

Supplementary Table S2  
Results of Chemical compounds screening

Name	Class	Action	Selectivity	Ratio(DMSO)
Emetine dihydrochloride hydrate	Apoptosis	Activator		2.260
Vincristine sulfate	Cytoskeleton and ECM	Inhibitor	Tubulin	2.212
Podophyllotoxin	Cytoskeleton and ECM	Inhibitor	Tubulin	2.180
Vinblastine sulfate salt	Cytoskeleton and ECM	Inhibitor	Tubulin	2.057
Colchicine	Cytoskeleton and ECM	Inhibitor	Tubulin	1.809
Thiocolchicine	Apoptosis	Inducer		1.708
Thapsigargin	Intracellular Calcium	Releaser		1.609
Phorbol 12-myristate 13-acetate	Phosphorylation	Activator	PKC	1.509
Gemcitabine hydrochloride	Apoptosis and Cell Cycle			1.494
Quabain	Ion Pump	Inhibitor	Na+/K+ ATPase	1.382
RepSox	Neuroscience	Inhibitor		1.287
SB743921 hydrochloride	Cell Cycle	Inhibitor	KSP	1.283
Brequinar sodium salt hydrate	DNA-RNA transcription regulators	Inhibitor	DHODH	1.272
Diphenylethidium chloride	Nitric Oxide	Inhibitor	eNOS	1.248
CID 11210285 hydrochloride	Gene Regulation	Agonist	Wnt	1.218
Idarubicin	DNA Metabolism	Inhibitor		1.213
Rotenone	Cell Stress	Modulator	Mitochondria	1.211
(-)-Epinephrine bitartrate	Adrenoceptor	Agonist		1.195
BMS-195614	Gene regulation	Antagonist	RARa	1.193
Oltipraz metabolite M2	Lipid Signaling	Inhibitor	LXRa	1.164
SU 5416	Phosphorylation	Inhibitor	VEGFR PTK	1.156
KRN633	Kinase	Inhibitor	VEGFR	1.153
Sodium Taurocholate hydrate	Multi-Drug Resistance	Modulator	Conjugate Pathway	1.150
YM 976	Cyclic nucleotides	Inhibitor	PDE 4	1.145
Calcimycin	Intracellular Calcium		Ca2+	1.145
DL-2-Amino-5-phosphopentanoic acid	Glutamate	Antagonist	NMDA	1.144
Ethopropazine hydrochloride	Neurotransmission	Inhibitor	Butyrylcholinesterase	1.140
Cefazolin sodium	Antibiotic		Cell wall synthesis	1.136
IC 261	Phosphorylation	Inhibitor	CK-1delta/epsilon	1.134
Nylidrin hydrochloride	Adrenoceptor	Agonist	beta	1.133
GR 113808	Serotonin	Antagonist	5-HT4	1.132
Pifithrin-mu	Apoptosis	Inhibitor	p53 binding	1.122
EGTA	Biochemistry	Inhibitor	Carboxypeptidase B	1.122
DMH4	Kinase/Phosphatase	Inhibitor	VEGF	1.118
L(-)-Norepinephrine bitartrate	Adrenoceptor	Agonist	alpha, beta1	1.118
SU 1498	Tyrosine Kinase	Inhibitor		1.114
Phenylephrine hydrochloride	Adrenoceptor	Agonist	alpha1	1.113
Epibestatin hydrochloride	Biochemistry	Inhibitor	Metalloprotease	1.113
BAY 61-3606 hydrochloride hydrate	Phosphorylation	Inhibitor	Tyrosine kinase	1.111
Capsazepine	Vanilloid	Agonist		1.108
Ro 41-0960	Neurotransmission	Inhibitor	COMT	1.105
Piribedil maleate	Dopamine	Agonist	D3	1.102
SIB 1757	Glutamate	Antagonist	mGluR5	1.102
Albuterol hemisulfate	Adrenoceptor	Agonist	beta2	1.101
erythro-9-(2-Hydroxy-3-nonyl)adenine hydrochloride	Adenosine	Inhibitor	Adenosine deaminase	1.101
CYM50769	Cytokines	Antagonist	NPBWR1	1.101
CNQX disodium	Glutamate	Antagonist	AMPA/Kainate	1.099
Nocodazole	Cytoskeleton and ECM	Inhibitor	beta-tubulin	1.099
Carmofur	Apoptosis			1.098
(-)-alpha-Methylnorepinephrine	Adrenoceptor	Agonist		1.095
(+/-)-Anisodamine	Cholinergic	Antagonist	muscarinic	1.094
5-(N,N-Dimethyl)amiloride hydrochloride	Ion Pump	Blocker	Na+/H+ Antiporter	1.093
Spiperone hydrochloride	Dopamine	Antagonist	D2	1.090
Epinephrine hydrochloride	Adrenoceptor	Agonist		1.090
BMS-299897	Cell Biology	Inhibitor	alpha-secretase	1.088
K145 hydrochloride	Kinase Phosphatase	Inhibitor	SphK2	1.087
L2-b	Cell Biology	Chelator		1.087
Tetraethylthiuram disulfide	Biochemistry	Inhibitor	Alcohol Dehydrogenase	1.086
SCH-50911	GABAergics	Antagonist	GABA <sub>B</sub>	1.086
4-Imidazoleacrylic acid	Histamine	Inhibitor	Histidine ammonia-lyase/ decarboxylase	1.085
Spermidine trihydrochloride	Glutamate	Ligand	NMDA-Polyamine	1.083
Auranofin	Phosphorylation	Inhibitor		1.083
BPTES	Oxidative Stress	Inhibitor	GLS1	1.083
Prilocaine hydrochloride	Na+ Channel	Blocker		1.082
Mevastatin	Antibiotic	Inhibitor	Ras, Rho	1.081
LP44	Serotonin	Agonist	5-HT7	1.080
Trifluoperidol hydrochloride	Dopamine	Antagonist	D1/D2	1.079
SCH-202676 hydrobromide	G protein	Modulator	GPCR	1.079
p-Chlorophenylalanine	Neurotransmission	Inhibitor	Tryptophan hydroxylase	1.077
Domperidone	Dopamine	Antagonist	D2	1.077
(6R)-5,6,7,8-Tetrahydro-L-biopterin hydrochloride	Neurotransmission	Cofactor	Tyrosine & tryptophan hydroxylase, NOS	1.076
SB-525334	Phosphorylation	Inhibitor	Aik5	1.076
cis(+/-)-8-OH-PBZI hydrobromide	Dopamine	Agonist	D3	1.075
Bupropion hydrochloride	Dopamine	Blocker	Reuptake	1.075
TBBz	Phosphorylation	Inhibitor	CK2	1.072
Tyrphostin 51	Phosphorylation	Inhibitor	EGFR	1.071
cis-Piperidine-2,3-dicarboxylic acid	Glutamate	Agonist	NMDA	1.069
3'-Azido-3'-deoxythymidine	Immune System	Inhibitor	Reverse transcriptase	1.069
Daurisoline	Ion Channels	Modulator		1.069
Terutroban	Cell Signaling and Neuroscience	Inhibitor	TPr	1.068
CCT137690	Kinase/Phosphatase Biology	Inhibitor	Aurora A, B and C	1.068
S-Methylisothiourea hemisulfate	Nitric Oxide	Inhibitor	iNOS	1.068
BMS-193885	Neurotransmission	Antagonist	Y1	1.067
Stattic	Gene Regulation	Inhibitor	STAT3	1.067
L-Mimosine from Koa hoale seeds	Apoptosis	Inhibitor		1.067
Procainamide hydrochloride	Na+ Channel	Antagonist		1.066
GR 79236X	Adenosine	Agonist	A1	1.066
Octoclotheptin maleate	Dopamine	Antagonist	D2	1.065
(-)-Sulpiride	Dopamine	Antagonist	D2	1.065
Propionylpromazine hydrochloride	Dopamine	Antagonist	D2	1.065
Isotharine mesylate	Adrenoceptor	Agonist	beta	1.064
Genistein	Phosphorylation	Inhibitor	Tyrosine kinase	1.064
Nisoxetine hydrochloride	Adrenoceptor	Blocker	Reuptake	1.064
4-Hydroxyphenethylamine hydrochloride	Dopamine	Agonist		1.064
NSC405020	Extracellular Matrix	Inhibitor	MT1-MMP	1.063
Alaproclate hydrochloride	Serotonin	Inhibitor	Reuptake	1.063
Procaine hydrochloride	Na+ Channel	Blocker		1.062
Cystamine dihydrochloride	Glutamate	Inhibitor	Transglutaminase	1.062
(+)-Chlorpheniramine maleate	Histamine	Antagonist	H1	1.062
CP466722	Kinase/Phosphatase	Inhibitor	ATM	1.062
Lubiprostone	Ion Channels	Channel Activator	CIC-2 and CFTR	1.061
Terfenadine	Histamine	Antagonist	H1	1.061
Succinylcholine chloride	Cholinergic	Antagonist	Nicotinic	1.060
3-Tropanyl-indole-3-carboxylate hydrochloride	Serotonin	Antagonist	5-HT3	1.060
2-Chloroadenosine	Adenosine	Agonist	A1 > A2	1.059
N6-Cyclopentyladenosine	Adenosine	Agonist	A1	1.059
Ribavirin	Cell Cycle	Inhibitor	IMP dehydrogenase	1.059
UK 14,304	Adrenoceptor	Agonist	alpha2	1.058
R(-)-Isoproterenol (+)-bitartrate	Adrenoceptor	Agonist	beta	1.058
Sulpiride	Dopamine	Antagonist	D2	1.058
Flumazenil	Benzodiazepine	Antagonist		1.058
6(SH)-Phenanthridinone	Transcription	Inhibitor	PARP	1.058
AC-55649	Gene Regulation	Agonist	RARbeta2	1.057
SDZ 220-581 hydrochloride	Neurotransmission	Antagonist	NMDA	1.057

Trimipramine maleate	Serotonin	Inhibitor	Reuptake	1.056
NS593 hydrochloride	Ca2+ Channel	Blocker	SK(Ca)	1.056
Promazine hydrochloride	Dopamine	Antagonist	D2	1.056
Clofibrate	Lipid	Modulator	Lipoprotein lipase	1.056
3,7-Dimethyl-1-propargylxanthine	Adenosine	Antagonist	A2	1.056
Quipazine, 6-nitro-, maleate	Serotonin	Inhibitor	Reuptake	1.056
TMPH hydrochloride	Cholinergic	Inhibitor	Nicotinic	1.055
NBQX disodium	Glutamate	Antagonist	AMPA/kainate	1.055
LDN-21417	Tyrosine kinase	Inhibitor	BMP	1.055
Chlorothiazide	Biochemistry	Inhibitor	Carbonic anhydrase	1.054
L-703,606 oxalate salt hydrate	Tachykinin	Antagonist	NK1	1.054
GANT61	Angiogenic Factors	Inhibitor	SF-1	1.054
Rutaecarpine	K+ Channel	Blocker		1.053
Bropiramine	Immunomodulators			1.053
Pergolide methanesulfonate	Dopamine	Agonist	D2/D1	1.053
Pancuronium bromide	Cholinergic	Antagonist		1.053
Pirenperone	Serotonin	Antagonist	5-HT2	1.053
S(-)-Eticlopride hydrochloride	Dopamine	Antagonist	D2	1.053
TPMPA	GABA	Antagonist	GABA-C	1.052
D(-)-2-Amino-5-phosphonopentanoic acid	Glutamate	Antagonist	NMDA-glycine	1.052
Pyrimilamine maleate	Histamine	Antagonist	H1	1.051
4-DAMP	Cholinergics	Antagonist	M3	1.051
Taurine	Glycine	Agonist		1.050
CCT007093	Apoptosis	Activator	PPM1D	1.050
5alpha-Pregnan-3alpha-ol-20-one	GABA	Modulator	GABA-A	1.049
Ro 04-6790 dihydrochloride	Serotonin	Antagonist	5-HT6	1.049
Rottlerin	Phosphorylation	Inhibitor	PKC / CaM Kinase III	1.049
Pirenzepine dihydrochloride	Cholinergic	Antagonist	M1	1.049
U-62066	Opioid	Agonist	kappa	1.048
Nitrendipine	Ca2+ Channel	Antagonist	L-type	1.048
Trequinsin hydrochloride	Cyclic Nucleotides	Inhibitor	PDE III	1.048
Aminophylline ethylenediamine	Adenosine	Antagonist	A1/A2	1.046
(-)-Quinpirole hydrochloride	Dopamine	Agonist	D2/D3	1.046
Cimetidine	Histamine	Antagonist	H2	1.046
L-732,138	Tachykinin	Antagonist	NK1 > NK2, NK3	1.046
Topotecan hydrochloride hydrate	Apoptosis and Cell Cycle	Inhibitor	topoisomerase I	1.046
Ritodrine hydrochloride	Adrenoceptor	Agonist	beta2	1.046
10058-F4	Apoptosis	Inhibitor	c-Myc	1.045
Spirolactone	Hormone	Antagonist	Mineralocorticoid	1.045
Tegafur	Apoptosis			1.044
IRAK-1/4 Inhibitor I	Phosphorylation	Inhibitor	IRAK-1/4	1.044
Estrone	Hormone		Estrogen	1.044
TCPOBOP	Transcription	Agonist	CAR	1.044
LP 12 hydrochloride hydrate	Serotonin	Agonist	5-HT7	1.044
Spermine tetrahydrochloride	Glutamate	Antagonist	NMDA-Polyamine	1.043
GW5074	Phosphorylation	Inhibitor	Raf1 kinase	1.043
Edrophonium chloride	Cholinergic	Inhibitor	Acetylcholinesterase	1.043
Tirofiban hydrochloride monohydrate	Cell Signaling	inhibitor	glycoprotein IIb/IIIa inhibitor	1.043
Pseudocantharidin C	Gene Regulation		PP2A	1.043
Synephrine	Adrenoceptor	Agonist	alpha	1.043
Lasofoxifene tartrate	Estrogen	Modulator		1.043
Eptifibatid acetate	Anticoagulants	Inhibitor	GPIIb/IIIa	1.043
Phenamil methanesulfonate	Na+ Channel	Inhibitor	Amiloride sensitive	1.042
Sulindac	Prostaglandin	Inhibitor	COX	1.042
Ro 11-1464	Lipid Signaling	Activator	apoA-1	1.042
Arecoline hydrobromide	Cholinergic	Agonist		1.042
R(+)-SCH-23390 hydrochloride	Dopamine	Antagonist	D1	1.041
Imipenem monohydrate	Antibiotic			1.041
PAC-1	Apoptosis	Activator	Caspase 3	1.040
(-)-Isoproterenol hydrochloride	Adrenoceptor	Agonist	beta	1.040
Cytosine-1-beta-D-arabinofuranoside hydrochloride	DNA Metabolism	Inhibitor		1.040
Chlormezanone	Neurotransmission	Modulator	Muscle relaxant	1.039
Isoliquirigenin	Cyclic Nucleotides	Activator	Guanylyl cyclase	1.038
CYM50358	Lipids	Antagonist	S1P4	1.038
Triflusal	Anticoagulants	Inhibitor	COX-1	1.037
Sulfaphenazole	Multi-Drug Resistance	Inhibitor	Cytochrome P4502C	1.037
Vanillic acid diethylamide	Vanilloid	Agonist		1.037
KB-R7493	Calcium Channel	Inhibitor	NCX	1.036
ARL 67156 trisodium salt	P2 Receptor	Inhibitor	ecto-ATPase	1.036
Disopyramide phosphate	K+ Channel	Modulator		1.036
SMER28	Cell Biology	Enhancer	Autophagy	1.036
Phaclofen	GABA	Antagonist	GABA-B	1.036
Riluzole	Glutamate	Antagonist	Release	1.036
N-p-Tosyl-L-phenylalanine chloromethyl ketone	Biochemistry	Inhibitor	Chymotrypsin alpha	1.036
beta-Estradiol	Hormone		Estrogen	1.035
CIQ	Neurotransmission	Modulator	NR2C/NR2D	1.035
BMS-189453	Gene Regulation	Agonist/Antagonist	RAR $\alpha$ , RAR $\beta$ and RAR $\gamma$	1.035
IMID-4F hydrochloride	K+ Channel	Blocker		1.035
Trifluoperazine dihydrochloride	Dopamine	Antagonist	D1/D2	1.034
Quinidine sulfate	Na+ Channel	Antagonist		1.034
Clomipramine hydrochloride	Serotonin	Inhibitor	Reuptake	1.034
Ranitidine hydrochloride	Histamine	Antagonist	H2	1.034
Amifostine	Cell Stress	Inhibitor	Cytoprotectant	1.034
Furegrelate sodium	Phosphorylation	Inhibitor	Thromboxane synthase	1.034
Bumetanide	Ion Pump	Inhibitor	Na+K+-2Cl- cotransporter	1.033
SR 142948A	Cell signaling	Antagonist	Neurotensin	1.033
1,3-Dimethyl-8-phenylxanthine	Adenosine	Antagonist	A1	1.033
(+)-MK-801 hydrogen maleate	Glutamate	Antagonist	NMDA	1.033
Ifenprodil tartrate	Glutamate	Blocker	Polyamine site NMDA	1.032
SB 206553 hydrochloride	Serotonin	Antagonist	5-HT2C/5-HT2B	1.032
S(-)-3PPP hydrochloride	Dopamine	Agonist	D2	1.032
SC 19220	Prostaglandin	Antagonist	EP1	1.032
BIA 2-093	Na+ Channels	Blocker		1.031
Quercetin dihydrate	Cyclic Nucleotides	Inhibitor	PDE	1.031
Semicarbazide hydrochloride	Neurotransmission	Inhibitor	MAO	1.031
Tetraethylammonium chloride	Cholinergic	Antagonist	Nicotinic	1.031
Uridine 5'-diphosphate sodium	P2 Receptor	Agonist	P2Y	1.031
ANA-12	Cytokines		TrkB	1.030
Roscovitine	Phosphorylation	Inhibitor	CDK	1.030
O-(Carboxymethyl)hydroxylamine hemihydrochloride	Biochemistry	Inhibitor	Aminotransferase	1.030
Quinolinic acid	Glutamate	Antagonist	NMDA	1.030
Anisotropine methyl bromide	Muscarinic	Antagonist		1.030
Phenylbutazone	Prostaglandin	Substrate	Prostaglandin peroxidase	1.029
JW74	Transcription	Inhibitor	b-catenin/GSK-3b/AXIN/APC/CK1	1.029
Ro 8-4304	Glutamate	Antagonist	NMDA-NR2B	1.029
VU0420373	Immune Signaling	Activator	HssRSmmonoamine oxidase	1.029
N-(2-[4-(4-Chlorophenyl)piperazin-1-yl]ethyl)-3-methoxybenzamide	Dopamine	Agonist	D4	1.029
Guvacine hydrochloride	GABA	Inhibitor	Uptake	1.029
Quinelorane dihydrochloride	Dopamine	Agonist	D2	1.029
Methazolamide	Enzyme Inhibitors	Inhibitor	Carbonic anhydrase	1.029
Isoproterenol hydrochloride	Adrenoceptor	Agonist	beta	1.029
Genipin	Cell Biology	Modulator	UCP2	1.029
Fluspirilene	Dopamine	Antagonist	D2/D1	1.029
Thalidomide	Cytoskeleton and ECM	Inhibitor	TNFalpha	1.029
R(+)-3PPP hydrochloride	Dopamine	Agonist	D2	1.028
Aminobenztrpine	Cholinergic	Ligand	Muscarinic	1.028
Epinastine hydrochloride	Histamine	Antagonist	H1	1.028

N-Phenylanthranilic acid	Cl- Channel	Blocker		1.028
Galloflavin potassium	Cell Stress	Inhibitor	LDN-A/B	1.028
Cephalothin sodium	Antibiotic		Cell wall synthesis	1.027
Methoctramine tetrahydrochloride	Cholinergic	Antagonist	M2	1.027
(±)-6-Chloro-PB hydrobromide	Dopamine	Agonist	D1	1.027
GW9508	Lipids	Agonist	FFA1/GPR40	1.026
Pregnenolone sulfate sodium	GABA	Antagonist	GABA-A	1.026
H2L5186303	Lipids	Inhibitor	LP2A	1.026
Protriptyline hydrochloride	Adrenoceptor	Blocker	Reuptake	1.025
O-Phospho-L-serine	Glutamate	Antagonist	NMDA	1.025
WIN 62,577	Tachykinin	Antagonist	NK1	1.025
Prazosin hydrochloride	Adrenoceptor	Antagonist	alpha1	1.025
1,10-Phenanthroline monohydrate	Biochemistry	Inhibitor	Metalloprotease	1.024
Molsidomine	Nitric Oxide	Donor		1.024
Gabaculine hydrochloride	GABA	Inhibitor	GABA transaminase	1.024
DL-alpha-Methyl-p-tyrosine	Neurotransmission	Inhibitor	Tyrosine hydroxylase	1.024
JS-K	Nitric Oxide	Donor		1.024
SKF 83959 hydrobromide	Dopamine	Agonist	D1	1.023
Ranolazine dihydrochloride	Lipid	Inhibitor	pFOX	1.023
SB 216763	Phosphorylation	Inhibitor	GSK-3	1.023
Nedocromil	Immune Signaling	Stabilizer	Mast cell	1.023
Aconitine	Ion Pump	Blocker	Na+/H+ Antiporter	1.023
Ruthenium red	Ion Pump	Inhibitor	Mitochondrial uniporter	1.022
DFU	Lipids	Inhibitor	COX-2	1.022
Tyrphostin AG 538	Apoptosis	Inhibitor	Pin-1	1.022
SC-514	Phosphorylation	Inhibitor	IKK-2	1.022
Tienilic acid	MultiDrug Resistance	Inhibitor	P450	1.022
alpha,beta-Methylene adenosine 5'-triphosphate dilithium	P2 Receptor	Agonist	P2X > P2Y	1.022
Phosphonoacetic acid	DNA	Inhibitor	DNA Polymerase	1.022
Vinpocetine	Cyclic Nucleotides	Inhibitor	PDE 1	1.021
Tyrphostin 1	Phosphorylation	Inhibitor	EGFR	1.021
Rilmenidine hemifumarate	Imidazole	Agonist	I1	1.021
Myricetin	Phosphorylation	Inhibitor	Casein Kinase II	1.021
N6-2-(4-Aminophenyl)ethyladenosine	Adenosine	Agonist	A3	1.021
D-609 potassium	Lipid	Inhibitor	PIPLC	1.021
7-Chloro-4-hydroxy-2-phenyl-1,8-naphthyridine	Adenosine	Antagonist	A1	1.021
YC-1	Cyclic Nucleotides	Activator	Guanylyl cyclase	1.021
Retinoic acid	Apoptosis	Activator		1.021
trans-(7)-ACPD	Glutamate	Agonist	Metabotropic	1.020
Trihexyphenidyl hydrochloride	Cholinergic	Antagonist	Muscarinic	1.020
Phosphoramidon disodium	Biochemistry	Inhibitor	Endopeptidase	1.020
Bendamustine hydrochloride	Apoptosis			1.019
7,8-Dihydroxyflavone hydrate	Cytokines, Growth Factors and Hormones	Agonist	TrkB	1.019
Moxonidine hydrochloride	Adrenoceptor	Agonist	alpha2A	1.019
Betaxolol hydrochloride	Adrenoceptor	Antagonist	beta1	1.019
Cirazoline hydrochloride	Adrenoceptor	Agonist	alpha1A	1.019
Pyrocatechol	Cell Cycle	Inhibitor		1.019
Nomifensine maleate	Dopamine	Inhibitor	Reuptake	1.019
Valproic acid sodium	Anticonvulsant			1.019
Amisulpride	Dopamine	Antagonist	D2/D3	1.019
Urapidil hydrochloride	Adrenoceptor	Antagonist	alpha1	1.019
Ezatiostat	Cell signaling	Inhibitor	GSTP1-1	1.018
(-)-Scopolamine methyl nitrate	Cholinergic	Antagonist	Muscarinic	1.018
1-Phenyl-3-(2-thiazolyl)-2-thiourea	Dopamine	Inhibitor	beta-Hydroxylase	1.018
JNJ-40418677	Neurobiology	Modulator	gamma-Secretase	1.018
Kenpaullone	Phosphorylation	Inhibitor	CDK1, CDK2, CDK5	1.017
5-Hydroxyindolacetic acid	Serotonin	Metabolite		1.017
1-Methylnicotinamide chloride	Inflammation	Metabolite		1.016
Steviol	Ion Channels	Inhibitor	hOAT1/hOAT3	1.016
RU-SKI 43 maleate	Cytokines	Inhibitor	Hhat	1.016
Amantadine hydrochloride	Dopamine	Releaser		1.016
Minocycline hydrochloride	Cell Cycle	Inhibitor		1.016
D-Serine	Glutamate	Agonist	NMDA-Glycine	1.016
Aminoguanidine hemisulfate	Nitric Oxide	Inhibitor	NOS	1.016
Bay 11-7082	Phosphorylation	Inhibitor	IKB-alpha	1.016
Lamotrigine isethionate	Cell Signaling and Neuroscience			1.015
JFD00244	Gene Regulation	Inhibitor	SIRT	1.015
Sanguinarine chloride	Ion Pump	Inhibitor	Na+/K+ ATPase	1.014
Metaproterenol hemisulfate	Adrenoceptor	Agonist	beta2	1.014
Tropicamide	Cholinergic	Antagonist	M4	1.014
Oxotremorine sesquifumarate salt	Cholinergic	Agonist	M2	1.014
Demeclocycline hydrochloride	Antibiotic		Protein synthesis	1.014
L-165,041	Lipid Signaling	Agonist	PPAR-gamma	1.014
Triprolidine hydrochloride	Histamine	Antagonist	H1	1.014
7,7-Dimethyl-(5Z,8Z)-eicosadienoic acid	Lipid	Inhibitor	PLA2 / Lipoxigenase	1.013
6-Methoxy-1,2,3,4-tetrahydro-9H-pyrido[3,4b] indole	Neurotransmission	Inhibitor	MAO	1.013
Tetrabenazine	Neurotransmission	Inhibitor	VMAT	1.013
DL-threo-beta-hydroxyaspartic acid	Glutamate	Inhibitor	Transport	1.012
Bexarotene	Gene Regulation	Agonist	RXR	1.012
Gilipizide	K+ Channel	Blocker	ATP-sensitive	1.012
5-Hydroxy-L-tryptophan	Serotonin	Precursor		1.012
Zanamivir	Antiviral		Viral neuraminidase	1.011
2,3-Butanedione	Cytoskeleton and ECM	Inhibitor	Myosin ATPase	1.011
Acetylthiocholine chloride	Cholinergic	Agonist	Nicotinic	1.011
Hydrochlorothiazide	Biochemistry	Inhibitor	Carbonic anhydrase	1.011
6-Hydroxymelatonin	Melatonin	Metabolite		1.011
SDZ-205,557 hydrochloride	Serotonin	Antagonist	5-HT4	1.011
3-alpha,21-Dihydroxy-5-alpha-pregnan-20-one	GABA	Modulator	GABA-A	1.011
(-)-Scopolamine hydrobromide	Cholinergic	Antagonist	Muscarinic	1.011
S(+)-Raclopride L-tartrate	Dopamine	Antagonist	D2	1.011
Hexamethonium dichloride	Cholinergic	Antagonist	Nicotinic	1.011
SR 27897 hydrate	Cholecystokinin	Antagonist	CCK1	1.010
Pivmecillinam	Antibiotics	Inhibitor	PBP2	1.010
DL-p-Chlorophenylalanine methyl ester hydrochloride	Neurotransmission	Inhibitor	Tryptophan hydroxylase	1.009
GABA	GABA	Agonist		1.009
Tetraoisopropyl pyrophosphoramidate	Biochemistry	Inhibitor	Butyrylcholinesterase	1.009
Verapamil hydrochloride	Ca2+ Channel	Modulator	L-type	1.009
SKF 95282 dimaleate	Histamine	Antagonist	H2	1.008
1-Phenylbiguanide	Serotonin	Agonist	5-HT3	1.008
Forskolin	Cyclic Nucleotides	Activator	Adenylate cyclase	1.008
Benzamil hydrochloride	Ion Pump	Blocker	Na+/H+, Na+/Ca2+ Pump	1.008
3-Aminopropylphosphonic acid	GABA	Agonist	GABA-B	1.008
N-Acetylprocainamide hydrochloride	Na+ Channel	Blocker		1.008
Ibandronate sodium	Lipid Signaling	Inhibitor	Farnesyl diphosphate synthase	1.008
ML-9	Phosphorylation	Inhibitor	MLCK	1.007
5-hydroxydecanoic acid sodium	K+ Channel	Blocker		1.007
Tetrahydrozoline hydrochloride	Adrenoceptor	Agonist	alpha	1.006
Filbanserin	Serotonin	Agonist/Antagonist	5-HT1A /5-HT2A	1.006
Alloxazine	Adenosine	Antagonist	A2b	1.006
(-)-Scopolamine,n-Butyl- bromide	Cholinergic	Antagonist	Muscarinic	1.006
U-74389G maleate	Cell Stress	Inhibitor		1.006
GR 5562 dihydrobromide	Serotonin	Antagonist	5-HT1B/1D	1.006
5,5-Dimethyl-1-pyrroline-N-oxide	Cell Stress	Inhibitor	Antioxidant	1.006
INDY	Kinase/Phosphatase	Inhibitor	Dyrk1A and Dyrk1B	1.006
ML 230	Multi-drug resistance	Inhibitor	BCRP	1.006
XCT790	Gene Regulation	Inverse Agonist	ERRalpha	1.005
Dobutamine hydrochloride	Adrenoceptor	Agonist	beta1	1.005

(S)-Propranolol hydrochloride	Adrenoceptor	Blocker	beta	1.005
Thiopropamide maleate	Histamine	Antagonist	H3	1.005
Ro 25-6981 hydrochloride	Glutamate	Antagonist	NMDA-NR2B	1.005
CPCCOEt	Cell Signaling and Neuroscience	Antagonist	mGluR1	1.004
Azathioprine	P2 Receptor	Inhibitor	Purine synthesis	1.004
Carbamazepine	Anticonvulsant			1.004
Rollipram	Cyclic Nucleotides	Inhibitor	PDE IV	1.004
Phloretin	Ca2+ Channel	Blocker	L-Type	1.004
Tomoxetine	Adrenoceptor	Inhibitor	Reuptake	1.004
L-2-aminoadipic acid	Glutamate	Inhibitor	Glutamine synthetase	1.004
L-798106	Lipids	Antagonist	EP3	1.004
Mecamylamine hydrochloride	Cholinergic	Antagonist	Nicotinic	1.003
SB 200646 hydrochloride	Serotonin	Antagonist	5-HT2C/2B	1.003
ATPA	Glutamate	Agonist	Kainate	1.003
cDPCP	Cell Cycle		DNA-N7 of guanosine	1.003
Bicalutamide (CDX)	Gene Regulation	Antagonist	AR	1.003
Cantharidic Acid	Phosphorylation	Inhibitor	PP1 / PP2A	1.003
SB 415286	Phosphorylation	Inhibitor	GSK-3	1.003
Py6	Calcium Channel Modulator	Inhibitor	STIM1/Orai1	1.003
L-DOPS	Adrenergics	Agonist		1.003
17alpha-hydroxyprogesterone	Hormone	Metabolite	Progesterone	1.003
Tetramisole hydrochloride	Phosphorylation	Inhibitor	Phosphatase	1.003
Dantrolene sodium	Intracellular Calcium	Inhibitor	Release	1.002
A-68930 hydrochloride	Dopamine	Agonist	D1	1.002
Sepiapterin	Nitric Oxide	Cofactor	NOS	1.002
Acetylsalicylic acid	Prostaglandin	Inhibitor	COX-3 > COX-1 > COX-2	1.002
Ancitabine hydrochloride	DNA Metabolism	Inhibitor		1.002
(+)-CP-99994 dihydrochloride	Tachykinins	Antagonist	NK-1	1.002
Sodium Oxamate	Biochemistry	Inhibitor	Lactate Dehydrogenase	1.002
Quinacrine dihydrochloride	Neurotransmission	Inhibitor	MAO	1.002
5-Carboxamidotryptamine maleate	Serotonin	Agonist	5-HT7	1.002
Tyrphostin AG 112	Phosphorylation	Inhibitor	Tyrosine kinase	1.001
MK-912	Adrenoceptor	Agonist	alpha2A	1.001
Propranolol hydrochloride	Adrenoceptor	Antagonist	beta	1.001
Cortisone 21-acetate	Hormone		Cortisol	1.001
Sumanriole maleate	Dopaminergics	Agonist	D2	1.001
Lorglumide sodium	Cholecystokinin	Antagonist	CCK-A	1.000
SB 204741	Serotonin	Antagonist	5-HT2B	1.000
AEG 3482	Heat Shock Proteins		HSP90	0.999
Memantine hydrochloride	Glutamate	Antagonist	NMDA	0.999
SNC80	Opioid	Agonist	delta	0.999
DL-Thiorphan	Neurotransmission	Inhibitor	Enkephalinase	0.999
(-)-Cotinine	Cholinergic	Metabolite	Nicotinic	0.999
CID2858522	Gene Regulation	Inhibitor	NF-kB	0.999
Doxycycline hydrochloride	Antibiotic		Protein synthesis	0.999
Piperlongumine	Apoptosis	inhibitor	GSTP1	0.999
Valganciclovir hydrochloride hydrate	Antiviral	Inhibitor	DNA Polymerase	0.999
Altretamine	DNA Metabolism	Inhibitor		0.999
Clotrimazole	K+ Channel	Inhibitor	Ca2+-activated K+ channel	0.999
Reactive Blue 2	P2 Receptor	Antagonist	P2Y	0.999
Cyclobenzaprine hydrochloride	Serotonin	Antagonist	5-HT2	0.999
FAUC 213	Dopamine	Antagonist	D4	0.999
Imipramine hydrochloride	Serotonin	Blocker	Reuptake	0.998
R(+)-6-Bromo-APB hydrobromide	Dopamine	Agonist	D1/D5	0.998
Donitriptan monohydrochloride	Neurotransmission	Agonist	5-HT1B/1D	0.998
NSC 95397	Phosphorylation	Inhibitor	Cdc25	0.998
p-Benzoguinone	DNA Repair	Inhibitor	G:C site	0.998
Ceftriaxone sodium	Antibiotic		Cell wall synthesis	0.998
AB-MECA	Adenosine	Agonist	A3	0.997
9-Amino-1,2,3,4-tetrahydroacridine hydrochloride	Cholinergic	Inhibitor	Cholinesterase	0.997
Carbetapentane citrate	Opioid	Ligand	sigma1	0.997
KT203	Neurotransmission,	Inhibitor	ABHD6	0.997
(-)-Perillic acid	G protein	Inhibitor	p21 Ras	0.997
S-(+)-Fluoxetine hydrochloride	Serotonin	Inhibitor	Reuptake	0.997
Promethazine hydrochloride	Histamine	Antagonist	H1	0.997
Rivastigmine tartrate	Cholinergics	Inhibitor	cholinesterase	0.997
Tetracaine hydrochloride	Na+ Channel	Modulator		0.997
Phenytoin sodium	Anticonvulsant			0.997
Vanillylmandelic acid	Adrenoceptor	Metabolite		0.997
Hexahydro-sila-difenidol hydrochloride, p-fluoro analog	Cholinergic	Antagonist	M3>M1>M2	0.997
N-Methylhistadipriden dioxalate salt	Histamine	Agonist	H1	0.996
Brinzolamide	anhydrases	Inhibitor	anhydrase II	0.996
Picrotoxin	GABA	Antagonist	GABA-C	0.996
Mifamurtide	Immune cell signaling	immunostimulant		0.996
Carbachol	Cholinergic	Agonist		0.996
Methapyrilene hydrochloride	Histamine	Antagonist	H1	0.995
Citalopram hydrobromide	Serotonin	Inhibitor	Reuptake	0.995
Ganaxolone	GABA	Modulator	GABA-A	0.995
Hydroquinone	Leukotriene	Inhibitor	Arachidonate 12-Lipoxygenase	0.995
SB 205384	GABA	Modulator	GABA-A	0.995
Cantharidin	Phosphorylation	Inhibitor	PP2A	0.995
Tranylcypromine hydrochloride	Neurotransmission	Inhibitor	MAO	0.995
Felbamate	Glutamate	Antagonist		0.995
WAY-100635 maleate	Serotonin	Antagonist	5-HT1A	0.994
Tetradecylthioacetic acid	Transcription	Agonist	PPAR-alpha	0.994
Terbutaline hemisulfate	Adrenoceptor	Agonist	beta	0.994
Na-p-Tosyl-L-lysine chloromethyl ketone hydrochloride	Cyclic Nucleotides	Inhibitor	Adenylyl cyclase	0.994
DL-Cycloserine	Sphingolipid	Inhibitor	Ketosphinganine synthase, Alanine aminotransferase	0.994
GYKI 52466 hydrochloride	Glutamate	Antagonist	AMPA/kainate	0.994
p-Aminoglutethimide	Biochemistry	Inhibitor	P450-dependent hydroxylation	0.994
THIP hydrochloride	GABA	Agonist	GABA-A	0.994
Acetohexamide	Hormone	Releaser	Insulin	0.994
BRL 54443 maleate	Serotonin	Agonist	5-HT1E/1F	0.994
Dofequidar fumarate	Mult-Drug Resistance	Inhibitor	MDR-1	0.994
alpha-Lipoic Acid	Cell Stress	Coenzyme	Pyruvate dehydrogenase	0.994
Pheniramine maleate	Histamine	Antagonist	H1	0.993
8-(4-Chlorophenylthio)-cAMP sodium	Cyclic Nucleotides	Activator		0.993
Efavirenz	Gene Regulation	Inhibitor	Reverse transcriptase	0.993
Tyrphostin 23	Phosphorylation	Inhibitor	EGFR	0.993
Cephalosporin C zinc salt	Antibiotic		Cell wall synthesis	0.993
Ibuprofen	Prostaglandin	Inhibitor	COX	0.992
Phentolamine mesylate	Adrenoceptor	Antagonist	alpha	0.992
Hypotaurine	Cell Stress	Inhibitor	Antioxidant	0.992
Acepromazine maleate	neurotransmission	Antagonist		0.992
Nimodipine	Ca2+ Channel	Antagonist	L-type	0.992
Tulobuterol hydrochloride	Adrenoceptor	Agonist	beta	0.991
Mifepristone	Hormone	Antagonist	Progesterone	0.991
CYM-5520	Neurotransmission	Agonist	S1PR2;	0.991
A-77636 hydrochloride	Dopamine	Agonist	D1	0.990
Eliprodil	Glutamate	Antagonist	NMDA-polyamine	0.990
Cefsulodin sodium salt hydrate	Antibiotic		Cell wall synthesis	0.990
(±)-7-Hydroxy-DPAT hydrobromide	Dopamine	Agonist	D3	0.990
EMPA	Orexin	Antagonist	OXR2	0.990
Acetamide	Biochemistry	Inhibitor	Carbonic anhydrase	0.990
Imidazole-4-acetic acid hydrochloride	GABA	Antagonist	GABA-C	0.990
GNF-5	Phosphorylation	Inhibitor	BRC-Abi	0.990
L-741,626	Dopamine	Antagonist	D2	0.990

Psora-4	K+ Channel	Inhibitor	Kv1.3	0.990
Pyrazinocarboxamide	Antibiotic			0.990
Labetalol hydrochloride	Adrenoceptor	Antagonist	beta	0.989
Resveratrol	Prostaglandin	Inhibitor	COX	0.989
Cefotaxime sodium	Antibiotic		Cell wall synthesis	0.989
L-Histidine hydrochloride	Histamine	Precursor		0.989
Tolbutamide	Hormone	Releaser	Insulin	0.989
3,4-Dihydroxyphenylacetic acid	Dopamine	Metabolite		0.989
Cefaclor	Antibiotic		Cell wall synthesis	0.989
N-Acetyl-L-Cysteine	Glutamate	Antagonist		0.989
CNS-1102	Glutamate	Antagonist	NMDA	0.989
L-Hyoscyamine	Cholinergic	Antagonist		0.988
N-(4-Amino-2-chlorophenyl)phthalimide	Anticonvulsant			0.988
Guanabenz acetate	Adrenoceptor	Agonist	alpha2	0.988
4-DAMP methiodide	Cholinergic	Antagonist	M3	0.988
Fenoldopam bromide	Dopamine	Agonist	D1	0.988
D-ribofuranosylbenzimidazole	Transcription	Inhibitor		0.988
Piceatannol	Phosphorylation	Inhibitor	Syk / Lck	0.988
L-Beta-threo-benzyl-aspartate	Neurotransmission	Antagonist	EAAT3	0.988
5-Bromo-2'-deoxyuridine	DNA Metabolism	Inhibitor		0.988
Mitoxantrone	DNA Metabolism	Inhibitor		0.988
Ivermectin	Cholinergic	Modulator	alpha7 nACh	0.987
5-(N-Ethyl-N-isopropyl)amiloride	Ion Pump	Blocker	Na+/H+ Antiporter	0.987
Sertraline hydrochloride	Serotonin	Inhibitor	Reuptake	0.987
AMT hydrochloride	Nitric Oxide	Inhibitor	iNOS	0.987
Diazoxide	K+ Channel	Activator	ATP-sensitive	0.987
Granisetron hydrochloride	Serotonin	Antagonist	5-HT3	0.987
Diacylglycerol Kinase Inhibitor II	Phosphorylation	Inhibitor	Diacylglycerol kinase	0.987
Naftopidil dihydrochloride	Adrenoceptor	Antagonist	alpha1	0.987
Ritanserine	Serotonin	Antagonist	5-HT2/5-HT1C	0.987
Caffeic acid phenethyl ester	Cell Cycle	Inhibitor	NFkB	0.987
RX 821002 hydrochloride	Adrenoceptor	Antagonist	alpha2	0.987
Cyproheptadine hydrochloride	Serotonin	Antagonist	5-HT2	0.987
Tolazamide	Hormone	Releaser	Insulin	0.987
(-)-Physostigmine	Cholinergic	Inhibitor	Cholinesterase	0.986
(-)-MK-801 hydrogen maleate	Glutamate	Antagonist	NMDA	0.986
rac BHEF	Neurotransmission	modulator	GABA-B	0.986
Bisdemethoxycurcumin	Ion Channels	Inhibitor		0.986
9-cyclopentyladenine	Cyclic Nucleotides	Inhibitor	Adenylate cyclase	0.986
Chloroquine diphosphate	DNA	Intercalator	DNA	0.986
YS-035 hydrochloride	Ca2+ Channel	Blocker	L-type	0.986
Olanzapine	Dopaminergics	Antagonists	5-HT2, D1/D2	0.986
L-allylglycine	Biochemistry	Inhibitor	Glutamic acid decarboxylase	0.986
DL-Homatropine hydrobromide	Cholinergic	Antagonist	Muscarinic	0.985
6-Aminoheptanoic acid	Immune System	Inhibitor	Blood Clotting	0.985
ODQ	Cyclic Nucleotides	Inhibitor	NO-sensitive guanylyl cyclase	0.985
Fenoterol hydrobromide	Adrenoceptor	Agonist	beta2	0.985
Benzamide	Apoptosis	Inhibitor	PARS	0.985
SB 269970 hydrochloride	Serotonin	Antagonist	5-HT7	0.985
Bethanechol chloride	Cholinergic	Agonist	Muscarinic	0.985
N-Acetyl-5-hydroxytryptamine	Melatonin	Precursor		0.985
Oxymetazoline hydrochloride	Adrenoceptor	Agonist	alpha2A	0.985
Proprantheline bromide	Cholinergic	Antagonist	Muscarinic	0.984
Theophylline	Adenosine	Antagonist	A1 > A2	0.984
Indomethacin	Prostaglandin	Inhibitor	COX	0.984
Pentamidine isethionate	Glutamate	Antagonist	NMDA	0.984
Droxinostat	Gene Regulation	Inhibitor	HDAC3, HDAC6, and HDAC8	0.984
Cortisolone	Hormone	Precursor	Cortisol	0.984
Xylazine hydrochloride	Adrenoceptor	Agonist	alpha2	0.984
Orphenadrine hydrochloride	Cholinergic	Antagonist	Muscarinic	0.984
2,3-Dimethoxy-1,4-naphthoquinone	Cell Stress	Modulator		0.984
Chloro-APB hydrobromide	Dopamine	Agonist	D1	0.984
BW 723C86	Serotonin	Agonist	5-HT2B	0.984
NS-1619	K+ Channel	Activator	Ca2+ activated	0.984
U0126	Phosphorylation	Inhibitor	MEK1/MEK2	0.984
Triflupromazine hydrochloride	Dopamine	Antagonist	D2	0.984
IMS2186	Cell Cycle	Inhibition	G2	0.983
(-)-Eseroline fumarate	Cholinergic	Inhibitor	Cholinesterase	0.983
Artemether	Immunomodulators and Antib			0.983
Fenobam	Glutamate	Antagonist	mGluR5	0.983
2-Phenylaminoadenosine	Adenosine	Agonist	A2 > A1	0.983
Felodipine	Ca2+ Channel	Blocker	L-type	0.983
Caroverine hydrochloride	Glutamatergics	Antagonist	NMDA/AMPA	0.983
Mianserin hydrochloride	Serotonin	Antagonist		0.983
Nestorone	Lipid Signaling	Agonist	Progesterone receptor	0.983
CP-31398 dihydrochloride hydrate	Apoptosis and Cell Cycle		p53	0.983
Progesterone	Hormone		Progesterone	0.982
Ro 20-1724	Cyclic Nucleotides	Inhibitor	cAMP phosphodiesterase	0.982
Enalaprilat dihydrate	Neurotransmitters	Inhibitor		0.982
HEMADO	Adenosine	Agonist	A3	0.982
Oxybutynin Chloride	Cholinergic	Antagonist	Muscarinic	0.982
Retinoic acid p-hydroxyanilide	Cell Cycle	Inhibitor		0.982
Acetazolamide	Biochemistry	Inhibitor	Carbonic anhydrase	0.982
Yohimbine hydrochloride	Adrenoceptor	Antagonist	alpha2	0.982
Telenzepine dihydrochloride	Cholinergic	Antagonist	M1	0.982
ZM 39923 hydrochloride	Phosphorylation	Inhibitor	JNK-3	0.982
Raloxifene hydrochloride	Hormone	Modulator	ER	0.981
Biperiden hydrochloride	Cholinergic	Antagonist	muscarinic	0.981
BRL 37344 sodium	Adrenoceptor	Agonist	beta3	0.981
Sotalol hydrochloride	Adrenoceptor	Antagonist	beta	0.981
L-Arginine	Nitric Oxide	Precursor		0.981
N-Oleoyl ethanolamine	Sphingolipid	Inhibitor	Ceramidase	0.981
Ammonium pyrrolidinedithiocarbamate	Nitric Oxide	Modulator	NOS	0.981
Amiodarone hydrochloride	Adrenoceptor	Agonist	alpha/beta	0.981
1-Allyl-3,7-dimethyl-8-p-sulphophenylxanthine	Adenosine	Antagonist	A2	0.980
Dipropylidopamine hydrobromide	Dopamine	Agonist		0.980
R(-)-Desmethyldiprenyl hydrochloride	Neurotransmission	Inhibitor	MAO-B	0.980
Palonosetron hydrochloride	Serotonergics	Antagonist	5-HT3	0.980
Paliperidone	Neurotransmission	Antipsychotic		0.980
Xylometazoline hydrochloride	Adrenoceptor	Agonist	alpha	0.980
Baclofen	GABA	Agonist	GABA-B	0.980
Ro 61-8048	Neuroscience	Inhibitor	KMO	0.980
CGS-15943	Adenosine	Antagonist	A1	0.980
Auraptene	Cell Signaling	Modulator/Inhibitor	ACAT	0.980
U-99194A maleate	Dopamine	Antagonist	D3	0.979
Zoledronic acid monohydrate	Kinase	Inhibitor	FPP synthase	0.979
Decamethonium dibromide	Cholinergic	Agonist	Nicotinic	0.979
Hydroxylamine hydrochloride	Neurotransmission	Inhibitor	MAO	0.979
PRE-084	Opioid	Agonist	sigma1	0.978
Acetyl-beta-methylcholine chloride	Cholinergic	Agonist	M1	0.978
Captopril	Neurotransmission	Inhibitor	ACE	0.978
Lithium Chloride	Neurotransmission	Inhibitor	Inositol monophosphatase	0.978
Ziprasidone hydrochloride monohydrate	Neurotransmission	Antipsychotic		0.978
1,7-Dimethylxanthine	Adenosine	Antagonist	A1 > A2	0.978
S(-)-Atenolol	Adrenoceptor	Antagonist	beta1	0.978
1-(2-Methoxyphenyl)piperazine hydrochloride	Serotonin	Agonist	5-HT1 > 5-HT2	0.978
SB 222200	Tachykinin	Antagonist	NK3	0.978

Adenosine 3',5'-cyclic monophosphate	Phosphorylation	Activator	PKA	0.978
Hexamethonium bromide	Cholinergic	Antagonist	Nicotinic	0.977
Serotonin hydrochloride	Serotonin	Agonist		0.977
Amlexanox				0.977
Sertaconazole nitrate	Antifungal	Inhibitor	P450	0.977
Thioridazine hydrochloride	Dopamine	Antagonist	D1/D2	0.977
Clemastine fumarate	Histamine	Antagonist	H1	0.977
Tiapride hydrochloride	Dopamine	Antagonist	D2/D3	0.976
Propafenone hydrochloride	K+ Channel	Blocker	hKv1.5	0.976
Paromomycin sulfate	Antibiotic		Protein synthesis	0.976
Remodelin hydrobromide	Gene Regulation	Inhibitor	NAT10	0.976
GSK2578215A	Phosphorylation	Inhibitor	LRRK2	0.976
Ciproxifan hydrochloride	Histamine	Antagonist	H3	0.976
SR-58611A	Adrenergics	Agonist	b3	0.976
Dipyridamole	Adenosine	Inhibitor		0.976
Mexiletene hydrochloride	Na+ Channel	Blocker		0.976
Centrophoxine hydrochloride	Nootropic			0.976
Cyclosporin A	Phosphorylation	Inhibitor	Calcineurin phosphatase	0.976
8-Hydroxy-DPAT hydrobromide	Serotonin	Agonist	5-HT1A	0.976
Harmaline	Imidazoline	Agonist	I1	0.975
SKF-525A hydrochloride	Multi-Drug Resistance	Inhibitor	Microsomal oxidation	0.975
Droperidol	Dopamine	Antagonist	D1/D2	0.975
Nicosamide	Antibiotic		Protonophore	0.975
8-(3-Chlorostyryl)caffeine	Adenosine	Antagonist	A2A	0.975
Apomorphine hydrochloride hemihydrate	Dopamine	Agonist		0.975
Aurothioglucose	Phosphorylation	Inhibitor	rac1	0.975
Cephalexin hydrate	Antibiotic		Cell wall synthesis	0.975
Entecavir	Cell Signaling	Inhibitor		0.975
CCCI-01	Apoptosis	Inducer		0.975
Bisoprolol hemifumarate salt	Adrenoceptor	Antagonist	Beta1	0.974
Diphenhydramine hydrochloride	Histamine	Antagonist	H1	0.974
Clodronic acid	Cytoskeleton and ECM	Inhibitor	MMP1 / collagenase	0.974
NAN-190 hydrobromide	Serotonin	Antagonist	5-HT1A	0.974
Lomequatrib	Gene Regulation	Inhibitor	MGMT	0.974
Lubuluzole dihydrochloride	Glutamate	Antagonist	NMDA	0.974
Pyridostigmine bromide	Cholinergic	Inhibitor	Cholinesterase	0.974
Vancomycin hydrochloride from Streptomyces orientalis	Antibiotic		Cell wall synthesis	0.974
Sandoz 58-035	Lipid	Inhibitor	ACAT	0.974
2',3'-dideoxycytidine	Immune System	Inhibitor	Reverse Transcriptase	0.974
CRANAD 2	Alzheimer's disease	fluorescent probe	A <sup>+</sup> plaque	0.973
N-Oleoyldopamine	Neurotransmission	Ligand	CB1	0.973
A-315456	Adrenoceptor	Antagonist	alpha1D	0.973
(-)-trans-(1S,2S)-U-50488 hydrochloride	Opioid	Agonist	kappa	0.973
Hispidin	Phosphorylation	Inhibitor	PKC-beta	0.973
Primidone	Anticonvulsant			0.973
(+)-Hydrastine	GABA	Antagonist	GABA-A	0.973
N,N-Dihexyl-2-(4-fluorophenyl)indole-3-acetamide	Benzodiazepine	Ligand	Mitochondria	0.973
L-Canavanine sulfate	Nitric Oxide	Inhibitor	iNOS	0.973
Pirfenidone	Immune System	Inhibitor		0.972
Alprenolol hydrochloride	Adrenoceptor	Antagonist	beta	0.972
TTNPB	Transcription	Ligand	RAR-alpha, beta, gamma	0.972
Indinavir sulfate salt hydrate	immune cell signaling	Inhibitor	HIV	0.972
2,3-Butanedione monoxide	K+ Channel	Blocker	ATP-sensitive	0.972
Arecaidine propargyl ester hydrobromide	Cholinergic	Agonist	M2	0.972
Phenserine	Neurotransmission	Inhibitor	Acetylcholinesterase	0.972
Clozapine	Dopamine	Antagonist	D4 > D2, D3	0.972
SB-366791	Vanilloid	Antagonist	VR1	0.972
PD 98,059	Phosphorylation	Inhibitor	MEK2	0.972
SU 4312	Phosphorylation	Inhibitor	KDR	0.971
SBI-0087702	Cell Signaling and Neuroscience	Inhibitor	ATF2	0.971
Disopyramide	Na+ Channel	Blocker		0.971
4-Aminobenzamide dihydrochloride	Biochemistry	Inhibitor	Trypsin	0.971
Daphnetin	Phosphorylation	Inhibitor	PK	0.971
1-Methylhistamine dihydrochloride	Histamine	Metabolite		0.971
Fosmidomycin sodium salt hydrate	Arachidonic Acid Cascade	Inhibitor	DXR	0.971
CGP 20712A methanesulfonate	Adrenoceptor	Antagonist	beta1	0.971
Methoxamine hydrochloride	Adrenoceptor	Agonist	alpha1	0.970
Atropine methyl bromide	Cholinergic	Antagonist	Muscarinic	0.970
L-3,4-Dihydroxyphenylalanine	Dopamine	Precursor		0.970
2-methoxyestradiol	Hormone	Metabolite	Estrogen	0.970
Atglstatin	Lipids	Inhibitor	ATGL	0.970
Theobromine	Adenosine	Antagonist	A1 > A2	0.970
ICI 204,448 hydrochloride	Opioid	Agonist	kappa	0.970
ML277	Ion Channels	Activator	KCNQ1 > KCNQ2, KCNQ4	0.970
M-110	Kinase/Phosphatase	Inhibitor	PIM-3	0.969
R(+)-Butylindazole	Ion Pump	Inhibitor	K+/Cl- transport	0.969
Notriptyline hydrochloride	Adrenoceptor	Inhibitor	Uptake	0.969
Leukadherin-1	Cell Signaling and Neuroscience	Agonist	CD11b/CD18	0.969
Corticosterone	Hormone		Glucocorticoid	0.969
Bromoacetylcholine bromide	Cholinergic	Ligand		0.969
Lercanidipine hydrochloride hemihydrate	Calcium Channel	Antagonist	Cav1.2b	0.969
Atenolol	Adrenoceptor	Antagonist	beta1	0.969
SKF 38393, N-allyl-, hydrobromide	Dopamine	Agonist	D1	0.969
4-Hydroxy-3-methoxyphenylacetic acid	Dopamine	Metabolite		0.968
KT185	Cell Signaling and Neuroscience	Agonist	P2	0.968
Desipramine hydrochloride	Adrenoceptor	Inhibitor	Uptake	0.968
2-Hydroxysaclofen	GABA	Antagonist	GABA-B	0.968
Clonidine hydrochloride	Adrenoceptor	Agonist	alpha2	0.968
Venlafaxine hydrochloride	Serotonin	Reuptake	5-HT and NE	0.968
p-Aminoclonidine hydrochloride	Adrenoceptor	Agonist	alpha2	0.967
4-Imidazolemethanol hydrochloride	Histamine	Inhibitor	Histidin Dehydrogenase	0.967
AA-861	Leukotriene	Inhibitor	5-lipoxygenase	0.967
Tirapazamine	Apoptosis	Inducer		0.967
Zaprinas	Cyclic Nucleotides	Inhibitor	PDE V	0.967
Cilnidipine	Ca2+ Channels	Blocker	L-type	0.966
L-Canavanine	Cell Stress	Inhibitor	iNOS	0.966
threo-1-Phenyl-2-decanoilamino-3-morpholino-1-propanol hydrochloride	Sphingolipid	Inhibitor	Glucosylceramide synthase	0.966
Apigenin	Cell Cycle	Inhibitor		0.966
Azelaic acid	DNA Metabolism	Inhibitor		0.966
Fusaric acid	Dopamine	Inhibitor	Dopamine beta-hydroxylase	0.966
Dihydrokainic acid	Glutamate	Blocker	Kainate	0.966
Histamine dihydrochloride	Histamine	Agonist		0.966
1,4-Dideoxy-1,4-imino-D-arabinitol	Phosphorylation	Inhibitor	Glycogen phosphorylase	0.966
PF-429242 dihydrochloride	Gene Regulation	Inhibitor	S1P	0.966
K114	Neurotransmission	Amyloid probe		0.966
Benzamide hydrochloride	Biochemistry	Inhibitor	Peptidase	0.965
Tamoxifen citrate	Phosphorylation	Inhibitor	PKC	0.965
Lumefantrine	Immunomodulators and Antibiotics			0.965
Naltrexone hydrochloride	Opioid	Antagonist		0.965
1,3-Dipropyl-8-p-sulfophenylxanthine	Adenosine	Antagonist	A1 > A2	0.965
Phenelzine sulfate	Neurotransmission	Inhibitor	MAO-A/B	0.965
Hydroxyurea	DNA Metabolism	Inhibitor	Ribonucleoside reductase	0.965
Taxifolin	Cell Stress	Inhibitor	Antioxidant	0.965
Ebastine	Histaminergics	Antagonist	H1	0.965
DM 235	Nootropic			0.965
Cisplatin	DNA	Intercalator		0.965
2-Chloroadenosine triphosphate tetrasodium	P2 Receptor	Agonist	P2Y	0.965

ML324	Gene Regulation	Inhibitor	JMJD2	0.964
Octopamine hydrochloride	Adrenoceptor	Agonist	alpha	0.964
Nordihydroguaiaretic acid from Larrea divaricata (creosote bush)	Leukotriene	Inhibitor	Lipoxygenase	0.964
Teriflunomide	Immune Signaling	Inhibitor	dihydroorotate dehydrogenase	0.964
PPADS	P2 Receptor	Antagonist	P2	0.964
NNGH	Extracellular Matrix	Inhibitor	MMP-3	0.964
MNS	Phosphorylation	Inhibitor	Src/Syk	0.964
3-Aminopropionitrile fumarate	Multi-Drug Resistance	Substrate	CYP450	0.964
Urapidil, 5-Methyl-	Adrenoceptor	Antagonist	alpha1A	0.964
Varespladib	Lipids	Inhibitor	sPLA2	0.964
Candesartan cilexetil	Cell Signaling	Antagonist		0.963
Argatroban monohydrate	Cell signaling	Inhibitor	Thrombin	0.963
N,N,N',N'-Tetramethylazodicarboxamide	Cell Stress	Modulator	Thiols	0.963
1-Aminobenzotriazole	Multi-Drug Resistance	Inhibitor	CYP450, chloroperoxidase	0.963
Clostimamide	Cyclic Nucleotides	Inhibitor	PDE III	0.963
Prochlorperazine dimaleate	Dopamine	Antagonist		0.963
7-Cyclopentyl-5-(4-phenoxy)phenyl-7H-pyrrolo[2,3-d]pyrimidin-4-ylamine	Phosphorylation	Inhibitor	Ick	0.963
Normetanephrine hydrochloride	Adrenoceptor	Metabolite	Norepinephrine	0.963
p-Fluoro-L-phenylalanine	Neurotransmission	Substrate	Tyrosine Hydroxylase	0.962
Chelidamic acid	Glutamate	Inhibitor	L-glutamic decarboxylase	0.962
SR 59230A oxalate	Adrenoceptor	Antagonist	beta3	0.962
Tyrphostin AG 879	Phosphorylation	Inhibitor	TrkA	0.962
(-)-Scopolamine methyl bromide	Cholinergic	Antagonist	Muscarinic	0.962
4-Hydroxybenzhydrazide	Biochemistry	Inhibitor		0.962
Protoporphyrin IX disodium	Cyclic Nucleotides	Activator	Guanylyl cyclase	0.962
Fluphenazine dihydrochloride	Dopamine	Antagonist	D1/D2	0.962
L-azetidine-2-carboxylic acid	Biochemistry	Inhibitor	Collagen	0.962
Histamine, R(-)-alpha-methyl-, dihydrochloride	Histamine	Agonist	H3	0.962
Mitiglinide calcium	Ion channels	Antagonist	KATP	0.961
Benztropine mesylate	Cholinergic	Antagonist	Muscarinic	0.961
SIB 1893	Glutamate	Antagonist	mGluR5	0.961
P1,P4-Di(adenosine-5')tetraphosphate triammonium	Biochemistry	Inhibitor		0.961
AMG 9810	Ion Channels	Antagonist	TRPV1	0.961
Metergoline	Serotonin	Antagonist	5-HT2/5-HT1D	0.961
cis-4-Aminocrotonic acid	GABA	Agonist	GABA-C	0.961
Danshensu sodium salt	Cell Stress	Cardioprotectant		0.961
Ofloxacin	Antibiotic		DNA Synthesis	0.961
L-Buthionine-sulfoximine	Multi-Drug Resistance	Inhibitor		0.961
Opipramol dihydrochloride	Sigma receptor	Agonist	1, 2	0.961
Dihydroouabain	Ion Pump	Inhibitor	Na+/K+ Pump	0.961
Progulimide	Cholecystokinin	Antagonist		0.960
Methiohepin mesylate	Serotonin	Antagonist	5-HT1E, 5-HT1F, 5-HT6	0.960
Amitriptyline hydrochloride	Adrenoceptor	Inhibitor	Uptake	0.960
Psoralidin	Apoptosis	Inhibitor	PTP1B	0.960
cis-(Z)-Flupenthixol dihydrochloride	Dopamine	Antagonist		0.960
Metolazone	Na+ Channel	Inhibitor	Na+/Cl- cotransporter	0.960
Dihydroergotamine methanesulfonate	Serotonin	Antagonist		0.960
1-Amino-1-cyclohexanecarboxylic acid hydrochloride	Neurotransmission	Substrate		0.960
(S)-MAP4 hydrochloride	Glutamate	Antagonist	mGluR4,6,7	0.959
Cinoxacin	Antibiotic	Inhibitor		0.959
3-Amino-1-propanesulfonic acid sodium	GABA	Agonist	GABA-A	0.959
4-(2-Aminoethyl)benzenesulfonyl fluoride hydrochloride	Biochemistry	Inhibitor	Serine Protease	0.959
2-(2-Aminoethyl)isothioureia dihydrobromide	Nitric Oxide	Inhibitor	NOS	0.959
Ketanserin tartrate	Serotonin	Antagonist	5-HT2	0.959
Emodin	Phosphorylation	Inhibitor	p56lck TK	0.959
GR-89696 fumarate	Opioid	Agonist	kappa	0.959
Chlorzoxazone	Nitric Oxide	Inhibitor	iNOS	0.958
Imazodan	Cyclic Nucleotides	Inhibitor	PDE II	0.958
(+)-Catechin Hydrate	Cell Stress	Inhibitor	Antioxidant	0.958
Enclomiphene hydrochloride	Cytokines	Antagonist		0.958
U-73343	G-protein		PLC	0.958
S(+)-Ibuprofen	Prostaglandin	Inhibitor	COX	0.958
DCEBIO	K+ Channel	Activator	hK1	0.958
Cephadrine	Antibiotic		Cell wall synthesis	0.958
Daidzein	Cell Cycle	Inhibitor	Aldehyde dehydrogenase	0.958
Aurintricarboxylic acid	Apoptosis	Inhibitor	TopoII	0.958
Flutamide	Hormone	Inhibitor	Androgen	0.958
NG-Nitro-L-arginine methyl ester hydrochloride	Nitric Oxide	Inhibitor	NOS	0.958
Suramin sodium salt	P2 Receptor	Antagonist	P2X, P2Y	0.958
3-Iodo-L-tyrosine	Neurotransmission	Inhibitor	Tyrosine hydroxylase	0.958
2-Chloro-2-deoxy-D-glucose	Biochemistry	Analog	Glucose	0.958
Trazodone hydrochloride	Serotonin	Inhibitor	Reuptake	0.958
KU-55933	Kinase/Phosphatase	Inhibitor	(A-T) mutated (ATM) kinase	0.957
McN-A-343	Cholinergic	Agonist	M1	0.957
Nitisinone	Cell Stress	Inhibitor	4-Hydroxyphenylpyruvate oxidase	0.957
Oxiracetam	Nootropic			0.957
(+)-Butaclamol hydrochloride	Dopamine	Antagonist		0.957
5,5-Diphenylhydantoin	Anticonvulsant			0.957
GSK-650394	Cell signaling	Antagonist	SGK1	0.956
Meloxicam sodium	Prostaglandin	Inhibitor	COX-2	0.956
Methysergide maleate	Serotonin	Antagonist		0.956
5-Fluorindole-2-carboxylic acid	Glutamate	Antagonist	NMDA-Glycine	0.956
Zofenopril calcium	Angiotensin	Inhibitor	ACE	0.955
Quazone	Cyclic Nucleotides	Inhibitor	PDE III	0.955
Calmidazolium chloride	Intracellular Calcium	Inhibitor	Ca2+ATPase	0.955
L-Dopa ethyl ester	Dopaminergics			0.955
Clofazolin	Cyclic Nucleotides	Inhibitor	PDE III	0.955
Quinine sulfate	K+ Channel	Antagonist		0.955
Pramipexole dihydrochloride	Dopaminergics	Agonist	D3/D2	0.955
GSK1838705A	Tyrosine Kinase	Inhibitor	IGF-IR, IR ALK	0.954
Imetit dihydrobromide	Histamine	Agonist	H3	0.954
Imiloxan hydrochloride	Adrenoceptor	Antagonist	alpha2B	0.954
ABT-418 hydrochloride	Cholinergic	Agonist	nicotinic	0.954
Gabapentin	Anticonvulsant			0.954
Milrinone	Cyclic Nucleotides	Inhibitor	PDE III	0.954
Fenofibrate	Transcription	Agonist	PPAR-alpha	0.953
Sulindac sulfone	Prostaglandin	Inhibitor		0.953
DL-alpha-Difluoromethylornithine hydrochloride	Angiogenesis	Inhibitor	ODC	0.953
Pyridostatin trifluoroacetate salt	Gene Regulation	Stabilizer	G-quadruplex	0.953
Hydralazine hydrochloride	Neurotransmission	Inhibitor	MAO-A/B	0.953
Fluoxetine hydrochloride	Serotonin	Inhibitor	Reuptake	0.953
Isonipetric acid	GABA	Agonist	GABA-A	0.953
1,3-Dipropyl-7-methylxanthine	Adenosine	Antagonist	A2	0.952
S(-)-Pindolol	Adrenergic	Antagonist	beta	0.952
Carvedilol	Adrenoceptor	Blocker	alpha1/beta	0.952
1-Aminocyclopropanecarboxylic acid hydrochloride	Glutamate	Agonist	NMDA-Glycine	0.952
UCL 2077	Ion Channels	Blocker	sAHP	0.952
2,2'-Bipyridyl	Biochemistry	Inhibitor	Metalloprotease	0.952
Brompheniramine maleate	Histamine	Antagonist	H1	0.952
Cibenzoline succinate	K+ Channels	Blocker	ATP-sensitive	0.952
Perphenazine	Dopamine	Antagonist	D2	0.952
Dopamine hydrochloride	Dopamine	Agonist		0.951
Indatraline hydrochloride	Dopamine	Inhibitor	Reuptake	0.951
1-Deoxyynjirimycin hydrochloride	Biochemistry	Inhibitor	alpha-glucosidase	0.951
Atropine sulfate	Cholinergic	Antagonist	Muscarinic	0.951
L-Cysteinesulfonic Acid	Glutamate	Ligand		0.951
3-Morpholinolysynonimine hydrochloride	Nitric Oxide	Donor		0.950

PMEG hydrate	Apoptosis and Cell Cycle	Inhibitor	DNA polymerase	0.950
Norepinephrine (+)bitartrate	Adrenoceptor	Agonist		0.950
CCG-50014	Cell Signaling and Neuroscience	Inhibitor	RGS4 and RGS8	0.950
Adaphostin	Tyrosine kinase	Inhibitor	p210bcrr/abl	0.950
Parthenolide	Serotonin	Inhibitor		0.950
Atreleuton	Cell Signaling	Inhibitor	5-lipoxygenase	0.949
Chlorpheniramine maleate	Histamine	Antagonist	H1	0.949
Loxiglumide	Cholinergics	Antagonist	CCKA	0.949
1,3,5-tris(4-hydroxyphenyl)-4-propyl-1H-pyrazole	Hormone	Agonist	ER-alpha	0.949
Nialamide	Neurotransmission	Inhibitor	MAO	0.949
HA155	Cell Signaling and Neuroscience	Inhibitor	autotaxin	0.949
DL-2-Amino-3-phosphonopropionic acid	Glutamate	Antagonist	NMDA	0.949
U-101956 maleate	Dopamine	Antagonist	D4	0.949
Haloperidol	Dopamine	Antagonist	D2/D1	0.949
S-Nitroso-N-acetylpenicillamine	Nitric Oxide	Donor		0.949
1,1-Dimethyl-4-phenyl-piperazinium iodide	Cholinergic	Agonist		0.949
(E)-4-amino-2-butenic acid	GABA	Agonist	GABA-C	0.949
Iofetamine hydrochloride	Neurotransmission			0.949
MCC-555	Cell signaling and neuroscience	Inhibitor		0.948
3-MFA	Ion Channels	Blocker	TRPM2	0.948
Agmatine sulfate	Imidazoline	Agonist		0.948
SANT-1	Angiogenesis	Inhibitor	Smo	0.948
Gardiquimod	Immune Signaling	Agonist	TLR7/TLR8	0.948
Chlormethiazole hydrochloride	GABA	Agonist	GABA(A)	0.948
CGP-12177A hydrochloride	Adrenoceptor	Agonist	beta	0.948
Aniracetam	Glutamate	Agonist	AMPA	0.947
Triamterene	Na+ Channel	Blocker		0.947
8-(p-Sulfophenyl)theophylline	Adenosine	Antagonist	A1 > A2	0.947
NSC 617145	Gene Regulation	Inhibitor	WRN	0.947
TIC10 angular	Gene Regulation	Antagonist	Akt and ERK	0.947
Cyproterone acetate	Hormone	Antagonist	Androgen	0.947
Amoxapine	Adrenoceptor	Inhibitor	Uptake	0.946
AIDA	Glutamate	Antagonist	mGluR1	0.946
Fulvestrant	Hormone	SERD	Estrogen Receptor	0.946
alpha-Lobeline hydrochloride	Cholinergic	Agonist	Nicotinic	0.946
Trimethoprim	Antibiotic	Inhibitor	Dihydrofolate reductase	0.946
Nepicastat hydrochloride	Dopamine	Inhibitor	dopamine +hydroxylase	0.946
ONO-RS-082	Lipids	Inhibitor	phospholipase A2	0.946
5-azacytidine	DNA Metabolism	Inhibitor	DNA methyltransferase	0.946
Benazoline oxalate	Imidazoline	Agonist	i2	0.946
MHPG piperazine	Adrenoceptor	Metaboliite		0.946
D-Cycloserine	Glutamate	Agonist	NMDA-Glycine	0.946
MG 624	Cholinergic	Antagonist	Nicotinic	0.945
Rofecoxib	Lipid Signaling	Inhibitor	COX-2	0.945
Bestatin hydrochloride	Biochemistry	Inhibitor	Aminopeptidase	0.945
NADPH tetrasodium	Nitric Oxide	Cofactor		0.945
Alfuzosin hydrochloride	Adrenoceptor	Blocker		0.945
alpha-Methyl-DL-tyrosine methyl ester hydrochloride	Neurotransmission	Inhibitor	Tyrosine hydroxylase	0.945
Pargyline hydrochloride	Neurotransmission	Inhibitor	MAO-B	0.944
Cefmetazole sodium	Antibiotic		Cell wall synthesis	0.944
L-Glutamic acid, N-phthaloyl-	Glutamate	Agonist	NMDA	0.944
CGS-12066A maleate	Serotonin	Agonist	5-HT1B	0.944
Acyclovir	Immune System	Inhibitor	Viral DNA synthesis	0.944
p-Iodoclonidine hydrochloride	Adrenoceptor	Agonist	alpha2	0.944
Pinacidil	K+ Channel	Activator		0.944
Paroxetine hydrochloride hemihydrate (MW = 374.83)	Serotonin	Inhibitor	Reuptake	0.943
Ipratropium bromide	Cholinergic	Antagonist	Muscarinic	0.943
6-Hydroxy-DL-DOPA	Adrenoceptor	Neurotoxin		0.943
1-(5-Isouquinolinesulfonyl)-2-methylpiperazine dihydrochloride	Phosphorylation	Inhibitor	PKA / PKC	0.943
NNC 55-0396	Ca2+ Channel	Inhibitor	T-type	0.943
Lomefloxacin hydrochloride	Antibiotic	Inhibitor	DNA Gyrase	0.943
Salirasib	Cell signaling and Neuroscience	Inhibitor	RAS	0.943
Trovaloxacin mesylate	Immunomodulators and Antibiotics	Inhibitor	DNA gyrase and topoisomerase IV	0.943
Bay K 8644	Ca2+ Channel	Agonist	L-type	0.942
Fiduxosin hydrochloride	Adrenoceptor	Antagonist	alpha1	0.942
CPNQ	Neurotransmission	Neuroprotectant		0.942
R-(+)-8-Hydroxy-DPAT hydrobromide	Serotonin	Agonist	5-HT1A	0.942
(S)-(+)-Camptothecin	Apoptosis	Inhibitor	Topol	0.942
MK-677	Cytokines	Agonist	ghrelin	0.942
Hemicholinium-3	Cholinergic	Blocker	Uptake	0.942
Flunarizine dihydrochloride	Ion Pump	Blocker	Na+/Ca2+ channel	0.942
BMV 7378 dihydrochloride	Serotonin	Agonist	5-HT1A	0.941
Tizanidine hydrochloride	Adrenoceptor	Agonist	alpha2	0.941
AS-252424	Phosphorylation	Inhibitor	P13Kgamma	0.941
(+)-Cyclazocine	Opioid	Antagonist		0.941
gamma-Acetylinic GABA	GABA	Inhibitor	GABA transaminase	0.941
8-Methoxymethyl-3-isobutyl-1-methylxanthine	Cyclic Nucleotides	Inhibitor	PDE 1	0.941
Cinnarizine	Ca2+ Channel	Blocker		0.941
Noscaphine hydrochloride	Opioid	Ligand		0.941
R-(+)-7-Hydroxy-DPAT hydrobromide	Dopamine	Agonist	D3	0.940
Idazoxan hydrochloride	Imidazoline	Ligand	I1 / I2	0.940
N-omega-Methyl-5-hydroxytryptamine oxalate salt	Serotonin	Ligand		0.940
Nipecotic acid	GABA	Inhibitor	Uptake	0.940
GW7647	Transcription	Agonist	PPAR-alpha	0.940
N6-Cyclohexyladenosine	Adenosine	Agonist	A1	0.940
13-cis-retinoic acid	Transcription	Regulator	RAR-alpha, beta	0.940
Sematilide monohydrochloride monohydrate	K+ Channel Modulator	Blocker	Kir	0.940
loxoprofen	Prostaglandin	Inhibitor	COX	0.940
Pimozide	Dopamine	Antagonist	D2	0.940
Oxaprozin	Prostaglandin	Inhibitor		0.940
Buspirone hydrochloride	Serotonin	Agonist	5-HT1A	0.940
Tranilast	Leukotriene	Inhibitor	LTC4	0.940
Lamotrigine	Anticonvulsant			0.939
6,7-ADTN hydrobromide	Dopamine	Agonist		0.939
Chlorpromazine hydrochloride	Dopamine	Antagonist		0.939
Clemizole hydrochloride	Histamine	Antagonist	H1	0.939
AGK2	Gene Regulation	Inhibitor	SIRT2	0.939
Oleic Acid	Phosphorylation	Activator	PKC	0.939
Zonisamide sodium	Anticonvulsant			0.939
IB-MECA	Adenosine	Agonist	A3	0.939
Isoxanthopterin	Cell Stress	Metabolite		0.939
Naratriptan hydrochloride	Serotonin	Agonist	5-HT1B/1D	0.939
ML-7	Phosphorylation	Inhibitor	MLCK	0.939
Mibefradil dihydrochloride	Ca2+ Channel	Blocker	T-type	0.938
PK 11195	GABA	Antagonist	Benzodiazepine	0.938
Doxepin hydrochloride	Adrenoceptor	Inhibitor	Uptake	0.938
SANT-2	Gene Regulation	Inhibitor	SMO	0.938
GSK137647A	Lipids	Agonist	FFA4/GPR120	0.938
BIO	Phosphorylation	Inhibitor	GSK-3alpha/beta	0.938
R(+)-JAA-94	Cl- Channel	Inhibitor		0.938
S15535	Serotonin	Agonist	5-HT1A	0.938
Oxotremorine methiodide	Cholinergic	Agonist	Muscarinic	0.938
5,7-Dichlorokynurenic acid	Glutamate	Antagonist	NMDA-glycine	0.938
CX 546	Glutamate	Modulator	AMPA	0.938
Pentoxifylline	Cyclic Nucleotides	Inhibitor	PDE	0.938
Naltrindole hydrochloride	Opioid	Antagonist	delta	0.938
L-Tryptophan	Serotonin	Precursor		0.938



Atropine methyl nitrate	Cholinergic	Antagonist	Muscarinic	0.937
LY-310,762 hydrochloride	Serotonin	Antagonist	5-HT1D	0.937
Rabeprazole sodium	Ion Channels	Inhibitor	Proton pump	0.937
Nicardipine hydrochloride	Ca2+ Channel	Antagonist	L-type	0.937
2-Cyclooctyl-2-hydroxyethylamine hydrochloride	Neurotransmission	Inhibitor	PNMT	0.937
Dolasetron mesylate hydrate	Serotonergic	Antagonist	5-HT3	0.936
PAPP	Serotonin	Agonist	5-HT1A	0.936
Eprosartan mesylate	Angiotensins	Antagonist	AT 1	0.936
3-(1H-Imidazol-4-yl)propyl di(p-fluorophenyl)methyl ether hydrochloride	Histamine	Antagonist	H3	0.936
ZD 7114 hydrochloride	Adrenergics	Agonist	Beta-three	0.935
3-Isobutyl-1-methylxanthine	Adenosine	Inhibitor	Phosphodiesterase	0.935
Darunavir	Protease	Inhibitor	HIV protease	0.935
Ropinrole hydrochloride	Dopamine	Agonist	D3	0.935
Putrescine dihydrochloride	Glutamate	Agonist	NMDA-Polyamine	0.935
(-)-cis-(1S,2R)-U-50488 tartrate	Neurotransmission	Ligand	Sigma receptor	0.934
L-3,4-Dihydroxyphenylalanine methyl ester hydrochloride	Dopamine	Precursor		0.934
Aminoguanidine hydrochloride	Nitric Oxide	Inhibitor	NOS	0.934
Caffeic Acid	Cell Stress	Inhibitor	Antioxidant	0.934
N-Methyl-1-deoxyojirrimycin	Biochemistry	Inhibitor	Glucosidase	0.934
L-745,870 hydrochloride	Dopamine	Antagonist	D4	0.934
Norcatharidin	Phosphorylation	Inhibitor	PP2A	0.934
Kainic acid	Glutamate	Agonist	Kainate	0.934
Olprinone hydrochloride	Phosphodiesterase	Inhibitor	PDE3	0.934
4-Aminopyridine	K+ Channel	Blocker	A-type	0.934
Icaritin	PPAR	Modulator		0.933
Clorgyline hydrochloride	Neurotransmission	Inhibitor	MAO-A	0.933
Ibudilast	Cyclic Nucleotides	Inhibitor	PDE IV	0.933
Molindone hydrochloride	Dopamine	Antagonist	D2	0.933
Muscarine chloride	Cholinergic	Agonist	Muscarinic	0.933
Loxapine succinate	Dopamine	Antagonist		0.933
Metolazone	Ion Pump	Inhibitor	Na+/Cl- transporter	0.933
GR 127935 hydrochloride hydrate	Serotonin	Antagonist	5-HT1B/1D	0.933
Pindolol	Adrenoceptor	Antagonist	beta	0.932
Cysteamine hydrochloride	Somatostatin	Deleter		0.932
Ketotifen fumarate	Histamine	Antagonist	H1	0.932
Clonixin	Inflammation	Inhibitor		0.932
Benztropine mesylate	Cell Signaling and Neuroscience	Antagonist	muscarinic acetylcholine receptor / DAT	0.932
Lidocaine N-ethyl bromide quaternary salt	Na+ Channel	Antagonist		0.932
Metoprolol (+)-tartrate	Adrenoceptor	Antagonist	beta1	0.931
Betaine aldehyde chloride	Cholinergic	Metabolite	Choline dehydrogenase	0.931
(-)-Tetramisole hydrochloride	Phosphorylation	Inhibitor		0.931
MRS 1523	Adenosine	Antagonist	A3	0.931
Cambinol	Gene Regulation	Inhibitor	SIRT1/2	0.931
NG-Monomethyl-L-arginine acetate	Nitric Oxide	Inhibitor	NOS	0.931
Piroxicam	Prostaglandin	Inhibitor	COX	0.931
Actinonin	Biochemistry	Inhibitor	Leucine aminopeptidase	0.931
TMB-8 hydrochloride	Intracellular Calcium	Antagonist		0.930
Retro-2	Cell Signaling and Neuroscience	Inhibitor		0.930
Amiloride hydrochloride	Na+ Channel	Blocker	Epithelial	0.930
(±)-2-Amino-4-phosphonobutyric acid	Glutamate	Antagonist	NMDA	0.930
2',3'-didehydro-3'-deoxythymidine	Immune System	Inhibitor	Reverse Transcriptase	0.929
Metoclopramide hydrochloride	Dopamine	Antagonist	D2	0.929
Niflumic acid	Prostaglandin	Inhibitor	COX-2	0.929
SR-95531	GABA	Antagonist	GABA-A	0.929
4-Amidinophenylmethanesulfonyl fluoride hydrochloride	Biochemistry	Inhibitor	Serine protease	0.929
1,10-Diaminodecane	Glutamate	Agonist (inverse)	NMDA-polyamine	0.929
HI-TOPK-032	Kinase inhibitors	Inhibitor	TPOK	0.929
Ethosuximide	Anticonvulsant			0.929
Ketoprofen	Prostaglandin	Inhibitor	COX-1	0.928
PNU-282987	Cholinergic	Agonist	Nicotinic alpha7	0.928
Ara-G hydrate	Apoptosis	inducer		0.928
Isoguvacine hydrochloride	GABA	Agonist	GABA(A)	0.928
Cetirizine dihydrochloride	Histamine	Antagonist	H1	0.927
DBO-83	Cholinergic	Agonist	Nicotinic	0.927
6-Nitroso-1,2-benzopyrone	Gene Regulation	Inhibitor	GLUT1	0.927
AMN082	Glutamate	Agonist	mGluR7	0.927
5-Fluorouracil	Cell Cycle	Inhibitor	Thymidylate synthetase	0.926
Esomeprazole magnesium dihydrate	Ion Channel	Inhibitor		0.926
S(-)-Carbidopa	Biochemistry	Inhibitor	L-aromatic amino acid decarboxylase	0.926
5-(N,N-hexamethylene)amiloride	Ion Pump	Inhibitor	Na+/H+ Antipporter	0.926
Stevioside	Ion Channels	Transport inhibitor	PAH	0.926
Lometrexol hydrate	Apoptosis	Inhibitor	GARFTase	0.926
(S)-3,5-Dihydroxyphenylglycine	Glutamate	Agonist	mGluR1	0.926
Darglitazone sodium salt	Gene Regulation	Agonist	PPAR/RXR	0.926
BTCP hydrochloride	Dopamine	Blocker	Reuptake	0.925
Icilin	Neurotransmission	Agonist	CMR1	0.925
Agomelatine	Melatonins	Agonist	MT1/MT2	0.925
Doxylamine succinate	Histamine	Antagonist	H1	0.924
K 185	Melatonin	Antagonist		0.924
Oxolinic acid	Antibiotic	Inhibitor	DNA Gyrase	0.923
OBAA	Phospholipases	Inhibitor		0.923
Adenosine	Adenosine	Agonist		0.923
NO-711 hydrochloride	GABA	Inhibitor	Uptake	0.923
N-Bromoacetamide	Na+ Channel	Modulator		0.923
MTEP hydrochloride	Excitatory Amino Acids	Antagonist	mGluR5	0.922
L-655,708	Benzodiazepine	Ligand	GABA-A	0.922
L-alpha-Methyl DOPA	Biochemistry	Inhibitor	Aromatic amino acid decarboxylase	0.922
Iproniazid phosphate	Neurotransmission	Inhibitor	MAO	0.922
Lidocaine hydrochloride	Na+ Channel	Modulator		0.922
Maprotiline hydrochloride	Adrenoceptor	Inhibitor	Reuptake	0.922
1-(m-Chlorophenyl)-biguanide hydrochloride	Serotonin	Agonist	5-HT3	0.922
S(-)-Timolol maleate	Adrenoceptor	Antagonist	beta	0.922
Arbidol hydrochloride	Antiviral	Inhibitor		0.922
Loperamide hydrochloride	Opioid	Ligand		0.921
GBR-12909 dihydrochloride	Dopamine	Inhibitor	Reuptake	0.921
Praziquantel	Antibiotic		Ca2+ Ionophore	0.921
Benserazide hydrochloride	Biochemistry	Inhibitor	Decarboxylase	0.921
Iodoacetamide	Biochemistry	Inhibitor		0.920
8-Cyclopentyl-1,3-dimethylxanthine	Adenosine	Antagonist	A1	0.920
Bay 11-7085	Cell Cycle	Inhibitor	IkB-alpha	0.920
Ellipticine	Cell Cycle	Inhibitor	CYP1A1 / Topol	0.920
U-69593	Opioid	Agonist	kappa	0.920
(-)-Naproxen sodium	Prostaglandin	Inhibitor	COX	0.919
Palmitoyl-DL-Carnitine chloride	Phosphorylation	Modulator	PKC	0.919
Imperatorin	Phosphorylation	Modulator	p38 / ERK	0.919
beta-Lapachone	Apoptosis	Activator		0.919
Dihydrocapsaicin	Vanilloid	Agonist		0.919
Cyclothiazide	Glutamate	Agonist	AMPA	0.919
Mephetyl tetrazole	K+ Channel	Blocker	Kv1.5	0.918
Minoxidil	K+ Channel	Activator	ATP sensitive	0.918
Rosuvastatin calcium	Cell Signaling and Neuroscience	Inhibitor	HMG-CoA	0.918
Aprindine hydrochloride	K+ Channel	Blocker	HERG	0.918
TNP	Ion Channels	Inhibitor	IP3K	0.918
Pilocarpine nitrate	Cholinergic	Agonist	Muscarinic	0.917
Rizatriptan benzoate salt	Neurotransmission	Agonist	5HT-1B/1D	0.917
SCH 58261	Purinoceptor	Antagonist	alpha2A	0.917
Debrisoquin sulfate	Neurotransmission	Antihypertensive		0.917

Lansoprazole	Ion Pump	Inhibitor	H+ pump	0.917
Famciclovir	Immune Cell Signaling	Antiviral		0.917
Meclofenamic acid sodium	Prostaglandin	Inhibitor	COX / 5-Lipoxygenase	0.917
Tazarotene	Cell Biology	Inducer	TIG3	0.916
Reserpine	Serotonin	Inhibitor	Uptake	0.916
Flupirtine maleate	Glutamate	Antagonist	NMDA	0.916
CGP-7930	GABA	Modulator	GABA-B	0.915
Linopirdine	Cholinergic	Releaser		0.915
Butaclamol hydrochloride	Dopamine	Antagonist	D2-D1	0.914
CGP-13501	GABA	Modulator	GABA-B	0.914
gamma-Vinyl GABA	GABA	Inhibitor	Transaminase	0.914
O-Methylserotonin hydrochloride	Serotonin	Agonist		0.914
Furosemide	Ion Pump	Inhibitor	Na+,K+,Cl- cotransport	0.914
Efaroxan hydrochloride	Imidazoline	Antagonist	I1	0.914
CGS-21680 hydrochloride	Adenosine	Agonist	A2a	0.913
R(-)-Me5	Na+ Channel	Antagonist		0.913
Dilazep hydrochloride	Adenosine	Inhibitor	Uptake	0.912
Nefiracetam	Neurotransmission	Neotropic		0.912
Tryptamine hydrochloride	Serotonin	Ligand		0.912
NF 023	P2 Receptor	Antagonist	P2X1	0.912
SKF-89145 hydrobromide	Dopamine	Agonist	D1	0.911
Allopurinol	Cell Stress	Inhibitor	Xanthine oxidase	0.911
L-Aspartic acid	Glutamate	Agonist		0.911
CyPPA	K+ Channels	Modulator	SK3 and SK2	0.911
Imatinib mesylate	Tyrosine Kinase	Inhibitor	Bcr-Abl	0.911
TBB	Phosphorylation	Inhibitor	Casein kinase 2	0.911
Nalidixic acid sodium	Antibiotic	Inhibitor	DNA Gyrase	0.911
Capecitabine	Gene Regulation			0.911
Epalrestat	Cell Stress	Inhibitor	Aldose reductase	0.910
Furatylfline	Biochemistry	Inhibitor	P450IA2	0.910
5-Nitro-2-(3-phenylpropylamino)benzoic acid	Cl- Channel	Blocker		0.910
Gossypol	Apoptosis	Inducer		0.909
(+)-Brompheniramine maleate	Histamine	Antagonist	H1	0.909
Melatonin	Melatonin	Agonist		0.909
m-Iodobenzylguanidine hemisulfate	Apoptosis	Activator		0.909
Darifenacin hydrobromide	Cholinergics	Antagonist	M3	0.909
Lonidamine	Cell Stress	Inhibitor	Mitochondrial hexokinase	0.908
Metrazoline oxalate	Imidazoline	Ligand		0.908
CBIO	K+ Channel	Activator	CFTR / KCNN4	0.908
Pentylentetrazole	Neurotransmission	Modulator	CNS	0.908
Loratadine	Histamine	Antagonist	H1	0.908
SHPP-33	Cytoskeleton and extracellular matrix	Inhibitor	microtubules	0.907
Enoximone	Cyclic Nucleotides	Inhibitor	PDE III	0.907
1,5-Isoquinolinediol	Apoptosis	Inhibitor	PARS	0.907
(±)-3-(3,4-dihydroxyphenyl)-2-methyl-DL-alanine	Neurotransmission	Inhibitor	L-aromatic amino acid decarboxylase	0.907
Dequalinium chloride hydrate	K+ Channel	Blocker		0.907
Lorcainide hydrochloride	Ion Channel Modulator	Inhibitor	Nav1.5	0.907
CR 2249	Glutamate	Agonist	NMDA-Glycine	0.907
4-Methylpyrazole hydrochloride	Biochemistry	Inhibitor	Alcohol dehydrogenase	0.907
S 24795	Cholinergics	Agonist	a7-nAChR	0.907
O6-benzylguanine	DNA Repair	Inhibitor	O6-alkylguanine-DNA alkyltransferase	0.906
L-alpha-Methyl-p-tyrosine	Neurotransmission	Inhibitor	Tyrosine hydroxylase	0.905
alpha-Methyl-4-carboxyphenylglycine	Glutamate	Antagonist	Metabotropic	0.905
SQ 22536	Cyclic Nucleotides	Inhibitor	Adenylyl cyclase	0.905
6-Methyl-2-(phenylethynyl)pyridine hydrochloride	Glutamate	Antagonist	mGluR5	0.904
WWL113	Cell Signaling	Inhibitor	Mouse (Ces3)/human CES1	0.904
AS605240	Biochemistry	Inhibitor	P13K	0.903
Antozoline hydrochloride	Imidazoline	Agonist		0.903
BF-170 hydrochloride	Neurodegeneration	Binder	Tau	0.903
Aminopterin	Antibiotic	Inhibitor	Dihydrofolate reductase	0.902
(+)-Pilocarpine hydrochloride	Cholinergic	Agonist	Muscarinic	0.902
R(-)-2,10,11-Trihydroxy-N-propylhoraporphine hydrobromide	Dopamine	Agonist	D2	0.902
DFB	Glutamate	Modulator	mGluR5	0.901
BW 284c51	Cholinergic	Inhibitor	Acetylcholinesterase	0.901
8-Cyclopentyl-1,3-dipropylxanthine	Adenosine	Antagonist	A1	0.900
Moxisylyte hydrochloride	Adrenoceptor	Antagonist	alpha1	0.899
N-Methyl-D-aspartic acid	Glutamate	Agonist	NMDA	0.899
DL-Buthionine-[S,R]-sulfoximine	Multi-Drug Resistance	Inhibitor		0.899
Roslin 2				0.899
Fexofenadine hydrochloride	Histamine	Antagonist	H1	0.899
ML396	Neurotransmitters	Modulator	mGlu group III PAM	0.899
Diclofenac sodium	Prostaglandin	Inhibitor	COX	0.899
8-Bromo-cAMP sodium	Cyclic Nucleotides	Activator		0.898
(+)-Quisqualic acid	Glutamate	Agonist	AMPA	0.898
R(-)-N6-(2-Phenylisopropyl)adenosine	Adenosine	Agonist	A1	0.898
Ciprofibrate	Transcription	Ligand	PPAR-alpha	0.898
3-Nitropropionic acid	Cell Stress	Toxin		0.898
NCS-382	GABA	Antagonist	gamma-Hydroxybutyrate	0.897
Leflunomide	Immune System	Inhibitor		0.897
Diethylenetriamipentaacetic acid	Biochemistry	Inhibitor	Zn2+-dependent protease	0.897
GW9662	Transcription	Inhibitor	PPAR-gamma	0.896
Cortisone	Hormone		Corticosteroid	0.896
BIX	Cell signaling	inducer	GRP78	0.895
LDN-27219	Neurobiology	Inhibitor	TG2	0.895
alpha-Methyl-5-hydroxytryptamine maleate	Serotonin	Agonist	5-HT2	0.895
Piracetam	Glutamate	Modulator	AMPA	0.895
Zimelidine dihydrochloride	Serotonin	Inhibitor	Reuptake	0.895
Morin	Cell Stress	Inhibitor	Antioxidant	0.895
L-Cycloserine	Sphingolipid	Inhibitor	Ketosphinganine synthetase	0.894
CGP 55845 hydrochloride	GABA	Antagonist	GABA-B	0.894
Tocainide hydrochloride	Na+ Channel	Blocker		0.894
Ketoconazole	Multi-Drug Resistance	Inhibitor	Cytochrome P450c17	0.892
4-Amino-1,8-naphthalimide	Apoptosis	Inhibitor	FARP	0.891
L-Glutamine	Glutamate	Agonist		0.891
IPA-3	Phosphorylation	Inhibitor	Pak1	0.891
Dicyclomine hydrochloride	Cholinergic	Antagonist	Muscarinic	0.891
3-Morpholinylsodnonimine hydrochloride	Nitric Oxide	Donor		0.891
R(-)-Apocodine hydrochloride	Dopamine	Agonist		0.891
3,4-Dichloroisocoumarin	Biochemistry	Inhibitor	Serine Protease	0.890
Nilutamide	Hormone	Inhibitor	Androgen	0.890
RS504393	Cytokines	Antagonist	CCR2	0.889
JW55	Gene Regulation	Inhibitor	TNKS1/2	0.889
LE 300	Dopamine	Antagonist	D1	0.889
Methylergonovine maleate	Dopamine	Antagonist		0.889
Nimustine hydrochloride	DNA	Intercalator		0.889
S-Nitrosoglutathione	Nitric Oxide	Donor		0.889
Amsacrine hydrochloride	DNA Repair	Inhibitor	Topoll	0.888
Anagrelide hydrochloride	Phosphodiesterase inhibitors	inhibitor		0.888
Formoterol	Adrenoceptor	Agonist	beta2	0.887
FPL 64176	Ca2+ Channel	Activator	L-type	0.886
Ro 90-7501	Neurodegeneration	Inhibitor	amyloid beta42 fibril formation	0.886
AZ191	Cell Cycle	Inhibitor	DYRK1B	0.886
Papaverine hydrochloride	Cyclic Nucleotides	Inhibitor	PDE	0.886
WB-4101 hydrochloride	Adrenoceptor	Antagonist	alpha1A	0.885
SB 674042	Cytokines	Antagonist	OX1R	0.885
Nitidine chloride	Apoptosis	Inducer		0.885
CB 1954	DNA	Intercalator		0.885

Triamcinolone	Hormone	Agonist	Glucocorticoid	0.884
Kynurenic acid	Glutamate	Antagonist	NMDA-Glycine	0.883
Nimesulide	Prostaglandin	Inhibitor	COX-2	0.883
Carboplatin	DNA	Intercalator		0.883
BTO-1	Phosphorylation	Inhibitor	Plk	0.882
DNQX	Glutamate	Antagonist	Kainate/quisqualate	0.882
Sorbinil	Antioxidants and Cytoprotectants	Inhibitor	AR	0.882
GSK1210151A	Gene Regulation	Inhibitor	BET	0.881
S-(4-Nitrobenzyl)-6-thiinosine	Adenosine	Inhibitor	Uptake	0.881
MDL 28170	Cell Cycle	Inhibitor	Calpain I / II	0.880
p-MPPF dihydrochloride	Serotonin	Antagonist	5-HT1A	0.880
Ketorolac tris salt	Prostaglandin	Inhibitor	COX	0.879
Naphazoline hydrochloride	Adrenoceptor	Agonist	alpha	0.879
Arcaine sulfate	Glutamate	Antagonist	NMDA-Polyamine	0.879
B-HT 933 dihydrochloride	Adrenoceptor	Agonist	alpha2	0.879
Methoxyverapamil hydrochloride	Ca2+ Channel	Antagonist	L-type	0.878
ET-18-OCH3	Lipid	Inhibitor	PIPLC	0.878
Diltiazem hydrochloride	Ca2+ Channel	Antagonist	L-type	0.878
Gallamine triethiodide	Cholinergic	Antagonist	M2	0.878
Y-27632 dihydrochloride	Phosphorylation	Inhibitor	ROCK	0.877
T0070907	Gene Regulation	Antagonist	PPAR gamma	0.876
Perifosine	Phosphorylation	Inhibitor	PKB/Akt	0.874
NS5806	Ion Channels	Modulator	Kv4.3	0.874
NBI 27914	Neurotransmission	Antagonist	CRF1	0.874
Phosphomycin disodium	Antibiotic		Cell wall synthesis	0.873
Naloxone hydrochloride	Opioid	Antagonist		0.872
L-687,384 hydrochloride	Opioid	Agonist	sigma1	0.872
SCH-28080	Ion Channels	Inhibitor	H+/K+-ATPase	0.872
2,6-Difluoro-4-[2-(phenylsulfonfylamino)ethylthio]phenoxyacetamide	Glutamate	Agonist	AMPA	0.870
Tamoxifen	Antibiotics/Phosphorylation	Inhibitor	Protein Kinase C	0.870
L-Glutamic acid hydrochloride	Glutamate	Agonist		0.870
Supercinnamaldehyde	Ion Channels	Activator	TRPA1	0.870
2,4-Diamino-6-pyrimidinone	Phosphorylation	Inhibitor	GTP cyclohydrolase I	0.870
Etodolac	Prostaglandin	Inhibitor	COX	0.869
S-Methyl-L-thiocitrulline acetate	Nitric Oxide	Inhibitor	NOS	0.869
Caffeine	Adenosine	Inhibitor	Phosphodiesterase	0.869
Nemadipine-A	Ca2+ Channels	Antagonist	L-type (alpha1)	0.868
L-Methionine sulfoximine	Glutamate	Inhibitor	Glutamine synthase	0.868
R(-)-Propylorapomorphine hydrochloride	Dopamine	Agonist	D2	0.867
5-fluoro-5'-deoxyuridine	DNA Metabolism	Inhibitor		0.867
Rufinamide	Neurotransmission	Anticonvulsant		0.867
7-Nitroindazole	Nitric Oxide	Inhibitor	nNOS	0.867
Bepridil hydrochloride	Ca2+ Channel	Blocker		0.866
Aurora-A Inhibitor I	kinase phosphatase	Inhibitor	Aurora kinase A	0.865
Etoposide	Apoptosis	Inhibitor	Topo II	0.865
Cyclophosphamide monohydrate	DNA	Intercalator		0.864
Moclobemide	Neurotransmission	Inhibitor	MAO	0.864
Doxazosin mesylate	Adrenoceptor	Blocker	alpha1	0.863
Levetiracetam	Neurotransmission	Anticonvulsant		0.863
MRS 2159	P2 Receptor	Antagonist	P2X1	0.862
Olvamil	Neurotransmission	Agonist	Vanilloid receptor	0.861
PD-407824	Kinase	Inhibitor	Wee1/Chk1	0.861
5-Aminovaleric acid hydrochloride	GABA	Antagonist	GABA-B	0.861
AC-93253 iodide	Hormone	Agonist	RAR(alpha)	0.861
SP600125	Phosphorylation	Inhibitor	c-JNK	0.861
Eupatorin	Cell Cycle	Inhibitor	CYP1A- family	0.860
LY-294,002 hydrochloride	Phosphorylation	Inhibitor	PI3K	0.859
3,5-Dinitrocatechol	Neurotransmission	Inhibitor	COMT	0.859
Choline bromide	Cholinergic	Substrate	Choline acetyltransferase	0.859
(+)-Bromocriptine methanesulfonate	Dopamine	Agonist	D2	0.859
Fluvoxamine maleate	Serotonin	Inhibitor	Reuptake	0.859
Cytidine 5'-diphosphocholine sodium salt hydrate	Lipid Signaling	Inhibitor	PLA2	0.859
E-64	Biochemistry	Inhibitor	Cysteine protease	0.858
(±) trans-U-50488 methanesulfonate	Opioid	Agonist	kappa	0.858
DPO-1	K+ Channel	Blocker	Ikur and Kv1.5	0.858
Fusidic acid sodium	Cell Cycle	Inhibitor		0.858
Betaine hydrochloride	Biochemistry	Metabolite		0.857
Sivelestat sodium salt hydrate	Biochemistry	Inhibitor	HNE	0.857
S-(+)-PD 123177 trifluoroacetate salt hydrate	Neurotransmission	Antagonist	AT2	0.857
Propofol	Cholinergic	Inhibitor	Muscarinic	0.857
1-[2-(Trifluoromethyl)phenyl]imidazole	Nitric Oxide	Inhibitor	NOS	0.856
L-701,324	Glutamate	Antagonist	NMDA-Glycine	0.855
ML 10302	Serotonin	Agonist	5-HT4	0.855
NG-Nitro-L-arginine	Nitric Oxide	Inhibitor	NOS	0.855
Glybenclamide	K+ Channel	Blocker	ATP-dependent	0.853
Torin2	Kinase/Phosphatase	Inhibitor	mTOR	0.853
Neostigmine bromide	Cholinergic	Inhibitor	Acetylcholinesterase	0.851
Chlorprothixene hydrochloride	Dopamine	Antagonist	D2	0.849
S-Ethylisothiourea hydrobromide	Nitric Oxide	Inhibitor	NOS	0.849
Nifedipine	Ca2+ Channel	Antagonist	L-type	0.848
SKF-38393 hydrochloride	Dopamine	Antagonist	D1	0.846
ISRIB	Serine/Threonine Kinase Inhibitors,	Inhibitor	eIF2a,PERK	0.846
(±)-2,3-Dichloro-alpha-methylbenzylamine hydrochloride	Neurotransmission	Inhibitor	PNMT	0.845
Bendipine hydrochloride	Ion Channel	Blocker	Calcium	0.841
Talnetant	Cell Signaling/Neuroscience	Antagonist	neurokinin 3	0.840
N-Methyl-beta-carboline-3-carboxamide	GABA	Antagonist	GABA-A	0.838
Benoxathian hydrochloride	Adrenoceptor	Antagonist	alpha1	0.837
G15	Bioactive Small Molecules	Antagonist	GPR30	0.836
Ganciclovir	Cell Cycle	Inhibitor	G2-M checkpoint	0.836
DAPH	Phosphorylation	Inhibitor	EGFR	0.836
Hydrocortisone	Hormone		Cortisol	0.836
Chlorpropamide	Hormone	Releaser	Insulin	0.835
N-Ethylmaleimide	Biochemistry	Inhibitor	Isocitrate dehydrogenase	0.831
BIX 01294 trihydrochloride hydrate	Gene Regulation	Inhibitor	HMT	0.829
1-(4-Chlorobenzyl)-5-methoxy-2-methylindole-3-acetic acid	Multi-Drug Resistance	Inhibitor	MRP1	0.829
Famotidine	Histamine	Antagonist	H2	0.812
Carmustine	DNA	Intercalator		0.807
Beclomethasone	Hormone		Glucocorticoid	0.805
Bezafibrate	Transcription	Agonist	PPAR	0.798
MKC-733	Serotonergic	Agonist	5-HT3	0.780
Fenspiride hydrochloride	Adrenoceptor	Antagonist	alpha	0.780
BWB70C	Leukotriene	Inhibitor	5-lipoxygenase	0.773
Betamethasone	Hormone		Glucocorticoid	0.769
Wiskostatin	Actin	Inhibitor	N-WASP	0.769
Budesonide	Hormone		Cortisol	0.724
Wortmannin from Penicillium funiculosum	Phosphorylation	Inhibitor	PI3K	0.724
GW2974	Phosphorylation	Inhibitor	EGFR / ErbB-2	0.647
ML240	Cell Signaling and Neuroscience	Inhibitor	AAA ATPase p97	0.608
PD 169316	Phosphorylation	Inhibitor	p38 MAP kinase	0.581
Tyrphostin AG 1478	Phosphorylation	Inhibitor	EGFR	0.580
PD153035 hydrochloride	Phosphorylation	Inhibitor	EGFR	0.557
SB 202190	Phosphorylation	Inhibitor	p38 MAPK	0.403
Brefeldin A from Penicillium brefeldianum	Cytoskeleton and ECM	Inhibitor	Golgi apparatus	0.360