

A PREDICTIVE LIGAND-BASED BAYESIAN MODEL FOR HUMAN DRUG INDUCED LIVER INJURY

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Drug Metabolism and Disposition

Supplemental Table 1

Training set

Chemical Name	Formula	PubChem_CID	DILI_Bins_Binary *
1,2,3,4,5,6-hexachlorocyclohexane	C6H6Cl6	727	1
3-Acetamidophenol (AMAP)	C8H9NO2	12,124	0
Acetaminophen	C8H9NO2	1,983	1
Acetazolamide	C4H6N4O3S2	1,986	1
Acetohexamide	C15H20N2O4S	1,989	1
Acetylcholine Chloride	C7H16ClNO2	187	0
Acitretin	C21H26O3	5,284,513	1
acivicin	C5H7ClN2O3	294,641	0
Adenosine	C10H13N5O4	60,961	0
Albendazole	C12H15N3O2S	2,082	1
Allopurinol	C5H4N4O	2,094	1
Alloxan Hydrate	C4H4N2O5	312,231	0
Amantadine HCl	C10H18ClN	2,130	0
Amiloride HCl	C6H9Cl2N7O	16,231	0
Aminobenzoate Potassium	C7H6KNO2	978	0
Aminoglutethimide	C13H16N2O2	2,145	0
Aminosalicylic Acid	C7H7NO3	4,649	1
amiodarone	C25H29I2NO3	2,157	1
Amitriptyline HCl	C20H24ClN	2,160	0
ammonium chloride	H4ClN	22,985	0
amoxapine	C17H16ClN3O	2,170	0
Amrinone	C10H9N3O	3,698	1
Amsacrine HCl	C21H20ClN3O3S	2,179	1
Ascorbate	C6H8O6	235	0
Aspirin	C9H8O4	2,244	0
Astemizole	C28H31FN4O	2,247	0

Atenolol	C14H22N2O3	2,249	0
atractyloside	C30H44K2O16S2	5,702,200	1
Azaserine	C5H7N3O4	5,284,344	1
Azathioprine	C9H7N7O2S	2,265	1
Aztreonam (Z-isomer)	C13H17N5O8S2	5,742,832	0
Bacitracin	C66H103N17O16S	6,474,109	0
Bambuterol	C18H29N3O5	54,766	0
Beclomethasone Dipropionate	C28H37ClO7	20,469	0
Benazepril	C24H28N2O5	5,362,124	0
Benzbromarone	C17H12Br2O3	2,333	1
Bepridil HCl	C24H35ClN2O	2,351	1
Betahistine DiHCl	C8H14Cl2N2	2,366	1
Betamethasone	C22H29FO5	9,782	0
Bezafibrate	C19H20ClNO4	39,042	0
Bicalutamide	C18H14F4N2O4S	56,069	1
Biotin	C10H16N2O3S	171,548	0
Brompheniramine Maleate	C20H23BrN2O4	6,834	0
Bumetanide	C17H20N2O5S	2,471	1
Bupivacaine	C18H31ClN2O2	2,474	0
Bupropion HCl	C13H19Cl2NO	444	0
Busulphan	C6H14O6S2	2,478	1
cadmium chloride	CdCl2	176	1
Calcium Pantothenate	C18H32CaN2O10	6,109	0
Captopril	C9H15NO3S	44,093	1
carbendazim	C9H9N3O2	25,429	1
Carbenoxolone Disodium	C34H48Na2O7	6,419,769	0
Carbidopa	C10H14N2O4	34,359	0
Cefoperazone Dihydrate	C25H31N9O10S2	6,420,003	0
Chenodiol	C24H40O4	10,133	1
Chloramphenicol Palmitate	C27H42Cl2N2O6	5,959	1
Chlorpheniramine Maleate	C20H23ClN2O4	2,725	1
chlorpromazine	C17H19ClN2S	2,726	1
Chlortetracycline HCl	C22H24Cl2N2O8	5,280,963	1
Chlorzoxazone	C7H4ClNO2	2,733	1
Ciclopirox	C12H17NO2	38,911	0
Cimetidine	C10H16N6S	2,756	0
Ciprofibrate	C13H14Cl2O3	2,763	1
Ciprofloxacin HCl	C17H19ClFN3O3	2,764	1

Flupenthixol	C23H25F3N2OS	5,281,881	0
Cisapride	C23H29ClFN3O4	2,769	0
citalopram	C20H21FN2O	2,771	0
Cladribine	C10H12ClN5O3	20,279	0
clinafloxacin	C17H17ClFN3O3	60,063	0
Clomiphene Citrate	C32H36ClNO8	3,033,832	1
Clomipramine	C19H23ClN2	2,801	1
Clonidine HCl	C9H10Cl3N3	2,803	1
Clotrimazole	C22H17ClN2	2,812	0
Clozapine	C18H19ClN4	2,818	1
Colchicine	C22H25NO6	6,167	0
Cromolyn	C23H16O11	2,882	0
Cyanocobalamin	C63H88CoN14O14P	5,460,135	0
Cyclophosphamide	C7H15Cl2N2O2P	2,907	1
cyclosporin A	C62H111N11O12	5,284,373	1
Cyproheptadine HCl	C21H22ClN	2,913	1
Cyproterone acetate	C24H29ClO4	5,284,537	1
Danazol	C22H27NO2	28,417	1
Dantrolene Sodium	C14H9N4NaO5	9,568,637	1
Dapsone	C12H12N2O2S	2,955	1
Deferoxamine Mesylate	C26H52N6O11S	2,973	1
Demeclocycline HCl	C21H22Cl2N2O8	5,281,008	1
desipramine	C18H22N2	2,995	0
Dexamethasone	C22H29FO5	5,743	0
Dextromethorphan HBr	C18H26BrNO	5,360,696	0
d-galactosamine	C6H13NO5	24,154	1
Didanosine	C10H12N4O3	50,599	1
Diethylcarbamazine	C10H21N3O	3,052	1
Diflunisal	C13H8F2O3	3,059	1
Digoxin	C41H64O14	30,322	0
diltiazem HCl	C22H27ClN2O4S	62,920	0
Diphenhydramine HCl	C17H22ClNO	3,100	0
Disopyramide Phosphate	C21H32N3O5P	107,858	1
Dobutamine HCl	C18H24ClNO3	36,811	0
Donepezil	C24H29NO3	3,152	0
Dopamine	C8H11NO2	681	0
Doxycycline hyclate	C46H58Cl2N4O18	5,281,011	1
Edrophonium Chloride	C10H16ClNO	3,202	0

Ergocalciferol	C28H44O	5,280,793	0
Ergonovine Maleate	C23H27N3O6	6,437,065	0
erythromycin	C37H67NO13	12,560	0
Erythromycin estolate (1)	C52H97NO18S	12,560	1
Eserine	C15H21N3O2	5,983	0
estradiol	C18H24O2	5,991	0
estradiol 17b glucuronide	C24H32O8	66,424	1
Estrone	C18H22O2	9,919	1
Ethinodiol Diacetate	C24H32O4	6,432,306	1
Etoposide	C29H32O13	36,462	1
Famotidine	C8H15N7O2S3	3,325	0
FCCP	C10H5F3N4O	3,330	1
Felbamate	C11H14N2O4	3,331	1
Fenofibrate	C20H21ClO4	3,339	1
Fenoprofen Sodium	C15H13NaO3	3,342	1
Fenoterol HBr	C17H22BrNO4	3,343	1
Flecainide Acetate	C19H24F6N2O5	41,022	1
Floxuridine	C9H11FN2O5	5,790	1
Fluconazole	C13H12F2N6O	3,365	1
Flucytosine	C4H4FN3O	3,366	1
Fludrocortisone Acetate	C23H31FO6	5,875	0
Flumazenil	C15H14FN3O3	3,373	0
fluoxetine	C17H18F3NO	3,386	0
Flurbiprofen	C15H13FO2	3,394	1
Flutamide	C11H11F3N2O3	3,397	1
Fluvastatin	C24H26FNO4	5,281,101	0
fluvoxamine	C15H21F3N2O2	5,324,346	1
Folate	C19H17N7O6	6,037	0
Furazolidone	C8H7N3O5	5,323,714	1
Furosemide	C12H11ClN2O5S	3,440	1
Gabapentin	C9H17NO2	3,446	0
Gallamine Triethiodide	C30H60I3N3O3	6,172	0
Gallium Nitrate Hydrate	H2GaN3O10	61,635	0
gatifloxacin	C19H22FN3O4	5,379	0
Gemfibrozil	C15H22O3	3,463	1
Glafenine	C19H17ClN2O4	3,474	1
Gliclazide	C15H21N3O3S	3,475	0
Glimepiride	C24H34N4O5S	3,476	0

Griseofulvin	C17H17ClO6	441,140	1
Hycanthone	C20H24N2O2S	3,634	1
Hydrochlorothiazide	C7H8ClN3O4S2	3,639	1
Hydrocortisone	C21H30O5	26,133	0
Hydroxyurea	CH4N2O2	3,657	1
Idarubicin HCl	C26H28ClNO9	107,865	0
Idoxuridine	C9H11N2O5	5,905	1
Imipramine HCl	C19H25ClN2	3,696	1
indomethacin	C19H16ClNO4	3,715	1
isoniazid	C6H7N3O	3,767	1
Isoproterenol HCl	C11H18ClNO3	3,779	0
Isotretinoin	C20H28O2	444,795	1
Isoxsuprine HCl	C18H24ClNO3	3,783	0
Kanamycin Sulfate	C18H38N4O15S	441,374	0
Ketorolac Tromethamine	C19H24N2O6	3,826	1
Ketotifen	C19H19NOS	3,827	0
Labetalol	C19H24N2O3	3,869	1
Lamivudine	C8H11N3O3S	60,825	0
L-arginine	C6H14N4O2	6,322	0
Leflunomide	C12H9F3N2O2	3,899	1
L-Ethionine	C6H13NO2S	25,674	1
Levodopa	C9H11NO4	6,047	0
levofloxacin	C18H20FN3O4	149,096	0
Lidocaine	C14H22N2O	3,676	0
Lisinopril	C21H31N3O5	5,362,119	1
Lithocholic acid	C24H40O3	9,903	1
Lomefloxacin HCl	C17H20ClF2N3O3	3,948	1
Loperamide HCl	C29H34Cl2N2O2	3,955	0
Lovastatin	C24H36O5	53,232	0
maleic acid	C4H4O4	21,954	1
Maprotiline	C20H23N	4,011	0
Mebendazole	C16H13N3O3	4,030	1
Meclofenamate Sodium	C14H12Cl2NNaO3	4,037	1
Medroxyprogesterone Acetate	C24H34O4	5,702,080	0
Mefenamic Acid	C15H15NO2	4,044	1
Melatonin	C13H16N2O2	896	0
Memantine	C12H21N	4,054	0
Mercaptopurine	C5H4N4S	667,490	1

Mesoridazine Besylate	C27H32N2O4S3	4,078	1
Metaproterenol Sulfate	C22H36N2O10S	4,086	1
Methacycline HCl	C22H23ClN2O8	5,281,092	1
Methicillin Sodium	C17H19N2NaO6S	23,689,098	1
Methimazole	C4H6N2S	1,349,907	1
Methotrexate	C20H22N8O5	126,941	1
Methoxamine HCl	C11H18ClNO3	6,082	0
Methylergonovine Maleate	C24H29N3O6	8,226	0
Methysergide Maleate	C21H27N3O2	9,681	0
Metoclopramide HCl	C14H23Cl2N3O2	4,168	1
Metronidazole	C6H9N3O3	4,173	1
Mexiletine HCl	C11H18ClNO	21,467	1
Miconazole	C18H14Cl4N2O	4,189	0
Mitoxantrone diHCl	C22H30Cl2N4O6	4,212	1
Molindone HCl	C16H25ClN2O2	23,897	1
Monocrotaline	C16H23NO6	104,764	1
montelukast	C35H36ClNO3S	5,281,040	0
Nadolol	C17H27NO4	39,147	0
Nalidixic Acid	C12H12N2O3	4,421	1
Nalmefene	C21H25NO3	5,284,594	0
Naltrexone	C20H23NO4	5,360,515	1
Niacin	C6H5NO2	938	1
Nicardipine HCl	C26H30ClN3O6	4,474	1
Nifedipine	C17H18N2O6	4,485	1
Nimesulide	C13H12N2O5S	4,495	1
Nimodipine	C21H26N2O7	4,497	1
Nisoldipine	C20H24N2O6	4,499	0
Nocodazole	C14H11N3O3S	4,122	0
nomifensine	C16H18N2	4,528	1
Norethindrone	C20H26O2	6,230	1
Norgestrel	C21H28O2	5,991	1
Nortriptyline HCl	C19H22ClN	4,543	1
Novobiocin	C31H36N2O11	4,546	1
Orphenadrine Citrate	C24H31NO8	4,601	0
oxybendazole	C12H15N3O3	4,622	1
Oxybutynin HCl	C22H32ClNO3	4,634	0
Oxyphenonium	C21H34NO3	5,749	0
Pamidronate	C3H9NNa2O7P2	73,351	0

Paromomycin Sulfate	C23H47N5O18S	165,580	0
Paroxetine	C19H20FNO3	43,815	0
p-bromophenol	C6H5BrO	7,808	1
Penicillin G Sodium	C16H17N2NaO4S	2,349	1
Perhexilene	C19H35N	4,746	1
Phenacetin	C10H13NO2	4,754	1
Phenazopyridine HCl	C11H12ClN5	4,756	1
phenelzine	C8H12N2	61,100	0
Phenoxybenzamine HCl	C18H23Cl2NO	4,768	0
Phentolamine Mesylate	C18H23N3O4S	91,430	1
Phenylbutazone	C19H20N2O2	4,781	1
Phenylpropanolamine HCl	C9H14ClNO	26,934	0
phenytoin	C15H12N2O2	1,775	1
Pilocarpine	C11H16N2O2	5,910	0
Pinacidil	C13H21N5O	4,826	0
Pindolol	C14H20N2O2	4,828	0
Piroxicam	C15H13N3O4S	5,280,452	1
potassium dichromate	Cr2K2O7	8,232	1
Praziquantel	C19H24N2O2	4,891	0
Prednisone	C21H26O5	5,865	0
Primaquine Phosphate	C15H27N3O9P2	4,908	0
Primidone	C12H14N2O2	4,909	0
Procarbazine HCl	C12H20ClN3O	4,915	1
Progesterone	C21H30O2	12,419	1
Promazine HCl	C17H21ClN2S	4,926	0
Promethazine HCl	C17H21ClN2S	4,927	0
Propafenone HCl	C21H28ClNO3	4,932	0
Pseudoephedrine HCl	C10H16ClNO	7,028	0
puromycin	C22H29N7O5	4,984	1
Pyrazinamide	C5H5N3O	1,046	1
Pyridostigmine Bromide	C9H13BrN2O2	4,991	0
Pyridoxine	C8H11NO3	1,054	0
Pyrimethamine	C12H13ClN4	4,993	1
Quinapril	C25H30N2O5	54,892	1
quinidine	C20H24N2O2	11,069	1
quinine	C20H24N2O2	8,549	1
raloxifene	C28H27NO4S	5,035	0
ranitidine	C13H22N4O3S	3,001,055	0

Retinoic Acid	C20H28O2	444,795	1
Ribavirin	C8H12N4O5	37,542	0
Riluzole	C8H5F3N2OS	5,070	1
Risperidone	C23H27FN4O2	5,073	1
Sertraline	C17H17Cl2N	68,617	0
Simvastatin	C25H38O5	54,454	0
Sorbitol	C6H12O6	5,780	0
Spironolactone	C24H32O4S	5,833	1
Stavudine	C10H12N2O4	18,283	1
Streptomycin Sulfate	C21H41N7O16S	19,649	0
Sulfasalazine	C18H14N4O5S	5,353,980	1
Sulindac	C20H17FO3S	1,548,887	1
Sumatriptan	C14H21N3O2S	5,358	0
tacrine	C13H14N2	1,935	0
tamoxifen	C26H29NO	2,733,526	1
telmisartan	C33H30N4O2	65,999	0
Temozolomide	C6H6N6O2	5,394	0
terfenadine	C32H41NO2	5,405	0
Tetracaine HCl	C15H25ClN2O2	8,695	0
tetracycline	C22H24N2O8	5,497,101	1
thioacetamide	C2H5NS	2,723,949	1
Thioguanine	C5H5N5S	2,723,601	1
Thiothixene	C23H29N3O2S2	941,651	0
tianeptine	C21H25ClN2O4S	68,870	1
Ticlopidine	C14H14ClNS	5,472	1
Timolol Maleate	C17H28N4O7S	5,478	1
Tolmetin	C15H15NO3	5,509	1
Tranylcypromine HCl	C9H12ClN	19,493	0
Trazodone HCl	C19H23Cl2N5O	5,533	1
trifluoperazine	C21H24F3N3S	5,566	1
Trimethadione	C6H9NO3	5,576	1
Trovafloxacin	C20H15F3N4O3	483,952	1
Ursodeoxycholic acid	C24H40O4	31,401	0
Vancomycin	C66H75Cl2N9O24	444,193	1
Vidarabine	C10H15N5O5	21,704	0
Warfarin	C19H16O4	6,691	0
Zafirlukast	C31H33N3O6S	5,717	1
Zalcitabine	C9H13N3O3	24,066	0

Zidovudine	C10H13N5O4	35,370	1
Zileuton	C11H12N2O2S	60,490	1
Zomepirac	C15H14ClNO3	5,733	0

Test set

Chemical Name	Formula	PubChem_CID	DILI_Bins_Binary *
sudoxicam	C13H11N3O4S2		1
meloxicam	C14H13N3O4S2		0
olmesartan	C29H30N6O6		0
celecoxib	C17H14F3N3O2S		1
lapatinib	C29H26ClFN4O4S		1
gefitinib	C22H24ClFN4O3		1
6-mercaptopurine	C5H4N4S		1
Abacavir	C14H18N6O		1
Acenocoumarol	C19H15NO6		1
Acetylcysteine	C5H9NO3S		0
Aclarubicin HCl	C42H54ClNO15		0
adriamycin	C27H30ClNO11		0
aflatoxin B1	C17H12O6		1
Allyl alcohol	C3H6O		1
allyl formate	C4H6O2		1
alpidem	C21H23Cl2N3O		1
Amineptine HCl	C22H28ClNO2		1
Aminocaproic Acid	C6H13NO2		0
Amodiaquine HCl	C20H23Cl2N3O		1
Amoxicillin	C16H19N3O5S		0
Amphotericin B	C47H73NO17		0
Ampicillin Sodium	C16H18N3NaO4S		0
Anileridine HCl	C22H29ClN2O2		0
ANIT (1-Naphthyl isothiocyanate)	C11H7NS		1
Arsenic Trioxide	As2O3		1
atomoxetine	C17H21NO		1
Auranofin	C19H32AuO9PS		1
Aurothioglucose	C6H11AuO5S		1
aurothiolamate	C4H3AuNa2O4S		1
Azacytidine	C8H12N4O5		1
Azatadine Maleate	C24H26N2O4		1
Azlocillin Sodium	C20H22N5NaO6S		0

BEA (bromoethanamine)	C2H6BrN	1
benoxaprofen	C16H12ClNO3	1
Betaine HCl	C5H12ClNO2	0
Bismuth Subsalicylate	C7H5BiO4	0
Bithionol	C12H6Cl4O2S	1
BNIT (2-Naphthyl isothiocyanate)	C11H7NS	0
Bosentan	C27H29N5O6S	1
bromfenac	C15H12BrNO3	1
Bromobenzene	C6H5Br	1
buthioninesulphoxime	C20H10Br4O10S2	1
Butoconazole Nitrate	C19H18Cl3N3O3S	0
Butylated hydroxytoluene	C15H24O	1
Caffeine	C8H10N4O2	0
Calcifediol	C27H44O2	1
candesartan	C24H20N6O3	0
Capsaicin	C18H27NO3	0
carbamzepine	C15H12N2O	1
carbon tetrachloride (2)	CCl4	1
Carboplatin	C6H12N2O4Pt	1
Cefadroxil	C16H19N3O6S	1
Cefamandole Sodium	C18H17N6NaO5S2	1
Cefotetan	C17H17N7O8S4	0
Cefotiam HCl	C18H24ClN9O4S3	1
Cefoxitin	C16H17N3O7S2	1
Ceftazidime	C22H22N6O7S2	0
Ceftriaxone Sodium E-Isomer	C18H17N8NaO7S3	1
cephaloridine	C19H17N3O4S2	1
Cephalothin Sodium	C16H15N2NaO6S2	1
Cephapirin Sodium	C17H16N3NaO6S2	0
Cephradine	C16H19N3O4S	0
cerivastatin	C26H34FNO5	1
Chloroform	CHCl3	1
Chloroquine Phosphate	C18H32ClN3O8P2	0
Chlorpropamide	C10H13ClN2O3S	1
Ciglitizone	C18H23NO3S	1
Cinchophen	C16H11NO2	1
cisplatin	H6Cl2N2Pt	1
Citicoline	C12H22N4O11P2	0

Clarithromycin	C38H69NO13	1
Clemastine Fumarate	C25H30ClNO5	0
Clindamycin HCl	C18H34Cl2N2O5S	1
Clofibrate	C12H15ClO3	1
Cloxacillin Sodium	C19H19ClN3NaO6S	1
Cyclizine	C18H22N2	1
Dacarbazine	C6H10N6O	1
Dactinomycin	C62H86N12O16	1
DCB (dichlorobenzene)	C6H4Cl2	1
Dextroamphetamine Sulfate	C18H28N2O4S	1
dichloroethylene	C2H4Cl2	1
dichlorophenyl succinimide	C9H10Cl2N2O	1
Dicloxacillin Sodium	C19H16Cl2N3NaO5S	1
Diethylhexylphthalate (phthalate ester)	C24H38O4	1
difluoropentane	C5H10F2	1
Dimercaprol	C3H8OS2	1
dimethylnitrosamine	C2H6N2O	1
dinitrophenol	C6H4N2O5	1
Di-n-pentyl-phthalate	C18H26O4	1
Diphenoxylate HCl	C30H33ClN2O2	0
Dipyridamole	C24H40N8O4	0
Diquat	C12H12Br2N2	1
Divalproex Sodium	C16H31NaO4	1
d-limonene	C10H16	1
Doxorubicin HCl	C27H30ClNO11	1
Econazole Nitrate	C18H16Cl3N3O4	0
entacapone	C14H15N3O5	0
Epirubicin	C27H29NO11	0
eprosartan	C23H24N2O4S	0
Ergotamine I-Tartrate	C37H41N5O11	0
Ethane Dimethane Sulfonate	C14H10Cl4	1
ethinyl estradiol	C20H24O2	1
Ethosuximide	C7H11NO2	1
ethylene glycol	C2H6O2	1
Fexofenadine	C32H39NO4	0
Fialuridine	C9H10FIN2O5	1
Fipexide	C20H21ClN2O4	1
Flufenamic Acid (Flufenamate)	C14H10F3NO2	0

flunoxapfen	C16H12FNO3	0
Fluorouracil	C4H3FN2O2	1
Fluspirilene	C29H31F2N3O	1
Foscarnet	CH3O5P	0
Glutethimide	C13H15NO2	1
grepafloxacin	C19H22FN3O3	1
Guanethidine Sulfate	C10H24N4O4S	1
Hexachlorophene	C13H6Cl6O2	1
Hydrazine	H4N2	1
Hyoscyamine Sulfate	C17H25NO7S	1
Ibufenac	C12H16O2	1
Ibuprofen	C13H18O2	0
Ifosfamide	C7H15Cl2N2O2P	1
indacrinone	C18H14Cl2O4	1
indinavir sulphate	C36H49N5O8S	0
Iopamidol	C17H22I3N3O8	1
iproniazid	C9H13N3O	1
irbesartan	C25H28N6O	0
Isocarboxazid	C12H13N3O2	0
Isosorbide dinitrate	C6H8N2O8	0
Isoxicam	C14H13N3O5S	0
Ketoconazole	C26H28Cl2N4O4	1
ketoprofen	C16H14O3	0
Lactose	C12H22O11	0
Leucovorin Calcium	C20H21CaN7O7	0
Liothyronine	C15H12I3NO4	0
Loracarbef	C16H18ClN3O5	0
losartan	C22H23ClN6O	1
Lumiracoxib	C15H13ClFNO2	1
Menadione	C11H8O2	1
Mephobarbital	C13H14N2O3	1
Meproamate	C9H18N2O4	1
Mestranol	C21H26O2	1
Metformin	C4H11N5	0
Methapyrilene	C14H19N3S	1
Methapyrilene	C14H19N3S	1
Methoxyacetic Acid	C3H6O3	1
Methyldopa	C10H13NO4	1

methylene dianiline	C16H18ClN3S	1
Methylphenidate	C14H19NO2	1
Metolazone	C16H16ClN3O3S	1
Mezlocillin Sodium	C21H24N5NaO8S2	1
mianserin	C18H20N2	1
Mibefradil	C29H38FN3O3	0
Microcystin-LR	C49H74N10O12	1
Minocycline HCl	C23H28ClN3O7	1
Mometasone Furoate	C27H30Cl2O6	0
Moricizine HCl	C22H26ClN3O4S	1
Moxalactam Disodium	C20H18N6Na2O9S	0
Myo-inositol	C6H12O6	0
N-acetyl cysteine	C5H9NO3S	0
Nafcillin Sodium	C21H21N2NaO5S	0
naproxen	C14H14O3	0
Nitrofurantoin	C8H6N4O5	1
o-bromophenol	C6H5BrO	1
Octyl Methoxycinnamate	C18H26O3	1
Oxaprozin	C18H15NO3	1
Oxyquinoline Sulfate	C9H9NO5S	1
Paclitaxel	C47H51NO14	1
PAP (para-aminophenol)	C18H24NO5PS2	0
paraquat	C14H20N2O8S2	1
Pargyline	C11H13N	0
pemoline	C9H8N2O2	1
Penbutolol Sulfate	C36H60N2O8S	1
Pentanoic Acid	C5H10O2	0
Permethrin	C21H20Cl2O3	0
phenothiazine	C12H9NS	1
phenyl isothiocyanate	C7H5NS	1
Pimozide	C28H29F2N3O	0
Pirprofen	C13H14ClNO2	1
probenecid	C13H19NO4S	0
Probucol	C31H48O2S2	0
Prochlorperazine Maleate	C28H32ClN3O8S	1
Propofol	C12H18O	0
Quinine Sulfate	C40H50N4O8S	1
ragaglitazar	C25H25NO5	0

Retinyl palmitate	C36H58O3	1
Rifabutin	C46H62N4O11	1
Rifampicin	C43H58N4O12	0
ritonavir	C37H48N6O5S2	1
rotenone	C23H22O6	1
Saquinavir base / mesylate	C38H50N6O5	1
Spectinomycin HCl	C14H25ClN2O7	1
Streptomycin	C21H39N7O12	0
Streptozocin	C8H15N3O7	0
Sulconazole Nitrate	C18H16Cl3N3O3S	0
Sulfabenzamide	C13H12N2O3S	0
Sulfamethizole	C9H10N4O2S2	1
Sulfanilamide	C6H8N2O2S	1
Sulfapyrazone	C23H20N2O3S	1
Tasosartan	C23H21N7O	1
telenzepine	C19H22N4O2S	0
Temafloxacin	C21H18F3N3O3	1
Terbutaline Sulfate	C24H40N2O10S	1
Tetraethylthiuran	C10H20N2S4	0
Theophylline	C7H8N4O2	0
Thiamine	C12H17ClN4OS	0
ticrynafen	C13H8Cl2O4S	1
Tobramycin	C18H37N5O9	1
Tolazamide	C14H21N3O3S	1
Tolbutamide	C12H18N2O3S	1
tolcapone	C14H11NO5	1
Tolrestat	C16H14F3NO3S	1
Topiramate	C12H21NO8S	0
trichloroethylene	C2HCl3	1
Trientine HCl	C6H19ClN4	1
Trimethobenzamide HCl	C21H29ClN2O5	1
Trimethoprim	C14H18N4O3	1
Tripelennamine HCl	C16H22ClN3	1
Troleandomycin	C41H67NO15	1
Tromethamine	C4H11NO3	0
TUDC (tauroursodeoxycholic acid)	C26H45NO5S	1
Uracil Mustard	C8H11Cl2N3O2	1
Valproic Acid	C8H16O2	1

Verapamil HCl	C27H39ClN2O4		0
Vinblastine Sulfate	C46H60N4O13S		0
Vincristine Sulfate	C46H58N4O14S		1
Ximelagatran	C24H35N5O5		1
zolpidem	C19H21N3O		0
Azithromycin	C38H72N2O12	447,043	0
buspirone	C21H31N5O2	2,477	0
diclofenac	C14H11Cl2NO2	3,033	1
Nefazodone	C25H32ClN5O2	4,449	1
Pioglitazone	C19H20N2O3S	4,829	0
Propranolol	C16H21NO2	4,946	0
Rosiglitazone	C18H19N3O3S	77,999	0
telithromycin	C43H65N5O10	3,002,190	1
trogliatzone	C24H27NO5S	5,591	1
valsartan	C24H29N5O3	60,846	0