

Ref.	Compound	canonical SMILES	Technique	Kpuu	Animal	In refined dataset?
[1]	6-mercaptopurine	<chem>Sc1[n]c[n]c2[n]c[nH]c21</chem>	MD	0,0413	Rat	YES
[2]	Acetaminophen/Paracetamol	<chem>CC(=O)Nc1ccc(O)cc1</chem>	MD	0,73	Rat	NO
[3]	Alprenolol	<chem>CC(C)NCC(O)COc1ccccc1CC=C</chem>	Slice	0,38	Rat	YES
[2]	Amantadine	<chem>NC12CC3CC(C1)CC(C3)C2</chem>	Homog	3,01	Rat	NO
[4]	Amitriptyline	<chem>CN(C)CCC=C1c2ccccc2CCc2ccccc21</chem>	Slice	0,73	Rat	NO
[2]	Amoxapine	<chem>C1C1C=CC2=C(C=1)C(=NC1=CC=CC=C1O2)N1CCNCC1</chem>	Homog	0,35	Rat	NO
[5]	Anastrozole	<chem>CC(C)(C#N)c1cc(C[n]2c[n]c[n]2)cc(c1)C(C)(C)C#N</chem>	MD	0,118	Mice	YES
[6]	Antipyrine	<chem>C[n]1c(C)cc(=O)[n]1-c1ccccc1</chem>	MD	1,38	Rat	YES
[7]	Apomorphine	<chem>CN1CCc2cccc3c2C1Cc1ccc(O)c(O)c1-3</chem>	MD	5	Rat	YES
[2]	aricept/donepezil	<chem>COC1=C(OC)C=C2C(=O)C(CC3CCN(CC4=CC=CC=C4)CC3)CC2=C1</chem>	Homog	1,77	Rat	NO
[37]	Aripiprazole	<chem>O=C1CCC2C=CC(=CC=2N1)OCCCCN1CCN(C2C(Cl)=C(Cl)C=CC=2)CC1</chem>	Homog	0,19	Rat	NO
[3]	Atenolol	<chem>CC(C)NCC(O)COc1ccc(CC(N)=O)cc1</chem>	Slice	0,026	Rat	NO
[8]	Atomoxetine	<chem>Cc1ccccc1OC(CCNC)c1ccccc1</chem>	MD	0,7	Rat	YES
[9]	Baclofen	<chem>NCC(CC(O)=O)c1ccc(Cl)cc1</chem>	MD	0,027	Rat	YES
[10]	Benzylpenicillin	<chem>CC1(C)SC2C(NC(=O)Cc3ccccc3)C(=O)N2C1C(O)=O</chem>	Slice	0,0264	Rat	YES
[2]	Bupropion	<chem>CC(C)(C)NC(C)C(=O)c1ccc(Cl)c1</chem>	MD	3,3	Rat	YES
[10]	Buspirone	<chem>O=C1CC2(CC(=O)N1CCCCN1CCN(CC1)c1[n]ccc[n]1)CCCC2</chem>	Slice	0,612	Rat	YES
[11]	Caffeine	<chem>C[n]1c(=O)c2c([n]c[n]2C)[n](C)c1=O</chem>	MD	0,9551	Rat	NO
[6]	Carbamazepine	<chem>NC(=O)N1c2ccccc2C=Cc2ccccc12</chem>	MD	0,643	Rat	NO
[4]	Carisoprodol	<chem>CCCC(C)(COC(N)=O)COC(=O)NC(C)C</chem>	Slice	0,95	Rat	YES
[12]	Cefadroxil	<chem>CC1CSC2C(NC(=O)C(N)c3ccc(O)cc3)C(=O)N2C=1C(O)=O</chem>	MD	0,033	Rat	YES
[36]	celecoxib	<chem>C1(C(F)(F)F)C=C(C2=CC=C(C)C=C2)N(C2=CC=C(S(=O)(=O)N)C=C2)N=1</chem>	Homog	0,4164	Rat	NO
[10]	Cephalexin	<chem>CC1CSC2C(NC(=O)C(N)c3ccccc3)C(=O)N2C=1C(O)=O</chem>	Slice	0,016	Rat	YES

[4]	Cetirizine	<chem>OC(=O)COCCN1CCN(CC1)C(c1ccc(Cl)cc1)c1ccccc1</chem>	Slice	0,01	Rat	YES
[4]	Chlorpromazine	<chem>CN(C)CCCN1c2ccccc2Sc2ccc(Cl)cc12</chem>	Slice	0,49	Rat	NO
[36]	ciglitazone	<chem>O=C1SC(C(=O)N1)CC1C=CC(OCC2(CCCCC2)C)=CC=1</chem>	Homog	6,932	Rat	NO
[10]	Cimetidine	<chem>Cc1[nH]c[n]c1CSCCNC(NC#N)=NC</chem>	Slice	0,00981	Rat	YES
[13]	Citalopram	<chem>CN(C)CCCC1(OCc2cc(ccc12)C#N)c1ccc(F)cc1</chem>	MD	1	Rat	NO
[2]	Clozapine	<chem>CN1CCN(CC1)C1=Nc2cc(Cl)ccc2Nc2ccccc21</chem>	MD	2,16	Rat	NO
[14]	Codeine	<chem>COc1ccc2CC3C4C=CC(O)C5Oc1c2C45CCN3C</chem>	MD	1,06	Rat	YES
[15]	Colchicine	<chem>CC(=O)NC1CCc2cc(OC)c(OC)c(OC)c2-c2ccc(OC)c(=O)cc21</chem>	MD	0,001	Rat	NO
[10]	Daidzein	<chem>Oc1ccc(cc1)-c1coc2cc(O)ccc2c1=O</chem>	Slice	0,0667	Rat	YES
[16]	DAMGO	<chem>CC(NC(=O)C(N)Cc1ccc(O)cc1)C(=O)NCC(=O)N(C)C(Cc1ccccc1)C(=O)NCCO</chem>	MD	0,09	Rat	YES
[10]	Dantrolene	<chem>[O-][N+](=O)c1ccc(cc1)-c1ccc(C=NN2CC(=O)NC2=O)o1</chem>	Slice	0,0297	Rat	YES
[3]	Delavirdine	<chem>CS(=O)(=O)Nc1cc2cc([nH]c2cc1)C(=O)N1CCN(CC1)c1[n]cccc1NC(C)C</chem>	Slice	0,043	Rat	YES
[6]	Desloratadine	<chem>Clc1cc2CCc3ccc[n]c3C(c2cc1)=C1CCNCC1</chem>	MD	0,018	Rat	YES
[13]	Desmethylclozapine	<chem>Clc1ccc2Nc3ccccc3C(=Nc2c1)N1CCNCC1</chem>	MD	0,075	Rat	YES
[17]	Dexamethasone	<chem>CC1CC2C3CCC4=CC(=O)C=CC4(C)C3(F)C(O)CC2(C)C1(O)C(=O)CO</chem>	Slice	0,0933	Mice	NO
[18]	Diazepam	<chem>CN1C(=O)CN=C(c2cc(Cl)ccc12)c1ccccc1</chem>	MD	0,982	Rat	NO
[36]	diclofenac	<chem>N(C1C=CC=CC=1CC(=O)O)C1=C(C=CC=C1Cl)Cl</chem>	Homog	0,0927	Rat	NO
[17]	Digoxin	<chem>CC12CCC(CC1CCC1C2CC(O)C2(C)C(CCC21O)C1COC(=O)C=1)OC1CC(O)C(OC2CC(O)C(OC3CC(O)C(O)C(C)O3)C(C)O2)C(C)O1</chem>	Slice	0,00469	Mice	NO
[19]	Diphenhydramine	<chem>CN(C)CCOC(c1ccccc1)c1ccccc1</chem>	MD	3,85	Rat	YES
[2]	Doxepin	<chem>C1(=CCCN(C)C)C2=CC=CC=C2OCC2=CC=CC=C12</chem>	Homog	3,11	Rat	NO
[6]	E2074	<chem>C[n]1c(=O)[n](CC(F)CN2C3CC(CC2CC3)OCc2cc(F)ccc2)[n]c1C</chem>	MD	0,178	Rat	YES

[20]	EAB 515	<chem>NC(Cc1cc(cc(CP(O)(O)=O)c1)-c1ccccc1)C(O)=O</chem>	MD	0,119	Rat	YES
[2]	Ergotamine	<chem>[H][C@@]12CCCN1C(=O)[C@H](CC1=CC=CC=C1)N1C(=O)[C@](C)(NC(=O)[C@H]3CN(C)[C@]4([H])CC5=CNC6=C5C(=CC=C6)C4=C3)O[C@@]</chem>	Homog	0,02	Rat	NO
[2]	Ethosuximide	<chem>O=C1C(C)(CC)CC(N1)=O</chem>	Homog	1,5	Rat	NO
[3]	Ethyl-2-phenylmalonami	<chem>CCC(c1ccccc1)(C(N)=O)C(N)=O</chem>	Slice	1,3	Rat	YES
[21]	Etoposide	<chem>CC1OC2C(CO1)OC(OC1C3COC(=O)C3C(c3cc4OCOc4cc31)c1cc(OC)c(O)c(c1)OC)C(O)C2O</chem>	MD	0,36	Rat	NO
[36]	etoricoxib	<chem>ClC1C=NC(C2=CC=C(C)N=C2)=C(C=1)C1C=CC(=CC=1)S(C)(=O)=O</chem>	Homog	0,38754	Rat	NO
[4]	Fexofenadine	<chem>CC(C)(c1ccc(cc1)C(O)CCCN1CCC(CC1)C(O)(c1ccccc1)c1ccccc1)C(O)=O</chem>	Slice	0,04	Rat	NO
[10]	Flavopiridol	<chem>CN1CC(O)C(CC1)c1c2oc(cc(=O)c2c(O)cc1O)-c1ccccc1Cl</chem>	Slice	0,0525	Rat	NO
[22]	Fleroxacin	<chem>CN1CCN(CC1)c1c(F)c2c(cc1F)c(=O)c(c[n]2CCF)C(O)=O</chem>	MD	0,147	Rat	YES
[23]	Fluorescein	<chem>Oc1cc2Oc3cc(O)ccc3C3(OC(=O)c4ccccc34)c2cc1</chem>	MD	0,06	Rat	YES
[4]	Fluoxetine	<chem>CNCCC(Oc1ccc(cc1)C(F)(F)F)c1ccccc1</chem>	Slice	1	Rat	YES
[2]	Fluphenazine	<chem>S1C2C=CC=CC=2N(CCCN2CCN(CCO)CC2)C2C=C(C=CC1=2)C(F)(F)F</chem>	Homog	1,58	Rat	NO
[36]	flurbiprofen	<chem>O=C(C(C1C=C(F)C(C2C=CC=CC=2)=CC=1)C)O</chem>	Homog	0,2056	Rat	NO
[39]	FRM-1	<chem>[H]N([C@H]1CN2CCC1CC2)C(=O)C1=CC2=C(S1)C(F)=CC=C2</chem>	Homog	0,69	Rat	NO
[39]	FRM-2	<chem>O=C(NC1CN2CCC1CC2)C1=CC2=CC=CC(C#N)=C2S1</chem>	Homog	0,08	Rat	NO
[13]	Gabapentin	<chem>NCC1(CC(O)=O)CCCC1</chem>	MD	0,021	Rat	YES
[24]	Ganciclovir	<chem>Nc1[nH]c(=O)c2[n]c[n](COC(CO)CO)c2[n]1</chem>	MD	0,07320	Rat	YES
[10]	Genistein	<chem>Oc1cc(O)cc2occ(c(=O)c12)-c1ccc(O)cc1</chem>	Slice	0,181	Rat	YES
[4]	Haloperidol	<chem>OC1(CCN(CCCC(=O)c2ccc(F)cc2)CC1)c1ccc(Cl)cc1</chem>	Slice	1,1	Rat	NO
[4]	Hydroxyzine	<chem>OCCOCCN1CCN(CC1)C(c1ccc(Cl)cc1)c1ccccc1</chem>	Slice	0,86	Rat	YES
[36]	ibuprofen	<chem>O=C(C(C)C1C=CC(CC(C)C)=CC=1)O</chem>	Homog	0,55575	Rat	NO

[17]	Indinavir	<chem>CC(C)(C)NC(=O)C1CN(Cc2c[n]ccc2)CCN1CC(O)CC(Cc1cccc1)C(=O)NC1C(O)Cc2cccc21</chem>	Slice	0,119	Mice	NO
[3]	Indomethacin	<chem>Cc1c(CC(O)=O)c2cc(ccc2[n]1C(=O)c1ccc(Cl)cc1)OC</chem>	Slice	0,11	Rat	NO
[2]	Isocarboxazid	<chem>O1C(C)=CC(C(NNCC2C=CC=CC=2)=O)=N1</chem>	Homog	0,18	Rat	NO
[36]	ketorolac	<chem>OC(C1C2=CC=C(C(C3=CC=CC=C3)=O)N2CC1)=O</chem>	Homog	0,08338	Rat	NO
[11]	L-tryptophan	<chem>NC(Cc1c[nH]c2cccc21)C(O)=O</chem>	MD	0,0609	Rat	YES
[6]	Lamotrigine	<chem>Nc1[n]c(N)c([n][n]1)-c1cccc(Cl)c1Cl</chem>	MD	0,643	Rat	NO
[5]	Letrozole	<chem>N#Cc1ccc(cc1)C(c1ccc(cc1)C#N)[n]1c[n]c[n]1</chem>	Slice	0,208	Mice	YES
[25]	Levetiracetam	<chem>CCC(C(N)=O)N1CCCC1=O</chem>	MD	0,5	Rat	NO
[3]	Levofloxacin	<chem>CN1CCN(CC1)c1c(F)cc2c3c1OCC(C)[n]3cc(C(O)=O)c2=O</chem>	Slice	0,12	Rat	NO
[38]	Levomilnacipran	<chem>O=C([C@@]1(C2C=CC=CC=2)C[C@H]1CN)N(CC)CC</chem>	Homog	0,038	Mice	NO
[3]	Loperamide	<chem>CN(C)C(=O)C(CCN1CCC(O)(CC1)c1ccc(Cl)cc1)(c1cccc1)c1cccc1</chem>	Slice	0,007	Rat	NO
[17]	Loratadine	<chem>CCOC(=O)N1CCC(CC1)=C1c2[n]cccc2CCc2cc(Cl)ccc21</chem>	Slice	0,74	Mice	YES
[2]	Loxapine	<chem>ClC1C=CC2=C(C=1)C(=NC1=CC=CC=C1O2)N1CCN(C)CC1</chem>	Homog	2,95	Rat	NO
[11]	Mannitol	<chem>OC(CO)C(O)C(O)C(O)CO</chem>	MD	0,0141	Rat	NO
[2]	Maprotiline	<chem>CNCCCC12C3=CC=CC=C3C(C3=CC=CC=C13)CC2</chem>	Homog	0,98	Rat	NO
[19]	Memantine	<chem>CC12CC3CC(N)(CC(C)(C3)C1)C2</chem>	MD	1,8	Rat	YES
[2]	Meprobamate	<chem>O(C(N)=O)CC(C)(CCC)COC(N)=O</chem>	Homog	0,77	Rat	NO
[2]	Mesoridazine	<chem>C1(N)C2N=C(CN(C)C3=CC=C(C(N[C@@H](CCC(=O)O)C(=O)O)=O)C=C3)C=NC=2N=C(N)N=1</chem>	Homog	0,1	Rat	NO
[3]	Methotrexate	<chem>CN(Cc1c[n]c2[n]c(N)[n]c(N)c2[n]1)c1ccc(cc1)C(=O)NC(CCC(O)=O)C(O)=O</chem>	Slice	0,0061	Rat	NO
[6]	Metoclopramide	<chem>COc1cc(N)c(Cl)cc1C(=O)NCCN(CC)CC</chem>	MD	0,669	Rat	YES

[3]	Metoprolol	<chem>CC(C)NCC(O)COc1ccc(CCOC)cc1</chem>	Slice	0,64	Rat	NO
[6]	Midazolam	<chem>Cc1[n]cc2CN=C(c3ccccc3F)c3cc(Cl)ccc3-[n]21</chem>	MD	0,652	Rat	NO
[2]	Mirtazapine	<chem>N12CCN(C)CC1C1C=CC=CC=1CC1=CC=CN=C21</chem>	Homog	3,85	Rat	NO
[26]	Morphine	<chem>CN1CCC23C4Oc5c2c(CC1C3C=CC4O)ccc5O</chem>	MD	0,29	Rat	NO
[27]	Morphine-3-glucuronide	<chem>CN1CCC23C4C=CC(O)C2Oc2c3c(CC14)ccc2OC1OC(C(O)C(O)C1O)C(O)=O</chem>	MD	0,1	Rat	YES
[3]	Morphine-6-glucuronide	<chem>CN1CCC23C4Oc5c2c(CC1C3C=CC4OC1OC(C(O)C(O)C1O)C(O)=O)ccc5O</chem>	Slice	0,0084	Rat	YES
[3]	Moxalactam	<chem>C[n]1[n][n][n]c1SCC1COC2N(C=1C(O)=O)C(=O)C2(NC(=O)C(c1ccc(O)cc1)C(O)=O)OC</chem>	Slice	0,019	Rat	YES
[37]	N-desmethyl-venlafaxine	<chem>[H]N(C)CC(C1=CC=C(OC)C=C1)C1(O)CCCC1</chem>	Homog	0,34	Rat	NO
[3]	Nadolol	<chem>CC(C)(C)NCC(O)COc1cccc2CC(O)C(O)Cc21</chem>	Slice	0,037	Rat	NO
[13]	Naltrexone	<chem>OC12CCC(=O)C3Oc4c5c(CC1N(CC1CC1)CCC253)ccc4O</chem>	MD	0,61	Rat	YES
[36]	naproxen	<chem>O(C)C1C=CC2C=C(C=CC=2C=1)[C@H](C)C(O)=O</chem>	Homog	0,6018	Rat	NO
[3]	Nelfinavir	<chem>Cc1c(cccc1O)C(=O)NC(CSc1ccccc1)C(O)CN1CC2CCCC2CC1C(=O)NC(C)(C)C</chem>	Slice	0,019	Rat	NO
[3]	Nitrofurantoin	<chem>[O-][N+](=O)c1ccc(C=NN2CC(=O)NC2=O)o1</chem>	Slice	0,011	Rat	NO
[22]	Norfloxacin	<chem>CC[n]1cc(C(O)=O)c(=O)c2cc(F)c(cc12)N1CCNCC1</chem>	MD	0,034	Rat	YES
[4]	Nortriptyline	<chem>CNCCC=C1c2ccccc2CCc2ccccc21</chem>	Slice	1	Rat	YES
[37]	O-desmethyl-venlafaxine	<chem>CN(CC(C1(CCCCC1)O)C1=CC=C(O)C=C1)C</chem>	Homog	0,38	Rat	NO
[40]	Olanzapine	<chem>CN1CCN(C2C3C=C(C)SC=3NC3C=CC=CC=3N=2)CC1</chem>	Homog	1,8	Rat	NO
[6]	Ondansetron	<chem>C[n]1c2ccccc2c2c1CCC(C[n]1cc[n]c1C)C2=O</chem>	MD	0,283	Rat	YES

[3]	Oxprenolol	<chem>CC(C)NCC(O)COc1cccc1OCC=C</chem>	Slice	0,2	Rat	YES
[19]	Oxycodone	<chem>COc1ccc2CC3N(C)CCC45C(Oc1c42)C(=O)CCC53O</chem>	MD	1,69	Rat	YES
[3]	Oxymorphone	<chem>CN1CCC23C4Oc5c2c(CC1C3(O)CCC4=O)ccc5O</chem>	Slice	0,79	Rat	YES
[3]	Paclitaxel	<chem>CC1(C)C2C(OC(C)=O)C(=O)C3(C)C(C(OC(=O)c4cccc4)C1(O)CC(OC(=O)C(O)C(NC(=O)c1cccc1)c1cccc1)C=2C)C1(COC1CC3O)OC(C)=O</chem>	Slice	0,0073	Rat	NO
[6]	Paliperidone/9-OH Risperidone	<chem>Cc1[n]c2C(O)CCC[n]2c(=O)c1CCN1CCC(CC1)c1[n]oc2cc(F)ccc21</chem>	MD	0,06	Rat	YES
[4]	Paroxetine	<chem>Fc1ccc(cc1)C1CCNCC1COc1cc2OCOc2cc1</chem>	Slice	0,53	Rat	YES
[22]	Pefloxacin	<chem>CN1CCN(CC1)c1cc2c(cc1F)c(=O)c(c[n]2CC)C(O)=O</chem>	MD	0,147	Rat	YES
[28]	Pemetrexed	<chem>Nc1[nH]c2[nH]cc(Cc3ccc(cc3)C(=O)NC(CCC(O)=O)C(O)=O)c2c(=O)[n]1</chem>	MD	0,106	Rat	YES
[2]	Pemoline	<chem>O1C(N)=NC(C1C1C=CC=CC=1)=O</chem>	Homog	0,55	Rat	NO
[2]	Pergolide	<chem>S(C)C[C@H]1CN(CCC)[C@]2([H])CC3=CNC4C=CC=C(C3=4)[C@@]2([H])C1</chem>	Homog	3,19	Rat	NO
[41]	Perphenazine	<chem>OCCN1CCN(CCCN2C3=CC(=CC=C3SC3C=CC=CC2=3)Cl)CC1</chem>	Homog	7,12	Rat	NO
[2]	Phenelzine	<chem>N(CCC1C=CC=CC=1)N</chem>	Homog	1,48	Rat	NO
[29]	Phenytoin	<chem>O=C1NC(=O)C(N1)(c1cccc1)c1cccc1</chem>	MD	0,52170	Human	NO
[3]	Pindolol	<chem>CC(C)NCC(O)COc1cccc2[nH]ccc12</chem>	Slice	0,5	Rat	YES
[36]	pioglitazone	<chem>S1C(NC(C1CC1C=CC(=CC=1)OCCC1=CC=C(CC)C=N1)=O)=O</chem>	Homog	0,5611	Rat	NO
[2]	Primidone	<chem>O=C1C(CC)(C(NCN1)=O)C1C=CC=CC=1</chem>	Homog	0,38	Rat	NO
[30]	Probenecid	<chem>CCCN(CCC)S(=O)(=O)c1ccc(cc1)C(O)=O</chem>	MD	0,199	Rat	YES
[31]	Propranolol	<chem>CC(C)NCC(O)COc1cccc2ccccc12</chem>	MD	0,947	Monkey	NO
[19]	Pyrilamine	<chem>CN(C)CCN(Cc1ccc(cc1)OC)c1cccc[n]1</chem>	MD	2,5	Rat	YES

[40]	Quetiapine	<chem>OCCOCCN1CCN(C2C3=CC=CC=C3SC3=CC=CC=C3N=2)CC1</chem>	Homog	0,63	Rat	NO
[32]	Quinidine	<chem>COc1ccc2[n]ccc(C(O)C3CC4CCN3CC4C=C)c2c1</chem>	MD	0,324	Rat	NO
[3]	Rifampicin	<chem>CN1CCN(CC1)N=Cc1c2NC(=O)C(C)=CC=CC(C)C(O)C(C)C(O)C(C)C(OC(C)=O)C(C)C(C=COC3(C)Oc4c(c(c2O)c(O)c4C)c1O)C3=O)OC</chem>	Slice	0,035	Rat	NO
[6]	Risperidone	<chem>Cc1[n]c2CCCC[n]2c(=O)c1CCN1CCC(CC1)c1[n]oc2cc(F)ccc21</chem>	MD	0,119	Rat	NO
[2]	Rizatriptan	<chem>CN(CCC1C2C=C(CN3N=CN=C3)C=CC=2NC=1)C</chem>	Homog	0,04	Rat	NO
[30]	Salicylic acid	<chem>Oc1ccccc1C(O)=O</chem>	MD	0,126	Rat	NO
[3]	Saquinavir	<chem>CC(C)(C)NC(=O)C1CC2CCCC2CN1CC(O)C(Cc1ccccc1)NC(=O)C(CC(N)=O)NC(=O)c1ccc2ccccc2[n]1</chem>	Slice	0,055	Rat	NO
[2]	Selegiline	<chem>C1C=C(C=CC(=C1)[C@@H]1CC[C@@H](C2=CC=CC=C12)NC)Cl</chem>	Homog	1,08	Rat	NO
[10]	Sertraline	<chem>CNC1CCC(c2ccccc21)c1cc(Cl)c(Cl)cc1</chem>	Slice	1,85	Rat	YES
[33]	Stavudine	<chem>Cc1c[n](C2C=CC(CO)O2)c(=O)[nH]c1=O</chem>	MD	0,33	Rat	YES
[4]	Sulpiride	<chem>CCN1CCCC1CNC(=O)c1cc(ccc1OC)S(N)(=O)=O</chem>	Slice	0,05	Rat	YES
[4]	Sumatriptan	<chem>CNS(=O)(=O)Cc1cc2c(cc1)[nH]cc2CCN(C)C</chem>	Slice	0,07	Rat	NO
[3]	Tacrine	<chem>Nc1c2ccccc2[n]c2CCCCc21</chem>	Slice	0,78	Rat	YES
[2]	Temazepam	<chem>C1C1=CC=C2C(=C1)C(C1C=CC=CC=1)=NC(C(N2C)=O)O</chem>	Homog	0,8	Rat	NO
[24]	Thiopental	<chem>CCC1(C(C)CCC)C(=O)NC(=S)NC1=O</chem>	MD	1,0158	Rat	YES
[3]	Thioridazine	<chem>CN1CCCC1CCN1c2cc(ccc2Sc2ccccc12)SC</chem>	Slice	0,45	Rat	YES
[2]	Thiothixene	<chem>S(C1C=CC2=C(C=1)/C=C\CCN1CCN(C)CC1)/C1C=CC=CC=1S2)(N(C)C)(=O)=O</chem>	Homog	0,13	Rat	NO
[2]	Tiagabine	<chem>OC([C@]1(CN(CC/C=C/C2=C(C)C=CS2)\C2=C(C)C=CS2)CCC1)[H])=O</chem>	Homog	0,62	Rat	NO
[3]	Topiramate	<chem>CC1(C)OC2C3OC(C)(C)OC3COC2(COS(N)(=O)=O)O1</chem>	Slice	0,33	Rat	YES

[34]	Tramadol	<chem>COc1cc(ccc1)C1(O)CCCC1CN(C)C</chem>	MD	2,3	Rat	YES
[2]	Trazodone	<chem>C1C=CC=C(C=1)N1CCN(CC1)CCCN1C(N2C=CC=CC2=N1)=O</chem>	Homog	1,54	Rat	NO
[4]	Trifluoperazine	<chem>CN1CCN(CCCN2c3ccccc3Sc3ccc(cc23)C(F)(F)F)CC1</chem>	Slice	1	Rat	YES
[36]	valdecoxib	<chem>O=S(=O)(N)C1C=CC(C2C(C3C=CC=CC=3)=NOC=2C)=CC=1</chem>	Homog	0,2224	Rat	NO
[2]	Venlafaxine	<chem>COC1=CC=C(C(C2(CCCC2)O)CN(C)C)C=C1</chem>	Homog	1,91	Rat	NO
[6]	Verapamil	<chem>CN(CCC1cc(OC)c(cc1)OC)CCCC(C#N)(C(C)C)c1cc(OC)c(cc1)OC</chem>	MD	0,0718	Rat	NO
[38]	Vilazodone	<chem>O=C(N)C1OC2=CC=C(N3CCN(CCCCC4C5C=C(C=CC=5NC=4)C#N)CC3)C=C2C=1</chem>	Homog	0,27	Mice	NO
[17]	Vinblastine	<chem>CN1C2C3(CCN4CC=CC(CC)(C34)C(OC(C)=O)C2(O)C(=O)OC)c2cc(c(cc12)OC)C1(CC2CC(O)(CN(C2)CCc2c1[nH]c1ccccc21)CC)C(=O)OC</chem>	Slice	0,0248	Mice	NO
[36]	vioxx	<chem>C1C=CC=CC=1C1=C(C2C=CC(S(=O))(=O)C)=CC=2)COC1=O</chem>	Homog	0,74620	Rat	NO
[5]	Vorozole	<chem>C[n]1[n][n]c2ccc(cc12)C(c1ccc(Cl)cc1)[n]1c[n]c[n]1</chem>	Slice	0,297	Mice	YES
[38]	Vortioxetine	<chem>S(C1=CC=C(C)C=C1C)C1C=CC=CC=1N1CCNCC1</chem>	Homog	1,2	Mice	NO
[35]	YM992	<chem>Fc1ccc(OCC2CNCCO2)c2CCCC21</chem>	MD	1,42	Rat	YES
[2]	Zaleplon	<chem>O=C(C)N(CC)C1C=CC=C(C=1)C1=CC=NC2=C(C#N)C=NN12</chem>	Homog	0,59	Rat	NO
[33]	Zidovudine	<chem>Cc1c[n](C2CC(N=[N+]=[N-])C(CO)O2)c(=O)[nH]c1=O</chem>	MD	0,15	Rat	NO
[2]	Ziprasidone	<chem>C1C=CC2=C(CC(N2)=O)C=C1CCN1CCN(CC1)C1C2C=CC=CC=2SN=1</chem>	Homog	0,75	Rat	NO
[4]	Zolpidem	<chem>CN(C)C(=O)Cc1c([n]c2ccc(C)c[n]21)-c1ccc(C)cc1</chem>	Slice	0,42	Rat	YES

#### REFERENCES

- [1] Deguchi, Y et al. Life Sci., 66 (2000) 649.  
[2] Summerfield, SG et al. J. Pharmacol. Exp. Ther., 358 (2016) 294.  
[3] Fridén, M et al. J. Med. Chem., 52 (2009) 6233.



- [4] Culot, M et al. PLoS One, 8 (2013) e80634.
- [5] Miyajima, M et al. J. Pharm. Sci., 102 (2013) 3309.
- [6] Nagaya, Y et al. Drug Metab. Pharmacokinet., 31 (2016) 57.
- [7] Sam, E et al. Eur. J. Pharmacol., 329 (1997) 9.
- [8] Kielbasa, W et al. Drug Metab. Dispos., 37 (2009) 137.
- [9] Deguchi, Y et al. Pharm. Res., 12 (1995) 1838.
- [10] Kodaira, H et al. J. Pharmacol. Exp. Ther., 339 (2011) 935.
- [11] Hansen, DK et al. J. Pharm. Biomed. Anal., 27 (2002) 945.
- [12] Chen, X et al. Fluids Barriers CNS, 11 (2014) 25.
- [13] Deshmukh, G et al. Drug Metab. Dispos., 43 (2015) 1123.
- [14] Xie, R et al. Pharm. Res., 15 (1998) 570.
- [15] Desrayaud, S et al. Life Sci., 61 (1997) 153.
- [16] Lindqvist, A et al. Mol. Pharm., 10 (2013) 1533.
- [17] Uchida, Y et al. J. Pharmacol. Exp. Ther., 339 (2011) 579.
- [18] Dubey, RK et al. J. Clin. Invest., 84 (1989) 1155.
- [19] Kitamura, A et al. J. Pharm. Sci., 105 (2016) 935.
- [20] Malhotra, BK et al. Pharm. Res., 11 (1994) 1223.
- [21] Burgio, DE et al. Biochem. Pharmacol., 51 (1996) 987.
- [22] Ooie, T et al. Drug Metab. Dispos., 25 (1997) 784.
- [23] Sun, H et al. Pharm. Res., 18 (2001) 1542.
- [24] Liu, X et al. Drug Metab. Dispos., 37 (2009) 787.
- [25] Tong, X et al. Br. J. Pharmacol., 133 (2001) 867.
- [26] Tunblad, K et al. Pharm. Res., 20 (2003) 618.
- [27] Xie, R et al. Br. J. Pharmacol., 131 (2000) 1784.
- [28] Dai, H et al. J. Pharmacol. Exp. Ther., 315 (2005) 222.
- [29] Scheyer, RD et al. Epilepsy Res., 18 (1994) 227.
- [30] Deguchi, Y et al. J. Pharmacol. Exp. Ther., 280 (1997) 551.
- [31] Nagaya, Y et al. Drug Metab. Pharmacokinet., 29 (2014) 419.

- [32] Durk, MR et al. Pharm. Res., 32 (2015) 1128.
- [33] Yang, Z et al. Pharm. Res., 14 (1997) 865.
- [34] Kitamura, A et al. J. Pharm. Sci., 103 (2014) 3335.
- [35] Mano, Y et al. Biopharm. Drug Dispos., 23 (2002) 351.
- [36] Summerfield, SG et al. J. Pharmacol. Exp. Ther., 316 (2006) 1282.
- [37] Bundgaard, C et al. Drug Metab Dispos 40 (2012) 461.
- [38] Bundgaard, C et al. Neuropharmacol., 103 (2016) 104.
- [39] Tang, C et al. Biochem Pharmacol 15 (2014) 543.
- [40] Loryan, I et al. Mol. Psychiatry, 21 (2016) 1527.
- [41] Zhang, YY et al. Mol. Pharm., 13 (2016) 1540.