

Online Resource List of compounds used in model construction

Compound name	Data set		Observed		Predicted M/P _{AUC} classification		Ref.
	affiliation		M/P _{AUC}	M/P _{AUC} classification	ANN model (confidence)	SVM model	
	ANN model	SVM model					
Acetaminophen	Tr	V	1.6 ^a	H	H (95%)	H	(1)
Acyclovir	Tr	Tr	2.69 ^a	H	H (73%)	H	(2)
Alphamethyldopa	Tr	Tr	0.22	L	L (98%)	L	(3)
Alprazolam	Te	Tr	0.36	L	L (60%)	L	(4)
Amitriptyline	V	Tr	0.83 ^b	L	L (98%)	L	(5)
Apixaban	V	Tr	2.61	H	H (87%)	H	(6)
Atenolol	Te	Tr	5.7	H	H (53%)	H	(7)
Baclofen	Tr	Tr	0.72 ^b	L	L (98%)	L	(8)
Budesonide	Te	Te	0.5	L	L (98%)	L	(9)
Buprenorphine	Tr	Tr	1.73	H	H (95%)	H	(10)
Caffeine	Tr	Tr	0.7	L	L (98%)	L	(11)
Candesartan	Tr	Tr	0.02	L	L (77%)	L	(12)
Cefprozil	Tr	Te	0.6	L	L (98%)	L	(13)
Celecoxib	Tr	Tr	0.18	L	L (81%)	L	(14)
Chlorprothixene	V	Tr	1.31	H	H (77%)	H	(15)
Chlorprothixene sulphoxide	Tr	V	0.67 ^b	L	L (94%)	L	(15)
Citalopram	V	V	1.8	H	H (95%)	H	(16)
Clarithromycin	V	V	0.25	L	L (88%)	L	(17)
Codeine	Tr	Tr	2.16	H	H (62%)	H	(18)
Colchicine	Tr	Tr	0.52 ^a	L	L (98%)	L	(19)
Cotinine	Tr	Tr	1.2	H	H (95%)	H	(20)
Dapivirine	Tr	Tr	1.8	H	H (77%)	H	(21)
Dehydronitrendipine	Tr	Te	0.6	L	L (98%)	L	(22)
Demethylcitalopram	Te	Te	1.8	H	H (95%)	H	(16)
Descarboethoxyloratadine	Te	Tr	0.8	L	L (74%)	L	(23)
Desmethylmirtazapine	Tr	Tr	0.45 ^a	L	L (98%)	L	(24)
Dexamphetamine	Tr	Tr	2.2	H	H (95%)	H	(25)
Digoxin	Tr	Tr	0.85	L	L (94%)	L	(26)
Diltiazem	Tr	Tr	0.99 ^a	L	L (98%)	L	(27)
Disopyramide	Tr	Tr	0.41	L	L (69%)	L	(28)
Doxazosin	Tr	Tr	0.1	L	L (98%)	L	(29)
Doxorubicin	Tr	Tr	1.19	H	H (95%)	H	(30)
Doxorubicinol	V	V	9.71	H	H (95%)	H	(30)
Drospirenone	Tr	Tr	0.18	L	L (91%)	L	(31)
Duloxetine	Tr	Tr	0.27	L	L (98%)	L	(32)

Efavirenz	Tr	Tr	0.84 ^a	L	L (60%)	L	(33)
Emtricitabine	Tr	Tr	3.01	H	H (87%)	H	(34)
Escitalopram	Tr	Tr	2.2	H	H (95%)	H	(35)
Ethanol	Tr	Te	0.99 ^a	L	L (60%)	L	(36)
Etravirine	V	V	3.47 ^b	H	H (59%)	H	(37)
Fexofenadine	Tr	Tr	0.21	L	L (98%)	L	(38)
Fluconazole	Tr	Te	0.77 ^b	L	H (62%)	L	(39)
Fluoxetine	V	V	0.52	L	L (88%)	L	(40)
Flurbiprofen	Tr	Tr	0.02	L	L (94%)	L	(41)
Fluvoxamine	Te	Te	1.32 ^a	H	H (62%)	L	(42)
Hydrochlorothiazide	Tr	V	0.46 ^a	L	L (77%)	L	(43)
14-Hidroxcylarithromycin	Tr	Tr	0.66	L	L (88%)	L	(17)
Hydroxynefazodone	V	V	0.07	L	L (94%)	L	(44)
Imatinib Mesylate	Tr	Tr	0.37 ^a	L	L (70%)	L	(45)
Labetalol	Tr	V	0.8	L	L (76%)	L	(46)
Lamivudine	V	V	1.31	H	H (95%)	H	(47)
Levodopa	V	V	0.32	L	L (98%)	L	(48)
Levonorgestrel	V	V	0.26	L	L (79%)	L	(49)
Lopinavir	Tr	Tr	0.19	L	L (98%)	L	(50)
Loratadine	Tr	Tr	1.2	H	H (87%)	H	(23)
m-Chlorophenylpiperazine	Tr	Tr	0.19	L	H (82%)	L	(44)
Metformin	Tr	Te	0.4	L	L (64%)	L	(51)
(R)-Methadone	Tr	Tr	0.47	L	L (88%)	L	(52)
(S)-Methadone	V	V	0.27	L	L (88%)	L	(52)
Methotrexate	Te	Tr	0.04 ^a	L	L (94%)	L	(53)
Metoprolol	Tr	Tr	2.4	H	H (82%)	H	(54)
Minoxidil	V	Tr	0.75 ^b	L	H (47%)	L	(55)
Minoxidil Glucuronide	Tr	V	0.12 ^b	L	L (98%)	L	(55)
Mirtazapine	Te	Tr	1.43 ^a	H	L (86%)	H	(24)
Monomethyl 2,6-dimethyl-4-(2-nitrophenyl)-3,5-pyridinedicarboxylate	V	Te	0.88 ^a	L	L (98%)	L	(56)
Morphine	Te	Te	2.45	H	H (65%)	H	(57)
Moxidectin	Tr	Tr	1.77	H	L (83%)	H	(58)
Nadolol	Tr	Tr	4.6	H	H (95%)	H	(59)
N-Desalkyl-2-oxoquazepam	V	Te	0.09	L	L (98%)	L	(60)
N-Desmethyl Imatinib	V	V	0.71 ^a	L	L (70%)	L	(45)
N-Desmethylsertraline	Tr	V	1.64	H	H (70%)	H	(61)
Nefazodone	Tr	Tr	0.27	L	L (94%)	L	(44)
Nevirapine	V	V	0.95	L	L (98%)	L	(62)
Nicotine	Tr	Tr	1.5	H	H (95%)	H	(20)

Nifedipine	V	V	0.74 ^a	L	L (98%)	L	(56)
Nimodipine	Te	Te	0.11	L	L (86%)	L	(63)
Nitrendipine	Tr	Tr	0.82	L	L (98%)	L	(22)
Nitrofurantoin	Tr	Tr	6.2	H	H (69%)	H	(64)
N-Monodesalkylidisopyramide	V	V	5.99	H	H (73%)	L	(65)
Norbuprenorphine	V	V	0.73	L	H (56%)	L	(10)
Norfluoxetine	Tr	Tr	0.42	L	L (81%)	L	(40)
Nortriptyline	V	Tr	0.65 ^b	L	L (98%)	L	(5)
Norverapamil	Tr	Tr	0.16	L	L (98%)	L	(66)
Noscapine	V	V	0.34	L	L (98%)	L	(67)
Olanzapine	Tr	Tr	0.38	L	L (76%)	L	(68)
2-Oxoquazepam	Tr	Tr	2.01	H	H (47%)	H	(60)
Paliperidone	Tr	Tr	0.24	L	L (98%)	L	(69)
Pantoprazole	V	Tr	0.03	L	L (98%)	L	(70)
Paraxanthine	Tr	Tr	0.52	L	L (98%)	L	(11)
Penicillin V	Tr	Tr	0.15	L	L (98%)	L	(71)
Phenacetin	V	Tr	0.67	L	L (65%)	L	(18)
Pilsicainide	Tr	Tr	1.75	H	H (95%)	H	(28)
Praziquantel	V	V	0.35	L	H (45%)	L	(72)
Prednisolone	Tr	Tr	0.03	L	L (98%)	L	(73)
Predonisone	V	V	0.55	L	L (98%)	L	(73)
Pregabalin	V	V	0.76	L	L (98%)	L	(74)
Propafenone	V	Tr	0.25	L	L (86%)	L	(28)
Propranolol	Tr	V	0.32 ^b	L	L (64%)	L	(75)
Propylthiouracil	Tr	Tr	0.09 ^a	L	L (91%)	L	(76)
Pseudoephedrine	V	V	2.48	H	H (95%)	H	(77)
Quazepam	Te	V	4.18	H	H (45%)	H	(60)
Quetiapine	V	V	0.29	L	L (88%)	L	(78)
Quinapril	V	Tr	0.12	L	L (98%)	L	(79)
Ranitidine	Tr	Tr	9.83 ^b	H	H (56%)	H	(80)
Reboxetine	Tr	Tr	0.06	L	L (76%)	L	(81)
Risperidone	V	V	0.42	L	L (98%)	L	(69)
Ritonavir	V	V	0.2	L	L (98%)	L	(50)
Rivaroxaban	Tr	V	0.27	L	L (88%)	L	(6)
Rofecoxib	Tr	V	0.25	L	L (98%)	L	(82)
Rosaramicin	Tr	V	0.12	L	L (98%)	L	(83)
Roxithromycin	Te	Te	0.03	L	L (83%)	L	(84)
Saccharin	Tr	Tr	0.72	L	L (91%)	L	(85)
Salicylate	V	V	0.05	L	L (88%)	L	(18)
Sertraline	V	V	1.93	H	H (95%)	H	(61)

Sumatriptan	Tr	Tr	4.9	H	H (42%)	H	(86)
Suprofen	Tr	Tr	0.01	L	L (98%)	L	(87)
Tacrolimus	Tr	Tr	0.13	L	L (94%)	L	(88)
Tenofovir	Tr	Tr	0.02	L	L (67%)	L	(34)
Terbutaline	Tr	Tr	1.04	H	H (95%)	H	(89)
Theobromine	V	V	0.82	L	L (98%)	L	(11)
Theophylline	Te	Te	0.57	L	L (98%)	L	(11)
Thiopental Sodium	Tr	V	0.44 ^b	L	L (81%)	L	(90)
Tolmetin	V	V	0.01	L	L (98%)	L	(91)
Trazodone	Te	Te	0.14	L	L (81%)	L	(92)
Triazoledione	Tr	Te	0.02	L	L (98%)	L	(44)
Tripolidine	Tr	V	0.53	L	L (88%)	L	(77)
Verapamil	V	V	0.6	L	L (98%)	L	(66)
Zaleplon	Tr	Tr	0.5	L	L (94%)	L	(93)
Zidovudine	Tr	Tr	1.35	H	H (65%)	H	(50)

a : Value calculated by reproducing the graph using Degitizelt[®]

b : Value calculated using the trapezoidal method

H = High ($M/P_{AUC} \geq 1$), L = low ($M/P_{AUC} < 1$)

Tr: Training set, V: Verify set, Te: Test set

ANN; Artificial Neural Network, SVM; Support Vector Machine

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