

Computer-Aided Methods for Molecular Classification

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Table S1. Positive and negative effects of the molecules in Group 1, and the probabilities of their activities.

CID	Positive effects		Negative effects	
	<i>Pa</i>	Effect	<i>Pa</i>	Effect
9889172	0.473	Analgesic. non-opioid	0.445	Cyanosis
	0.462	Cannabinoid receptor antagonist	0.392	Nail discoloration
	0.448	Analgesic	0.354	Torsades de pointes
	0.425	Sigma receptor antagonist		
	0.386	Antineoplastic alkaloid		
	0.326	Glycosylphosphatidylinositol phospholipase D inhibitor		
	0.319	Lymphocytopoiesis inhibitor		
	0.319	Prostate disorders treatment		
	0.318	Peptide agonist		
	0.318	Thromboxane B2 antagonist		
	0.303	NADPH-cytochrome-c2 reductase inhibitor		
117587582	0.466	Chemosensitizer	0.481	Thrombocytopenia
	0.464	Pseudolysin inhibitor	0.479	Hypotension
	0.414	CYP1A2 substrate	0.469	Fibrillation. atrial
	0.397	Antineoplastic (breast cancer)	0.447	Sneezing
	0.38	Endopeptidase So inhibitor	0.441	Dyskinesia
	0.378	Glycosylphosphatidylinositol phospholipase D inhibitor	0.429	Neurotoxic
	0.366	Analgesic	0.429	Thrombophlebitis
	0.357	CYP1A substrate	0.428	Optic neuropathy
	0.352	Antiinfective	0.424	Toxic. respiration
	0.342	Glutamyl endopeptidase II inhibitor	0.417	Paralysis
	0.328	DNA synthesis inhibitor	0.406	Hepatotoxic
	0.321	Thromboxane B2 antagonist	0.406	Necrosis
	0.318	Peptide agonist	0.391	Dermatitis
	0.316	Antiviral (Picornavirus)	0.388	Ocular toxicity
	0.31	CYP2C8 substrate	0.38	Photoallergy dermatitis
	0.307	Venombin AB inhibitor	0.377	Endocrine disruptor
	0.303	NADPH-cytochrome-c2 reductase inhibitor	0.373	Optic neuritis
			0.372	Emetic
			0.348	Pulmonary edema
			0.341	Torsades de pointes

			0.341	Nail discoloration
			0.33	Fatty liver
			0.327	Keratopathy
			0.322	Nausea
			0.317	Gastrointestinal disturbance
			0.317	Toxic. gastrointestinal
			0.314	Allergic contact dermatitis
			0.301	Hematotoxic
10226340	0.491	Amyotrophic lateral sclerosis treatment	0.474	Choreoathetosis
	0.381	Histamine release stimulant	0.42	Torsades de pointes
	0.371	(R)-6-hydroxynicotine oxidase inhibitor	0.403	Paralysis
	0.363	CYP2H substrate	0.382	Urinary retention
	0.349	Neurotransmitter uptake inhibitor	0.381	Xerostomia
	0.341	Octopamine antagonist	0.376	Nephrotic syndrome
	0.326	Systemic lupus erythematosus treatment	0.36	Postural (orthostatic) hypotension
	0.315	Vascular (periferal) disease treatment	0.349	Bradycardic
	0.312	P-glycoprotein substrate	0.331	Dizziness
	0.305	Platelet adhesion inhibitor	0.328	Sensory disturbance
	0.303	Lymphocytopoiesis inhibitor	0.324	Asthma
	0.303	Antiviral (Picornavirus)	0.312	Photoallergy dermatitis
	0.301	Nicotinic alpha4beta2 receptor antagonist	0.307	Yawning
	0.301	Cognition disorders treatment	0.3	Laryngospasm
	0.301	Ovulation inhibitor		
57507911	0.487	CYP2C18 substrate	0.494	Hypotonia
	0.48	Prostate disorders treatment	0.489	Nephritis
	0.471	Ubiquinol-cytochrome-c reductase inhibitor	0.488	Urinary retention
	0.468	Acetylcholine neuromuscular blocking agent	0.482	Toxic. respiration
	0.46	CYP2D6 substrate	0.48	Choreoathetosis
	0.456	Platelet adhesion inhibitor	0.477	Hepatitis
	0.455	Polyporopepsin inhibitor	0.462	Bradycardic
	0.454	Oxidoreductase inhibitor	0.461	Sweating
	0.453	Lipid metabolism regulator	0.459	Edema
	0.451	Platelet aggregation stimulant	0.448	Postural (orthostatic) hypotension
	0.45	Sulfur reductase inhibitor	0.44	Dizziness
	0.449	Carboxypeptidase Taq inhibitor	0.439	Interstitial nephritis
	0.442	Antinociceptive	0.43	Optic neuropathy
	0.436	CYP2D substrate	0.429	Bronchoconstrictor
	0.434	Plastoquinol-plastocyanin reductase inhibitor	0.424	Optic neuritis
	0.431	Antihypoxic	0.421	Sensory disturbance
	0.431	Fructose 5-dehydrogenase inhibitor	0.415	Asthma
	0.429	Glycerol-ether monooxygenase inhibitor	0.41	Dysarthria
	0.429	Ovulation inhibitor	0.409	Visual acuity impairment
	0.429	Membrane permeability inhibitor	0.405	Stomatitis
	0.423	MMP9 expression inhibitor	0.404	Hypercholesterolemic
	0.418	2-Hydroxyquinoline 8-monooxygenase inhibitor	0.403	Gastrointestinal disturbance
	0.417	Antiviral (Picornavirus)	0.399	Cholestasis
	0.414	CYP2C9 substrate	0.395	Diarrhea
	0.41	Antiinfective	0.394	Ocular toxicity
	0.409	Fusarinine-C ornithinesterase inhibitor	0.392	Ulceration

	0.407	Gonadotropin antagonist	0.392	Necrosis
	0.399	Antineoplastic (uterine cancer)	0.39	Fatty liver
	0.389	CYP2C8 inhibitor	0.389	Nail discoloration
	0.387	Insulysin inhibitor	0.386	Torticollis
	0.384	CYP1A2 inhibitor	0.385	Sedative
	0.382	Leukotriene-C4 synthase inhibitor	0.38	Inflammation
	0.381	TNF expression inhibitor	0.38	Headache
	0.381	CYP2C substrate	0.379	Cardiodepressant
	0.381	4-Nitrophenol 2-monooxygenase inhibitor	0.379	Akathisia
	0.375	CYP1A inhibitor	0.377	Cataract
	0.374	Phobic disorders treatment	0.377	Excitability
	0.372	Eye irritation, inactive	0.374	Euphoria
	0.37	CYP2H substrate	0.372	Nephrotic syndrome
	0.367	ATP-binding cassette A1 stimulant	0.369	Weight loss
	0.367	Antineurogenic pain	0.368	Sleep disturbance
	0.367	CYP2C8 substrate	0.364	Paralysis
	0.366	Glycosylphosphatidylinositol phospholipase D inhibitor	0.363	Keratopathy
	0.364	N-methyl-2-oxoglutaramate hydrolase inhibitor	0.358	Withdrawal
	0.36	Nicotine dehydrogenase inhibitor	0.35	Retroperitoneal fibrosis
	0.359	Histamine release stimulant	0.349	Weight gain
	0.357	Antinephritic	0.348	Ulcer, gastric
	0.357	Membrane integrity antagonist	0.347	Porphyria
	0.357	CYP2J2 substrate	0.347	Chorea
	0.356	Caspase 8 stimulant	0.347	Pain
	0.355	Antiviral (Rhinovirus)	0.346	Hyperthermic
	0.352	5 Hydroxytryptamine uptake stimulant	0.344	Yawning
	0.351	Nitrate reductase (cytochrome) inhibitor	0.343	Weakness
	0.351	Octopamine antagonist	0.339	Acidosis
	0.349	Endopeptidase So inhibitor	0.337	Extrapyrasidal effect
	0.348	CYP2B10 substrate	0.333	Thrombocytopenia
	0.348	Electron-transferring-flavoprotein dehydrogenase inhibitor	0.331	Laryngospasm
	0.347	HERG 1 channel blocker	0.328	Galactorrhea
	0.347	HIF1A expression inhibitor	0.328	Depression
	0.347	Thioredoxin inhibitor	0.324	Ulcer, peptic
	0.346	27-Hydroxycholesterol 7alpha-monooxygenase inhibitor	0.321	Hypotension
	0.342	Intermittent claudication treatment	0.319	Hyperglycemic
	0.34	Interleukin 2 agonist	0.316	Anorexiant
	0.34	APOA1 expression enhancer	0.315	Multiple organ failure
	0.338	Sugar-phosphatase inhibitor	0.313	Piloerection
	0.337	Gluconate 5-dehydrogenase inhibitor	0.313	Endocrine disruptor
	0.336	CYP2E1 inducer	0.311	QT interval prolongation
	0.334	Pin1 inhibitor	0.308	Tachycardiac
	0.332	Pseudolysin inhibitor	0.306	Hypnotic
	0.33	Beta-adrenergic receptor kinase inhibitor	0.305	Palpitation
	0.33	G-protein-coupled receptor kinase inhibitor	0.3	Drowsiness
	0.329	Antiviral (Adenovirus)		
	0.329	1-Acylglycerol-3-phosphate O-acyltransferase inhibitor		

	0.329	All-trans-retinyl-palmitate hydrolase inhibitor		
	0.329	Hydroxylamine oxidase inhibitor		
	0.329	Spermidine dehydrogenase inhibitor		
	0.328	Inotropic		
	0.326	TRKB antagonist		
	0.326	MAP kinase stimulant		
	0.321	Mucositis treatment		
	0.319	Antineoplastic alkaloid		
	0.319	5 Hydroxytryptamine 2B agonist		
	0.319	CYP1A2 substrate		
	0.319	Oxygen scavenger		
	0.319	Macrophage colony stimulating factor agonist		
	0.317	Nicotinate dehydrogenase inhibitor		
	0.317	General pump inhibitor		
	0.316	Calcium channel activator		
	0.316	Sigma receptor agonist		
	0.316	Vanilloid 1 agonist		
	0.315	15-Hydroxyprostaglandin-D dehydrogenase (NADP+) inhibitor		
	0.315	CYP4A substrate		
	0.315	CYP2J substrate		
	0.314	CYP3A4 substrate		
	0.313	Antiprotozoal (Leishmania)		
	0.312	Indanol dehydrogenase inhibitor		
	0.312	Antiinflammatory. intestinal		
	0.312	Prion diseases treatment		
	0.309	1.4-Lactonase inhibitor		
	0.308	Phenol O-methyltransferase inhibitor		
	0.308	Vasodilator. peripheral		
	0.307	Caspase 3 stimulant		
	0.306	Reductant		
	0.306	Mediator release inhibitor		
	0.306	CYP3A3 substrate		
	0.306	CYP2D15 substrate		
	0.303	Neuropeptide Y2 antagonist		
	0.302	Urethanase inhibitor		
	0.302	Phosphatidylinositol diacylglycerol-lyase inhibitor		
	0.302	Glutathione thiolesterase inhibitor		
	0.301	Polarisation inhibitor		
	0.3	Choline-phosphate cytidyltransferase inhibitor		
	0.3	5 Hydroxytryptamine release inhibitor		
56841530	0.495	Platelet adhesion inhibitor	0.498	Xerostomia
	0.491	Saccharopepsin inhibitor	0.468	Dysphoria
	0.491	Chymosin inhibitor	0.466	Fibrosis. interstitial
	0.491	Acrocyllindropepsin inhibitor	0.466	Extrapyrarnidal effect
	0.49	Amine dehydrogenase inhibitor	0.466	Delirium
	0.476	CYP2C18 substrate	0.461	Pseudoporphyria

	0.449	Carboxypeptidase Taq inhibitor	0.461	Conjunctivitis
	0.448	Antihypoxic	0.449	Dystonia
	0.44	Prostate disorders treatment	0.448	Hypothermic
	0.438	Antineoplastic (uterine cancer)	0.444	Urinary retention
	0.433	CYP1A2 inhibitor	0.435	Nephritis
	0.423	CYP2D6 substrate	0.433	Hematuria
	0.422	CYP1A inhibitor	0.424	Cyanosis
	0.422	Sulfur reductase inhibitor	0.418	Hypercholesterolemic
	0.422	Antinociceptive	0.415	Fibrillation. atrial
	0.416	Platelet aggregation stimulant	0.407	Toxic. respiration
	0.415	Acetylcholine neuromuscular blocking agent	0.406	Bradycardic
	0.409	Fusarinine-C ornithinesterase inhibitor	0.397	Edema
	0.403	Polyporopepsin inhibitor	0.393	Hepatitis
	0.403	Ubiquinol-cytochrome-c reductase inhibitor	0.389	Weight gain
	0.402	CYP2D substrate	0.389	Postural (orthostatic) hypotension
	0.4	Gonadotropin antagonist	0.389	Nail discoloration
	0.4	Glyceryl-ether monooxygenase inhibitor	0.388	Torticollis
	0.393	Plastoquinol-plastocyanin reductase inhibitor	0.386	Weight loss
	0.393	Fructose 5-dehydrogenase inhibitor	0.385	Interstitial nephritis
	0.393	Antiviral (Picornavirus)	0.378	Bronchoconstrictor
	0.391	CYP2C9 substrate	0.375	Gastrointestinal disturbance
	0.388	Octopamine antagonist	0.374	Dizziness
	0.38	2-Hydroxyquinoline 8-monooxygenase inhibitor	0.371	Akathisia
	0.495	Platelet adhesion inhibitor	0.369	Visual acuity impairment
	0.491	Saccharopepsin inhibitor	0.367	Optic neuropathy
	0.491	Chymosin inhibitor	0.365	Cholestasis
	0.491	Acrocyllindropepsin inhibitor	0.365	Choreoathetosis
	0.49	Amine dehydrogenase inhibitor	0.364	Porphyria
	0.476	CYP2C18 substrate	0.364	Hypotonia
	0.449	Carboxypeptidase Taq inhibitor	0.362	Optic neuritis
	0.448	Antihypoxic	0.355	Ulcer. gastric
	0.44	Prostate disorders treatment	0.351	Excitability
	0.438	Antineoplastic (uterine cancer)	0.348	Endocrine disruptor
	0.433	CYP1A2 inhibitor	0.348	Euphoria
	0.423	CYP2D6 substrate	0.348	Depression
	0.422	CYP1A inhibitor	0.346	Sensory disturbance
	0.422	Sulfur reductase inhibitor	0.343	Stomatitis
	0.422	Antinociceptive	0.342	Cardiodepressant
	0.416	Platelet aggregation stimulant	0.341	Laryngospasm
	0.415	Acetylcholine neuromuscular blocking agent	0.34	Ocular toxicity
	0.409	Fusarinine-C ornithinesterase inhibitor	0.34	Asthma
	0.403	Polyporopepsin inhibitor	0.339	Ulceration
	0.403	Ubiquinol-cytochrome-c reductase inhibitor	0.339	Dysarthria
	0.402	CYP2D substrate	0.336	Acidosis
	0.4	Gonadotropin antagonist	0.336	Galactorrhea
	0.4	Glyceryl-ether monooxygenase inhibitor	0.333	Ulcer. peptic
	0.393	Plastoquinol-plastocyanin reductase inhibitor	0.328	Retroperitoneal fibrosis
	0.393	Fructose 5-dehydrogenase inhibitor	0.328	Nephrotic syndrome
	0.393	Antiviral (Picornavirus)	0.324	Sweating

	0.391	CYP2C9 substrate	0.322	Weakness
	0.388	Octopamine antagonist	0.32	Piloerection
	0.38	2-Hydroxyquinoline 8-monooxygenase inhibitor	0.32	Cataract
	0.379	Oxidoreductase inhibitor	0.318	Headache
	0.377	Ovulation inhibitor	0.315	Fasciculation
	0.375	Lipid metabolism regulator	0.315	Multiple organ failure
	0.374	Phobic disorders treatment	0.314	Sleep disturbance
	0.37	CYP2H substrate	0.31	Diarrhea
	0.366	Glycosylphosphatidylinositol phospholipase D inhibitor	0.308	Paralysis
	0.364	Leukotriene-C4 synthase inhibitor	0.306	Palpitation
	0.359	Histamine release stimulant	0.304	Fatty liver
	0.357	CYP2C8 inhibitor	0.303	Inflammation
	0.357	CYP2J2 substrate	0.301	Withdrawal
	0.352	5 Hydroxytryptamine uptake stimulant		
	0.351	4-Nitrophenol 2-monooxygenase inhibitor		
	0.35	Intermittent claudication treatment		
	0.349	Endopeptidase So inhibitor		
	0.348	Electron-transferring-flavoprotein dehydrogenase inhibitor		
	0.347	Membrane integrity antagonist		
	0.347	Thioredoxin inhibitor		
	0.344	ATP-binding cassette A1 stimulant		
	0.338	Sugar-phosphatase inhibitor		
	0.337	Gluconate 5-dehydrogenase inhibitor		
	0.335	MMP9 expression inhibitor		
	0.334	5 Hydroxytryptamine 2B agonist		
	0.334	Antithrombotic		
	0.334	Beta-adrenergic receptor kinase inhibitor		
	0.334	G-protein-coupled receptor kinase inhibitor		
	0.334	Antiviral (Rhinovirus)		
	0.332	Nicotine dehydrogenase inhibitor		
	0.332	APOA1 expression enhancer		
	0.332	Pseudolysin inhibitor		
	0.33	Aldehyde oxidase inhibitor		
	0.329	All-trans-retinyl-palmitate hydrolase inhibitor		
	0.329	Hydroxylamine oxidase inhibitor		
	0.328	Antiinfective		
	0.327	N-methyl-2-oxoglutaramate hydrolase inhibitor		
	0.327	TNF expression inhibitor		
	0.326	Vanilloid 1 agonist		
	0.325	Caspase 8 stimulant		
	0.325	CYP2C8 substrate		
	0.324	CYP2C substrate		
	0.324	Nitrate reductase (cytochrome) inhibitor		
	0.322	Eye irritation. inactive		
	0.322	1-Acylglycerol-3-phosphate O-acyltransferase inhibitor		
	0.322	5 Hydroxytryptamine release inhibitor		

	0.321	Prion diseases treatment		
	0.321	Mediator release inhibitor		
	0.321	Mucositis treatment		
	0.321	27-Hydroxycholesterol 7alpha-monooxygenase inhibitor		
	0.32	Cytoprotectant		
	0.319	Oxygen scavenger		
	0.319	Macrophage colony stimulating factor ago- nist		
	0.318	Antiinflammatory. intestinal		
	0.317	Antinephritic		
	0.316	Antiviral (Adenovirus)		
	0.315	CYP2J substrate		
	0.314	Antineurogenic pain		
	0.314	Antidyskinetic		
	0.311	TRKB antagonist		
	0.31	CYP2B10 substrate		
	0.31	CYP2E1 inducer		
	0.309	Antineoplastic alkaloid		
	0.308	Neuropeptide Y2 antagonist		
	0.308	Phenol O-methyltransferase inhibitor		
	0.307	Antiprotozoal (Trypanosoma)		
	0.307	Caspase 3 stimulant		
	0.306	Radioprotector		
	0.302	Urethanase inhibitor		
	0.302	Glutathione thiolesterase inhibitor		
	0.302	Interleukin 2 agonist		
	0.3	CYP1A2 substrate		
57507905	0.493	CYP2D6 substrate	0.499	Hepatitis
	0.486	Prostate disorders treatment	0.491	Sweating
	0.484	Gastrin inhibitor	0.483	Fibrillation. atrial
	0.482	CYP2C18 substrate	0.471	Bradycardic
	0.468	CYP2D substrate	0.466	Interstitial nephritis
	0.46	Fructose 5-dehydrogenase inhibitor	0.463	Toxic. respiration
	0.456	2-Hydroxyquinoline 8-monooxygenase in- hibitor	0.458	Hypercholesterolemic
	0.444	Ubiquinol-cytochrome-c reductase inhibitor	0.453	Dysarthria
	0.44	Fusarinine-C ornithinesterase inhibitor	0.45	Stomatitis
	0.438	Antinociceptive	0.444	Visual acuity impairment
	0.438	Platelet adhesion inhibitor	0.442	Edema
	0.436	Antihypoxic	0.441	Dizziness
	0.435	Sulfur reductase inhibitor	0.441	Optic neuritis
	0.432	Lipid metabolism regulator	0.439	Optic neuropathy
	0.431	CYP2C9 substrate	0.425	Fatty liver
	0.428	Platelet aggregation stimulant	0.424	Nail discoloration
	0.426	Polyporopepsin inhibitor	0.42	Bronchoconstrictor
	0.419	Antineoplastic (uterine cancer)	0.419	Sensory disturbance
	0.419	MMP9 expression inhibitor	0.41	Ulceration
	0.418	Oxidoreductase inhibitor	0.408	Cholestasis
	0.417	Ovulation inhibitor	0.406	Asthma
	0.414	Carboxypeptidase Taq inhibitor	0.406	Withdrawal
	0.411	Plastoquinol-plastocyanin reductase inhibi-	0.404	Extrapyramidal effect

		tor		
	0.411	4-Nitrophenol 2-monooxygenase inhibitor	0.404	Necrosis
	0.411	Antiviral (Picornavirus)	0.4	Nephrotic syndrome
	0.409	Gonadotropin antagonist	0.399	Chorea
	0.409	Insulysin inhibitor	0.398	Paralysis
	0.409	Glycosylphosphatidylinositol phospholipase D inhibitor	0.392	Sedative
	0.398	Membrane permeability inhibitor	0.392	Gastrointestinal disturbance
	0.397	CYP1A2 inhibitor	0.39	Akathisia
	0.389	Antiinfective	0.385	Headache
	0.388	CYP1A inhibitor	0.384	Cataract
	0.385	Nicotine dehydrogenase inhibitor	0.384	Ocular toxicity
	0.384	CYP2H substrate	0.383	Diarrhea
	0.383	Antineurogenic pain	0.38	Torticollis
	0.382	CYP2C substrate	0.379	Ulcer. gastric
	0.38	Thioredoxin inhibitor	0.376	Cardiodepressant
	0.379	CYP2C8 inhibitor	0.372	Retroperitoneal fibrosis
	0.378	ATP-binding cassette A1 stimulant	0.37	Excitability
	0.378	Glyceryl-ether monooxygenase inhibitor	0.369	Euphoria
	0.377	Electron-transferring-flavoprotein dehydrogenase inhibitor	0.361	Keratopathy
	0.372	Octopamine antagonist	0.36	Weight gain
	0.371	TNF expression inhibitor	0.358	Weight loss
	0.371	27-Hydroxycholesterol 7alpha-monooxygenase inhibitor	0.357	Ulcer. peptic
	0.37	HIF1A expression inhibitor	0.357	Yawning
	0.367	Leukotriene-C4 synthase inhibitor	0.357	Acidosis
	0.365	Sigma receptor agonist	0.356	Inflammation
	0.364	CYP2C8 substrate	0.355	Hyperglycemic
	0.362	Pin1 inhibitor	0.354	Porphyria
	0.359	Pseudolysin inhibitor	0.354	Sleep disturbance
	0.357	Spermidine dehydrogenase inhibitor	0.354	Thrombocytopenia
	0.356	HERG 1 channel blocker	0.35	Multiple organ failure
	0.355	Antinephritic	0.348	Depression
	0.353	APOA1 expression enhancer	0.348	Pain
	0.352	5 Hydroxytryptamine 2B agonist	0.345	Weakness
	0.351	MAP kinase stimulant	0.342	Hypomania
	0.347	Inotropic	0.342	Respiratory impairment
	0.345	Eye irritation. inactive	0.336	Palpitation
	0.345	Nicotinate dehydrogenase inhibitor	0.335	Piloerection
	0.345	Caspase 8 stimulant	0.335	Hyperthermic
	0.342	Phobic disorders treatment	0.334	Laryngospasm
	0.341	N-methyl-2-oxoglutaramate hydrolase inhibitor	0.325	Psychomotor impairment
	0.341	Phenol O-methyltransferase inhibitor	0.322	QT interval prolongation
	0.341	Glutathione thiolesterase inhibitor	0.322	Anorexiant
	0.34	5 Hydroxytryptamine uptake stimulant	0.321	Fasciculation
	0.339	CYP1A2 substrate	0.319	Tachycardiac
	0.338	Antineoplastic alkaloid	0.318	Hypnotic
	0.338	Indanol dehydrogenase inhibitor	0.316	Hypotension
	0.338	Nitrate reductase (cytochrome) inhibitor	0.316	Galactorrhea
	0.335	Intermittent claudication treatment	0.314	Coma

	0.335	Histamine release stimulant	0.307	Glaucoma
	0.334	TRKB antagonist	0.306	Endocrine disruptor
	0.332	CYP3A4 substrate	0.306	Sialorrhea
	0.332	1,4-Lactonase inhibitor		
	0.331	CYP2B10 substrate		
	0.33	CYP2J2 substrate		
	0.328	Antiviral (Rhinovirus)		
	0.327	Beta-adrenergic receptor kinase inhibitor		
	0.327	G-protein-coupled receptor kinase inhibitor		
	0.326	CYP2D15 substrate		
	0.324	Antiviral (Adenovirus)		
	0.323	Membrane integrity antagonist		
	0.323	Complement factor D inhibitor		
	0.322	1-Acylglycerol-3-phosphate O-acyltransferase inhibitor		
	0.322	Feruloyl esterase inhibitor		
	0.321	Steroid N-acetylglucosaminyltransferase inhibitor		
	0.321	CYP2E1 inducer		
	0.321	Endopeptidase So inhibitor		
	0.317	Interleukin 2 agonist		
	0.316	CYP2D2 inhibitor		
	0.315	Nicotinic alpha6beta3beta4alpha5 receptor antagonist		
	0.314	Mediator release inhibitor		
	0.311	CYP3A substrate		
	0.31	Prion diseases treatment		
	0.31	Sugar-phosphatase inhibitor		
	0.309	CF transmembrane conductance regulator agonist		
	0.309	Hydroxylamine oxidase inhibitor		
	0.309	JAK2 expression inhibitor		
	0.308	Trimethylamine-oxide aldolase inhibitor		
	0.307	Calcium channel activator		
	0.307	Gluconate 5-dehydrogenase inhibitor		
	0.307	Oxygen scavenger		
	0.306	Monoamine uptake inhibitor		
	0.306	Neuropeptide Y2 antagonist		
	0.306	Caspase 3 stimulant		
	0.306	General pump inhibitor		
	0.305	CYP3A3 substrate		
	0.305	Neurotransmitter antagonist		
	0.304	All-trans-retinyl-palmitate hydrolase inhib- itor		
	0.304	P-glycoprotein substrate		
	0.304	Macrophage colony stimulating factor ago- nist		
	0.304	Ribulose-phosphate 3-epimerase inhibitor		
	0.303	Lysase inhibitor		
	0.303	Mucositis treatment		
	0.302	Lysyl oxidase inhibitor		
	0.301	Polarization inhibitor		

56463	0.483	5 Hydroxytryptamine release stimulant	0.485	Hyperglycemic
	0.469	Sigma receptor agonist	0.464	Urinary retention
	0.469	Acetylcholine neuromuscular blocking agent	0.456	Hypomania
	0.457	Thromboxane B2 antagonist	0.441	Photoallergy dermatitis
	0.455	HIF1A expression inhibitor	0.44	Ulceration
	0.44	Rhinitis treatment	0.429	Asthma
	0.434	Antinociceptive	0.421	Allergic contact dermatitis
	0.431	Antiinflammatory	0.415	Choreoathetosis
	0.429	Lipid metabolism regulator	0.412	Fibrosis. interstitial
	0.415	Heat shock protein 27 antagonist	0.412	Xerostomia
	0.411	Cannabinoid receptor antagonist	0.411	Thrombocytopenia
	0.391	CYP2C19 inhibitor	0.41	Interstitial nephritis
	0.391	Transcription factor STAT inhibitor	0.402	Hypercholesterolemic
	0.38	Platelet adhesion inhibitor	0.4	Ulcer. gastric
	0.373	Histamine release stimulant	0.4	Weakness
	0.369	Glyoxylate reductase inhibitor	0.396	Hematuria
	0.365	Antihypoxic	0.388	Hypothermic
	0.363	Vasodilator. coronary	0.385	Weight loss
	0.363	Octopamine antagonist	0.384	Extrapyramidal effect
	0.362	Platelet aggregation inhibitor	0.381	Torsades de pointes
	0.36	Platelet aggregation stimulant	0.38	Sweating
	0.359	Vasodilator. peripheral	0.378	Bradycardic
	0.357	Antianginal	0.376	Stomatitis
	0.356	CYP2C18 substrate	0.374	Nephrotic syndrome
	0.349	Transcription factor STAT3 inhibitor	0.373	Ulcer. peptic
	0.347	HMGCS2 expression enhancer	0.371	Gastrointestinal hemorrhage
	0.347	General pump inhibitor	0.366	Hypotension
	0.339	Prostate disorders treatment	0.346	Laryngospasm
	0.335	Monoamine uptake inhibitor	0.339	Cardiodepressant
	0.335	MMP9 expression inhibitor	0.339	Retroperitoneal fibrosis
	0.334	Inotropic	0.339	Withdrawal
	0.329	CYP2D15 substrate	0.337	Hypotonia
	0.326	Antineoplastic (uterine cancer)	0.335	Hyperthermic
	0.324	4-Nitrophenol 2-monooxygenase inhibitor	0.335	Pain
	0.32	Spasmolytic. Papaverin-like	0.333	Thrombophlebitis
	0.319	Cyclohexanone monooxygenase inhibitor	0.332	Torticollis
	0.316	27-Hydroxycholesterol 7alpha-monooxygenase inhibitor	0.312	QT interval prolongation
	0.315	Antineurogenic pain	0.312	Glaucoma
	0.314	Imidazoline I1 receptor agonist	0.309	Akathisia
	0.314	Fibrinolytic	0.303	Pseudoporphyria
	0.312	Chemosensitizer		
	0.312	Antiviral (Picornavirus)		
	0.312	Fusarinine-C ornithinesterase inhibitor		
	0.31	Taurine dehydrogenase inhibitor		
	0.307	Mediator release inhibitor		
	0.305	Amine dehydrogenase inhibitor		
	0.303	Dementia treatment		
	0.303	1.4-Lactonase inhibitor		
	0.301	Antieczematic atopic		

Table S2. Positive and negative effects of the molecules in Group 2, and the probabilities of their activities.

44397641	0.485	Antiasthmatic	0.473	Euphoria
	0.483	Gastrin inhibitor	0.470	Myoclonus
	0.479	Polyporopepsin inhibitor	0.468	Weakness
	0.477	Saccharopepsin inhibitor	0.465	Hypercholesterolemic
	0.477	Chymosin inhibitor	0.459	Dysarthria
	0.477	Acrocylindropepsin inhibitor	0.458	Conjunctivitis
	0.474	Calcium channel (voltage-sensitive) activator	0.449	Weight gain
	0.465	Antinociceptive	0.448	Acidosis
	0.464	CYP2H substrate	0.443	Allergic contact dermatitis
	0.451	CYP2C18 substrate	0.438	Photoallergy dermatitis
	0.451	Amine dehydrogenase inhibitor	0.436	Akathisia
	0.444	Fibrinolytic	0.421	Bradycardic
	0.432	Platelet aggregation stimulant	0.417	Hypotension
	0.428	Platelet adhesion inhibitor	0.412	Fibrosis. interstitial
	0.422	Acetylcholine neuromuscular blocking agent	0.412	Hypotonia
	0.421	Plastoquinol-plastocyanin reductase inhibitor	0.410	Yawning
	0.418	Sulfur reductase inhibitor	0.409	Muscle weakness
	0.416	Gonadotropin antagonist	0.409	Gastrointestinal hemorrhage
	0.416	Antidyskinetic	0.399	Depression
	0.415	Prostate disorders treatment	0.399	Dizziness
	0.411	Ubiquinol-cytochrome-c reductase inhibitor	0.397	Sneezing
	0.408	Rhinitis treatment	0.393	Edema
	0.402	Antiviral (Picornavirus)	0.391	Tremor
	0.401	Ovulation inhibitor	0.388	Tachycardiac
	0.401	CYP2C8 inhibitor	0.385	Retroperitoneal fibrosis
	0.397	Benzoin aldolase inhibitor	0.385	Laryngospasm
	0.388	Glyceryl-ether monooxygenase inhibitor	0.384	Toxic. respiration
	0.387	Nicotinic alpha6beta3beta4alpha5 receptor antagonist	0.384	Reproductive dysfunction
	0.385	Histamine release stimulant	0.383	Nephritis
	0.383	Antipruritic	0.383	Fibrillation. atrial
	0.377	Antiviral (Rhinovirus)	0.381	Cholestasis
	0.375	Fructose 5-dehydrogenase inhibitor	0.381	Paralysis
	0.370	Antieczematic atopic	0.378	Xerostomia
	0.369	Carboxypeptidase Taq inhibitor	0.373	Dysphoria
	0.364	Leukotriene-C4 synthase inhibitor	0.373	Visual acuity impairment
	0.363	Membrane integrity antagonist	0.368	Hypomania
	0.360	Antiprotozoal (Leishmania)	0.367	Delirium
	0.358	Pin1 inhibitor	0.365	Interstitial nephritis

	0.357	1-Acylglycerol-3-phosphate O-acyltransferase inhibitor	0.363	Necrosis
	0.355	Endopeptidase So inhibitor	0.361	Cyanosis
	0.353	2-Hydroxyquinoline 8-monooxygenase inhibitor	0.360	Sensory disturbance
	0.351	Fusarinine-C ornithinesterase inhibitor	0.359	Ulcer. gastric
	0.347	ATP-binding cassette A1 stimulant	0.359	Torticollis
	0.343	Membrane permeability inhibitor	0.358	Inflammation
	0.342	Caspase 8 stimulant	0.350	Hepatitis
	0.340	27-Hydroxycholesterol 7alpha-monooxygenase inhibitor	0.347	Ulcer. peptic
	0.340	CYP2J2 substrate	0.344	Dependence
	0.339	15-Hydroxyprostaglandin-D dehydrogenase (NADP+) inhibitor	0.344	Dystonia
	0.339	MAP kinase stimulant	0.344	Asthma
	0.337	Antitussive. narcotic	0.342	Extrapyramidal effect
	0.337	Intermittent claudication treatment	0.339	Optic neuropathy
	0.336	CYP2C19 inhibitor	0.338	Ocular toxicity
	0.336	Dermatologic	0.337	Stomatitis
	0.335	HIV attachment inhibitor	0.332	Urinary retention
	0.334	5 Hydroxytryptamine release inhibitor	0.332	Galactorrhea
	0.333	CYP2D6 substrate	0.325	Piloerection
	0.333	CYP2C9 substrate	0.325	Palpitation
	0.329	Phospholipase A2 inhibitor	0.324	Sleep disturbance
	0.328	4-Nitrophenol 2-monooxygenase inhibitor	0.324	Nail discoloration
	0.325	Antinephritic	0.320	Thrombophlebitis
	0.325	Caspase 3 stimulant	0.318	Coma
	0.324	5 Hydroxytryptamine 7 agonist	0.317	Optic neuritis
	0.324	Sigma receptor agonist	0.316	Porphyria
	0.321	Monoamine uptake inhibitor	0.311	Sedative
	0.321	Mucomembranous protector	0.311	Keratopathy
	0.319	Mucositis treatment	0.309	Psychoses
	0.318	Steroid N-acetylglucosaminyltransferase inhibitor	0.308	Parkinsonism
	0.317	Cytoprotectant	0.307	Withdrawal
	0.315	Lactase inhibitor	0.305	Ataxia
	0.314	HERG 1 channel blocker	0.302	Fasciculation
	0.314	Nicotine dehydrogenase inhibitor	0.302	Sialorrhea
	0.313	Phospholipase inhibitor	0.300	Apnea
	0.313	CYP2D substrate	0.300	Toxic. vascular
	0.312	Octopamine antagonist		

	0.311	Prion diseases treatment		
	0.310	CYP4A substrate		
	0.310	Nitrate reductase (cytochrome) inhibitor		
	0.309	CYP4F2 substrate		
	0.307	5 Hydroxytryptamine uptake stimulant		
	0.306	CYP2B10 substrate		
	0.306	Antiinflammatory. intestinal		
	0.303	Nicotinic alpha2beta2 receptor antagonist		
	0.303	Pseudolysin inhibitor		
	0.300	Antipruritic. allergic		
44397500	0.498	HERG 1 channel blocker	0.499	Chorea
	0.491	Rhinitis treatment	0.485	Torticollis
	0.481	Antiasthmatic	0.483	Sneezing
	0.468	5 Hydroxytryptamine uptake stimulant	0.482	Xerostomia
	0.462	Antieczematic	0.480	Muscle weakness
	0.449	Carboxypeptidase Taq inhibitor	0.479	Dizziness
	0.437	CYP2C8 inhibitor	0.478	Sweating
	0.430	Nicotinic alpha6beta3beta4alpha5 receptor antagonist	0.472	Urinary retention
	0.429	Endopeptidase So inhibitor	0.472	Hypotonia
	0.426	Gastrin inhibitor	0.469	Bradycardic
	0.423	Sulfur reductase inhibitor	0.463	Tremor
	0.420	Preneoplastic conditions treatment	0.462	Extrapyramidal effect
	0.419	27-Hydroxycholesterol 7alpha-monooxygenase inhibitor	0.462	Conjunctivitis
	0.416	CYP2C19 inhibitor	0.458	Paralysis
	0.405	General pump inhibitor	0.456	Ataxia
	0.403	Antiviral (Picornavirus)	0.450	Acidosis
	0.403	Membrane permeability inhibitor	0.447	Torsades de pointes
	0.402	Mediator release inhibitor	0.442	Sensory disturbance
	0.401	Platelet aggregation stimulant	0.435	Allergic contact dermatitis
	0.400	Hydroxylamine oxidase inhibitor	0.432	Edema
	0.397	Prostate disorders treatment	0.432	Hepatitis
	0.397	Antidyskinetic	0.425	Laryngospasm
	0.396	Antieczematic atopic	0.424	Sleep disturbance
	0.394	GST A substrate	0.421	Photoallergy dermatitis
	0.385	Ubiquinol-cytochrome-c reductase inhibitor	0.413	Euphoria
	0.377	CYP2C18 substrate	0.413	Toxic. respiration
	0.377	Histidine kinase inhibitor	0.412	Keratopathy
	0.373	Pseudolysin inhibitor	0.408	Neutrophilic dermatosis

				(Sweet's syndrome)
	0.373	Calcium channel (voltage-sensitive) activator	0.395	Retroperitoneal fibrosis
	0.372	Amine dehydrogenase inhibitor	0.391	Gastrointestinal hemorrhage
	0.371	Leukotriene-C4 synthase inhibitor	0.390	Hypotension
	0.369	Dermatologic	0.389	Nail discoloration
	0.368	5-O-(4-coumaroyl)-D-quinic 3'-monooxygenase inhibitor	0.383	Cyanosis
	0.367	HIV attachment inhibitor	0.383	Occult bleeding
	0.364	Antiviral (Rhinovirus)	0.381	Cholestasis
	0.356	Fructose 5-dehydrogenase inhibitor	0.379	Myocarditis
	0.355	Benzoin aldolase inhibitor	0.375	Necrosis
	0.353	Monoamine uptake inhibitor	0.372	Tachycardiac
	0.352	CYP4A11 substrate	0.371	Gastrointestinal disturbance
	0.351	Fibrinolytic	0.365	Yawning
	0.350	Nicotinic alpha2beta2 receptor antagonist	0.363	Thrombophlebitis
	0.348	Electron-transferring-flavoprotein dehydrogenase inhibitor	0.359	Consciousness alteration
	0.347	Antitussive. narcotic	0.358	Sialorrhea
	0.346	Nitrate reductase (cytochrome) inhibitor	0.356	Drowsiness
	0.346	2-Hydroxyquinoline 8-monooxygenase inhibitor	0.355	Hypomagnesemia
	0.344	Glyceryl-ether monooxygenase inhibitor	0.355	Emetic
	0.342	Mucositis treatment	0.353	Anorexiant
	0.337	IgA-specific serine endopeptidase inhibitor	0.349	Respiratory impairment
	0.337	Gluconate 5-dehydrogenase inhibitor	0.345	Visual acuity impairment
	0.332	Phthalate 4.5-dioxygenase inhibitor	0.340	QT interval prolongation
	0.332	Polyporopepsin inhibitor	0.336	Dysphoria
	0.329	RNA-directed RNA polymerase inhibitor	0.335	Interstitial nephritis
	0.329	Diabetic neuropathy treatment	0.335	Coma
	0.328	Macrophage colony stimulating factor agonist	0.335	Ocular toxicity
	0.327	5 Hydroxytryptamine 2B agonist	0.335	Psychoses
	0.323	Intermittent claudication treatment	0.333	Headache
	0.322	Antiprotozoal (Leishmania)	0.332	Dyskinesia
	0.321	Antinociceptive	0.331	Sedative
	0.318	Botulin neurotoxin A light chain inhibitor	0.330	Dependence
	0.318	Cl--transporting ATPase inhibitor	0.330	Hyperglycemic
	0.317	Complement factor D inhibitor	0.325	Pure red cell aplasia
	0.315	CYP3A4 substrate	0.325	Asthma
	0.312	H+-exporting ATPase inhibitor	0.320	Endocrine disruptor
	0.312	CYP2A8 substrate	0.320	Nephritis
	0.312	Mucomembranous protector	0.319	Dermatitis

	0.311	CF transmembrane conductance regulator agonist	0.318	Stomatitis
	0.307	Thioredoxin inhibitor	0.315	Pain
	0.306	Sugar-phosphatase inhibitor	0.312	Adrenal cortex hypoplasia
	0.306	Fusarinine-C ornithinesterase inhibitor	0.307	Depression
	0.305	Antipruritic	0.304	Parkinsonism
	0.302	CYP3A substrate	0.302	Behavioral disturbance
	0.301	Coccolysin inhibitor	0.300	Spermicide
	0.300	Lysyl oxidase inhibitor		
44397540	0.489	Antiasthmatic	0.486	Excitability
	0.489	Aspulvinone dimethylallyltransferase inhibitor	0.482	Torsades de pointes
	0.473	Fibrinolytic	0.472	Extrapyramidal effect
	0.472	Platelet adhesion inhibitor	0.445	Conjunctivitis
	0.471	General pump inhibitor	0.440	Gastrointestinal hemorrhage
	0.452	Gastrin inhibitor	0.438	Pseudoporphyria
	0.447	Membrane permeability inhibitor	0.432	Weakness
	0.432	Rhinitis treatment	0.427	Hypercholesterolemic
	0.424	Antinociceptive	0.426	Tremor
	0.421	CYP2C18 substrate	0.426	Weight gain
	0.407	Antidyskinetic	0.419	Hypotension
	0.406	Acrocyllindropepsin inhibitor	0.417	Sweating
	0.406	Saccharopepsin inhibitor	0.391	Acidosis
	0.406	Chymosin inhibitor	0.389	Dizziness
	0.401	Amine dehydrogenase inhibitor	0.384	Photoallergy dermatitis
	0.401	Gonadotropin antagonist	0.382	Akathisia
	0.397	Calcium channel (voltage-sensitive) activator	0.381	Xerostomia
	0.396	Platelet aggregation stimulant	0.379	Muscle weakness
	0.396	CDP-glycerol glycerophosphotransferase inhibitor	0.376	Sneezing
	0.394	CYP2H substrate	0.375	Bradycardic
	0.391	Prostate disorders treatment	0.375	Myoclonus
	0.391	Sulfur reductase inhibitor	0.366	Ocular toxicity
	0.387	Nicotinic alpha6beta3beta4alpha5 receptor antagonist	0.362	Depression
	0.380	Plastoquinol-plastocyanin reductase inhibitor	0.362	Torticollis
	0.379	5 Hydroxytryptamine 2B agonist	0.353	Laryngospasm
	0.378	Benzoin aldolase inhibitor	0.352	Cyanosis
	0.377	Dermatologic	0.352	Nephritis
	0.377	Acetylcholine neuromuscular blocking agent	0.351	Edema
	0.375	Polyporopepsin inhibitor	0.350	Cholestasis

	0.369	Carboxypeptidase Taq inhibitor	0.350	Sensory disturbance
	0.364	CYP2D6 substrate	0.347	Euphoria
	0.360	Antieczematic atopic	0.344	Dysphoria
	0.359	Antiviral (Rhinovirus)	0.342	Allergic contact dermatitis
	0.358	Glycerol-ether monooxygenase inhibitor	0.341	Dysarthria
	0.357	Intermittent claudication treatment	0.339	Palpitation
	0.355	HIV attachment inhibitor	0.339	Retroperitoneal fibrosis
	0.354	Antiviral (Picornavirus)	0.337	Ulcer. gastric
	0.351	Fusarinine-C ornithinesterase inhibitor	0.335	Visual acuity impairment
	0.350	Male reproductive dysfunction treatment	0.332	Interstitial nephritis
	0.350	Caspase 3 stimulant	0.330	Fibrillation. atrial
	0.347	Antipruritic	0.329	Gastrointestinal disturbance
	0.347	Octopamine antagonist	0.327	Toxic. respiration
	0.346	Leukotriene-C4 synthase inhibitor	0.326	Tachycardiac
	0.346	Ubiquinol-cytochrome-c reductase inhibitor	0.325	Reproductive dysfunction
	0.344	Heat shock protein 27 antagonist	0.324	Nail discoloration
	0.343	Ovulation inhibitor	0.323	Cardiodepressant
	0.342	Fructose 5-dehydrogenase inhibitor	0.321	Behavioral disturbance
	0.341	CYP2D substrate	0.321	Dystonia
	0.340	5 Hydroxytryptamine antagonist	0.320	Fibrosis. interstitial
	0.340	CYP2J2 substrate	0.320	Paralysis
	0.337	Monoamine uptake inhibitor	0.317	Hypotonia
	0.334	Antitussive. narcotic	0.315	Ulcer. peptic
	0.334	Membrane integrity antagonist	0.309	Sleep disturbance
	0.334	Histamine release stimulant	0.308	Stomatitis
	0.331	1-Acylglycerol-3-phosphate O-acyltransferase inhibitor	0.307	Dependence
	0.327	Cytoprotectant	0.307	Sedative
	0.327	CYP2C8 inhibitor	0.305	Fasciculation
	0.324	ATP-binding cassette A1 stimulant	0.303	Optic neuropathy
	0.323	5 Hydroxytryptamine release inhibitor	0.301	Piloerection
	0.321	2-Hydroxyquinoline 8-monooxygenase inhibitor		
	0.316	27-Hydroxycholesterol 7alpha-monooxygenase inhibitor		
	0.315	Prion diseases treatment		
	0.312	Antiinflammatory. intestinal		
	0.311	5 Hydroxytryptamine 7 agonist		
	0.310	Phospholipase A2 inhibitor		
	0.310	Antiprotozoal (Leishmania)		
	0.308	Endopeptidase So inhibitor		

	0.307	5 Hydroxytryptamine uptake stimulant		
	0.305	Antiinflammatory		
	0.303	Caspase 8 stimulant		
	0.303	Nicotinic alpha2beta2 receptor antagonist		
	0.303	Pseudolysin inhibitor		
	0.302	CYP2C19 inhibitor		
	0.302	4-Nitrophenol 2-monooxygenase inhibitor		
	0.300	Vanilloid 1 agonist		
53494930	0.497	5 Hydroxytryptamine antagonist	0.479	Yawning
	0.462	Platelet adhesion inhibitor	0.463	Twitching
	0.455	Analgesic	0.416	Sneezing
	0.443	Rhinitis treatment	0.400	Torsades de pointes
	0.431	Acetylcholine neuromuscular blocking agent	0.386	Hyperglycemic
	0.428	Antineurotic	0.380	Parkinsonism
	0.425	Antiallergic	0.374	Palpitation
	0.425	Octopamine antagonist	0.351	Piloerection
	0.420	Ovulation inhibitor	0.348	Postural (orthostatic) hypotension
	0.404	Neurotransmitter antagonist	0.341	Torticollis
	0.389	Antinociceptive	0.326	Dystonia
	0.374	CYP2D2 inhibitor	0.325	Galactorrhea
	0.372	Antihistaminic	0.319	Tremor
	0.369	Histamine antagonist	0.317	Hypothermic
	0.366	Systemic lupus erythematosus treatment	0.316	Akathisia
	0.364	Male reproductive dysfunction treatment	0.315	Psychoses
	0.358	Antitussive. narcotic	0.313	Shivering
	0.354	Cognition disorders treatment	0.312	Euphoria
	0.349	Neurotransmitter uptake inhibitor	0.310	Choreoathetosis
	0.339	Vascular (periferal) disease treatment	0.310	Xerostomia
	0.337	Nicotinic alpha4beta2 receptor antagonist	0.309	Excitability
	0.337	Histamine release stimulant	0.301	Paralysis
	0.330	HIV attachment inhibitor		
	0.327	HERG 1 channel blocker		
	0.323	Benzoin aldolase inhibitor		
	0.323	Alzheimer's disease treatment		
	0.321	MAP kinase stimulant		
	0.318	Heat shock protein 27 antagonist		
	0.316	5 Hydroxytryptamine 2B agonist		
	0.310	Antiasthmatic		
	0.308	4-Nitrophenol 2-monooxygenase inhibitor		

	0.305	Sleep disorders treatment		
	0.304	Antiischemic. cerebral		
11616723	0.499	CYP2C19 inhibitor	0.499	Nail discoloration
	0.497	CYP2J2 substrate	0.485	Tachycardiac
	0.488	HERG 1 channel blocker	0.485	Nephritis
	0.481	Platelet aggregation stimulant	0.483	Necrosis
	0.465	Rhinitis treatment	0.482	Tremor
	0.462	Antiasthmatic	0.480	Interstitial nephritis
	0.453	Antinociceptive	0.479	Pseudoporphyria
	0.452	All-trans-retinyl-palmitate hydrolase inhibitor	0.478	Hepatitis
	0.450	Nicotinic alpha6beta3beta4alpha5 receptor antagonist	0.475	Torsades de pointes
	0.441	Polyporopepsin inhibitor	0.474	Toxic. respiration
	0.437	General pump inhibitor	0.472	Stomatitis
	0.434	Chlordecone reductase inhibitor	0.472	Fibrillation. atrial
	0.434	Gluconate 2-dehydrogenase (acceptor) inhibitor	0.469	Hypothermic
	0.421	Fibrinolytic	0.467	Edema
	0.418	Prostate disorders treatment	0.463	Reproductive dysfunction
	0.418	Pseudolysin inhibitor	0.463	Dizziness
	0.417	Gluconate 5-dehydrogenase inhibitor	0.462	Choreoathetosis
	0.415	Dermatologic	0.462	Cholestasis
	0.415	Platelet adhesion inhibitor	0.462	Dysarthria
	0.409	Glycerol-ether monooxygenase inhibitor	0.458	Sensory disturbance
	0.408	Glycosylphosphatidylinositol phospholipase D inhibitor	0.457	Delirium
	0.407	Electron-transferring-flavoprotein dehydrogenase inhibitor	0.456	Psychoses
	0.407	Ubiquinol-cytochrome-c reductase inhibitor	0.454	Multiple organ failure
	0.400	Histidine kinase inhibitor	0.450	Asthma
	0.400	Trimethylamine-oxide aldolase inhibitor	0.447	Keratopathy
	0.398	27-Hydroxycholesterol 7alpha-monooxygenase inhibitor	0.446	Allergic contact dermatitis
	0.395	Antidyskinetic	0.442	Gastrointestinal hemorrhage
	0.393	CYP2C8 inhibitor	0.442	Retroperitoneal fibrosis
	0.390	Glutamyl endopeptidase II inhibitor	0.435	Akathisia
	0.384	Antiviral (Picornavirus)	0.434	Sleep disturbance
	0.383	5 Hydroxytryptamine release stimulant	0.433	Photoallergy dermatitis
	0.382	Antipruritic	0.432	Neutrophilic dermatosis (Sweet's syndrome)
	0.380	Sulfur reductase inhibitor	0.432	Myoclonus

	0.379	Macrophage colony stimulating factor agonist	0.429	Respiratory impairment
	0.376	Antieczematic atopic	0.429	Thrombophlebitis
	0.376	Nicotinic alpha2beta2 receptor antagonist	0.427	Cyanosis
	0.375	Benzoin aldolase inhibitor	0.426	Inflammation
	0.374	Alkylacetylgllycerophosphatase inhibitor	0.425	Ataxia
	0.372	Amine dehydrogenase inhibitor	0.425	Ocular toxicity
	0.372	Membrane integrity antagonist	0.424	Hypotension
	0.372	Sugar-phosphatase inhibitor	0.423	Respiratory failure
	0.371	Histamine release inhibitor	0.421	Hyperthermic
	0.371	Thioredoxin inhibitor	0.418	Gastrointestinal disturbance
	0.368	Plastoquinol-plastocyanin reductase inhibitor	0.417	Emetic
	0.365	Preneoplastic conditions treatment	0.414	Coma
	0.360	Fusarinine-C ornithinesterase inhibitor	0.413	Fibrosis. interstitial
	0.359	Membrane permeability inhibitor	0.413	Extrapyramidal effect
	0.357	Antitussive. narcotic	0.412	Torticollis
	0.355	Ecdysone 20-monooxygenase inhibitor	0.412	Withdrawal
	0.354	Hydroxylamine oxidase inhibitor	0.410	Dyskinesia
	0.354	Insulin promoter	0.408	Dystonia
	0.352	CYP2C9 substrate	0.401	Hyperglycemic
	0.351	Phosphatidylcholine-retinol O-acyltransferase inhibitor	0.398	Sedative
	0.350	Antiviral (Rhinovirus)	0.395	Dysphoria
	0.348	Nitrate reductase (cytochrome) inhibitor	0.393	Depression
	0.345	Fatty-acyl-CoA synthase inhibitor	0.391	Drowsiness
	0.345	Chymosin inhibitor	0.390	Behavioral disturbance
	0.345	Acrocyllindropepsin inhibitor	0.390	Sialorrhea
	0.345	Saccharopepsin inhibitor	0.389	Apnea
	0.344	Oxidizing agent	0.387	Fasciculation
	0.344	CYP2C18 substrate	0.383	Laryngospasm
	0.344	5 Hydroxytryptamine release inhibitor	0.383	Anorexiant
	0.344	Calcium channel (voltage-sensitive) activator	0.383	Visual acuity impairment
	0.343	Phospholipase A2 inhibitor	0.381	Yawning
	0.343	CYP2F1 substrate	0.380	Chorea
	0.342	Phenol O-methyltransferase inhibitor	0.379	Dependence
	0.341	HIV attachment inhibitor	0.379	Bronchoconstrictor
	0.340	Phospholipase inhibitor	0.378	Cleft palate
	0.340	5 Hydroxytryptamine uptake stimulant	0.378	Urinary retention
	0.336	Protein-S-isoprenylcysteine O-methyltransferase inhibitor	0.375	Hypercholesterolemic
	0.334	Leukotriene-C4 synthase inhibitor	0.373	Nausea

	0.333	Antiviral (Adenovirus)	0.372	Dermatitis
	0.332	Prostaglandin-A1 DELTA-isomerase inhibitor	0.372	Headache
	0.329	Mucomembranous protector	0.371	Acidosis. lactic
	0.328	Urethanase inhibitor	0.368	Hypotonia
	0.323	Glutathione thiolesterase inhibitor	0.365	Acneiform eruption
	0.323	Lysine 2.3-aminomutase inhibitor	0.365	Leukopenia
	0.323	Ovulation inhibitor	0.363	Thrombocytopenia
	0.322	Leukotriene-B4 20-monooxygenase inhibitor	0.361	Pulmonary edema
	0.322	Glucan endo-1.3-beta-D-glucosidase inhibitor	0.359	Hypomagnesemia
	0.320	Monoamine uptake inhibitor	0.359	Splenomegaly
	0.320	Gonadotropin antagonist	0.358	Hypocalcaemic
	0.320	Oxygen scavenger	0.357	Vasopressor
	0.319	CYP4A11 substrate	0.356	Pure red cell aplasia
	0.319	Aspulvinone dimethylallyltransferase inhibitor	0.355	Mydriatic
	0.318	Alkane 1-monooxygenase inhibitor	0.355	Dyspnea
	0.318	CF transmembrane conductance regulator agonist	0.354	Demyelination
	0.317	Omptin inhibitor	0.353	Neurotoxic
	0.315	Octopamine antagonist	0.349	Ulcer. gastric
	0.308	Caspase 8 stimulant	0.349	Skin irritation. corrosive
	0.308	Antiinflammatory	0.348	Cardiodepressant
	0.308	Testosterone 17beta-dehydrogenase (NADP+) inhibitor	0.347	Porphyria
	0.307	CYP2C29 substrate	0.345	Hypomania
	0.306	Tryptophan 2.3-dioxygenase inhibitor	0.345	Irritation
	0.306	NADPH-cytochrome-c2 reductase inhibitor	0.343	Bullous pemphigoid
	0.305	Ribulose-phosphate 3-epimerase inhibitor	0.342	Hypnotic
	0.304	FMO3 substrate	0.340	Pneumotoxic
	0.303	Acetylesterase inhibitor	0.339	Hypothermic
	0.303	Insulysin inhibitor	0.336	Fibrillation. atrial
	0.302	CYP2C9 inducer	0.335	Delirium
	0.302	Erythropoiesis stimulant	0.335	Torticollis
	0.301	Chloride channel blocker	0.335	Chorea
	0.301	Intermittent claudication treatment	0.335	Reproductive dysfunction
	0.300	Venombin AB inhibitor	0.333	Weakness
			0.332	Sneezing
			0.331	Muscle weakness
			0.330	Torsades de pointes
			0.330	Sweating
			0.329	Tremor

			0.328	Urinary retention
			0.328	Dizziness
			0.325	Xerostomia
			0.325	Hypotonia
			0.322	Bradycardic
			0.321	Ataxia
			0.320	Extrapyramidal effect
			0.320	Paralysis
			0.320	Acidosis
			0.319	Allergic contact dermatitis
			0.318	Laryngospasm
			0.317	Photoallergy dermatitis
			0.315	Retroperitoneal fibrosis
			0.315	Edema
			0.312	Sensory disturbance
			0.310	Conjunctivitis
			0.307	Keratopathy
			0.304	Sleep disturbance
			0.304	Hepatitis
			0.302	Euphoria
			0.302	Myocarditis
			0.300	Cholestasis
11493740	0.492	Antiasthmatic	0.499	Euphoria
	0.486	Gastrin inhibitor	0.481	Hypercholesterolemic
	0.463	Antinociceptive	0.480	Myoclonus
	0.448	Calcium channel (voltage-sensitive) activator	0.461	Weakness
	0.446	CYP2H substrate	0.456	Allergic contact dermatitis
	0.444	Polyporopepsin inhibitor	0.449	Conjunctivitis
	0.442	CYP2C18 substrate	0.448	Gastrointestinal hemorrhage
	0.435	Chymosin inhibitor	0.440	Acidosis
	0.435	Acrocylindropepsin inhibitor	0.434	Fibrillation. atrial
	0.435	Saccharopepsin inhibitor	0.431	Hypotension
	0.431	Acetylcholine neuromuscular blocking agent	0.427	Dysarthria
	0.424	Fibrinolytic	0.425	Bradycardic
	0.413	Antidyskinetic	0.424	Photoallergy dermatitis
	0.413	CYP2C8 inhibitor	0.418	Akathisia
	0.409	Amine dehydrogenase inhibitor	0.408	Hypotonia
	0.404	Prostate disorders treatment	0.406	Depression
	0.403	Rhinitis treatment	0.405	Muscle weakness
	0.402	Platelet aggregation stimulant	0.402	Tremor

	0.397	Platelet adhesion inhibitor	0.399	Dizziness
	0.392	Gonadotropin antagonist	0.394	Edema
	0.391	Sulfur reductase inhibitor	0.386	Tachycardiac
	0.389	Plastoquinol-plastocyanin reductase inhibitor	0.383	Laryngospasm
	0.388	Benzoin aldolase inhibitor	0.382	Paralysis
	0.380	Antiviral (Rhinovirus)	0.381	Weight gain
	0.377	1-Acylglycerol-3-phosphate O-acyltransferase inhibitor	0.378	Dysphoria
	0.377	Histamine release stimulant	0.378	Sneezing
	0.368	Antieczematic atopic	0.377	Hypomania
	0.367	Glycerol-ether monooxygenase inhibitor	0.377	Fibrosis. interstitial
	0.367	Antiviral (Picornavirus)	0.372	Xerostomia
	0.364	Antiprotozoal (Leishmania)	0.371	Reproductive dysfunction
	0.364	Antipruritic	0.366	Ulcer. gastric
	0.361	Ovulation inhibitor	0.365	Yawning
	0.360	Membrane integrity antagonist	0.364	Nephritis
	0.359	MAP kinase stimulant	0.363	Retroperitoneal fibrosis
	0.353	Caspase 8 stimulant	0.363	Cyanosis
	0.353	Ubiquinol-cytochrome-c reductase inhibitor	0.361	Sensory disturbance
	0.353	Nicotinic alpha6beta3beta4alpha5 receptor antagonist	0.360	Necrosis
	0.350	Fructose 5-dehydrogenase inhibitor	0.359	Delirium
	0.346	Leukotriene-C4 synthase inhibitor	0.356	Cholestasis
	0.342	Steroid N-acetylglucosaminyltransferase inhibitor	0.356	Toxic. respiration
	0.340	Dermatologic	0.351	Ulcer. peptic
	0.338	Intermittent claudication treatment	0.351	Inflammation
	0.338	CYP2D6 substrate	0.350	Dystonia
	0.337	ATP-binding cassette A1 stimulant	0.348	Palpitation
	0.337	Mucomembranous protector	0.348	Hepatitis
	0.335	5 Hydroxytryptamine 7 agonist	0.347	Galactorrhea
	0.333	Caspase 3 stimulant	0.344	Ocular toxicity
	0.333	Carboxypeptidase Taq inhibitor	0.342	Piloerection
	0.331	Pin1 inhibitor	0.342	Visual acuity impairment
	0.331	Mucositis treatment	0.338	Interstitial nephritis
	0.330	Sigma receptor agonist	0.333	Dependence
	0.327	Phospholipase A2 inhibitor	0.332	Optic neuropathy
	0.326	Antinephritic	0.331	Torticollis
	0.325	Monoamine uptake inhibitor	0.328	Sleep disturbance
	0.325	CYP2C9 substrate	0.325	Urinary retention

	0.324	2-Hydroxyquinoline 8-monooxygenase inhibitor	0.323	Fasciculation
	0.324	Fusarinine-C ornithinesterase inhibitor	0.321	Stomatitis
	0.323	HIV attachment inhibitor	0.317	Toxic. vascular
	0.323	CYP2C19 inhibitor	0.314	Psychoses
	0.323	5 Hydroxytryptamine release inhibitor	0.311	Asthma
	0.322	Antitussive. narcotic	0.310	Coma
	0.322	Cytoprotectant	0.307	Sedative
	0.321	CYP4A substrate	0.307	Optic neuritis
	0.318	Phospholipase inhibitor	0.304	Psychomotor impairment
	0.318	Endopeptidase So inhibitor	0.304	Sialorrhea
	0.317	Vanilloid 1 agonist	0.303	Apnea
	0.317	Prion diseases treatment	0.300	Ataxia
	0.317	27-Hydroxycholesterol 7alpha-monooxygenase inhibitor		
	0.316	5 Hydroxytryptamine 2B agonist		
	0.316	CYP2D substrate		
	0.312	15-Hydroxyprostaglandin-D dehydrogenase (NADP+) inhibitor		
	0.308	CYP1A2 inhibitor		
	0.308	CYP2J2 substrate		
	0.307	CYP1A inhibitor		
	0.307	Lactase inhibitor		
	0.306	Feruloyl esterase inhibitor		
	0.306	Membrane permeability inhibitor		
	0.304	4-Nitrophenol 2-monooxygenase inhibitor		
	0.302	HERG 1 channel blocker		
	0.300	Lysyl oxidase inhibitor		
53394099	0.493	5 Hydroxytryptamine antagonist	0.499	Sweating
	0.466	Fibrinolytic	0.457	Excitability
	0.461	CYP2H substrate	0.447	Twitching
	0.460	General pump inhibitor	0.413	Akathisia
	0.457	Antinociceptive	0.408	Torsades de pointes
	0.450	Antieczematic	0.398	Withdrawal
	0.437	Male reproductive dysfunction treatment	0.387	Shivering
	0.423	Heat shock protein 27 antagonist	0.387	Tremor
	0.402	Pin1 inhibitor	0.370	Respiratory impairment
	0.400	HIV attachment inhibitor	0.363	Yawning
	0.399	MAP kinase stimulant	0.361	Urinary retention
	0.397	Mediator release inhibitor	0.360	Piloerection
	0.396	Prostate disorders treatment	0.342	Palpitation

	0.388	Rhinitis treatment	0.341	Laryngospasm
	0.387	Neurotransmitter uptake inhibitor	0.337	Photoallergy dermatitis
	0.376	Cardiovascular analeptic	0.334	Dizziness
	0.372	Benzoin aldolase inhibitor	0.333	Depression
	0.368	5 Hydroxytryptamine 2B agonist	0.323	Gastrointestinal hemorrhage
	0.367	Sigma receptor agonist	0.319	Paralysis
	0.364	Calcium channel (voltage-sensitive) activator	0.316	Tachycardiac
	0.356	Neuropeptide Y2 antagonist	0.311	Conjunctivitis
	0.349	Chlordecone reductase inhibitor	0.307	Myoclonus
	0.348	Antitussive, narcotic	0.307	Xerostomia
	0.348	Aspulvinone dimethylallyltransferase inhibitor	0.305	Sensory disturbance
	0.343	Octopamine antagonist	0.499	Sweating
	0.339	Histamine release stimulant		
	0.334	Dermatologic		
	0.333	Spasmolytic, urinary		
	0.333	Platelet adhesion inhibitor		
	0.328	Caspase 3 stimulant		
	0.326	Nicotinic alpha4beta4 receptor agonist		
	0.320	Antiviral (Picornavirus)		
	0.319	Antieczematic atopic		
	0.315	Antiviral (Rhinovirus)		
	0.310	27-Hydroxycholesterol 7alpha-monooxygenase inhibitor		
	0.309	4-Nitrophenol 2-monooxygenase inhibitor		
	0.308	Chloride channel blocker		
	0.303	Thromboxane B2 antagonist		