.0	4 / 30

B



C

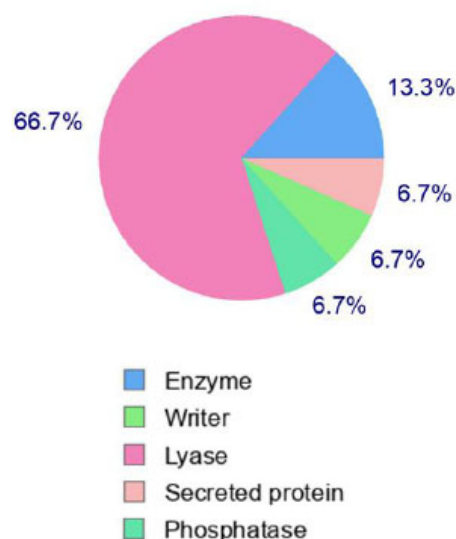


Fig. (S1). Predicted proteins in the human body that can be targeted by phytochemicals and compounds reported in different parts of *Helianthus tuberosus* (*H. tuberosus*) with antidiabetic characteristics. **A:** The results of the SwissTargetPrediction online tool, **B:** The 2D structure of compounds derived from *H. Tuberosus* that can target proteins in the human body, **C:** The class of proteins that compounds can target, originating from *H. Tuberosus*

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