

Journal of Pharmacology and Experimental Therapeutics

Molecular Determinants of Ligand Selectivity for the Human Multidrug And Toxin Extrusion Proteins, MATE1 and MATE-2K

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Supplemental Table 1. Compounds selected by the common features pharmacophore after searching a database of 2690 FDA approved compounds (www.collaboratedrug.com).

FitValue	Common Name	Indication
3.93897	PYRIMETHAMINE	Antimalarial
3.3167	naloxone Naloxone Hydrochloride	Antidote
3.27622	DEXMEDETOMIDINE	Anxiolytic
3.2407	Chlordantoin	Antifungal
3.1776	NALORPHINE Nalorphine Hydrochloride	Antidote
3.15108	Perfosfamide	Antineoplastic
3.11759	Cinchonidine Sulfate Cinchonidine	Antimalarial
3.10352	Cinchonine Sulfate Cinchonine	Antimalarial
3.07469	METHOHEXITAL	Anesthetic
3.06799	PROGUANIL PROGUANIL HYDROCHLORIDE 100MG	Antimalarial
3.05018	TOPIRAMATE	Anticonvulsant
3.04366	MIDODRINE Midodrine Hydrochloride	Antihypertensive
2.98558	Chlorbetamide	Antiamebic
2.98463	TRIMETHOPRIM	Antibiotic Antibacterial
2.98457	ZILEUTON	Antiinflammatory
2.94205	AMINOMETRADINE	Diuretic
2.89284	SCOPOLAMINE ScopolamineHydrobromide	Antispasmodic

2.88791	ARTICAINE	Anesthetic
2.84534	RITODRINE	Tocolytic
2.82357	MITOBRONITOL Mitolactol	Antineoplastic
2.81033	LORAZEPAM	Anxiolytic
2.74943	ETHOHEXADIOL	Insecticide
2.64902	METHOXAMINE Methoxamine Hydrochloride	Antihypotensive
2.63216	URACIL MUSTARD	Antineoplastic
2.62879	SECOBARBITAL secobarbital sodium	Sedative
2.62336	Methitural	Sedative
2.6233	THIAMYLAL	Anesthetic
2.62264	METHYLDOPATE Methyldopate Hydrochloride	Antiseptic
2.59665	ISOCARBOXAZID	Antidepressant
2.5942	FAMOTIDINE	Antiulcerative
2.57673	Peldesine	Antineoplastic
2.55252	vorinostat	Antineoplastic
2.53092	OXYBENZONE	Dermatologic
2.50659	Dichlorophen Dichlorophene	Anthelminthic
2.44664	Oxamide	Anxiolytic
2.42605	QUINIDINE GLUCONATE	Antimalarial
2.42605	QUINIDINE POLYGALACTURONATE 275MG Quinidine Polygalacturonate	Antimalarial
2.42594	NIALAMIDE	Antidepressant
2.42406	PENTOBARBITAL	Sedative
2.41611	THIOPENTAL Thiopental Sodium	Anesthetic
2.40768	ETHAMBUTOL Ethambutol Hydrochloride	Antibacterial

2.37852	Dioxybenzone	Dermatologic
2.37222	Ubiquinol	
2.35757	QUINETHAZONE	Diuretic
2.34956	TRICHLORMETHIAZIDE	Diuretic
2.30659	EFAVIRENZ	Antiviral
2.30277	IMIQUIMOD	Antiviral
2.28689	DIHYDROCODEINE	
2.28689	DihydrocodeineBitartrate	Analgesic
2.25638	PHENTOLAMINE Phentolamine Hydrochloride	Antihypertensive
2.25153	CARISOPRODOL	Muscle relaxant (skeletal)
2.24775	STAVUDINE	Antiviral
2.23961	NEPAFENAC	Antiinflammatory
2.19761	2-cyano-3-hydroxy-N-[4-(trifluoromethyl)phenyl]hept-6-ynamide (2Z)-2-cyano-3-hydroxy-N-[4-(trifluoromethyl)phenyl]-2-hepten-6-ynamide	
2.19309	ALKANET	Antiseptic
2.18273	CODEINE	Antitussive
2.18273	Codeine Phosphate	Antitussive
2.16503	MEFENAMIC ACID	Antiinflammatory
2.15091	OXPRENOLOL oxprenolol hydrochloride	Antihypertensive
2.15023	TROPICAMIDE	Mydriatic Ophthalmic
2.13938	Meclofenamic Acid MECLOFENAMATE Meclofenamate Sodium	Antiinflammatory
2.1224	Iopydol	Diagnostic aid
2.10354	Brivaracetam	Nootropic
2.07716	Remacemide Remacemide Hydrochloride	Anticonvulsant
2.02021	Almecillin	Antibiotic

2.00987	HYDROXYPHENAMATE	Anxiolytic
2.00066	CIMETIDINE	Antiulcerative
1.97202	ABACAVIR Abacavir Sulfate	Antiviral
1.95059	Modafinil Armodafinil	Nootropic
1.85633	IFOSFAMIDE	Antineoplastic
1.84656	TYBAMATE	Anxiolytic
1.841	MEPROBAMATE	Sedative
1.82933	CHLORTHALIDONE	Diuretic
1.82785	Vinbarbital	Sedative
1.82602	ISOETHARINE IsoetharineMesylate	Bronchodilator
1.76184	morphine sulfate Morphine sulfate concentrate (preservative free)	
1.76184	MORPHINE Morphine Hydrochloride	Analgesic
1.73457	ACRISORCIN	Antifungal
1.73457	HEXYLRESORCINOL	Anthelminthic
1.72351	CICLOPIROX OLAMINE	Antifungal
1.72233	CICLOPIROX	Antifungal
1.6687	METHYCLOTHIAZIDE	Diuretic
1.66708	RAMELTEON	Anxiolytic
1.59483	METHOCARBAMOL	Muscle relaxant Muscle relaxant (skeletal)
1.58606	AMOBARBITAL Amobarbital Sodium	Sedative
1.54448	ETHOTOIN	Anticonvulsant. Anticonvulsant
1.53768	TALBUTAL	Sedative
1.48706	PHENYRAMIDOL Phenylramidol Hydrochloride	Analgesic

1.46098	MAZINDOL	Anorexic
1.42678	ETHYL VANILLATE NG Ethyl Vanillate	Antiseptic
1.39667	VILOXAZINE Viloxazine Hydrochloride	Antidepressant
1.38498	Methylphenidate DEXMETHYLPHENIDATE Dexmethylphenidate Hydrochloride	Nootropic
1.34472	TRAMADOL Tramadol hydrochloride	Analgesic
1.3286	1,3-DIMETHYLBUTYL SALICYLATE 5.0% 1,3 Dimethylbutyl Salicylate	Antiinflammatory
1.32048	OXAZEPAM	Anxiolytic
1.29591	MELPHALAN	Antineoplastic
1.29194	Allobarbitol	Sedative
1.27263	FUROSEMIDE	Diuretic
1.25673	OXCARBAZEPINE	Anticonvulsant
1.25425	GUAIFENESIN	Expectorant
1.23631	BUTALBITAL	Sedative
1.20772	DEZOCINE	Analgesic
1.17107	LEVETIRACETAM Etiracetam	Anticonvulsant
1.13128	CYCLOPHOSPHAMIDE	Antineoplastic
0.994299	CARBAMAZEPINE	Anticonvulsant
0.990726	LEFLUNOMIDE	Antirheumatic
0.966053	PRAMIPEXOLE	Antiparkinsonian
0.920325	BUTABARBITAL	Sedative
0.834914	ALOSETRON Alosetron Hydrochloride	Antidiarrheal
0.813755	ETHAMIVAN	Nootropic
0.808493	HEXYLCAINE	Anesthetic

	Hexylcaine Hydrochloride	
0.781187	Lofexidine Hydrochloride Lofexidine	Antihypertensive
0.713663	METHALLATAL 0.15GM Methallatal	Antiemetic
0.696448	MONOCTANOIN Monoctanoïn	Anticholelithogenic
0.633994	BENZOIN TINCTURE, COMPOUND 0.5OZ" BENZOIN Benzoin Tincture Bitter Tincture	Antiseptic Therapeutic plant extract
0.612587	MEBUTAMATE	Antihypertensive
0.596225	DICLOFENAC Diclofenac Sodium	Antiinflammatory
0.446284	HEPTABARBITAL	Sedative
0.441581	PHENPROCOUMON	Anticoagulant
0.392467	GALANTAMINE	Nootropic
0.27683	HOMATROPINE	Mydriatic
0.27683	HomatropineHydrobromide	Mydriatic
0.262311	APROBARBITAL	Sedative
0.249796	BROMFENAC Bromfenac Sodium	Antiinflammatory
0.073764	Metabutethamine Hydrochloride Metabutethamine	Anesthetic
0.043867	GLUTETHIMIDE	Sedative