

Supplementary Material

Surface Functionalization of Magnetite Nanoparticles with Multipotent Antioxidant as Potential Magnetic Nanoantioxidants and Antimicrobial Agents

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Table S1. Part of the Predicted Biological Activity Spectra of the MPAO based on PASS Prediction Software.

Pa	Pi	Biological Activity
0.884	0.004	Skin irritation, inactive
0.861	0.008	Antiseborrheic
0.811	0.016	Mucomembranous protector
0.778	0.006	Lipoprotein lipase inhibitor
0.738	0.008	Radioprotector
0.727	0.004	Acaricide
0.726	0.005	Eye irritation, inactive
0.678	0.016	Hypolipemic
0.671	0.017	Fucoesterol-epoxide lyase inhibitor
0.651	0.013	Cholesterol antagonist
0.620	0.019	Lipid metabolism regulator
0.605	0.019	Linoleate diol synthase inhibitor
0.624	0.042	Alkenylglycerophosphocholine hydrolase inhibitor
0.602	0.024	General pump inhibitor
0.652	0.079	Aspulvinone dimethylallyltransferase inhibitor
0.583	0.014	Hepatoprotectant
0.595	0.033	Antiinflammatory
0.573	0.013	Antiulcerative
0.571	0.014	Anesthetic general
0.568	0.036	Feruloyl esterase inhibitor

0.550	0.020	TNF expression inhibitor
0.538	0.014	Acetylgalactosaminyl-O-glycosyl-glycoprotein beta-1,3-N-acetylglucosaminyltransferase inhibitor
0.538	0.041	Phosphatidylcholine-retinol O-acyltransferase inhibitor
0.509	0.015	Antiparasitic
0.537	0.045	Venombin AB inhibitor
0.542	0.051	Cytoprotectant
0.545	0.058	Acute neurologic disorders treatment
0.507	0.025	1-Alkylglycerophosphocholine O-acetyltransferase inhibitor
0.503	0.024	Reductant
0.586	0.113	Ubiquinol-cytochrome-c reductase inhibitor
0.499	0.035	Kinase inhibitor
0.542	0.084	Antiischemic, cerebral
0.504	0.050	Lysine 2,3-aminomutase inhibitor
0.477	0.025	Antihypercholesterolemic
0.456	0.013	Free radical scavenger
0.449	0.006	ICAM1 expression inhibitor
0.489	0.047	Membrane integrity antagonist
0.474	0.033	Antiallergic
0.481	0.047	Antianginal
0.462	0.038	Antisecretoric
0.458	0.042	Alkenylglycerophosphoethanolamine hydrolase inhibitor
0.469	0.057	Leukopoiesis stimulant
0.414	0.005	Retinoprotector
0.436	0.033	Antimyopathies
0.417	0.016	Ethanolaminephosphotransferase inhibitor
0.402	0.009	Antidote
0.430	0.043	All-trans-retinyl-palmitate hydrolase inhibitor
0.470	0.083	Protein-disulfide reductase (glutathione) inhibitor
0.447	0.063	Thromboxane B2 antagonist
0.412	0.035	Atherosclerosis treatment
0.402	0.027	Vanilloid 1 agonist
0.372	0.014	Anticataract
0.378	0.021	Ubiquitin thiolesterase inhibitor
0.366	0.013	ErbB-1 antagonist
0.394	0.043	1-Acylglycerol-3-phosphate O-acyltransferase inhibitor
0.354	0.002	Glycine receptor agonist
0.364	0.013	Expectorant
0.375	0.028	Ophthalmic drug
0.444	0.100	Proteasome ATPase inhibitor
0.352	0.010	Restenosis treatment
0.353	0.014	Anti-Helicobacter pylori
0.428	0.091	NADPH peroxidase inhibitor

0.347	0.012	Antiprotozoal (Trichomonas)
0.428	0.095	Mannotetraose 2-alpha-N-acetylglucosaminyltransferase inhibitor
0.401	0.070	Alcohol O-acetyltransferase inhibitor
0.406	0.076	Trimethylamine-oxide aldolase inhibitor
0.364	0.046	Phosphatidylinositol diacylglycerol-lyase inhibitor
0.320	0.006	Lipoxygenase inhibitor
0.315	0.003	Antidote, heavy metal
0.401	0.090	Histamine release inhibitor
0.401	0.091	Alkylacetylglycerophosphatase inhibitor
0.344	0.041	Carboxypeptidase D inhibitor
0.351	0.049	Lipid peroxidase inhibitor
0.297	0.007	Phospholipase A2 inhibitor
0.374	0.086	Ecdysone 20-monooxygenase inhibitor
0.312	0.023	Retinol dehydrogenase inhibitor
0.331	0.044	Antinephritic
0.303	0.016	Poly(3-hydroxybutyrate) depolymerase inhibitor
0.330	0.043	Antiinflammatory, ophthalmic
0.395	0.114	Glyceryl-ether monooxygenase inhibitor
0.365	0.086	Pancreatic elastase inhibitor
0.329	0.050	Acidifying agent non gastric
0.282	0.004	VCAM1 expression inhibitor
0.310	0.034	Antipruritic, non-allergic
0.291	0.015	Gastric antisecretory
0.288	0.015	Protein-S-isoprenylcysteine O-methyltransferase inhibitor
0.303	0.030	Alpha-amylase inhibitor
0.286	0.015	Mucolytic
0.384	0.116	Chlordecone reductase inhibitor
0.317	0.052	Anticarcinogenic
0.366	0.101	Apyrase inhibitor
0.278	0.016	Endoglycosylceramidase inhibitor
0.285	0.026	Antioxidant
0.327	0.069	Antidiabetic
0.409	0.152	Fusarinine-C ornithinesterase inhibitor
0.273	0.018	Cystinyl aminopeptidase inhibitor
0.320	0.067	Nitrite reductase (NO-forming) inhibitor
0.327	0.074	Mediator release inhibitor
0.410	0.158	Chymosin inhibitor
0.410	0.158	Acrocylindropepsin inhibitor
0.410	0.158	Saccharopepsin inhibitor
0.383	0.132	Sugar-phosphatase inhibitor
0.289	0.038	Chemoprotective
0.273	0.025	Lipoprotein disorders treatment

0.365	0.119	1,4-Lactonase inhibitor
0.265	0.020	Leukotriene synthesis inhibitor
0.284	0.039	Antiseptic
0.297	0.052	Levansucrase inhibitor
0.253	0.013	Stromelysin 2 inhibitor
0.287	0.047	Non-steroidal antiinflammatory agent
0.329	0.090	Phenol O-methyltransferase inhibitor
0.318	0.079	Dermatologic
0.322	0.083	Retinoic acid metabolism inhibitor
0.307	0.069	FMO3 substrate
0.384	0.150	TP53 expression enhancer
0.267	0.034	Protein-tyrosine sulfotransferase inhibitor
0.335	0.102	Peptide agonist
0.274	0.042	Choleretic
0.289	0.058	Maillard reaction inhibitor
0.241	0.011	Antiemphysemic
0.333	0.103	Caspase 8 stimulant
0.324	0.094	N-acetylneuraminate 7-O(or 9-O)-acetyltransferase inhibitor
0.233	0.003	Prostaglandin EP4 antagonist
0.279	0.050	Pediculicide
0.241	0.015	Phospholipase inhibitor
0.301	0.076	Antipsoriatic
0.284	0.059	Methane monooxygenase inhibitor
0.346	0.121	Acylcarnitine hydrolase inhibitor
0.307	0.085	Antiasthmatic
0.261	0.041	Acyl-CoA oxidase inhibitor
0.282	0.062	Photosensitizer
0.278	0.061	CYP2E1 substrate
0.235	0.019	Arachidonic acid antagonist
0.253	0.038	Histone acetyltransferase inhibitor
0.252	0.037	Antinaupathic
0.262	0.049	Anesthetic
0.346	0.133	Preneoplastic conditions treatment
0.240	0.028	Diacylglycerol cholinephosphotransferase inhibitor
0.318	0.108	Superoxide dismutase inhibitor
0.291	0.082	Neuropeptide Y2 antagonist
0.236	0.026	Retinyl-palmitate esterase inhibitor
0.267	0.058	Ferredoxin hydrogenase inhibitor
0.237	0.028	Microtubule formation inhibitor
0.230	0.022	Methylglutamate dehydrogenase inhibitor
0.215	0.007	5-Lipoxygenase inhibitor
0.284	0.078	4-Coumarate-CoA ligase inhibitor

0.268	0.061	Hepatic disorders treatment
0.232	0.026	Calcium channel blocker
0.270	0.064	CYP2E substrate
0.424	0.219	Phobic disorders treatment
0.308	0.104	Peptidoglycan glycosyltransferase inhibitor
0.339	0.135	Aspartyltransferase inhibitor
0.272	0.069	Arylesterase inhibitor
0.205	0.003	Prostaglandin E2 agonist
0.337	0.141	Oxygen scavenger
0.346	0.150	NADPH-cytochrome-c2 reductase inhibitor
0.264	0.068	Clavamate synthase inhibitor
0.227	0.034	Aldehyde dehydrogenase inhibitor
0.215	0.023	O-acetylhomoserine aminocarboxypropyltransferase inhibitor
0.361	0.170	Glycosylphosphatidylinositol phospholipase D inhibitor
0.261	0.071	Undecaprenyl-phosphate mannosyltransferase inhibitor
0.299	0.110	Antihelmintic (Nematodes)
0.265	0.077	Dextranase inhibitor
0.259	0.072	Phosphatidylcholine-sterol O-acyltransferase inhibitor
0.333	0.146	Glucan endo-1,3-beta-D-glucosidase inhibitor
0.309	0.122	Apoptosis agonist
0.247	0.061	Shikimate O-hydroxycinnamoyltransferase inhibitor
0.206	0.022	Leishmanolysin inhibitor
0.210	0.026	Skin whitener
0.310	0.126	GST A substrate
0.217	0.035	Antiglaucomic
0.232	0.050	Vanilloid agonist
0.230	0.048	Inorganic diphosphatase inhibitor
0.261	0.080	Antitoxic
0.274	0.094	Methylenetetrahydrofolate reductase (NADPH) inhibitor
0.291	0.112	CYP3A4 inducer
0.275	0.096	CYP2C19 substrate
0.235	0.056	Glycine dehydrogenase (decarboxylating) inhibitor
0.311	0.132	5 Hydroxytryptamine release inhibitor
0.241	0.063	Cutinase inhibitor
0.285	0.108	Mucinamylserine mucinaminidase inhibitor
0.222	0.044	Aldehyde dehydrogenase (NADP+) inhibitor
0.296	0.120	Antipruritic
0.383	0.207	Phosphatase inhibitor
0.240	0.065	Sclerosant
0.307	0.133	Hydrogen dehydrogenase inhibitor
0.221	0.048	Penicillin amidase inhibitor
0.279	0.106	HMOX1 expression enhancer

0.289	0.117	CDP-diacylglycerol-serine O-phosphatidyltransferase inhibitor
0.276	0.105	Phosphoinositide 5-phosphatase inhibitor
0.268	0.097	Antifungal
0.276	0.106	Plastoquinol-plastocyanin reductase inhibitor
0.205	0.035	Pectate lyase inhibitor
0.259	0.091	Pyruvate decarboxylase inhibitor
0.190	0.022	Adenylate cyclase stimulant
0.240	0.073	Lactose synthase inhibitor
0.192	0.025	Lactoylglutathione lyase inhibitor
0.380	0.213	Antieczematic
0.235	0.069	Di-trans,poly-cis-decaprenylcistransferase inhibitor
0.277	0.113	CYP3A inducer
0.261	0.096	Steroid N-acetylglucosaminyltransferase inhibitor
0.337	0.172	Electron-transferring-flavoprotein dehydrogenase inhibitor
0.335	0.172	Membrane integrity agonist
0.270	0.108	Cardioprotectant
0.271	0.110	3-Cyanoalanine hydratase inhibitor
0.199	0.038	Insecticide
0.284	0.123	CYP2A4 substrate
0.290	0.130	N-hydroxyarylamine O-acetyltransferase inhibitor
0.340	0.181	CYP2C8 inhibitor
0.258	0.099	Mannose isomerase inhibitor
0.237	0.078	Prolyl aminopeptidase inhibitor
0.164	0.006	Leukotriene antagonist
0.221	0.063	Cyclopropane-fatty-acyl-phospholipid synthase inhibitor
0.284	0.127	Transcription factor NF kappa B stimulant
0.284	0.127	Transcription factor stimulant
0.194	0.038	Melanin inhibitor
0.188	0.033	Carboxylesterase inhibitor
0.229	0.074	Thiol protease inhibitor
0.299	0.144	Antipruritic, allergic
0.317	0.162	APOA1 expression enhancer
0.343	0.189	5-O-(4-coumaroyl)-D-quinic 3'-monooxygenase inhibitor
0.157	0.005	Adenine nucleotide translocase inhibitor
0.180	0.029	Agmatinase inhibitor
0.189	0.039	Antihyperlipoproteinemic
0.191	0.041	Pyroglutamyl-peptidase I inhibitor
0.228	0.080	Dactylisin inhibitor
0.245	0.097	Pullulanase inhibitor
0.279	0.132	Sphinganine kinase inhibitor
0.212	0.065	Lipoprotein lipase stimulant
0.180	0.033	Alcohol dehydrogenase substrate

0.278	0.132	Leukotriene-C4 synthase inhibitor
0.352	0.206	Kidney function stimulant
0.176	0.031	Thiol S-methyltransferase inhibitor
0.180	0.035	Aspartyl aminopeptidase inhibitor
0.213	0.070	Antiuremic
0.243	0.100	Monodehydroascorbate reductase (NADH) inhibitor
0.145	0.003	Free fatty acid receptor 1 agonist
0.285	0.144	Benzoate-CoA ligase inhibitor
0.272	0.130	Manganese peroxidase inhibitor
0.289	0.148	Fragilysin inhibitor
0.204	0.064	Coenzyme-B sulfoethylthiotransferase inhibitor
0.268	0.127	Bilirubin oxidase inhibitor
0.221	0.082	UGT1A6 substrate
0.329	0.191	Ribulose-phosphate 3-epimerase inhibitor
0.215	0.078	CDP-diacylglycerol-glycerol-3-phosphate 3-phosphatidyltransferase inhibitor
0.196	0.060	Sterol 3-beta-glucosyltransferase inhibitor
0.232	0.097	Gamma-glutamyltransferase inhibitor
0.185	0.052	Cytosol alanyl aminopeptidase inhibitor
0.278	0.145	S-formylglutathione hydrolase inhibitor
0.242	0.110	Immunomodulator
0.205	0.073	Endopeptidase inhibitor
0.162	0.032	Caspase 3 inhibitor
0.189	0.059	Deoxyribonuclease I inhibitor
0.219	0.090	[acyl-carrier-protein] S-acetyltransferase inhibitor
0.163	0.034	Cyclooxygenase 1 inhibitor
0.197	0.068	Lymphocytopoiesis inhibitor
0.241	0.112	RNA synthesis inhibitor
0.175	0.047	Phosphoinositide phospholipase C inhibitor
0.132	0.004	Prostaglandin EP1 antagonist
0.153	0.025	Homocysteine S-methyltransferase inhibitor
0.230	0.103	Aspergillus nuclease S1 inhibitor
0.192	0.066	Anthrax lethal factor inhibitor
0.224	0.098	Antibacterial
0.197	0.071	Proteasome endopeptidase complex inhibitor
0.341	0.218	Nicotinic alpha4beta4 receptor agonist
0.233	0.111	UGT1A9 substrate
0.127	0.004	Prostaglandin EP2 antagonist
0.186	0.064	Isopenicillin-N synthase inhibitor
0.227	0.106	2-Hydroxymuconate-semialdehyde hydrolase inhibitor
0.235	0.115	N-formylmethionyl-peptidase inhibitor
0.160	0.040	Sarcosine oxidase inhibitor
0.204	0.085	Fumarate reductase (NADH) inhibitor

0.205	0.086	Pappalysin-1 inhibitor
0.177	0.059	Keratolytic
0.247	0.129	Dolichyl-diphosphooligosaccharide-protein glycotransferase inhibitor
0.270	0.154	Arginine 2-monooxygenase inhibitor
0.370	0.255	CYP2H substrate
0.244	0.129	Aldehyde oxidase inhibitor
0.144	0.029	Aldehyde dehydrogenase substrate
0.217	0.103	NOS2 expression inhibitor
0.186	0.074	Malate dehydrogenase inhibitor
0.267	0.155	Malate dehydrogenase (acceptor) inhibitor
0.267	0.156	GABA aminotransferase inhibitor
0.148	0.038	Aspartate kinase inhibitor
0.158	0.047	Cyclooxygenase inhibitor
0.162	0.052	3-Ketovalidoxylamine C-N-lyase inhibitor
0.194	0.085	Levanase inhibitor
0.123	0.014	Glutathione S-transferase inhibitor
0.235	0.128	4-Hydroxymandelate oxidase inhibitor
0.177	0.070	Glyoxylate reductase (NADP+) inhibitor
0.231	0.126	Urethanase inhibitor
0.205	0.099	Dopamine release stimulant
0.212	0.109	Long-chain-aldehyde dehydrogenase inhibitor
0.176	0.073	2,3-Dihydroxyindole 2,3-dioxygenase inhibitor
0.224	0.122	Transcription factor NF kappa A inhibitor
0.177	0.075	Aureolysin inhibitor
0.181	0.080	CYP4F2 substrate
0.180	0.080	3-Demethylubiquinone-9 3-O-methyltransferase inhibitor
0.197	0.097	Glutaminase inhibitor
0.334	0.235	Polyporopepsin inhibitor
0.167	0.067	Gametolysin inhibitor
0.194	0.095	Antiviral (Hepatitis B)
0.281	0.181	2-Dehydropantoate 2-reductase inhibitor
0.107	0.008	Prostaglandin agonist
0.182	0.084	Polygalacturonase inhibitor
0.306	0.209	Trans-acenaphthene-1,2-diol dehydrogenase inhibitor
0.193	0.096	Oryzin inhibitor
0.299	0.204	Fibrinolytic
0.196	0.101	Ceramide glucosyltransferase inhibitor
0.195	0.101	Thiopurine S-methyltransferase inhibitor
0.136	0.042	Pyrimidine-deoxynucleoside 2'-dioxygenase inhibitor
0.251	0.157	CYP2C9 substrate
0.224	0.130	Phosphopantothenoylcysteine decarboxylase inhibitor
0.215	0.122	Phospholipase C inhibitor

0.244	0.151	Antithrombotic
0.142	0.051	Thromboxane synthase stimulant
0.128	0.037	UDP-N-acetylglucosamine 1-carboxyvinyltransferase inhibitor
0.213	0.123	Flavin-containing monooxygenase substrate
0.157	0.068	Peptidylamidoglycolate lyase inhibitor
0.181	0.093	Phospholipase A1 inhibitor
0.173	0.087	Metallocoarboxypeptidase D inhibitor
0.211	0.125	Angiogenesis stimulant
0.136	0.049	Calcium channel (voltage-sensitive) blocker
0.187	0.101	Peroxidase inhibitor
0.172	0.086	Polyneuridine-aldehyde esterase inhibitor
0.199	0.114	Antipyretic
0.312	0.228	Antiviral (Rhinovirus)
0.254	0.169	CYP3A5 substrate
0.258	0.174	Biotinidase inhibitor
0.188	0.106	UDP-glucuronosyltransferase substrate
0.120	0.039	tRNA (guanine-N1-)-methyltransferase inhibitor
0.204	0.123	Catenin beta inhibitor
0.239	0.158	Fatty-acyl-CoA synthase inhibitor
0.224	0.143	Arylsulfate sulfotransferase inhibitor
0.158	0.078	Alkylator
0.252	0.173	Gonadotropin antagonist
0.152	0.073	Thioredoxin reductase inhibitor
0.159	0.080	4-Hydroxybenzoate nonaprenyltransferase inhibitor
0.133	0.054	Kexin inhibitor
0.188	0.110	Diabetic nephropathy treatment
0.133	0.055	Furin inhibitor
0.319	0.241	Testosterone 17beta-dehydrogenase (NADP+) inhibitor
0.227	0.149	Antiinflammatory, intestinal
0.158	0.081	Licheninase inhibitor
0.274	0.197	UDP-N-acetylglucosamine 4-epimerase inhibitor
0.151	0.075	Shikimate 5-dehydrogenase inhibitor
0.163	0.088	Glycine C-acetyltransferase inhibitor
0.235	0.160	MMP9 expression inhibitor
0.125	0.050	Glycerol-3-phosphate dehydrogenase (NAD+) inhibitor
0.286	0.211	Gastrin inhibitor
0.110	0.036	Chelator
0.239	0.165	NAD(P)+-arginine ADP-ribosyltransferase inhibitor
0.288	0.214	Alopecia treatment
0.151	0.077	Homoserine dehydrogenase inhibitor
0.087	0.014	Leukotriene B4 antagonist
0.188	0.115	O-aminophenol oxidase inhibitor

0.244	0.171	Histidine N-acetyltransferase inhibitor
0.097	0.024	Dihydrodipicolinate synthase inhibitor
0.142	0.070	Ganglioside galactosyltransferase inhibitor
0.170	0.099	Tauropine dehydrogenase inhibitor
0.178	0.107	Antitussive
0.217	0.146	D-lactaldehyde dehydrogenase inhibitor
0.196	0.126	Saluretic
0.181	0.111	Cyclohexyl-isocyanide hydratase inhibitor
0.185	0.115	Calpain inhibitor
0.251	0.182	Nitrate reductase (cytochrome) inhibitor
0.210	0.141	CYP2A5 substrate
0.148	0.079	Procollagen C-endopeptidase inhibitor
0.203	0.134	Lysostaphin inhibitor
0.140	0.071	UGT1A7 substrate
0.161	0.093	Mannitol-1-phosphatase inhibitor
0.274	0.206	Mucositis treatment
0.074	0.006	Prostaglandin E2 antagonist
0.160	0.092	Nitric oxide scavenger
0.185	0.118	Nardilysin inhibitor
0.199	0.132	Glycerol-3-phosphate dehydrogenase inhibitor
0.295	0.228	Macrophage colony stimulating factor agonist
0.124	0.057	Keratosis actinic (solar) treatment
0.261	0.194	Glycerol-3-phosphate oxidase inhibitor
0.254	0.187	CYP2A1 substrate
0.164	0.097	N-(long-chain-acyl)ethanolamine deacylase inhibitor
0.134	0.068	Succinic dehydrogenase inhibitor
0.197	0.131	Antidiabetic symptomatic
0.115	0.050	Serine O-acetyltransferase inhibitor
0.134	0.069	Diisopropyl-fluorophosphatase inhibitor
0.096	0.031	Thromboxane antagonist
0.154	0.090	Chemopreventive
0.146	0.082	Lactaldehyde reductase inhibitor
0.250	0.186	Insulysin inhibitor
0.213	0.150	4-Methoxybenzoate monooxygenase (O-demethylating) inhibitor
0.167	0.104	Galactolipase inhibitor
0.257	0.195	Muramoyltetrapeptide carboxypeptidase inhibitor
0.160	0.098	Antiparkinsonian, tremor relieving
0.135	0.074	Cellulase inhibitor
0.121	0.061	Pectin lyase inhibitor
0.125	0.065	Neurotrophic factor
0.078	0.018	Cruzipain inhibitor
0.207	0.147	Hematopoietic inhibitor

0.157	0.098	ADP-ribosylarginine hydrolase inhibitor
0.094	0.034	High-mannose-oligosaccharide beta-1,4-N-acetylglucosaminyltransferase inhibitor
0.229	0.170	Formaldehyde transketolase inhibitor
0.126	0.067	Gelatinase inhibitor
0.207	0.149	Methylumbelliferyl-acetate deacetylase inhibitor
0.257	0.199	Lactase inhibitor
0.224	0.166	Glyoxylate reductase inhibitor
0.253	0.196	Calcium regulator
0.176	0.119	Proliferative diseases treatment
0.239	0.182	UGT2B12 substrate
0.272	0.215	Aminobutyraldehyde dehydrogenase inhibitor
0.192	0.136	Immunostimulant
0.153	0.097	Dynein ATPase inhibitor
0.138	0.083	Acylaminoacyl-peptidase inhibitor
0.190	0.134	Leukotriene-B4 20-monooxygenase inhibitor
0.134	0.078	Glucan 1,4-beta-glucosidase inhibitor
0.072	0.017	Prostaglandin antagonist
0.378	0.323	Gluconate 2-dehydrogenase (acceptor) inhibitor
0.078	0.023	Leukotriene C antagonist
0.166	0.111	Xylan endo-1,3-beta-xylosidase inhibitor
0.206	0.152	N-benzyloxycarbonylglycine hydrolase inhibitor
0.250	0.197	Beta-adrenergic receptor kinase inhibitor
0.250	0.197	G-protein-coupled receptor kinase inhibitor
0.111	0.058	Squalene epoxidase inhibitor
0.241	0.188	CYP3A1 substrate
0.115	0.062	Glycerol-3-phosphate O-acyltransferase inhibitor
0.059	0.007	Carbonic anhydrase XIV inhibitor
0.135	0.082	Tripeptide aminopeptidase inhibitor
0.185	0.134	Coccolysin inhibitor
0.074	0.023	Peroxisome proliferator-activated receptor agonist
0.121	0.070	Xanthine oxidase inhibitor
0.157	0.106	Alkylglycerophosphoethanolamine phosphodiesterase inhibitor
0.242	0.191	Aspartate-phenylpyruvate transaminase inhibitor
0.228	0.178	CYP2C substrate
0.134	0.084	Magnesium-protoporphyrin IX methyltransferase inhibitor
0.235	0.186	Cyanoalanine nitrilase inhibitor
0.129	0.080	Interleukin 1 antagonist
0.181	0.132	Glucan 1,4-alpha-maltotetraohydrolase inhibitor
0.069	0.020	Vanilloid 4 antagonist
0.127	0.079	Acylglycerone-phosphate reductase inhibitor
0.055	0.006	VCAM-1 antagonist
0.204	0.156	CYP2C18 substrate

0.054	0.007	VCAM antagonist
0.151	0.104	Myeloblastin inhibitor
0.077	0.030	SULT1A2 substrate
0.083	0.036	Long-chain-fatty-acid-CoA ligase inhibitor
0.254	0.207	CF transmembrane conductance regulator agonist
0.069	0.023	Homoserine O-acetyltransferase inhibitor
0.116	0.069	Glycerone-phosphate O-acyltransferase inhibitor
0.067	0.021	Retinoid X alpha receptor agonist
0.114	0.068	Monophenol monooxygenase inhibitor
0.107	0.062	Pantothenase inhibitor
0.119	0.074	Adenylate cyclase inhibitor
0.090	0.045	Ornithine decarboxylase inhibitor
0.100	0.056	CDC25A inhibitor
0.246	0.202	Carboxypeptidase Taq inhibitor
0.169	0.125	Anthelmintic
0.072	0.029	Antihypermotility
0.091	0.048	Protein-tyrosine phosphatase 1B inhibitor
0.199	0.157	NADPH-ferrihemoprotein reductase inhibitor
0.158	0.117	Mucorpepsin inhibitor
0.124	0.083	Interleukin 4 antagonist
0.221	0.180	Acetylcholinesterase inhibitor
0.117	0.076	Malate-CoA ligase inhibitor
0.085	0.045	[acyl-carrier-protein] S-malonyltransferase inhibitor
0.117	0.077	N-(5-amino-5-carboxypentanoyl)-L-cysteinyl-D-valine synthase inhibitor
0.053	0.013	Carbonic anhydrase VII inhibitor
0.333	0.293	Nootropic
0.159	0.120	Dihydroxy-acid dehydratase inhibitor
0.060	0.021	Calcium channel L-type blocker
0.185	0.147	Platelet aggregation inhibitor
0.231	0.193	JAK2 expression inhibitor
0.254	0.216	Dementia treatment
0.141	0.103	1,4-Alpha-glucan branching enzyme inhibitor
0.215	0.178	Antiprotozoal (Leishmania)
0.093	0.056	Cytokine release inhibitor
0.054	0.017	Alpha-amino-acid esterase inhibitor
0.068	0.031	1-Alkyl-2-acetylgllycerol O-acyltransferase inhibitor
0.057	0.020	Lysophosphatidic acid receptor antagonist
0.224	0.187	Histidine kinase inhibitor
0.166	0.129	PfA-M1 aminopeptidase inhibitor
0.288	0.251	Platelet aggregation stimulant
0.177	0.141	TRPA1 agonist
0.257	0.222	Caspase 3 stimulant

0.124	0.088	Cysteine synthase inhibitor
0.202	0.167	FMO1 substrate
0.040	0.005	Juvenile-hormone esterase inhibitor
0.173	0.139	Linoleoyl-CoA desaturase inhibitor
0.102	0.069	Palmitoyl-CoA hydrolase inhibitor
0.102	0.069	Acyl-CoA hydrolase inhibitor
0.244	0.210	CYP2C8 substrate
0.126	0.093	D-xylulose reductase inhibitor
0.099	0.066	Sorbose dehydrogenase inhibitor
0.102	0.070	Dimethylhistidine N-methyltransferase inhibitor
0.180	0.148	H ⁺ -exporting ATPase inhibitor
0.137	0.105	Styrene-oxide isomerase inhibitor
0.253	0.221	Pin1 inhibitor
0.115	0.084	Glycosylphosphatidylinositol diacylglycerol-lyase inhibitor
0.053	0.022	Peroxisome proliferator-activated receptor alpha agonist
0.130	0.098	NAD ⁺ synthase (glutamine-hydrolysing) inhibitor
0.256	0.225	Sulfur reductase inhibitor
0.073	0.042	3-Dehydroquinate synthase inhibitor
0.110	0.079	Glucosamine-6-phosphate deaminase inhibitor
0.116	0.086	Bcl2 antagonist
0.178	0.148	Acetylserotonin O-methyltransferase inhibitor
0.126	0.096	Corticosteroid antagonist
0.192	0.162	Amyotrophic lateral sclerosis treatment
0.288	0.259	CYP2J2 substrate
0.084	0.055	Sporulation kinase A inhibitor
0.184	0.155	Thyroxine 5-deiodinase inhibitor
0.143	0.114	Sedoheptulose-bisphosphatase inhibitor
0.099	0.070	Phosphoglycerate mutase inhibitor
0.199	0.170	Hydroxylamine reductase (NADH) inhibitor
0.186	0.158	ADP-thymidine kinase inhibitor
0.100	0.072	Site-specific DNA-methyltransferase (adenine-specific) inhibitor
0.085	0.057	Interleukin 1b antagonist
0.127	0.099	IgA-specific metalloendopeptidase inhibitor
0.088	0.061	Pantetheine-phosphate adenylyltransferase inhibitor
0.126	0.098	Cysteamine dioxygenase inhibitor
0.211	0.184	Antineurogenic pain
0.275	0.249	Complement factor D inhibitor
0.070	0.044	Anesthetic inhalation
0.224	0.199	Glycogen synthase stimulant
0.166	0.141	Fructan beta-fructosidase inhibitor
0.091	0.066	Acyloxyacyl hydrolase inhibitor
0.097	0.073	Protein-tyrosine phosphatase inhibitor

0.057	0.033	CDC25B inhibitor
0.198	0.175	Venom exonuclease inhibitor
0.263	0.240	Neurotransmitter antagonist
0.099	0.076	Sulfotransferase substrate
0.075	0.053	Amino-acid racemase inhibitor
0.089	0.067	Arylformamidase inhibitor
0.061	0.039	Mannosidase inhibitor
0.090	0.068	4-Alpha-glucanotransferase inhibitor
0.103	0.081	Protein phosphatase inhibitor
0.150	0.128	Glycerol 2-dehydrogenase (NADP+) inhibitor
0.124	0.103	Sphinganine-1-phosphate aldolase inhibitor
0.048	0.026	tRNA (adenine-N1-)-methyltransferase inhibitor
0.179	0.158	Endothelial growth factor antagonist
0.060	0.040	N-acetylmuramoyl-L-alanine amidase inhibitor
0.101	0.081	NAD+ kinase inhibitor
0.133	0.113	N-methyl-2-oxoglutaramate hydrolase inhibitor
0.043	0.023	Leukotriene C4 antagonist
0.186	0.167	Antiischemic
0.137	0.118	Protein-Npi-phosphohistidine-sugar phosphotransferase inhibitor
0.180	0.161	Antiparkinsonian, rigidity relieving
0.028	0.010	Retinoic acid receptor agonist
0.076	0.057	mRNA (guanine-N7-)-methyltransferase inhibitor
0.020	0.002	Eukaryotic elongation factor 2 kinase inhibitor
0.256	0.238	2-Hydroxyquinoline 8-monooxygenase inhibitor
0.144	0.127	2-Oxoaldehyde dehydrogenase (NADP+) inhibitor
0.144	0.126	Prenyl-diphosphatase inhibitor
0.058	0.041	Angiotensin-converting enzyme inhibitor
0.047	0.030	Phospholipase A2 IIa inhibitor
0.143	0.127	Vitamin-K-epoxide reductase (warfarin-insensitive) inhibitor
0.020	0.004	Prostaglandin EP12 antagonist
0.157	0.141	S-alkylcysteine lyase inhibitor
0.133	0.117	[phosphorylase] phosphatase inhibitor
0.069	0.053	Pantoate-beta-alanine ligase inhibitor
0.039	0.023	Prostacyclin antagonist
0.166	0.151	Uroporphyrinogen-III synthase inhibitor
0.183	0.168	Vascular dementia treatment
0.125	0.111	HMG CoA synthase inhibitor
0.099	0.085	Asparaginase inhibitor
0.195	0.181	Dehydro-L-gulonate decarboxylase inhibitor
0.177	0.163	tRNA-pseudouridine synthase I inhibitor
0.229	0.216	Sulfite dehydrogenase inhibitor
0.147	0.134	Ketol-acid reductoisomerase inhibitor

0.233	0.219	3-Hydroxybenzoate 6-monooxygenase inhibitor
0.036	0.022	Leukotriene D4 antagonist
0.201	0.188	Adenylyl-sulfate reductase inhibitor
0.193	0.180	Exoribonuclease II inhibitor
0.132	0.119	Envelysin inhibitor
0.165	0.153	Antineoplastic enhancer
0.051	0.040	Magnolysin inhibitor
0.182	0.170	Glucan 1,4-alpha-maltotriohydrolase inhibitor
0.161	0.150	Glutathione dehydrogenase (ascorbate) inhibitor
0.194	0.184	Peptide-N4-(N-acetyl-beta-glucosaminyl)asparagine amidase inhibitor
0.249	0.239	Prion diseases treatment
0.102	0.092	Steroid 9alpha-monooxygenase inhibitor
0.012	0.003	Apolipoprotein A inhibitor
0.252	0.243	Rubredoxin-NAD+ reductase inhibitor
0.183	0.175	Peptide alpha-N-acetyltransferase inhibitor
0.216	0.207	Hydroxylamine oxidase inhibitor
0.051	0.042	D-Serine ammonia-lyase inhibitor
0.071	0.063	S-methyl-5-thioribose kinase inhibitor
0.126	0.117	L-glucuronate reductase inhibitor
0.047	0.039	Cysteine dioxygenase inhibitor
0.046	0.039	Secretory phospholipase A2 inhibitor
0.012	0.004	Factor IXa inhibitor
0.033	0.026	Dopamine precursors
0.162	0.155	Peroxidase substrate
0.063	0.057	L-3-cyanoalanine synthase inhibitor
0.127	0.121	Phosphatidylglycerophosphatase inhibitor
0.224	0.219	CYP3A substrate
0.077	0.071	Retinoic acid beta receptor agonist
0.183	0.177	AR expression inhibitor
0.114	0.109	Guanidinoacetate N-methyltransferase inhibitor
0.154	0.149	Sorbitol-6-phosphate 2-dehydrogenase inhibitor
0.077	0.072	Cyclooxygenase 2 inhibitor
0.107	0.102	Phosphoenolpyruvate-protein phosphotransferase inhibitor
0.012	0.007	Caspase 7 inhibitor
0.284	0.279	Glutamyl endopeptidase II inhibitor
0.128	0.124	Paraoxonase substrate
0.112	0.108	Farnesyltranstransferase inhibitor
0.107	0.103	Radical formation agonist
0.042	0.038	Elastase inhibitor
0.040	0.037	Acetyl-CoA transferase 2 inhibitor
0.065	0.062	Acetate-CoA ligase inhibitor
0.100	0.097	Beta lactamase inhibitor

0.175	0.173	Xenobiotic-transporting ATPase inhibitor
0.087	0.085	6-Methylsalicylate decarboxylase inhibitor
0.114	0.113	Phenol 2-monooxygenase inhibitor
0.164	0.163	1,2-alpha-L-fucosidase inhibitor
0.079	0.077	Glycine hydroxymethyltransferase inhibitor
0.158	0.157	Diuretic
0.111	0.110	Phenylacetate-CoA ligase inhibitor
0.179	0.178	Antihypertensive
0.122	0.120	Arylacetonitrilase inhibitor
0.211	0.210	Antiprotozoal (Amoeba)
0.084	0.083	Homocysteine desulfhydrase inhibitor
0.190	0.189	Gluconate 5-dehydrogenase inhibitor
0.163	0.163	3-Methylbutanal reductase inhibitor