

Pub-Name	Set	Target Mechanism	MW	CLOGP	TPSA	CLOGD	HBD	PKA	LE	LLE	LELP	Papp Op	Papp Mean	Papp SD
Acamprosate	Drugs	Glutamate receptors	181.2	-2.5	83.5	-6.1	2	1.0	0.41	9.32	-6.07			
Alprazolam	Drugs	Gaba Receptors	308.8	2.6	43.1	2.5	0	1.9	0.55	6.14	4.65			
Amfebutamone	Drugs	Dopaminergic GPCR	239.7	3.2	29.1	3.3	1	7.2	0.56	3.11	5.75	=	32.1	3.7
Amisulpride	Drugs	Dopaminergic GPCR	369.5	1.8	101.7	-0.2	3	9.0	0.50	9.12	3.62	=	1.1	0.0
Amphetamine	Drugs	Reuptake Inhibitors	135.2	1.7	26.0	-0.6	2	9.9	1.06	8.22	1.64			
Aniracetam	Drugs		219.2	0.7	46.6	0.3	0	1.0						
Apomorphine	Drugs	Dopaminergic GPCR	267.3	2.5	43.7	2.5	2	7.9	0.59	5.93	4.21	=	2.7	0.0
Aprepitant	Drugs		534.4	4.6	83.2	4.1	2	4.0	0.37	5.60	12.52	=	4.4	3.2
Aripiprazole	Drugs	Dopaminergic GPCR	448.4	5.3	44.8	5.5	1	6.7	0.43	3.59	12.47			
Atomoxetine	Drugs	Reuptake Inhibitors	255.4	3.9	21.3	0.7	1	10.1	0.61	7.59	6.44	=	16.7	9.8
Bromazepam	Drugs	Gaba Receptors	316.2	1.7	54.4	2.1	1	2.0	0.54	5.29	3.15	=	27.5	0.0
Bromocriptine	Drugs	Dopaminergic GPCR	654.6	6.6	118.2	5.1	3	6.7	0.28	3.63	23.25	=	5.5	3.5
Brotizolam	Drugs	Gaba Receptors	393.7	2.7	43.1	2.3	0	2.2	0.52	5.81	5.22	=	30.8	0.0
Budipine	Drugs	Calcium Channels	293.4	5.6	3.2	2.4	0	9.7	0.27	1.85	20.76			
Buprenorphine	Drugs	Opioid Receptor	467.6	4.0	62.2	2.5	2	8.3	0.41	7.50	9.73			
Buspirone	Drugs	Serotonergic GPCR	385.5	2.2	69.6	3.4	0	6.7	0.38	4.23	5.75	=	30.0	4.6
Cabergoline	Drugs	Dopaminergic GPCR	451.6	4.2	71.7	0.0	2	9.4	0.38	9.03	10.90	=	1.3	0.1
Caffeine	Drugs	Serotonergic GPCR	194.2	0.0	61.8	-0.1	0	1.0	0.50	5.11	-0.08	=	37.4	0.0
Carbamazepine	Drugs	Reuptake Inhibitors	236.3	2.4	46.3	2.7	2	1.0	0.34	1.67	7.06	=	36.1	2.2
Carisoprodol	Drugs		260.3	2.3	90.7	2.2	3	1.0						
Chlorpromazine	Drugs	Dopaminergic GPCR	318.9	5.3	6.5	2.9	0	9.4	0.53	5.13	9.94			
Citalopram	Drugs	Serotonergic GPCR	324.4	3.1	36.3	0.4	0	9.6	0.50	8.13	6.30	=	15.1	3.9
Clomipramine	Drugs	Serotonergic GPCR	314.9	5.9	6.5	3.5	0	9.5	0.63	6.31	9.44	=	1.9	0.7
Clonazepam	Drugs	Gaba Receptors	315.7	2.4	84.6	2.3	1	1.6	0.57	6.56	4.21	=	31.1	0.0
Clozapine	Drugs	Serotonergic GPCR	326.8	3.7	30.9	3.4	1	7.1	0.52	5.24	7.11	=	6.8	2.9
Cyclobenzaprine	Drugs		275.4	5.1	3.2	3.3	0	9.2						
Dexmethylphenidate	Drugs	Dopaminergic GPCR	233.3	2.6	38.3	-0.3	1	10.6						
Dextropropoxyphene	Drugs	Opioid Receptor	339.5	5.2	29.5	3.7	0	9.2	0.55	6.23	9.41			
Diazepam	Drugs	Gaba Receptors	284.7	3.0	32.7	3.0	0	3.4	0.45	3.52	6.53			
Donepezil	Drugs	Enzyme	379.5	4.6	38.8	3.3	0	8.8	0.38	4.34	12.04	=	21.9	8.2
Dronabinol	Drugs	Cannabinoids	314.5	7.2	29.5	7.7	1	1.0	0.47	-0.01	15.50			
Duloxetine	Drugs	Serotonergic GPCR	297.4	4.3	21.3	1.2	1	10.0	0.61	7.86	7.02			
Eletriptan	Drugs	Serotonergic GPCR	382.5	3.4	53.2	0.3	1	10.4	0.45	8.48	7.38	=	9.1	4.0
Escitalopram	Drugs	Serotonergic GPCR	324.4	3.1	36.3	0.4	0	9.6	0.52	8.56	6.00	=	16.1	0.8
Eszopiclone	Drugs	Gaba Receptors	388.8	1.3	91.8	0.7	0	6.8	0.36	6.34	3.46			
Ethosuximide	Drugs	Calcium Channels	141.2	0.4	46.2	0.4	1	1.0	0.88	5.88	0.45			
Felbamate	Drugs	Gaba Receptors	238.2	0.5	104.6	1.2	4	1.0						

Pub-Name	Set	Target Mechanism	MW	CLOGP	TPSA	CLOGD	HBD	PKA	LE	LLE	LELP	Papp Op	Papp Mean	Papp SD
Fentanyl	Drugs	Opioid Receptor	336.5	3.6	23.6	2.5	0	9.1	0.48	6.01	7.57			
Flumazenil	Drugs	Gaba Receptors	303.3	1.3	64.4	0.9	0	1.1	0.59	8.44	2.18	=	30.8	4.3
Fluoxetine	Drugs	Serotonergic GPCR	309.3	4.6	21.3	1.6	1	10.1	0.57	7.40	8.01	=	2.1	1.3
Fluvoxamine	Drugs	Serotonergic GPCR	318.3	3.3	56.8	1.2	2	9.4	0.55	7.49	6.04	=	7.5	3.6
Gabapentin	Drugs	Calcium Channels	171.2	-0.7	63.3	-1.3	3	10.3	0.77	7.91	-0.86			
Galantamine	Drugs	Enzyme	287.4	1.0	41.9	1.1	1	7.9	0.62	8.24	1.64	=	15.6	0.0
Haloperidol	Drugs	Dopaminergic GPCR	375.9	3.8	40.5	2.1	1	8.3	0.47	6.65	8.22			
Hydrocodone	Drugs	Opioid Receptor	299.4	1.1	38.8	0.7	0	8.5				=	29.5	0.0
Indeloxazine	Drugs	Reuptake Inhibitors	231.3	2.2	30.5	0.4	1	8.5	0.64	7.31	3.46	=	25.2	0.0
Lamotrigine	Drugs	Reuptake Inhibitors	256.1	2.5	90.7	-0.2	4	5.4	0.44	5.19	5.79	=	24.7	4.0
Levetiracetam	Drugs	Calcium Channels	170.2	-0.3	63.4	-0.7	2	1.0	0.56	5.50	-0.61			
Levomethadyl Acetate	Drugs	Opioid Receptor	353.5	4.6	29.5	3.5	0	9.4						
Lofexidine	Drugs		259.1	3.5	33.6	1.7	1	9.8						
Lorazepam	Drugs	Gaba Receptors	321.2	2.4	61.7	2.5	2	1.0	0.58	6.27	4.06	=	24.7	2.4
Meprobamate	Drugs		218.3	0.9	104.6	0.7	4	1.0						
Methylphenidate	Drugs	Dopaminergic GPCR	233.3	2.6	38.3	-0.3	1	10.6	0.58	7.36	4.38	=	28.3	0.0
Metoclopramide	Drugs		299.8	2.2	67.6	0.0	3	9.7						
Midazolam	Drugs	Gaba Receptors	325.8	3.4	30.2	3.9	0	5.6	0.53	4.85	6.41			
Milnacipran	Drugs	Serotonergic GPCR	246.3	1.9	46.3	-1.5	2	10.4	0.54	8.43	3.55			
Minaprine	Drugs	Enzyme	298.4	3.2	50.3	1.2	1	7.1				=	36.6	0.0
Mirtazapine	Drugs		265.4	2.8	19.4	2.1	0	8.1				=	25.9	7.0
Moclobemide	Drugs	Enzyme	268.7	2.2	41.6	0.7	1	6.9	0.27	2.73	8.11	=	35.2	13.9
Modafinil	Drugs	Dopaminergic GPCR	273.4	0.9	60.2	1.2	2	1.0						
Morphine	Drugs	Opioid Receptor	285.3	0.6	52.9	-0.4	2	8.3	0.61	9.55	0.94			
Nalmefene	Drugs	Opioid Receptor	339.4	2.6	52.9	2.1	2	7.7	0.50	6.90	5.24			
Naltrexone	Drugs	Opioid Receptor	341.4	0.4	70.0	1.4	2	7.5	0.56	8.61	0.64	=	20.4	3.7
Nemonapride	Drugs	Dopaminergic GPCR	387.9	4.2	53.6	2.0	2	8.4	0.56	8.83	7.46	=	20.6	0.0
Nicergoline	Drugs		484.4	4.1	56.6	3.8	0	7.8						
Nicotrol	Drugs	Nicotinic Receptor	162.2	0.9	16.1	-0.5	0	8.0	1.05	9.47	0.84	=	28.1	4.2
Nimodipine	Drugs	Calcium Channels	418.4	4.0	117.0	3.9	1	2.8	0.17	-0.17	23.30	=	15.4	0.0
Nortriptyline	Drugs		263.4	4.3	12.0	3.2	1	10.0						
Olanzapine	Drugs	Dopaminergic GPCR	312.4	3.0	30.9	2.5	1	7.8	0.51	5.50	5.91	=	18.8	11.8
Oxcarbazepine	Drugs	Reuptake Inhibitors	252.3	1.2	63.4	1.3	2	1.0	0.28	2.54	4.31			
Oxycodone	Drugs	Opioid Receptor	315.4	0.0	59.0	1.2	1	7.6	0.45	6.15	-0.09	=	28.3	0.0
Paliperidone	Drugs	Dopaminergic GPCR	426.5	1.1	84.4	1.0	1	7.9	0.39	7.59	2.78	=	21.5	0.0
Paroxetine	Drugs	Serotonergic GPCR	329.4	4.2	39.7	1.2	1	10.3	0.61	9.21	6.99	=	1.0	0.2
Pergolide	Drugs	Dopaminergic GPCR	314.5	4.4	19.0	2.2	1	9.7	0.49	5.55	8.95	=	9.7	6.3

Pub-Name	Set	Target Mechanism	MW	CLOGP	TPSA	CLOGD	HBD	PKA	LE	LLE	LELP	Papp Op	Papp Mean	Papp SD
Perospirone	Drugs	Dopaminergic GPCR	426.6	3.8	56.8	2.4	0	8.4	0.43	6.85	8.73			
phenytoin	Drugs	Reuptake Inhibitors	252.3	2.1	58.2	2.5	2	1.0	0.67	6.54	3.13	=	28.6	2.6
Piracetam	Drugs		142.2	-1.2	63.4	-1.6	2	1.0						
Pramipexole	Drugs	Dopaminergic GPCR	211.3	1.2	50.9	-0.5	3	9.5	0.93	9.84	1.25	=	12.8	0.0
Pregabalin	Drugs	Calcium Channels	159.2	-0.9	63.3	-1.4	3	11.3	0.88	8.30	-1.04			
Propofol	Drugs		178.3	3.9	20.2	4.2	1	1.0						
Propoxyphene	Drugs		339.5	5.2	29.5	3.7	0	9.2						
Quazepam	Drugs	Gaba Receptors	386.8	3.2	15.6	4.1	0	1.0	0.43	3.59	7.42			
Quetiapine	Drugs	Serotonergic GPCR	383.5	3.0	48.3	1.6	1	5.8	0.36	5.41	8.29	=	21.8	1.4
Ramelteon	Drugs	Melatonin Receptor	259.3	2.5	38.3	2.6	1	1.0	0.80	8.29	3.11	=	33.4	1.9
Rasagiline	Drugs	Enzyme	171.2	2.5	12.0	1.9	1	7.5	0.85	5.93	2.98			
Reboxetine	Drugs	Reuptake Inhibitors	313.4	3.3	39.7	1.8	1	8.4	0.49	6.25	6.66	=	12.2	0.0
Remifentanyl	Drugs	Opioid Receptor	376.4	2.0	76.2	2.0	0	6.6						
Riluzole	Drugs	Reuptake Inhibitors	234.2	3.2	48.1	2.8	2	3.6	0.41	1.55	7.89	=	30.4	5.3
Rimonabant	Drugs	Cannabinoids	463.8	6.5	50.2	6.0	1	3.2	0.38	2.20	16.88	=	3.5	1.8
Risperidone	Drugs	Dopaminergic GPCR	410.5	2.7	64.2	2.3	0	7.9	0.44	7.23	6.10	=	23.2	10.9
Rivastigmine	Drugs	Enzyme	250.3	2.1	32.8	0.9	0	8.6	0.43	4.65	4.83	=	27.3	4.8
Ropinirole	Drugs	Dopaminergic GPCR	260.4	2.8	32.3	1.2	1	9.5	0.60	6.94	4.66	=	26.9	7.0
Ropivacaine	Drugs		274.4	3.2	32.3	2.6	1	8.2				=	43.4	0.0
Selegiline	Drugs	Enzyme	187.3	3.0	3.2	2.6	0	7.5	0.82	5.59	3.70	=	25.9	0.0
Sertindole	Drugs	Serotonergic GPCR	440.9	5.3	40.5	3.8	1	9.1	0.45	6.05	11.84	=	0.1	0.0
Sertraline	Drugs	Serotonergic GPCR	306.2	5.3	12.0	2.8	1	9.5	0.67	6.82	7.97	=	2.2	0.0
Sinequan	Drugs	Serotonergic GPCR	279.4	4.1	12.5	2.1	0	9.2	0.50	5.49	8.11	=	10.4	0.0
Sulpiride	Drugs	Dopaminergic GPCR	341.4	1.1	101.7	-1.4	3	9.0	0.50	9.57	2.23	=	0.3	0.0
Tacrine	Drugs	Enzyme	198.3	3.3	38.9	1.1	2	9.6	0.70	6.47	4.66	=	30.1	7.5
Talipexole	Drugs	Dopaminergic GPCR	209.3	1.1	42.2	1.0	2	7.2	0.63	5.29	1.82	=	22.9	6.7
Terguride	Drugs	Dopaminergic GPCR	340.5	2.8	51.4	1.4	2	9.8	0.53	8.00	5.25			
Thiopental	Drugs	Gaba Receptors	242.3	1.8	58.5	-0.7	1	1.0						
Tiagabine	Drugs	Gaba Receptors	375.5	2.8	40.5	3.2	1	9.4	0.39	3.79	7.12	=	20.7	1.9
Tianeptine	Drugs	Reuptake Inhibitors	437.0	1.5	86.7	0.4	2	7.5				=	22.7	5.2
Topiramate	Drugs	Enzyme	339.4	0.0	115.5	3.0	2	1.0	0.58	6.09	0.07			
Tramadol	Drugs	Reuptake Inhibitors	263.4	3.1	32.7	0.5	1	9.6	0.46	5.71	6.78			
Trazodone	Drugs	Serotonergic GPCR	371.9	3.9	45.8	1.6	0	6.7	0.43	6.31	9.03			
Tropisetron	Drugs	Serotonergic GPCR	284.4	2.9	45.3	1.0	1	10.0	0.58	7.66	4.97			
Valproic Acid	Drugs		144.2	2.8	37.3	0.2	1	1.0						
Varenicline	Drugs	Nicotinic Receptor	211.3	0.9	37.8	-1.3	1	9.6	0.87	11.29	1.03	=	24.6	0.0
Venlafaxine	Drugs	Serotonergic GPCR	277.4	3.3	32.7	1.2	1	9.3	0.52	6.27	6.26	=	20.7	6.1

Pub-Name	Set	Target Mechanism	MW	CLOGP	TPSA	CLOGD	HBD	PKA	LE	LLE	LELP	Papp Op	Papp Mean	Papp SD
Verapamil	Drugs	Calcium Channels	454.6	4.5	64.0	2.3	0	9.0	0.38	6.52	11.89			
Vigabatrin	Drugs	Gaba Receptors	129.2	-2.2	63.3	-2.6	3	10.6	0.40	5.19	-5.51			
Vinpocetine	Drugs		350.5	4.8	34.5	4.6	0	7.8				=	4.7	1.6
Zaleplon	Drugs	Gaba Receptors	305.3	1.4	74.3	0.9	0	1.0	0.45	6.47	3.21	=	37.1	0.0
Ziprasidone	Drugs	Dopaminergic GPCR	412.9	4.2	48.5	3.1	1	8.4	0.45	5.85	9.44	=	10.3	0.0
Zolpidem	Drugs	Gaba Receptors	307.4	3.0	37.6	2.9	0	6.6	0.47	4.85	6.44	=	80.3	0.0
Zonisamide	Drugs	Enzyme	212.2	-0.4	86.2	-0.1	2	1.0	0.83	8.40	-0.44	=	29.1	0.0
Zotepine	Drugs	Serotonergic GPCR	331.9	5.1	12.5	5.2	0	8.7	0.55	3.35	9.35			
Candidate-001	Candidates	Glutamate receptors	276.2	-0.5	112.1	0.3	2	6.9	0.50	6.83	-0.91			
Candidate-002	Candidates	Reuptake Inhibitors	255.3	3.7	21.3	1.7	1	9.1	0.62	6.25	5.93	=	7.8	5.6
Candidate-003	Candidates	Reuptake Inhibitors	326.2	5.5	21.3	2.7	1	10.1	0.57	5.94	9.55	=	11.4	8.2
Candidate-004	Candidates	Serotonergic GPCR	391.5	2.0	78.5	0.0	2	10.3	0.40	7.78	4.92			
Candidate-005	Candidates	Enzyme	375.5	3.9	58.4	2.1	1	8.8	0.48	7.47	8.23			
Candidate-006	Candidates	Peptide GPCR	379.5	2.6	53.6	0.2	2	9.9	0.50	9.83	5.23	=	8.4	1.4
Candidate-007	Candidates	Enzyme	311.4	4.1	51.4	2.3	2	8.7	0.46	5.22	8.97	=	1.0	0.0
Candidate-008	Candidates	Calcium Channels	159.2	-0.8	63.3	-1.1	3	10.6	0.96	8.59	-0.89			
Candidate-009	Candidates	Nicotinic Receptor	269.1	1.0	34.0	-2.2	1	10.2	0.90	11.81	1.10			
Candidate-010	Candidates	Opioid Receptor	372.5	4.7	49.4	2.3	1	9.4	0.48	6.59	9.76	=	18.4	0.3
Candidate-011	Candidates	Dopaminergic GPCR	436.5	3.7	87.2	3.1	1	6.6	0.40	5.75	9.23			
Candidate-012	Candidates	Peptide GPCR	459.6	5.5	80.2	5.4	1	5.1	0.33	2.64	16.65	=	5.0	1.8
Candidate-013	Candidates	Enzyme	378.5	5.3	33.2	3.0	0	8.8	0.43	5.25	12.42	=	11.4	0.0
Candidate-014	Candidates	Opioid Receptor	396.5	3.3	45.9	1.8	0	9.9	0.35	5.44	9.52	=	19.9	0.0
Candidate-015	Candidates	Nicotinic Receptor	271.3	1.7	58.4	-0.9	1	9.1	0.62	9.70	2.69			
Candidate-016	Candidates	Gaba Receptors	336.4	2.0	61.4	2.2	0	6.2	0.48	6.40	4.15	=	31.5	2.9
Candidate-017	Candidates	Enzyme	468.5	2.2	105.8	0.3	1	5.7	0.40	9.38	5.48	=	20.6	14.0
Candidate-018	Candidates	Cannabinoids	436.3	5.6	38.1	4.9	0	1.0	0.45	4.28	12.60	=	6.1	1.9
Candidate-019	Candidates	Peptide GPCR	392.9	6.0	80.7	6.3	2	4.0	0.42	1.94	14.04	=	7.8	0.0
Candidate-020	Candidates	Glutamate receptors	402.5	3.2	66.3	2.2	1	8.1	0.41	6.05	7.75	=	14.9	0.0
Candidate-021	Candidates	Enzyme	315.4	3.1	60.6	1.1	2	8.6	0.47	6.55	6.56	=	5.4	5.1
Candidate-022	Candidates	Enzyme	489.6	5.6	71.0	2.1	3	10.4	0.36	6.85	15.66	=	0.5	0.8
Candidate-023	Candidates	Nicotinic Receptor	227.2	2.6	12.0	-0.2	1	10.0	0.76	8.93	3.47	=	12.8	12.7
Candidate-024	Candidates	Calcium Channels	187.3	0.1	63.3	-0.3	3	11.2	0.88	8.48	0.16			
Candidate-025	Candidates	Reuptake Inhibitors	319.8	4.5	21.3	1.5	1	10.3	0.53	6.79	8.52			
Candidate-026	Candidates	Serotonergic GPCR	322.8	2.9	50.3	3.8	1	7.8	0.58	5.25	4.95	=	3.3	1.0
Candidate-027	Candidates	Serotonergic GPCR	447.6	4.1	57.9	1.5	0	8.7	0.37	7.30	10.93	=	4.1	5.4
Candidate-028	Candidates	Histaminergic GPCR	322.4	2.4	32.3	0.0	1	9.2	0.53	8.75	4.54	=	51.5	0.0
Candidate-029	Candidates	Glutamate receptors	327.4	1.8	63.9	0.8	3	8.2	0.47	7.36	3.79	=	26.5	0.0

Pub-Name	Set	Target Mechanism	MW	CLOGP	TPSA	CLOGD	HBD	PKA	LE	LLE	LELP	Papp Op	Papp Mean	Papp SD
Candidate-030	Candidates	Peptide GPCR	296.4	3.4	33.3	0.8	2	9.9	0.56	8.01	6.08	=	15.3	3.1
Candidate-031	Candidates	Serotonergic GPCR	383.5	1.9	69.6	2.0	0	6.7	0.39	5.91	4.84	=	32.8	8.1
Candidate-032	Candidates	Gaba Receptors	310.4	1.1	61.4	2.3	0	6.5	0.47	5.00	2.34	=	26.0	5.3
Candidate-033	Candidates	Opioid Receptor	426.6	3.1	69.6	0.8	2	10.3	0.45	8.72	6.98	=	15.7	1.1
Candidate-034	Candidates	Reuptake Inhibitors	308.4	3.5	41.1	3.3	1	7.1	0.53	5.48	6.59	=	4.0	3.8
Candidate-035	Candidates	Calcium Channels	185.3	-0.2	63.3	-0.9	3	10.3	0.86	8.90	-0.21			
Candidate-036	Candidates	Peptide GPCR	326.5	7.6	34.2	7.1	1	7.2	0.50	1.51	15.13			
Candidate-037	Candidates	Gaba Receptors	324.3	2.5	74.3	-2.8	2	12.4	0.51	11.59	4.95			
Candidate-038	Candidates	Serotonergic GPCR	417.5	5.1	26.8	3.6	0	7.8	0.39	4.68	13.16			
Candidate-039	Candidates	Glutamate receptors	462.9	5.6	51.0	4.0	0	8.5	0.30	3.13	18.51	=	3.3	0.0
Candidate-040	Candidates	Enzyme	395.5	-1.5	101.8	-0.7	1	7.9	0.39	8.75	-3.79	=	38.4	0.0
Candidate-041	Candidates	Peptide GPCR	380.4	4.6	42.5	1.9	2	9.9	0.54	8.43	8.54	=	8.4	4.0
Candidate-042	Candidates	Serotonergic GPCR	304.8	2.9	50.3	2.8	1	7.4	0.61	6.32	4.76			
Candidate-043	Candidates	Peptide GPCR	394.9	2.1	50.1	0.7	0	8.7	0.42	7.81	5.02			
Candidate-044	Candidates	Serotonergic GPCR	355.4	3.3	37.4	2.5	1	8.2	0.47	6.32	7.01	=	2.9	1.0
Candidate-045	Candidates	Cannabinoids	510.4	4.1	102.0	2.7	3	7.0	0.36	6.30	11.37	=	9.3	5.5
Candidate-046	Candidates	Serotonergic GPCR	448.4	5.7	26.8	4.8	0	7.7	0.46	4.80	12.19	=	3.9	0.0
Candidate-047	Candidates	Calcium Channels	187.3	0.1	63.3	-0.2	3	10.3	0.85	8.05	0.09			
Candidate-048	Candidates	Dopaminergic GPCR	430.5	5.2	57.7	4.8	1	7.1	0.40	4.32	12.88			
Candidate-049	Candidates	Serotonergic GPCR	455.0	5.7	48.5	3.5	1	8.4	0.44	6.37	12.80	=	6.0	0.4
Candidate-050	Candidates	Gaba Receptors	373.4	2.5	83.2	-0.1	3	9.3	0.46	9.07	5.27	=	1.7	0.1
Candidate-051	Candidates	Reuptake Inhibitors	363.3	3.7	48.3	1.9	1	8.3	0.45	6.52	8.20	=	2.5	1.7
Candidate-052	Candidates	Enzyme	385.3	3.1	52.2	5.0	1	1.0	0.39	2.30	7.93			
Candidate-053	Candidates	Nicotinic Receptor	227.2	2.6	12.0	-0.2	1	10.0	0.82	9.57	3.23	=	31.0	1.7
Candidate-054	Candidates	Opioid Receptor	319.5	6.4	3.2	5.3	0	8.6	0.39	1.34	16.32			
Candidate-055	Candidates	Enzyme	388.5	5.1	34.5	2.6	0	8.8	0.38	5.31	13.40	=	7.5	6.8
Candidate-056	Candidates	Enzyme	392.5	3.8	52.8	3.5	0	4.3	0.44	5.84	8.79	=	7.8	2.1
Candidate-057	Candidates	Dopaminergic GPCR	391.5	4.3	39.5	4.7	0	7.3	0.42	4.04	10.15	=	4.9	0.0
Candidate-058	Candidates	Peptide GPCR	614.7	6.0	149.6	2.2	5	1.0	0.28	6.70	21.74	=	0.5	0.0
Candidate-059	Candidates	Dopaminergic GPCR	480.9	4.9	61.5	5.8	1	6.7	0.36	2.70	13.71			
Candidate-060	Candidates	Serotonergic GPCR	464.6	5.3	45.0	1.5	0	9.7	0.35	6.98	15.21	=	3.4	0.0
Candidate-061	Candidates	Histaminergic GPCR	350.4	3.4	32.3	0.9	1	9.2	0.50	8.10	6.64	=	42.7	8.0
Candidate-062	Candidates	Dopaminergic GPCR	433.5	4.9	44.8	3.3	1	6.8	0.37	5.17	13.15			
Candidate-063	Candidates	Nicotinic Receptor	288.3	1.7	50.8	-0.7	1	9.7	0.54	8.75	3.07	=	3.8	1.0
Candidate-064	Candidates	Serotonergic GPCR	275.7	3.7	21.3	1.4	1	9.0	0.64	6.81	5.86	=	9.5	0.0
Candidate-065	Candidates	Peptide GPCR	417.3	6.2	63.0	3.8	2	6.3	0.48	5.06	12.93	=	14.9	0.0
Candidate-066	Candidates	Serotonergic GPCR	436.6	3.3	59.9	2.2	1	7.8	0.39	6.74	8.50	=	18.7	2.8

Pub-Name	Set	Target Mechanism	MW	CLOGP	TPSA	CLOGD	HBD	PKA	LE	LLE	LELP	Papp Op	Papp Mean	Papp SD
Candidate-067	Candidates	Dopaminergic GPCR	463.5	5.4	69.7	4.3	2	6.8	0.36	4.58	14.82			
Candidate-068	Candidates	Serotonergic GPCR	469.0	6.2	48.5	4.8	1	8.4	0.42	4.86	14.71	=	2.8	0.0
Candidate-069	Candidates	Reuptake Inhibitors	300.2	5.1	21.3	3.4	1	9.0	0.63	5.13	8.09	=	9.3	0.0
Candidate-070	Candidates	Dopaminergic GPCR	221.3	1.3	42.2	1.1	2	7.0	0.66	6.00	1.96	=	20.4	0.0
Candidate-071	Candidates	Reuptake Inhibitors	376.9	1.7	41.4	-0.9	0	10.1	0.43	8.81	4.04	=	13.2	0.0
Candidate-072	Candidates	Dopaminergic GPCR	360.4	3.1	41.5	4.1	0	7.8	0.46	4.41	6.71	=	8.2	0.0
Candidate-073	Candidates	Gaba Receptors	323.3	2.2	84.1	4.1	2	1.0	0.50	4.41	4.48	=	5.8	0.0
Candidate-074	Candidates	Peptide GPCR	327.5	7.6	31.4	6.2	0	5.6	0.52	2.67	14.60			
Candidate-075	Candidates	Nicotinic Receptor	271.3	1.7	58.4	-1.2	1	9.5	0.51	8.40	3.27	=	18.3	4.5
Candidate-076	Candidates	Nicotinic Receptor	258.3	1.6	45.4	0.4	0	8.9	0.61	7.94	2.55	=	22.7	1.0
Candidate-077	Candidates	Gaba Receptors	316.3	2.0	71.2	1.4	2	1.0	0.52	7.03	3.97	=	21.2	8.6
Candidate-078	Candidates	Reuptake Inhibitors	335.3	2.9	39.7	1.5	1	8.3	0.51	7.24	5.70	=	15.8	3.7
Candidate-079	Candidates	Calcium Channels	187.3	0.2	63.3	0.0	3	10.5	0.82	7.61	0.26			
Candidate-080	Candidates	Dopaminergic GPCR	367.4	3.0	65.3	3.4	0	7.2	0.46	5.46	6.48	=	12.6	0.0
Candidate-081	Candidates	Serotonergic GPCR	382.5	2.8	39.7	2.3	0	7.2	0.43	6.40	6.50	=	32.4	0.0
Candidate-082	Candidates	Gaba Receptors	297.4	1.2	74.0	-1.9	3	9.6	0.49	9.66	2.52	=	2.6	3.7
Candidate-083	Candidates	Cannabinoids	452.3	5.8	47.4	5.1	0	1.0	0.42	4.00	13.59	=	7.1	0.0
Candidate-084	Candidates	Gaba Receptors	360.4	2.6	72.3	3.1	0	4.0	0.44	5.44	5.90	=	31.2	8.0
Candidate-085	Candidates	Reuptake Inhibitors	294.4	3.2	52.6	1.5	1	8.4	0.53	6.54	6.07			
Candidate-086	Candidates	Muscarinic Receptor	270.3	2.5	34.1	3.9	0	5.5	0.54	3.91	4.59	=	23.0	0.0
Candidate-087	Candidates	Cannabinoids	496.4	4.3	101.4	2.2	3	5.7	0.40	7.48	10.70	=	3.7	0.0
Candidate-088	Candidates	Dopaminergic GPCR	357.8	3.5	44.8	2.3	1	5.8	0.49	6.41	7.17	=	16.7	0.0
Candidate-089	Candidates	Enzyme	271.4	2.2	60.2	0.3	3	9.4	0.53	7.22	4.23	=	9.6	2.0
Candidate-090	Candidates	Glutamate receptors	359.4	1.6	73.2	1.1	3	6.8	0.42	6.63	3.82	=	18.2	0.0
Candidate-091	Candidates	Gaba Receptors	330.4	2.5	71.2	2.0	2	1.0	0.46	5.97	5.44	=	19.9	6.6
Candidate-092	Candidates	Reuptake Inhibitors	360.3	3.1	50.2	0.6	1	8.1	0.41	7.00	7.55	=	11.9	0.0
Candidate-093	Candidates	Muscarinic Receptor	269.2	5.2	15.6	2.3	0	7.3	0.56	4.51	9.38	=	23.3	0.0
Candidate-094	Candidates	Dopaminergic GPCR	420.5	4.9	44.3	3.7	1	7.8	0.36	4.32	13.58	=	6.8	5.4
Candidate-095	Candidates	Gaba Receptors	321.3	2.9	68.5	0.9	1	2.1	0.49	7.55	5.90			
Candidate-096	Candidates	Serotonergic GPCR	419.6	4.1	47.0	2.3	1	7.8	0.41	6.86	9.88	=	36.0	0.0
Candidate-097	Candidates	Reuptake Inhibitors	309.8	4.9	30.5	3.1	1	8.6	0.57	5.47	8.53	=	7.5	5.6
Candidate-098	Candidates	Enzyme	460.5	4.1	52.8	4.8	0	4.1	0.36	4.02	11.34	=	1.7	0.0
Candidate-099	Candidates	Peptide GPCR	412.6	5.6	24.5	3.5	1	10.0	0.45	6.49	12.39	=	5.7	2.5
Candidate-100	Candidates	Enzyme	400.3	8.6	49.3	5.4	2	1.0	0.30	0.42	28.68			
Candidate-101	Candidates	Dopaminergic GPCR	434.6	5.2	48.5	3.7	1	8.4	0.40	5.11	13.06			
Candidate-102	Candidates	Serotonergic GPCR	450.6	4.1	69.9	3.7	0	8.0	0.39	5.60	10.29	=	15.1	10.4
Candidate-103	Candidates	Dopaminergic GPCR	329.5	6.4	3.2	5.0	0	8.4	0.48	3.65	13.31			

Pub-Name	Set	Target Mechanism	MW	CLOGP	TPSA	CLOGD	HBD	PKA	LE	LLE	LELP	Papp Op	Papp Mean	Papp SD
Candidate-104	Candidates	Peptide GPCR	419.6	3.2	53.6	1.2	2	9.9	0.46	9.05	7.03	=	10.7	6.8
Candidate-105	Candidates	Gaba Receptors	298.3	2.4	71.2	1.5	2	1.3	0.52	6.66	4.58	=	12.7	5.6
Candidate-106	Candidates	Peptide GPCR	493.6	5.8	103.5	4.6	4	1.0				=	16.8	0.0
Candidate-107	Candidates	Calcium Channels	173.3	-0.3	63.3	-0.5	3	10.5	0.88	8.07	-0.36			
Candidate-108	Candidates	Nicotinic Receptor	209.2	2.5	12.0	0.2	1	10.1	0.88	9.17	2.90	=	28.9	1.1

Pub-Name	Set	Target Mechanism	Papp CV	Papp SEM	Papp Up95	Papp Low95	Papp N	Pgp OP	Pgp Mean	Pgp SD	Pgp CV	Pgp SEM	Pgp Up95
Acamprosate	Drugs	Glutamate receptors					0						
Alprazolam	Drugs	Gaba Receptors						=	1.4	0.0	0.0	0.0	1.4
Amfebutamone	Drugs	Dopaminergic GPCR	11.5	2.1	41.2	23.0	3	=	1.2	0.3	23.3	0.1	1.6
Amisulpride	Drugs	Dopaminergic GPCR	0.0	0.0	1.1	1.1	1	>	9.2	9.4	102.3	5.4	32.6
Amphetamine	Drugs	Reuptake Inhibitors											
Aniracetam	Drugs							=	1.1	0.0	0.0	0.0	1.1
Apomorphine	Drugs	Dopaminergic GPCR	0.0	0.0	2.7	2.7	1	=	6.9	8.6	123.7	6.1	83.8
Aprepitant	Drugs		73.2	2.3	33.2	-24.4	2	>	5.5	1.8	33.4	0.7	7.4
Aripiprazole	Drugs	Dopaminergic GPCR					0						
Atomoxetine	Drugs	Reuptake Inhibitors	58.7	6.9	104.6	-71.2	2	=	2.5	0.9	33.8	0.5	4.7
Bromazepam	Drugs	Gaba Receptors	0.0	0.0	27.5	27.5	1	=	1.2	0.0	0.0	0.0	1.2
Bromocriptine	Drugs	Dopaminergic GPCR	64.0	1.8	11.1	-0.1	4	=	5.8	0.0	0.0	0.0	5.8
Brotizolam	Drugs	Gaba Receptors	0.0	0.0	30.8	30.8	1	=	1.3	0.2	15.0	0.1	1.8
Budipine	Drugs	Calcium Channels											
Buprenorphine	Drugs	Opioid Receptor											
Buspirone	Drugs	Serotonergic GPCR	15.3	2.7	41.4	18.6	3	=	1.3	0.2	16.0	0.1	1.5
Cabergoline	Drugs	Dopaminergic GPCR	5.3	0.1	2.0	0.7	2	=	14.3	5.9	41.3	2.9	23.7
Caffeine	Drugs	Serotonergic GPCR	0.0	0.0	37.4	37.4	1						
Carbamazepine	Drugs	Reuptake Inhibitors	6.1	1.6	55.8	16.4	2	=	1.0	0.1	13.9	0.1	1.2
Carisoprodol	Drugs							=	1.2	0.0	0.0	0.0	1.2
Chlorpromazine	Drugs	Dopaminergic GPCR						=	5.7	0.0	0.0	0.0	5.7
Citalopram	Drugs	Serotonergic GPCR	25.6	2.7	50.0	-19.7	2	=	1.9	0.4	20.4	0.2	2.5
Clomipramine	Drugs	Serotonergic GPCR	36.1	0.5	8.1	-4.3	2	>	10.9	7.9	72.4	4.0	23.6
Clonazepam	Drugs	Gaba Receptors	0.0	0.0	31.1	31.1	1	=	1.3	0.0	0.0	0.0	1.3
Clozapine	Drugs	Serotonergic GPCR	41.9	1.7	14.0	-0.3	3	=	2.5	0.9	36.3	0.3	3.3
Cyclobenzaprine	Drugs							=	2.8	0.0	0.0	0.0	2.8
Dexmethylphenidate	Drugs	Dopaminergic GPCR											
Dextropropoxyphene	Drugs	Opioid Receptor											
Diazepam	Drugs	Gaba Receptors											
Donepezil	Drugs	Enzyme	37.6	5.8	95.7	-51.9	2	=	1.6	0.4	21.5	0.2	2.5
Dronabinol	Drugs	Cannabinoids											
Duloxetine	Drugs	Serotonergic GPCR					0	=	1.8	2.0	114.0	1.4	20.0
Eletriptan	Drugs	Serotonergic GPCR	44.6	2.9	45.4	-27.3	2	=	22.6	6.6	29.3	1.6	25.9
Escitalopram	Drugs	Serotonergic GPCR	4.8	0.4	18.0	14.2	3	=	2.0	0.4	20.9	0.2	2.6
Eszopiclone	Drugs	Gaba Receptors											
Ethosuximide	Drugs	Calcium Channels											
Felbamate	Drugs	Gaba Receptors					0						



Pub-Name	Set	Target Mechanism	Papp CV	Papp SEM	Papp Up95	Papp Low95	Papp N	Pgp OP	Pgp Mean	Pgp SD	Pgp CV	Pgp SEM	Pgp Up95
Fentanyl	Drugs	Opioid Receptor											
Flumazenil	Drugs	Gaba Receptors	13.9	2.5	41.4	20.1	3	=	1.1	0.1	13.7	0.1	1.4
Fluoxetine	Drugs	Serotonergic GPCR	63.3	0.9	14.2	-9.9	2	=	5.2	4.9	94.1	2.5	13.1
Fluvoxamine	Drugs	Serotonergic GPCR	48.1	2.1	16.5	-1.5	3	=	3.1	2.1	66.8	0.9	5.8
Gabapentin	Drugs	Calcium Channels					0						
Galantamine	Drugs	Enzyme	0.0	0.0	15.6	15.6	1	=	1.0	0.1	12.4	0.1	1.3
Haloperidol	Drugs	Dopaminergic GPCR					0						
Hydrocodone	Drugs	Opioid Receptor	0.0	0.0	29.5	29.5	1	=	1.3	0.0	0.0	0.0	1.3
Indeloxazine	Drugs	Reuptake Inhibitors	0.0	0.0	25.2	25.2	1	=	1.4	0.0	0.0	0.0	1.4
Lamotrigine	Drugs	Reuptake Inhibitors	16.2	2.0	31.1	18.3	4	=	1.1	0.1	6.5	0.0	1.2
Levetiracetam	Drugs	Calcium Channels					0	=	1.3	0.0	0.0	0.0	1.3
Levomethadyl Acetate	Drugs	Opioid Receptor											
Lofexidine	Drugs							=	1.2	0.0	3.4	0.0	1.6
Lorazepam	Drugs	Gaba Receptors	9.8	1.7	46.4	3.0	2	=	1.2	0.0	1.6	0.0	1.3
Meprobamate	Drugs												
Methylphenidate	Drugs	Dopaminergic GPCR	0.0	0.0	28.3	28.3	1	=	1.1	0.0	0.0	0.0	1.1
Metoclopramide	Drugs												
Midazolam	Drugs	Gaba Receptors											
Milnacipran	Drugs	Serotonergic GPCR											
Minaprine	Drugs	Enzyme	0.0	0.0	36.6	36.6	1	=	1.2	0.2	14.4	0.1	1.7
Mirtazapine	Drugs		27.0	4.9	88.5	-36.8	2	=	1.2	0.1	8.8	0.0	1.4
Moclobemide	Drugs	Enzyme	39.5	9.8	159.7	-89.4	2	=	1.1	0.0	3.1	0.0	1.2
Modafinil	Drugs	Dopaminergic GPCR					0						
Morphine	Drugs	Opioid Receptor											
Nalmefene	Drugs	Opioid Receptor						=	1.1	0.0	4.0	0.0	1.3
Naltrexone	Drugs	Opioid Receptor	18.0	2.6	53.5	-12.7	2	=	1.1	0.1	7.5	0.0	1.3
Nemonapride	Drugs	Dopaminergic GPCR	0.0	0.0	20.6	20.6	1	=	1.6	0.1	7.8	0.1	1.9
Nicergoline	Drugs												
Nicotrol	Drugs	Nicotinic Receptor	15.0	3.0	66.0	-9.8	2	=	1.3	0.4	28.7	0.3	4.8
Nimodipine	Drugs	Calcium Channels	0.0	0.0	15.4	15.4	1	=	1.5	0.2	10.6	0.1	1.7
Nortriptyline	Drugs												
Olanzapine	Drugs	Dopaminergic GPCR	62.7	6.8	48.2	-10.5	3	=	2.0	0.6	28.3	0.2	2.5
Oxcarbazepine	Drugs	Reuptake Inhibitors						=	1.4	0.4	30.7	0.2	2.4
Oxycodone	Drugs	Opioid Receptor	0.0	0.0	28.3	28.3	1	=	1.1	0.0	0.0	0.0	1.1
Paliperidone	Drugs	Dopaminergic GPCR	0.0	0.0	21.5	21.5	1	=	4.1	0.8	18.5	0.4	5.9
Paroxetine	Drugs	Serotonergic GPCR	17.0	0.1	2.4	-0.5	2	=	5.5	3.8	69.1	1.9	11.6
Pergolide	Drugs	Dopaminergic GPCR	65.0	4.4	66.0	-46.7	2	=	1.6	0.2	13.7	0.1	2.1

Pub-Name	Set	Target Mechanism	Papp CV	Papp SEM	Papp Up95	Papp Low95	Papp N	Pgp OP	Pgp Mean	Pgp SD	Pgp CV	Pgp SEM	Pgp Up95
Perospirone	Drugs	Dopaminergic GPCR						=	7.8	2.0	26.2	1.2	12.9
phenytoin	Drugs	Reuptake Inhibitors	9.2	1.9	52.1	5.1	2	=	1.1	0.2	17.8	0.1	1.4
Piracetam	Drugs						0						
Pramipexole	Drugs	Dopaminergic GPCR	0.0	0.0	12.8	12.8	1	=	1.0	0.4	38.3	0.3	4.5
Pregabalin	Drugs	Calcium Channels					0						
Propofol	Drugs						0						
Propoxyphene	Drugs						0						
Quazepam	Drugs	Gaba Receptors											
Quetiapine	Drugs	Serotonergic GPCR	6.6	1.0	34.7	8.9	2	=	1.8	0.7	37.2	0.3	2.9
Ramelteon	Drugs	Melatonin Receptor	5.8	1.4	50.7	16.1	2	=	1.0	0.1	8.3	0.0	1.2
Rasagiline	Drugs	Enzyme						=	1.0	0.0	0.0	0.0	1.0
Reboxetine	Drugs	Reuptake Inhibitors	0.0	0.0	12.2	12.2	1	=	1.4	0.4	29.1	0.2	2.5
Remifentanyl	Drugs	Opioid Receptor											
Riluzole	Drugs	Reuptake Inhibitors	17.6	3.8	78.4	-17.7	2	=	1.5	0.5	31.1	0.3	2.6
Rimonabant	Drugs	Cannabinoids	52.1	1.3	20.1	-13.0	2	>	2.5	1.5	58.9	0.7	4.8
Risperidone	Drugs	Dopaminergic GPCR	47.1	6.3	50.3	-3.9	3	=	2.6	0.4	15.8	0.1	3.0
Rivastigmine	Drugs	Enzyme	17.5	3.4	70.4	-15.7	2	=	1.0	0.1	12.7	0.1	1.2
Ropinirole	Drugs	Dopaminergic GPCR	25.9	4.9	89.4	-35.7	2	=	1.3	0.3	21.9	0.1	1.6
Ropivacaine	Drugs		0.0	0.0	43.4	43.4	1	=	1.0	0.1	9.9	0.0	1.2
Selegiline	Drugs	Enzyme	0.0	0.0	25.9	25.9	1						
Sertindole	Drugs	Serotonergic GPCR	14.4	0.0	0.3	0.0	2	=	10.4	5.8	55.9	4.1	62.8
Sertraline	Drugs	Serotonergic GPCR	0.0	0.0	2.2	2.2	1	=	11.2	0.0	0.0	0.0	11.2
Sinequan	Drugs	Serotonergic GPCR	0.0	0.0	10.4	10.4	1	=	2.0	0.4	20.7	0.3	5.6
Sulpiride	Drugs	Dopaminergic GPCR	0.0	0.0	0.3	0.3	1						
Tacrine	Drugs	Enzyme	24.9	5.3	97.4	-37.3	2	=	1.3	0.6	46.1	0.3	2.0
Talipexole	Drugs	Dopaminergic GPCR	29.3	4.7	83.0	-37.2	2	=	1.2	0.2	20.6	0.1	1.7
Terguride	Drugs	Dopaminergic GPCR											
Thiopental	Drugs	Gaba Receptors											
Tiagabine	Drugs	Gaba Receptors	9.3	1.4	37.9	3.5	2	=	1.5	0.2	10.3	0.1	1.9
Tianeptine	Drugs	Reuptake Inhibitors	22.9	3.7	69.4	-24.0	2	=	1.5	0.1	9.8	0.1	1.8
Topiramate	Drugs	Enzyme					0	=	1.1	0.1	8.5	0.1	1.4
Tramadol	Drugs	Reuptake Inhibitors											
Trazodone	Drugs	Serotonergic GPCR						=	1.2	0.2	12.9	0.1	1.6
Tropisetron	Drugs	Serotonergic GPCR											
Valproic Acid	Drugs						0						
Varenicline	Drugs	Nicotinic Receptor	0.0	0.0	24.6	24.6	1	=	1.2	0.2	21.0	0.1	1.3
Venlafaxine	Drugs	Serotonergic GPCR	29.5	3.5	35.9	5.6	3	=	1.3	0.2	14.6	0.1	1.6

Pub-Name	Set	Target Mechanism	Papp CV	Papp SEM	Papp Upp95	Papp Low95	Papp N	Pgp OP	Pgp Mean	Pgp SD	Pgp CV	Pgp SEM	Pgp Upp95
Verapamil	Drugs	Calcium Channels						=	2.3	1.2	52.8	0.9	13.5
Vigabatrin	Drugs	Gaba Receptors											
Vinpocetine	Drugs		33.3	0.9	8.7	0.8	3	=	2.1	0.9	41.1	0.4	3.5
Zaleplon	Drugs	Gaba Receptors	0.0	0.0	37.1	37.1	1	=	1.4	0.0	0.0	0.0	1.4
Ziprasidone	Drugs	Dopaminergic GPCR	0.0	0.0	10.3	10.3	1	=	2.3	0.9	40.1	0.5	4.7
Zolpidem	Drugs	Gaba Receptors	0.0	0.0	80.3	80.3	1	=	1.2	0.0	0.0	0.0	1.2
Zonisamide	Drugs	Enzyme	0.0	0.0	29.1	29.1	1	=	1.0	0.0	4.7	0.0	1.1
Zotepine	Drugs	Serotonergic GPCR					0	=	5.1	0.0	0.0	0.0	5.1
Candidate-001	Candidates	Glutamate receptors					0						
Candidate-002	Candidates	Reuptake Inhibitors	72.1	2.8	16.8	-1.2	4	=	2.6	1.0	38.1	0.5	4.2
Candidate-003	Candidates	Reuptake Inhibitors	72.0	5.8	85.1	-62.3	2	=	6.2	2.2	35.8	1.6	25.9
Candidate-004	Candidates	Serotonergic GPCR											
Candidate-005	Candidates	Enzyme					0						
Candidate-006	Candidates	Peptide GPCR	16.8	1.0	21.1	-4.3	2						
Candidate-007	Candidates	Enzyme	0.0	0.0	1.0	1.0	1	>	6.3	1.9	29.8	0.8	8.7
Candidate-008	Candidates	Calcium Channels											
Candidate-009	Candidates	Nicotinic Receptor					0						
Candidate-010	Candidates	Opioid Receptor	1.6	0.2	21.1	15.8	2	=	1.9	0.0	1.0	0.0	2.0
Candidate-011	Candidates	Dopaminergic GPCR						=	2.3	0.0	0.9	0.0	2.5
Candidate-012	Candidates	Peptide GPCR	35.7	1.3	20.8	-10.9	2	=	2.9	0.9	29.6	0.5	5.1
Candidate-013	Candidates	Enzyme	0.0	0.0	11.4	11.4	1	=	5.6	7.3	130.0	2.1	10.0
Candidate-014	Candidates	Opioid Receptor	0.0	0.0	19.9	19.9	1	=	1.4	0.1	7.0	0.1	1.7
Candidate-015	Candidates	Nicotinic Receptor						=	1.2	0.1	10.8	0.1	1.5
Candidate-016	Candidates	Gaba Receptors	9.2	1.4	36.2	26.9	4	=	1.4	0.2	11.5	0.1	1.6
Candidate-017	Candidates	Enzyme	67.6	8.1	55.3	-14.0	3	=	3.1	0.0	0.0	0.0	3.1
Candidate-018	Candidates	Cannabinoids	30.5	1.1	10.8	1.5	3	=	2.3	0.3	12.2	0.1	2.7
Candidate-019	Candidates	Peptide GPCR	0.0	0.0	7.8	7.8	1	=	2.2	0.7	33.1	0.5	8.7
Candidate-020	Candidates	Glutamate receptors	0.0	0.0	14.9	14.9	1	=	3.0	0.0	0.0	0.0	3.0
Candidate-021	Candidates	Enzyme	95.0	2.9	18.0	-7.3	3	>	6.4	3.0	47.3	0.9	8.2
Candidate-022	Candidates	Enzyme	154.1	0.4	1.8	-0.8	4	=	13.8	1.9	14.1	1.1	18.6
Candidate-023	Candidates	Nicotinic Receptor	99.2	9.0	126.8	-101.2	2	=	1.2	0.2	16.6	0.1	1.5
Candidate-024	Candidates	Calcium Channels											
Candidate-025	Candidates	Reuptake Inhibitors						>	5.3	0.7	13.8	0.4	7.2
Candidate-026	Candidates	Serotonergic GPCR	30.0	0.7	12.2	-5.6	2	=	3.9	1.8	44.9	0.9	6.8
Candidate-027	Candidates	Serotonergic GPCR	132.7	2.7	12.8	-4.6	4	=	16.0	0.0	0.0	0.0	16.0
Candidate-028	Candidates	Histaminergic GPCR	0.0	0.0	51.5	51.5	1	=	1.2	0.1	7.2	0.0	1.3
Candidate-029	Candidates	Glutamate receptors	0.0	0.0	26.5	26.5	1	=	1.3	0.1	10.4	0.1	2.5

Pub-Name	Set	Target Mechanism	Papp CV	Papp SEM	Papp Upp95	Papp Low95	Papp N	Pgp OP	Pgp Mean	Pgp SD	Pgp CV	Pgp SEM	Pgp Upp95
Candidate-030	Candidates	Peptide GPCR	20.5	1.6	20.3	10.3	4	=	1.8	0.4	20.8	0.2	2.8
Candidate-031	Candidates	Serotonergic GPCR	24.7	4.7	52.9	12.7	3	=	1.1	0.1	7.2	0.0	1.2
Candidate-032	Candidates	Gaba Receptors	20.5	2.7	34.5	17.4	4	=	1.3	0.2	11.9	0.1	1.5
Candidate-033	Candidates	Opioid Receptor	7.1	0.8	25.7	5.7	2	=	2.8	0.8	29.6	0.2	3.3
Candidate-034	Candidates	Reuptake Inhibitors	93.6	2.7	37.8	-29.7	2	=	3.5	0.5	14.4	0.3	4.3
Candidate-035	Candidates	Calcium Channels					0						
Candidate-036	Candidates	Peptide GPCR					0						
Candidate-037	Candidates	Gaba Receptors					0	=	0.8	0.2	22.6	0.1	1.0
Candidate-038	Candidates	Serotonergic GPCR					0						
Candidate-039	Candidates	Glutamate receptors	0.0	0.0	3.3	3.3	1	>	5.5	1.4	25.5	0.5	6.6
Candidate-040	Candidates	Enzyme	0.0	0.0	38.4	38.4	1	=	1.3	0.0	0.0	0.0	1.3
Candidate-041	Candidates	Peptide GPCR	47.5	2.8	44.1	-27.4	2	>	6.6	8.1	121.3	1.6	10.1
Candidate-042	Candidates	Serotonergic GPCR						=	1.8	0.2	12.8	0.1	2.4
Candidate-043	Candidates	Peptide GPCR						=	2.4	0.2	6.4	0.1	2.8
Candidate-044	Candidates	Serotonergic GPCR	35.8	0.5	4.5	1.2	4	=	5.7	2.6	45.7	0.8	5.7
Candidate-045	Candidates	Cannabinoids	59.5	2.5	16.2	2.4	5	=	6.0	0.0	0.0	0.0	6.0
Candidate-046	Candidates	Serotonergic GPCR	0.0	0.0	3.9	3.9	1	>	9.7	18.2	187.0	6.1	23.7
Candidate-047	Candidates	Calcium Channels											
Candidate-048	Candidates	Dopaminergic GPCR						>	3.8	1.1	30.0	0.5	4.9
Candidate-049	Candidates	Serotonergic GPCR	7.1	0.3	9.8	2.2	2	=	3.5	0.7	19.8	0.2	4.1
Candidate-050	Candidates	Gaba Receptors	8.6	0.1	1.9	1.5	5	=	26.7	10.9	40.9	6.3	53.7
Candidate-051	Candidates	Reuptake Inhibitors	68.7	1.2	17.8	-12.8	2	=	4.3	0.9	21.4	0.5	6.6
Candidate-052	Candidates	Enzyme					0						
Candidate-053	Candidates	Nicotinic Receptor	5.5	1.2	46.2	15.8	2	=	1.2	0.1	10.2	0.0	1.3
Candidate-054	Candidates	Opioid Receptor					0						
Candidate-055	Candidates	Enzyme	91.7	4.8	68.9	-54.0	2	=	2.7	0.9	35.5	0.5	5.0
Candidate-056	Candidates	Enzyme	26.5	1.2	12.9	2.7	3	=	1.9	0.4	19.0	0.1	2.3
Candidate-057	Candidates	Dopaminergic GPCR	0.0	0.0	4.9	4.9	1						
Candidate-058	Candidates	Peptide GPCR	0.0	0.0	0.5	0.5	1	>	1.2	0.0	0.0	0.0	1.2
Candidate-059	Candidates	Dopaminergic GPCR											
Candidate-060	Candidates	Serotonergic GPCR	0.0	0.0	3.4	3.4	1						
Candidate-061	Candidates	Histaminergic GPCR	18.7	4.0	55.5	29.9	4	=	1.2	0.1	9.5	0.1	1.4
Candidate-062	Candidates	Dopaminergic GPCR						=	2.7	0.0	0.0	0.0	2.7
Candidate-063	Candidates	Nicotinic Receptor	25.4	0.6	6.2	1.4	3	=	3.5	1.0	27.3	0.6	5.9
Candidate-064	Candidates	Serotonergic GPCR	0.0	0.0	9.5	9.5	1	=	1.9	0.6	34.4	0.4	3.5
Candidate-065	Candidates	Peptide GPCR	0.0	0.0	14.9	14.9	1	=	1.8	0.4	19.6	0.2	2.7
Candidate-066	Candidates	Serotonergic GPCR	14.7	1.4	23.1	14.3	4	=	2.4	0.8	31.4	0.4	4.3

Pub-Name	Set	Target Mechanism	Papp CV	Papp SEM	Papp Up95	Papp Low95	Papp N	Pgp OP	Pgp Mean	Pgp SD	Pgp CV	Pgp SEM	Pgp Up95
Candidate-067	Candidates	Dopaminergic GPCR											
Candidate-068	Candidates	Serotonergic GPCR	0.0	0.0	2.8	2.8	1	<	1.0	0.0	0.0	0.0	1.0
Candidate-069	Candidates	Reuptake Inhibitors	0.0	0.0	9.3	9.3	1	=	4.3	0.3	7.4	0.2	5.1
Candidate-070	Candidates	Dopaminergic GPCR	0.0	0.0	20.4	20.4	1	=	0.9	0.1	8.8	0.1	1.5
Candidate-071	Candidates	Reuptake Inhibitors	0.0	0.0	13.2	13.2	1	=	4.1	1.1	27.1	0.6	5.9
Candidate-072	Candidates	Dopaminergic GPCR	0.0	0.0	8.2	8.2	1	=	1.9	0.2	10.2	0.1	2.4
Candidate-073	Candidates	Gaba Receptors	0.0	0.0	5.8	5.8	1	=	9.2	1.0	10.5	0.6	11.6
Candidate-074	Candidates	Peptide GPCR					0						
Candidate-075	Candidates	Nicotinic Receptor	24.7	3.2	58.9	-22.3	2	=	1.3	0.1	9.4	0.1	1.6
Candidate-076	Candidates	Nicotinic Receptor	4.5	0.5	24.3	21.1	4	=	1.2	0.1	4.9	0.0	1.4
Candidate-077	Candidates	Gaba Receptors	40.6	5.0	42.5	-0.1	3	=	1.3	0.2	14.2	0.1	1.8
Candidate-078	Candidates	Reuptake Inhibitors	23.3	2.1	25.0	6.7	3	=	1.8	0.3	18.4	0.1	2.1
Candidate-079	Candidates	Calcium Channels											
Candidate-080	Candidates	Dopaminergic GPCR	0.0	0.0	12.6	12.6	1	=	1.7	0.3	19.5	0.1	1.9
Candidate-081	Candidates	Serotonergic GPCR	0.0	0.0	32.4	32.4	1	=	1.6	0.2	13.3	0.1	1.9
Candidate-082	Candidates	Gaba Receptors	142.1	1.9	8.6	-3.3	4	=	2.6	1.1	42.0	0.6	5.4
Candidate-083	Candidates	Cannabinoids	0.0	0.0	7.1	7.1	1	=	2.0	0.6	28.2	0.3	3.5
Candidate-084	Candidates	Gaba Receptors	25.6	3.6	41.2	21.2	5	=	1.2	0.3	27.1	0.2	1.7
Candidate-085	Candidates	Reuptake Inhibitors						=	2.1	0.6	26.2	0.3	3.0
Candidate-086	Candidates	Muscarinic Receptor	0.0	0.0	23.0	23.0	1	=	1.2	0.1	9.1	0.1	1.5
Candidate-087	Candidates	Cannabinoids	0.0	0.0	3.7	3.7	1	>	1.5	0.0	0.0	0.0	1.5
Candidate-088	Candidates	Dopaminergic GPCR	0.0	0.0	16.7	16.7	1	=	2.4	1.2	49.0	0.7	5.3
Candidate-089	Candidates	Enzyme	21.3	1.2	14.6	4.5	3	=	3.2	0.4	11.3	0.1	3.4
Candidate-090	Candidates	Glutamate receptors	0.0	0.0	18.2	18.2	1	=	1.6	0.2	14.7	0.1	1.7
Candidate-091	Candidates	Gaba Receptors	33.3	3.8	36.3	3.4	3	=	1.4	0.2	13.6	0.1	1.9
Candidate-092	Candidates	Reuptake Inhibitors	0.0	0.0	11.9	11.9	1	=	3.9	1.9	49.3	0.8	6.0
Candidate-093	Candidates	Muscarinic Receptor	0.0	0.0	23.3	23.3	1	=	1.4	0.3	18.9	0.1	2.0
Candidate-094	Candidates	Dopaminergic GPCR	79.0	3.8	55.1	-41.5	2	=	3.5	1.2	35.4	0.5	4.7
Candidate-095	Candidates	Gaba Receptors					0	=	1.2	0.0	3.3	0.0	1.6
Candidate-096	Candidates	Serotonergic GPCR	0.0	0.0	36.0	36.0	1						
Candidate-097	Candidates	Reuptake Inhibitors	74.7	3.2	21.3	-6.4	3	=	3.3	0.6	16.6	0.3	4.7
Candidate-098	Candidates	Enzyme	2.0	0.0	2.0	1.4	2	=	2.4	0.2	8.8	0.1	2.8
Candidate-099	Candidates	Peptide GPCR	43.0	1.8	28.0	-16.5	2	=	10.0	4.3	43.1	1.1	12.3
Candidate-100	Candidates	Enzyme					0						
Candidate-101	Candidates	Dopaminergic GPCR						=	4.4	1.2	28.1	0.9	15.6
Candidate-102	Candidates	Serotonergic GPCR	68.8	7.3	108.2	-78.1	2	=	1.9	0.5	26.2	0.2	2.3
Candidate-103	Candidates	Dopaminergic GPCR					0						

Pub-Name	Set	Target Mechanism	Papp CV	Papp SEM	Papp Upp95	Papp Low95	Papp N	Pgp OP	Pgp Mean	Pgp SD	Pgp CV	Pgp SEM	Pgp Upp95
Candidate-104	Candidates	Peptide GPCR	64.1	3.9	27.6	-6.3	3	=	9.2	2.1	22.4	1.2	14.3
Candidate-105	Candidates	Gaba Receptors	43.8	2.8	21.6	3.8	4	=	1.5	0.2	14.5	0.1	2.1
Candidate-106	Candidates	Peptide GPCR	0.0	0.0	16.8	16.8	1	=	5.5	2.3	41.6	1.6	25.8
Candidate-107	Candidates	Calcium Channels					0						
Candidate-108	Candidates	Nicotinic Receptor	3.7	0.8	38.5	19.4	2	=	1.2	0.2	18.2	0.1	1.6

Pub-Name	Set	Target Mechanism	Pgp Low95	Pgp N	cFu,mi c	CLIA OP	CLIA Mean	CLIA SD	CLIA CV	CLIA SEM	CLIA Upp95	CLIA Low95	CLIA N	CLI_u
Acamprosate	Drugs	Glutamate receptors		0	0.984								0	
Alprazolam	Drugs	Gaba Receptors	1.4	1	0.779	<	7.6	0.4	4.9	0.2	8.5	6.6	3	9.7
Amfebutamone	Drugs	Dopaminergic GPCR	0.7	4	0.821	=	27.2	6.1	22.5	3.5	42.4	12.0	3	33.1
Amisulpride	Drugs	Dopaminergic GPCR	-14.2	3	0.614	<	13.9	12.8	91.6	6.4	34.4		4	22.7
Amphetamine	Drugs	Reuptake Inhibitors			0.741									
Aniracetam	Drugs		1.1	1	0.962								0	
Apomorphine	Drugs	Dopaminergic GPCR	-70.0	2	0.302	<	13.2	8.0	60.3	5.6	84.6		2	43.7
Aprepitant	Drugs		3.5	6	0.048	<	13.9	8.8	63.6	3.6	23.2	4.5	6	289.4
Aripiprazole	Drugs	Dopaminergic GPCR		0	0.030	=	31.7	11.5	36.2	4.3	42.1	21.3	7	1059.6
Atomoxetine	Drugs	Reuptake Inhibitors	0.4	3	0.486	=	138.6	30.1	21.7	17.4	213.3	63.9	3	285.2
Bromazepam	Drugs	Gaba Receptors	1.2	1	0.815	<	7.6				7.6	7.6	2	9.3
Bromocriptine	Drugs	Dopaminergic GPCR	5.8	1	0.046	>	265.2	64.4	24.3	37.2	425.0	105.5	3	5753.6
Brotizolam	Drugs	Gaba Receptors	0.8	3	0.845	=	15.2	8.0	52.6	3.6	25.3	5.2	5	18.1
Budipine	Drugs	Calcium Channels			0.065									
Buprenorphine	Drugs	Opioid Receptor			0.823									
Buspirone	Drugs	Serotonergic GPCR	1.0	6	0.812	=	147.5	30.8	20.9	12.6	180.2	114.8	6	181.7
Cabergoline	Drugs	Dopaminergic GPCR	4.8	4	0.570	=	49.6	6.9	13.9	3.1	58.2	40.9	5	86.9
Caffeine	Drugs	Serotonergic GPCR		0	0.980	<	6.9	0.5	7.9	0.3	8.3	5.6	3	7.1
Carbamazepine	Drugs	Reuptake Inhibitors	0.9	6	0.936	<	13.4	14.8	110.5	6.1	29.2		6	14.3
Carisoprodol	Drugs		1.2	1	0.977	<	7.9	0.5	5.8	0.3	12.0	3.8	2	8.1
Chlorpromazine	Drugs	Dopaminergic GPCR	5.7	1	0.114	=	61.2	14.5	23.7	7.2	84.4	38.0	4	538.4
Citalopram	Drugs	Serotonergic GPCR	1.3	4	0.690	<	13.8	7.7	56.2	3.9	26.2	1.4	4	20.0
Clomipramine	Drugs	Serotonergic GPCR	-1.7	4	0.047	=	38.8	27.6	71.1	13.8	83.1		4	835.4
Clonazepam	Drugs	Gaba Receptors	1.3	1	0.641	<	7.6				7.6	7.6	2	11.8
Clozapine	Drugs	Serotonergic GPCR	1.7	7	0.364	=	26.1	10.3	39.4	3.0	32.3	19.9	12	71.7
Cyclobenzaprine	Drugs		2.8	1	0.104	=	24.2	19.7	81.4	13.9	200.9		2	232.3
Dexmethylphenidate	Drugs	Dopaminergic GPCR			0.870									
Dextropropoxyphene	Drugs	Opioid Receptor		0	0.225	=	49.6	3.4	6.8	2.0	58.0	41.2	3	220.6
Diazepam	Drugs	Gaba Receptors			0.699	<	8.0	0.6	7.9	0.5	13.7	2.3	2	11.5
Donepezil	Drugs	Enzyme	0.8	3	0.642	<	9.6	3.7	38.1	1.6	14.3	5.0	5	15.0
Dronabinol	Drugs	Cannabinoids			0.004									
Duloxetine	Drugs	Serotonergic GPCR	-16.4	2	0.101	=	31.8	9.6	30.3	4.8	47.2	16.3	4	313.6
Eletriptan	Drugs	Serotonergic GPCR	19.4	18	0.897	=	29.3	11.0	37.4	4.5	41.0	17.7	6	32.7
Escitalopram	Drugs	Serotonergic GPCR	1.3	4	0.690	<	10.7	5.4	50.9	3.1	24.2		3	15.5
Eszopiclone	Drugs	Gaba Receptors			0.808									
Ethosuximide	Drugs	Calcium Channels			0.897									
Felbamate	Drugs	Gaba Receptors		0	0.992	<	7.6				7.6	7.6	1	7.6

Pub-Name	Set	Target Mechanism	Pgp Low95	Pgp N	cFu,mi c	CLIA OP	CLIA Mean	CLIA SD	CLIA CV	CLIA SEM	CLIA Upp95	CLIA Low95	CLIA N	CLI_u
Fentanyl	Drugs	Opioid Receptor			0.662	=	30.5	2.9	9.6	1.7	37.8	23.3	3	46.1
Flumazenil	Drugs	Gaba Receptors	0.7	3	0.951	<	10.0	3.9	38.7	1.9	16.1	3.8	4	10.5
Fluoxetine	Drugs	Serotonergic GPCR	-2.6	4	0.060	=	33.5	21.9	65.3	8.9	56.8	10.3	6	563.9
Fluvoxamine	Drugs	Serotonergic GPCR	0.5	5	0.349	<	20.8	14.1	67.6	5.3	33.6	8.1	7	59.7
Gabapentin	Drugs	Calcium Channels		0	0.973	<	6.6				6.6	6.6	1	6.8
Galantamine	Drugs	Enzyme	0.7	3	1.000	<	7.6				7.6	7.6	2	7.6
Haloperidol	Drugs	Dopaminergic GPCR		0	0.661	<	12.9	7.6	58.8	5.4	81.3		2	19.6
Hydrocodone	Drugs	Opioid Receptor	1.3	1	0.952	<	9.5	3.4	36.0	2.0	18.1	1.0	3	10.0
Indeloxazine	Drugs	Reuptake Inhibitors	1.4	1	0.882	<	7.6				7.6	7.6	2	8.6
Lamotrigine	Drugs	Reuptake Inhibitors	1.0	5	0.779	<	12.4	13.8	110.6	5.2	24.9		7	16.0
Levetiracetam	Drugs	Calcium Channels	1.3	1	0.975	<	6.6				6.6	6.6	1	6.8
Levomethadyl Acetate	Drugs	Opioid Receptor			0.304	=	45.5	3.5	7.6	2.0	54.1	36.9	3	149.7
Lofexidine	Drugs		0.8	2	0.758	<	11.0	2.9	26.9	1.7	18.3	3.6	3	14.5
Lorazepam	Drugs	Gaba Receptors	1.0	2	0.719	<	8.0	0.7	8.8	0.3	8.9	7.2	5	11.2
Meprobamate	Drugs				0.988									
Methylphenidate	Drugs	Dopaminergic GPCR	1.1	1	0.870	<	10.5	2.4	23.2	1.2	14.3	6.6	4	12.0
Metoclopramide	Drugs				0.895									
Midazolam	Drugs	Gaba Receptors			0.686	=	184.7	52.4	28.4	4.7	194.6	174.8	124	269.2
Milnacipran	Drugs	Serotonergic GPCR			0.927									
Minaprine	Drugs	Enzyme	0.8	3	0.747	=	122.5	12.4	10.1	7.1	153.2	91.8	3	163.9
Mirtazapine	Drugs		1.1	5	0.828	<	15.6	9.6	61.5	3.9	25.8	5.4	6	18.9
Moclobemide	Drugs	Enzyme	1.0	3	0.822	<	7.6				7.6	7.6	3	9.2
Modafinil	Drugs	Dopaminergic GPCR		0	0.891	<	7.6				7.6	7.6	1	8.5
Morphine	Drugs	Opioid Receptor			0.875	=	19.5	5.5	28.1	3.2	33.1	5.9	3	22.3
Nalmefene	Drugs	Opioid Receptor	1.0	3	0.867	=	11.4	1.4	12.0	0.8	14.8	8.0	3	13.1
Naltrexone	Drugs	Opioid Receptor	0.9	3	0.920	<	10.0	3.3	32.4	1.2	13.0	7.1	7	10.9
Nemonapride	Drugs	Dopaminergic GPCR	1.3	3	0.393	=	164.8	17.2	10.4	9.9	207.5	122.1	3	419.7
Nicergoline	Drugs				0.399									
Nicotrol	Drugs	Nicotinic Receptor	-2.1	2	0.832	=	18.6				18.6	18.6	1	22.4
Nimodipine	Drugs	Calcium Channels	1.2	4	0.271	>	302.2	0.5	0.2	0.2	302.7	301.7	8	1115.6
Nortriptyline	Drugs				0.230									
Olanzapine	Drugs	Dopaminergic GPCR	1.5	7	0.645	<	11.3	5.6	49.3	2.1	16.4	6.3	7	17.6
Oxcarbazepine	Drugs	Reuptake Inhibitors	0.3	3	1.000	<	8.9	1.1	12.9	0.7	11.7	6.0	3	8.9
Oxycodone	Drugs	Opioid Receptor	1.1	1	0.891	<	10.6	3.3	30.8	1.6	15.8	5.4	4	11.9
Paliperidone	Drugs	Dopaminergic GPCR	2.2	3	0.778	<	7.6				7.6	7.6	4	9.7
Paroxetine	Drugs	Serotonergic GPCR	-0.6	4	0.084	=	95.1	46.4	48.7	26.8	210.2		3	1126.7
Pergolide	Drugs	Dopaminergic GPCR	1.0	3	0.446	>	278.9	35.6	12.8	20.6	367.4	190.4	3	625.4



Pub-Name	Set	Target Mechanism	Pgp Low95	Pgp N	cFu,mi c	CLIA OP	CLIA Mean	CLIA SD	CLIA CV	CLIA SEM	CLIA Upp95	CLIA Low95	CLIA N	CLI_u
Perospirone	Drugs	Dopaminergic GPCR	2.7	3	0.388	>	296.6	10.1	3.4	5.8	321.7	271.5	3	763.8
phenytoin	Drugs	Reuptake Inhibitors	0.9	6	0.520	<	8.1	1.1	13.2	0.3	8.8	7.3	10	15.5
Piracetam	Drugs			0	0.977								0	
Pramipexole	Drugs	Dopaminergic GPCR	-2.5	2	0.859	<	11.7	7.2	61.5	4.2	29.6		3	13.6
Pregabalin	Drugs	Calcium Channels		0	0.975								0	
Propofol	Drugs			0	0.272								0	
Propoxyphene	Drugs				0.225									
Quazepam	Drugs	Gaba Receptors			0.348								0	
Quetiapine	Drugs	Serotonergic GPCR	0.7	4	0.556	=	125.9	49.7	39.4	20.3	178.6	73.2	6	226.6
Ramelteon	Drugs	Melatonin Receptor	0.8	3	0.820	=	49.8	9.8	19.7	4.9	65.5	34.2	4	60.8
Rasagiline	Drugs	Enzyme	1.0	1	0.890	=	22.5	5.0	22.0	2.9	34.9	10.2	3	25.3
Reboxetine	Drugs	Reuptake Inhibitors	0.4	3	0.647	<	12.0	6.8	56.5	3.4	22.8	1.2	4	18.5
Remifentanyl	Drugs	Opioid Receptor			0.962									
Riluzole	Drugs	Reuptake Inhibitors	0.3	3	0.633	=	21.6	9.4	43.2	4.7	36.6	6.7	4	34.1
Rimonabant	Drugs	Cannabinoids	0.1	4	0.015	=	58.8	30.8	52.5	15.4	108.1	9.4	4	3997.2
Risperidone	Drugs	Dopaminergic GPCR	2.3	9	0.782	=	36.6	5.2	14.3	1.6	36.6	36.6	11	46.8
Rivastigmine	Drugs	Enzyme	0.8	4	0.956	<	7.8	0.4	4.8	0.2	8.5	7.2	4	8.2
Ropinirole	Drugs	Dopaminergic GPCR	0.9	5	0.647	<	10.3	3.0	29.2	1.3	14.1	6.5	5	15.9
Ropivacaine	Drugs		0.8	4	0.927	=	42.2	7.1	16.9	3.6	53.6	30.8	4	45.5
Selegiline	Drugs	Enzyme			0.717									
Sertindole	Drugs	Serotonergic GPCR	-41.9	2	0.077	=	28.3	9.6	33.8	6.8	114.1		2	369.0
Sertraline	Drugs	Serotonergic GPCR	11.2	1	0.033	=	35.3	18.1	51.1	6.4	50.7	20.0	8	1064.6
Sinequan	Drugs	Serotonergic GPCR	-1.7	2	0.493	=	41.3	10.3	24.8	5.1	57.7	24.9	4	83.8
Sulpiride	Drugs	Dopaminergic GPCR			0.984								0	
Tacrine	Drugs	Enzyme	0.5	5	0.824	=	27.4	8.2	30.1	2.9	34.4	20.4	8	33.2
Talipexole	Drugs	Dopaminergic GPCR	0.6	3	0.994								0	
Terguride	Drugs	Dopaminergic GPCR			0.777									
Thiopental	Drugs	Gaba Receptors			0.917									
Tiagabine	Drugs	Gaba Receptors	1.1	3	0.832	<	8.1	1.2	14.7	0.5	9.6	6.6	5	9.7
Tianeptine	Drugs	Reuptake Inhibitors	1.1	3	0.861	<	7.6				7.6	7.6	3	8.8
Topiramate	Drugs	Enzyme	0.9	3	0.841	<	8.7	1.5	16.7	0.7	11.1	6.4	4	10.4
Tramadol	Drugs	Reuptake Inhibitors		0	0.840	<	7.6				7.6	7.6	2	9.0
Trazodone	Drugs	Serotonergic GPCR			0.597									
Tropisetron	Drugs	Serotonergic GPCR	0.8	3	0.708	=	15.6	7.8	49.9	4.5	35.0		3	22.1
Valproic Acid	Drugs			0	0.946								0	
Varenicline	Drugs	Nicotinic Receptor	1.0	15	1.000	<	10.1	5.1	50.4	2.5	18.3	2.0	4	10.1
Venlafaxine	Drugs	Serotonergic GPCR	1.0	4	0.492	<	11.9	5.7	48.1	2.3	17.9	5.8	6	24.1

Pub-Name	Set	Target Mechanism	Pgp Low95	Pgp N	cFu,mi c	CLIA OP	CLIA Mean	CLIA SD	CLIA CV	CLIA SEM	CLIA Upp95	CLIA Low95	CLIA N	CLI_u
Verapamil	Drugs	Calcium Channels	-8.8	2	0.420	=	97.0	31.2	32.1	5.4	108.4	85.6	33	231.3
Vigabatrin	Drugs	Gaba Receptors		0	0.972								0	
Vinpocetine	Drugs		0.7	4	0.334								0	
Zaleplon	Drugs	Gaba Receptors	1.4	1	0.562	=	14.4	4.5	31.4	2.3	21.6	7.2	4	25.6
Ziprasidone	Drugs	Dopaminergic GPCR	0.0	3	0.216	=	41.4	8.2	19.7	2.9	48.3	34.5	8	191.4
Zolpidem	Drugs	Gaba Receptors	1.2	1	0.807	<	8.5	1.4	16.8	0.7	10.7	6.2	4	10.5
Zonisamide	Drugs	Enzyme	0.9	3	0.894	<	10.0	6.0	60.0	2.5	16.4	3.6	6	11.2
Zotepine	Drugs	Serotonergic GPCR	5.1	1	0.030	=	48.2	25.4	52.7	14.7	111.4		3	1624.1
Candidate-001	Candidates	Glutamate receptors		0	0.865								0	
Candidate-002	Candidates	Reuptake Inhibitors	1.0	4	0.285	<	48.0	29.8	62.2	13.3	85.4	10.6	5	168.3
Candidate-003	Candidates	Reuptake Inhibitors	-13.6	2	0.078	=	37.3	19.8	53.1	9.9	69.0	5.6	4	479.7
Candidate-004	Candidates	Serotonergic GPCR			0.956									
Candidate-005	Candidates	Enzyme		0	0.451								0	
Candidate-006	Candidates	Peptide GPCR			0.739									
Candidate-007	Candidates	Enzyme	4.0	5	0.602	=	18.5	9.9	53.4	4.9	34.3	2.7	4	30.7
Candidate-008	Candidates	Calcium Channels		0	0.968								0	
Candidate-009	Candidates	Nicotinic Receptor		0	0.997	<	23.4	12.6	53.7	6.3	43.5	3.3	4	23.5
Candidate-010	Candidates	Opioid Receptor	1.9	3	0.609	=	25.2	3.3	13.2	2.4	55.1		2	41.4
Candidate-011	Candidates	Dopaminergic GPCR	2.1	2	0.297	=	71.2	74.8	105.0	37.4	190.8		4	239.5
Candidate-012	Candidates	Peptide GPCR	0.8	3	0.043	=	30.1	13.4	44.7	6.7	51.5	8.6	4	692.5
Candidate-013	Candidates	Enzyme	1.2	12	0.410	=	45.1				45.1	45.1	1	110.1
Candidate-014	Candidates	Opioid Receptor	1.2	3	0.678	=	36.4	1.5	4.2	1.1	50.1	22.6	2	53.6
Candidate-015	Candidates	Nicotinic Receptor	0.9	3	1.000	<	8.3	1.2	13.8	0.7	11.2	5.5	3	8.3
Candidate-016	Candidates	Gaba Receptors	1.2	5	0.982	<	9.9	2.7	27.3	0.9	12.0	7.8	9	10.1
Candidate-017	Candidates	Enzyme	3.1	1	0.795	<	7.6				7.6	7.6	1	9.5
Candidate-018	Candidates	Cannabinoids	1.8	4	0.064	<	12.8	9.2	71.7	3.7	22.5	3.1	6	201.1
Candidate-019	Candidates	Peptide GPCR	-4.3	2	0.087	=	44.2	7.1	16.1	4.1	61.8	26.5	3	509.5
Candidate-020	Candidates	Glutamate receptors	3.0	1	0.673	=	35.4	2.0	5.6	1.4	53.3	17.6	2	52.6
Candidate-021	Candidates	Enzyme	4.6	12	0.906	<	19.4	13.8	71.4	6.2	36.7	2.0	5	21.4
Candidate-022	Candidates	Enzyme	8.9	3	0.184	>	232.8	53.0	22.8	20.0	280.8	184.7	7	1263.6
Candidate-023	Candidates	Nicotinic Receptor	0.9	4	0.948	<	7.7	0.9	11.9	0.4	8.8	6.5	5	8.1
Candidate-024	Candidates	Calcium Channels		0	0.980								0	
Candidate-025	Candidates	Reuptake Inhibitors	3.5	3	0.066	=	74.9	20.6	27.5	11.9	126.1	23.8	3	1144.2
Candidate-026	Candidates	Serotonergic GPCR	1.1	4	0.082	=	49.4	49.8	100.8	18.8	94.5	4.2	7	603.1
Candidate-027	Candidates	Serotonergic GPCR	16.0	1	0.386	=	41.4	11.3	27.3	6.5	69.5	13.4	3	107.5
Candidate-028	Candidates	Histaminergic GPCR	1.0	4	0.938	<	12.3	4.9	39.5	1.7	16.5	8.2	8	13.2
Candidate-029	Candidates	Glutamate receptors	0.1	2	0.927	=	26.3	10.9	41.2	7.7	123.8		2	28.4

Pub-Name	Set	Target Mechanism	Pgp Low95	Pgp N	cFu, mi c	CLIA OP	CLIA Mean	CLIA SD	CLIA CV	CLIA SEM	CLIA Upp95	CLIA Low95	CLIA N	CLI_u
Candidate-030	Candidates	Peptide GPCR	0.9	3	0.811	=	229.2	20.8	9.1	12.0	280.8	177.6	3	282.6
Candidate-031	Candidates	Serotonergic GPCR	1.0	5	0.748	=	150.0	28.2	18.8	12.6	185.3	114.7	5	200.7
Candidate-032	Candidates	Gaba Receptors	1.0	4	0.992	<	13.7	7.4	53.9	3.7	25.4	1.9	4	13.8
Candidate-033	Candidates	Opioid Receptor	2.3	14	0.594	<	22.4	15.3	68.6	4.9	32.5	12.2	10	37.6
Candidate-034	Candidates	Reuptake Inhibitors	2.7	4	0.228	<	32.4	21.9	67.6	6.3	45.7	19.1	12	142.3
Candidate-035	Candidates	Calcium Channels		0	0.992								0	
Candidate-036	Candidates	Peptide GPCR		0	0.002								0	
Candidate-037	Candidates	Gaba Receptors	0.7	7	0.763	=	43.6	14.1	32.2	7.0	66.1	21.2	4	57.2
Candidate-038	Candidates	Serotonergic GPCR		0	0.164								0	
Candidate-039	Candidates	Glutamate receptors	4.5	9	0.195	=	77.7	6.2	8.0	3.6	93.2	62.2	3	399.2
Candidate-040	Candidates	Enzyme	1.3	1	0.559	<	7.2				7.2	7.2	1	12.8
Candidate-041	Candidates	Peptide GPCR	3.2	24	0.171	=	44.6	17.7	39.7	8.9	73.0	16.3	4	261.7
Candidate-042	Candidates	Serotonergic GPCR	1.2	3	0.220	<	19.9	30.3	151.9	11.5	47.4		7	90.7
Candidate-043	Candidates	Peptide GPCR	2.0	3	0.878	<	14.4	10.9	75.9	5.5	31.9		4	16.4
Candidate-044	Candidates	Serotonergic GPCR	5.7	11	0.115	=	58.5	45.5	77.8	18.6	106.9	10.2	6	507.1
Candidate-045	Candidates	Cannabinoids	6.0	1	0.123	=	22.3				22.3	22.3	1	181.8
Candidate-046	Candidates	Serotonergic GPCR	-4.2	9	0.068	=	86.3	23.8	27.5	10.6	116.0	56.5	5	1274.3
Candidate-047	Candidates	Calcium Channels			0.979	=	8.3				8.3	8.3	1	8.5
Candidate-048	Candidates	Dopaminergic GPCR	2.6	6	0.069	=	39.4	17.1	43.3	8.5	66.7	12.1	4	572.1
Candidate-049	Candidates	Serotonergic GPCR	3.0	9	0.080	=	90.2	35.6	39.5	13.5	122.6	57.9	7	1126.6
Candidate-050	Candidates	Gaba Receptors	-0.4	3	0.617	<	10.3	5.6	54.4	3.2	24.3		3	16.7
Candidate-051	Candidates	Reuptake Inhibitors	2.0	3	0.232	<	16.2	14.9	92.0	6.1	32.1	0.4	6	70.0
Candidate-052	Candidates	Enzyme		0	0.012								0	
Candidate-053	Candidates	Nicotinic Receptor	1.1	6	0.948	<	12.6	4.3	33.7	1.7	17.2	8.1	6	13.3
Candidate-054	Candidates	Opioid Receptor		0	0.028								0	
Candidate-055	Candidates	Enzyme	0.3	3	0.270	=	84.8	35.2	41.5	20.3	172.1		3	313.8
Candidate-056	Candidates	Enzyme	1.5	6	0.156	=	37.4	2.6	7.0	1.3	41.6	33.2	4	239.1
Candidate-057	Candidates	Dopaminergic GPCR		0	0.242								0	
Candidate-058	Candidates	Peptide GPCR	1.2	1	0.265	=	21.7	1.5	6.7	1.0	34.8	8.6	2	81.9
Candidate-059	Candidates	Dopaminergic GPCR		0	0.023	=	31.9				31.9	31.9	1	1417.9
Candidate-060	Candidates	Serotonergic GPCR		0	0.079	=	64.9	29.1	44.8	13.0	101.3	28.5	5	821.3
Candidate-061	Candidates	Histaminergic GPCR	1.1	4	0.869	<	11.3	6.5	57.2	2.9	19.5	3.2	5	13.1
Candidate-062	Candidates	Dopaminergic GPCR	2.7	1	0.083	=	37.4	21.4	57.2	10.7	71.6	3.2	4	451.0
Candidate-063	Candidates	Nicotinic Receptor	1.1	3	0.936	<	9.9	1.8	18.5	0.7	11.9	8.0	6	10.6
Candidate-064	Candidates	Serotonergic GPCR	0.3	3	0.320	<	46.7	30.8	65.9	15.4	96.0		4	145.9
Candidate-065	Candidates	Peptide GPCR	0.9	3	0.103	=	98.6	39.2	39.8	22.7	196.0	1.2	3	961.1
Candidate-066	Candidates	Serotonergic GPCR	0.5	3	0.641	=	134.5	34.7	25.8	20.0	220.6	48.3	3	209.9

Pub-Name	Set	Target Mechanism	Pgp Low95	Pgp N	cFu,mi c	CLIA OP	CLIA Mean	CLIA SD	CLIA CV	CLIA SEM	CLIA Upp95	CLIA Low95	CLIA N	CLI_u
Candidate-067	Candidates	Dopaminergic GPCR		0	0.016	=	45.8	14.4	31.5	7.2	68.9	22.7	4	2901.0
Candidate-068	Candidates	Serotonergic GPCR	1.0	1	0.024	>	248.8	92.8	37.3	53.6	479.3	18.3	3	10238.5
Candidate-069	Candidates	Reuptake Inhibitors	3.5	3	0.132	=	49.9	10.2	20.4	5.9	75.2	24.6	3	377.4
Candidate-070	Candidates	Dopaminergic GPCR	0.2	2	1.000	<	14.2	9.4	66.3	6.7	98.9		2	14.2
Candidate-071	Candidates	Reuptake Inhibitors	2.3	4	1.000	=	28.6	1.7	5.8	0.8	31.3	26.0	4	28.6
Candidate-072	Candidates	Dopaminergic GPCR	1.4	3	0.239	=	24.1				24.1	24.1	1	100.9
Candidate-073	Candidates	Gaba Receptors	6.8	3	0.785	=	14.6	2.5	17.2	0.9	16.8	12.3	7	18.5
Candidate-074	Candidates	Peptide GPCR		0	0.004	=	43.0				43.0	43.0	1	10476.8
Candidate-075	Candidates	Nicotinic Receptor	1.0	3	0.997	<	21.6	7.0	32.5	2.0	25.8	17.3	12	21.6
Candidate-076	Candidates	Nicotinic Receptor	1.1	3	0.795	<	10.4	5.7	54.8	2.9	19.5	1.3	4	13.1
Candidate-077	Candidates	Gaba Receptors	0.9	3	0.461	=	164.4	25.4	15.4	12.7	205.0	123.8	4	356.8
Candidate-078	Candidates	Reuptake Inhibitors	1.5	7	0.597	<	20.2	14.6	72.1	4.9	31.4	9.1	9	33.9
Candidate-079	Candidates	Calcium Channels		0	0.972	<	7.6				7.6	7.6	1	7.8
Candidate-080	Candidates	Dopaminergic GPCR	1.6	27	0.268	=	30.2				30.2	30.2	1	112.5
Candidate-081	Candidates	Serotonergic GPCR	1.2	4	0.642	=	28.2	15.5	55.1	6.3	44.7	11.7	6	43.9
Candidate-082	Candidates	Gaba Receptors	-0.1	3	0.850	<	13.4	10.1	75.2	5.8	38.3		3	15.7
Candidate-083	Candidates	Cannabinoids	0.6	3	0.061	<	12.7	5.2	40.7	3.0	25.5		3	206.5
Candidate-084	Candidates	Gaba Receptors	0.7	4	0.847	=	44.3	32.5	73.4	10.3	65.9	22.7	10	52.3
Candidate-085	Candidates	Reuptake Inhibitors	1.2	4	0.712	=	14.8	4.0	27.1	2.3	24.7	4.8	3	20.8
Candidate-086	Candidates	Muscarinic Receptor	1.0	3	0.871	=	38.5				38.5	38.5	1	44.2
Candidate-087	Candidates	Cannabinoids	1.5	1	0.015	=	21.0	9.2	43.7	6.5	103.3		2	1436.4
Candidate-088	Candidates	Dopaminergic GPCR	-0.5	3	0.287	=	15.5	4.2	27.0	3.0	53.2		2	54.2
Candidate-089	Candidates	Enzyme	3.0	16	0.933	<	15.4	6.9	44.9	4.0	32.6		3	16.5
Candidate-090	Candidates	Glutamate receptors	1.5	16	0.953	<	14.6	3.9	27.1	0.9	16.5	12.6	18	15.3
Candidate-091	Candidates	Gaba Receptors	0.9	3	0.431	=	28.3	5.8	20.5	2.6	35.5	21.0	5	65.5
Candidate-092	Candidates	Reuptake Inhibitors	1.9	6	0.417	<	10.6	5.7	53.9	3.3	24.7		3	25.4
Candidate-093	Candidates	Muscarinic Receptor	0.7	3	0.880	=	74.2	0.2	0.3	0.2	76.2	72.1	2	84.2
Candidate-094	Candidates	Dopaminergic GPCR	2.4	7	0.231	=	91.4	9.8	10.7	5.6	115.6	67.2	3	395.4
Candidate-095	Candidates	Gaba Receptors	0.9	2	0.709	=	93.4				93.4	93.4	1	131.7
Candidate-096	Candidates	Serotonergic GPCR			0.577									
Candidate-097	Candidates	Reuptake Inhibitors	2.0	3	0.150	=	86.9	32.8	37.7	12.4	116.6	57.1	7	579.1
Candidate-098	Candidates	Enzyme	2.1	4	0.033	<	43.3	33.5	77.3	13.7	78.8	7.8	6	1324.3
Candidate-099	Candidates	Peptide GPCR	7.7	15	0.330	=	35.5	12.0	33.8	6.9	65.3	5.7	3	107.5
Candidate-100	Candidates	Enzyme		0	0.003	=	30.3	3.6	11.8	2.5	62.2		2	8901.6
Candidate-101	Candidates	Dopaminergic GPCR	-6.8	2	0.143	<	59.5	73.4	123.4	51.9	718.5		2	414.6
Candidate-102	Candidates	Serotonergic GPCR	1.4	8	0.375	=	246.1	60.9	24.7	35.1	397.2	94.9	3	656.3
Candidate-103	Candidates	Dopaminergic GPCR		0	0.012								0	

Pub-Name	Set	Target Mechanism	Pgp Low95	Pgp N	cFu,mi c	CLIA OP	CLIA Mean	CLIA SD	CLIA CV	CLIA SEM	CLIA Upp95	CLIA Low95	CLIA N	CLI_u
Candidate-104	Candidates	Peptide GPCR	4.1	3	0.745	=	37.5	8.3	22.2	4.2	50.8	24.2	4	50.3
Candidate-105	Candidates	Gaba Receptors	1.0	3	0.410	=	122.0	10.9	8.9	6.3	149.0	95.0	3	297.4
Candidate-106	Candidates	Peptide GPCR	-14.9	2	0.168	>	302.4				302.4	302.4	2	1796.8
Candidate-107	Candidates	Calcium Channels		0	0.981								0	
Candidate-108	Candidates	Nicotinic Receptor	0.9	4	0.981	<	9.9	1.7	17.0	0.8	12.7	7.2	4	10.1

Pub-Name	Set	Target Mechanism	2D6 Inh (% @ 3uM) OP	2D6 Inh (% @ 3uM) Mean	2D6 Inh (% @ 3uM) SD	2D6 Inh (% @ 3uM) CV	2D6 Inh (% @ 3uM) SEM	2D6 Inh (% @ 3uM) Upp95	2D6 Inh (% @ 3uM) Low95	2D6 Inh (% @ 3uM) N	3A4 Inh (% @ 3uM) OP	3A4 Inh (% @ 3uM) Mean
Acamprosate	Drugs	Glutamate receptors	=	2.2	2.8	130.0	1.4	6.6	-2.3	4	=	1.6
Alprazolam	Drugs	Gaba Receptors	=	8.0	0.0	0.0	0.0	8.0	8.0	1	=	6.0
Amfebutamone	Drugs	Dopaminergic GPCR	=	4.4	5.3	120.9	2.7	12.9	-4.1	4	=	0.2
Amisulpride	Drugs	Dopaminergic GPCR	=	9.5	8.2	87.1	4.8	29.9	-11.0	3	=	0.9
Amphetamine	Drugs	Reuptake Inhibitors										
Aniracetam	Drugs		=	0.0	0.0	0.0	0.0	0.0	0.0	2	=	3.2
Apomorphine	Drugs	Dopaminergic GPCR	=	2.0	3.4	167.7	1.3	5.1	-1.1	7	=	5.0
Aprepitant	Drugs		=	4.6	4.6	99.1	1.9	9.4	-0.2	6	=	39.0
Aripiprazole	Drugs	Dopaminergic GPCR	=	14.8	10.4	70.2	3.9	24.3	5.4	7	=	0.0
Atomoxetine	Drugs	Reuptake Inhibitors	=	32.2	30.7	95.2	17.7	108.3	-43.9	3	=	2.3
Bromazepam	Drugs	Gaba Receptors	=	0.0	0.0	0.0	0.0	0.0	0.0	1	=	0.0
Bromocriptine	Drugs	Dopaminergic GPCR	=	5.6	4.8	86.8	2.8	17.6	-6.4	3	=	84.2
Brotizolam	Drugs	Gaba Receptors	=	0.8	1.1	145.5	0.6	3.5	-2.0	3	=	3.9
Budipine	Drugs	Calcium Channels										
Buprenorphine	Drugs	Opioid Receptor										
Buspirone	Drugs	Serotonergic GPCR	=	12.7	21.0	165.2	8.6	35.0	-9.6	6	=	6.3
Cabergoline	Drugs	Dopaminergic GPCR	=	7.0	8.0	114.4	3.6	16.9	-3.0	5	=	2.9
Caffeine	Drugs	Serotonergic GPCR	=	2.3	3.2	141.4	2.3	30.8	-26.3	2	=	10.3
Carbamazepine	Drugs	Reuptake Inhibitors	=	6.7	12.2	181.6	5.0	19.6	-6.2	6	=	11.4
Carisoprodol	Drugs		=	0.0	0.0	0.0	0.0	0.0	0.0	1	=	0.0
Chlorpromazine	Drugs	Dopaminergic GPCR	=	62.3	19.8	31.8	9.9	94.1	30.6	4	=	12.3
Citalopram	Drugs	Serotonergic GPCR	=	5.4	5.8	107.2	2.9	14.7	-3.9	4	=	3.8
Clomipramine	Drugs	Serotonergic GPCR	=	19.8	15.4	77.7	6.9	39.1	0.5	5	=	10.1
Clonazepam	Drugs	Gaba Receptors	=	0.0	0.0	0.0	0.0	0.0	0.0	1	=	0.0
Clozapine	Drugs	Serotonergic GPCR	=	6.7	7.3	108.3	2.4	12.3	1.1	9	=	3.6
Cyclobenzaprine	Drugs		=	25.5	0.0	0.0	0.0	25.5	25.5	1	=	18.5
Dexmethylphenidate	Drugs	Dopaminergic GPCR										
Dextropropoxyphene	Drugs	Opioid Receptor	=	2.8	0.0	0.0	0.0	2.8	2.8	1	=	36.8
Diazepam	Drugs	Gaba Receptors	=	0.0	0.0	0.0	0.0	0.0	0.0	1	=	0.0
Donepezil	Drugs	Enzyme	=	4.7	6.2	133.0	2.8	12.5	-3.1	5	=	3.3
Dronabinol	Drugs	Cannabinoids										
Duloxetine	Drugs	Serotonergic GPCR	=	55.7	21.9	39.3	9.8	83.2	28.3	5	=	12.0
Eletriptan	Drugs	Serotonergic GPCR	=	20.9	16.7	80.1	7.5	41.8	-0.1	5	=	16.6
Escitalopram	Drugs	Serotonergic GPCR	=	8.9	7.0	78.0	3.5	20.1	-2.2	4	=	1.3
Eszopiclone	Drugs	Gaba Receptors										
Ethosuximide	Drugs	Calcium Channels	=	1.6	3.6	223.6	1.6	6.1	-2.9	5	=	6.5
Felbamate	Drugs	Gaba Receptors	=	3.9	6.7	173.2	3.9	20.4	-12.7	3	=	5.7

Pub-Name	Set	Target Mechanism	2D6 Inh (% @ 3uM) OP	2D6 Inh (% @ 3uM) Mean	2D6 Inh (% @ 3uM) SD	2D6 Inh (% @ 3uM) CV	2D6 Inh (% @ 3uM) SEM	2D6 Inh (% @ 3uM) Upp95	2D6 Inh (% @ 3uM) Low95	2D6 Inh (% @ 3uM) N	3A4 Inh (% @ 3uM) OP	3A4 Inh (% @ 3uM) Mean
Fentanyl	Drugs	Opioid Receptor	=	0.8	1.5	200.0	0.8	3.2	-1.7	4	=	5.8
Flumazenil	Drugs	Gaba Receptors	=	76.0	6.7	8.8	2.1	80.4	71.6	10	=	-0.9
Fluoxetine	Drugs	Serotonergic GPCR	=	17.8	8.9	49.8	3.6	27.2	8.4	6	=	1.6
Fluvoxamine	Drugs	Serotonergic GPCR	=	3.6	6.5	180.1	2.3	9.1	-1.9	8	=	5.3
Gabapentin	Drugs	Calcium Channels	=	5.1	0.5	10.4	0.4	9.9	0.3	2	=	23.2
Galantamine	Drugs	Enzyme	=	17.8	3.9	21.9	2.8	52.7	-17.2	2	=	0.0
Haloperidol	Drugs	Dopaminergic GPCR	=	0.0	0.0	0.0	0.0	0.0	0.0	1	=	0.0
Hydrocodone	Drugs	Opioid Receptor	=	1.9	2.7	141.4	1.9	26.2	-22.4	2	=	1.8
Indeloxazine	Drugs	Reuptake Inhibitors	=	0.0	0.0	0.0	0.0	0.0	0.0	6	=	2.7
Lamotrigine	Drugs	Reuptake Inhibitors	=	1.4	1.6	112.3	0.7	3.3	-0.6	5	=	0.9
Levetiracetam	Drugs	Calcium Channels	=	47.9	10.4	21.8	7.4	141.6	-45.8	2	=	0.4
Levomethadyl Acetate	Drugs	Opioid Receptor	=	0.0	0.0	0.0	0.0	0.0	0.0	2	=	0.0
Lofexidine	Drugs	Gaba Receptors	=	0.2	0.3	141.4	0.2	3.4	-2.9	2	=	0.0
Lorazepam	Drugs	Dopaminergic GPCR	=	0.1	12.1	13284.6	1.8	3.9	-3.7	44	=	-53.7
Meprobamate	Drugs	Gaba Receptors	=	0.1	12.1	13284.6	1.8	3.9	-3.7	44	=	-53.7
Methylphenidate	Drugs	Dopaminergic GPCR	=	0.2	0.3	141.4	0.2	3.4	-2.9	2	=	0.0
Metoclopramide	Drugs	Dopaminergic GPCR	=	0.2	0.3	141.4	0.2	3.4	-2.9	2	=	0.0
Midazolam	Drugs	Gaba Receptors	=	0.1	12.1	13284.6	1.8	3.9	-3.7	44	=	-53.7
Milnacipran	Drugs	Serotonergic GPCR	=	17.7	13.2	74.3	9.3	136.2	-100.7	2	=	3.2
Minaprine	Drugs	Enzyme	=	3.1	3.7	117.4	1.6	7.7	-1.5	5	=	0.5
Mirtazapine	Drugs	Enzyme	=	7.9	10.2	129.7	5.9	33.2	-17.4	3	=	6.2
Moclobemide	Drugs	Enzyme	=	7.9	10.2	129.7	5.9	33.2	-17.4	3	=	6.2
Modafinil	Drugs	Dopaminergic GPCR	=	0.0	0.0	0.0	0.0	0.0	0.0	1	=	0.0
Morphine	Drugs	Opioid Receptor	=	0.0	0.0	0.0	0.0	0.0	0.0	1	=	0.0
Nalmefene	Drugs	Opioid Receptor	=	21.5	6.8	31.5	4.8	82.2	-39.3	2	=	0.4
Naltrexone	Drugs	Opioid Receptor	=	6.2	6.4	103.5	2.6	13.0	-0.6	6	=	1.4
Nemonapride	Drugs	Dopaminergic GPCR	=	73.6	6.4	8.7	3.7	89.5	57.7	3	=	13.3
Nicergoline	Drugs	Dopaminergic GPCR	=	73.6	6.4	8.7	3.7	89.5	57.7	3	=	13.3
Nicotrol	Drugs	Nicotinic Receptor	=	2.9	3.3	112.9	1.5	7.1	-1.2	5	=	3.6
Nimodipine	Drugs	Calcium Channels	=	4.2	3.8	91.7	1.5	7.7	0.7	7	=	30.8
Nortriptyline	Drugs	Calcium Channels	=	30.9	0.0	0.0	0.0	30.9	30.9	1	=	0.0
Olanzapine	Drugs	Dopaminergic GPCR	=	10.7	6.9	64.9	2.8	18.0	3.3	6	=	6.5
Oxcarbazepine	Drugs	Reuptake Inhibitors	=	0.0	0.0	0.0	0.0	0.0	0.0	2	=	6.8
Oxycodone	Drugs	Opioid Receptor	=	0.0	0.0	0.0	0.0	0.0	0.0	1	=	0.0
Paliperidone	Drugs	Opioid Receptor	=	0.0	0.0	0.0	0.0	0.0	0.0	1	=	0.0
Paliperidone	Drugs	Dopaminergic GPCR	=	0.0	0.0	0.0	0.0	0.0	0.0	2	=	0.0
Paroxetine	Drugs	Serotonergic GPCR	=	70.1	6.4	9.1	3.2	80.4	59.9	4	=	4.7
Pergolide	Drugs	Dopaminergic GPCR	=	94.7	1.3	1.4	0.8	97.9	91.5	3	=	2.4

Pub-Name	Set	Target Mechanism	2D6 Inh (% @ 3uM) OP	2D6 Inh (% @ 3uM) Mean	2D6 Inh (% @ 3uM) SD	2D6 Inh (% @ 3uM) CV	2D6 Inh (% @ 3uM) SEM	2D6 Inh (% @ 3uM) Upp95	2D6 Inh (% @ 3uM) Low95	2D6 Inh (% @ 3uM) N	3A4 Inh (% @ 3uM) OP	3A4 Inh (% @ 3uM) Mean
Perospirone	Drugs	Dopaminergic GPCR	=	9.8	3.5	35.7	2.5	41.0	-21.5	2	=	32.5
phenytoin	Drugs	Reuptake Inhibitors	=	4.1	5.2	126.1	1.7	8.1	0.1	9	=	6.8
Piracetam	Drugs		=	0.0	0.0	141.4	0.0	0.1	-0.1	2	=	0.5
Pramipexole	Drugs	Dopaminergic GPCR	=	0.0	0.0	0.0	0.0	0.0	0.0	4	=	0.0
Pregabalin	Drugs	Calcium Channels	=	1.0	1.4	141.4	1.0	13.6	-11.6	2	=	1.7
Propofol	Drugs		=	0.7	0.9	133.6	0.5	2.2	-0.8	4	=	1.4
Propoxyphene	Drugs											
Quazepam	Drugs	Gaba Receptors										
Quetiapine	Drugs	Serotonergic GPCR	=	0.8	1.8	223.6	0.8	3.0	-1.4	5	=	5.8
Ramelteon	Drugs	Melatonin Receptor	=	0.7	1.5	223.6	0.7	2.5	-1.2	5	=	2.8
Rasagiline	Drugs	Enzyme	=	5.3	0.0	0.0	0.0	5.3	5.3	1	=	2.7
Reboxetine	Drugs	Reuptake Inhibitors	=	21.8	12.4	57.1	7.2	52.7	-9.1	3	=	7.1
Remifentanyl	Drugs	Opioid Receptor										
Riluzole	Drugs	Reuptake Inhibitors	=	1.4	1.6	117.8	0.8	4.0	-1.2	4	=	0.9
Rimonabant	Drugs	Cannabinoids	=	1.4	2.4	173.2	1.4	7.2	-4.5	3	=	0.0
Risperidone	Drugs	Dopaminergic GPCR	=	17.3	11.4	65.9	3.8	26.1	8.6	9	=	11.5
Rivastigmine	Drugs	Enzyme	=	0.8	1.3	170.5	0.7	2.9	-1.3	4	=	2.8
Ropinirole	Drugs	Dopaminergic GPCR	=	13.7	7.3	53.2	3.7	25.4	2.0	4	=	0.6
Ropivacaine	Drugs		=	18.7	5.1	27.5	2.6	27.0	10.5	4	=	2.5
Selegiline	Drugs	Enzyme										
Sertindole	Drugs	Serotonergic GPCR	=	60.7	12.9	21.3	9.1	176.7	-55.3	2	=	5.2
Sertraline	Drugs	Serotonergic GPCR	=	33.4	18.4	55.1	6.5	49.1	17.8	8	=	10.3
Sinequan	Drugs	Serotonergic GPCR	=	31.8	19.4	61.1	9.7	62.8	0.7	4	=	5.1
Sulpiride	Drugs	Dopaminergic GPCR	=	0.0	0.0	0.0	0.0	0.0	0.0	1	=	1.0
Tacrine	Drugs	Enzyme	=	9.7	5.9	61.0	2.1	14.8	4.7	8	=	2.7
Talipexole	Drugs	Dopaminergic GPCR	=	1.9	3.7	200.0	1.9	7.8	-4.1	4	=	4.0
Terguride	Drugs	Dopaminergic GPCR										
Thiopental	Drugs	Gaba Receptors										
Tiagabine	Drugs	Gaba Receptors	=	0.2	0.4	200.0	0.2	0.9	-0.5	4	=	4.3
Tianeptine	Drugs	Reuptake Inhibitors	=	0.0	0.1	173.2	0.0	0.2	-0.1	3	=	0.0
Topiramate	Drugs	Enzyme	=	0.9	1.5	173.2	0.9	4.6	-2.9	3	=	0.0
Tramadol	Drugs	Reuptake Inhibitors	=	15.0	2.5	16.8	1.8	37.5	-7.6	2	=	4.8
Trazodone	Drugs	Serotonergic GPCR										
Tropisetron	Drugs	Serotonergic GPCR	=	26.2	5.8	22.0	4.1	77.9	-25.5	2	=	7.0
Valproic Acid	Drugs		=	1.3	2.3	173.2	1.3	7.1	-4.4	3	=	0.0
Varenicline	Drugs	Nicotinic Receptor	=	5.5	10.9	199.3	4.4	17.0	-6.1	6	=	5.3
Venlafaxine	Drugs	Serotonergic GPCR	=	9.3	7.8	84.4	3.2	17.5	1.0	6	=	4.3



Pub-Name	Set	Target Mechanism	2D6 Inh (% @ 3uM) OP	2D6 Inh (% @ 3uM) Mean	2D6 Inh (% @ 3uM) SD	2D6 Inh (% @ 3uM) CV	2D6 Inh (% @ 3uM) SEM	2D6 Inh (% @ 3uM) Upp95	2D6 Inh (% @ 3uM) Low95	2D6 Inh (% @ 3uM) N	3A4 Inh (% @ 3uM) OP	3A4 Inh (% @ 3uM) Mean
Verapamil	Drugs	Calcium Channels	=	4.6	12.1	264.1	2.0	8.8	0.3	36	=	19.1
Vigabatrin	Drugs	Gaba Receptors	=	2.1	0.4	18.0	0.3	5.6	-1.3	2	=	0.0
Vinpocetine	Drugs		=	4.4	4.1	93.0	2.0	10.8	-2.1	4	=	5.0
Zaleplon	Drugs	Gaba Receptors	=	0.0	0.0	0.0	0.0	0.0	0.0	1	=	4.0
Ziprasidone	Drugs	Dopaminergic GPCR	=	5.1	7.0	138.4	2.5	11.0	-0.9	8	=	17.7
Zolpidem	Drugs	Gaba Receptors	=	4.1	0.0	0.0	0.0	4.1	4.1	1	=	6.1
Zonisamide	Drugs	Enzyme	=	0.7	1.7	236.0	0.7	2.6	-1.1	6	=	1.9
Zotepine	Drugs	Serotonergic GPCR	=	40.5	11.5	28.4	6.6	69.1	11.9	3	=	9.3
Candidate-001	Candidates	Glutamate receptors	=	13.6	0.0	0.0	0.0	13.6	13.6	1	=	10.4
Candidate-002	Candidates	Reuptake Inhibitors	=	4.6	3.7	81.6	1.7	9.2	-0.1	5	=	3.2
Candidate-003	Candidates	Reuptake Inhibitors	=	92.0	1.8	2.0	1.0	96.5	87.5	3	=	5.5
Candidate-004	Candidates	Serotonergic GPCR										
Candidate-005	Candidates	Enzyme	=	18.6	0.0	0.0	0.0	18.6	18.6	1	=	1.3
Candidate-006	Candidates	Peptide GPCR										
Candidate-007	Candidates	Enzyme	=	1.0	1.3	128.1	0.6	3.1	-1.1	4	=	1.9
Candidate-008	Candidates	Calcium Channels	=	0.0	0.0	0.0	0.0	0.0	0.0	1	=	0.0
Candidate-009	Candidates	Nicotinic Receptor	=	3.9	5.8	151.5	2.4	10.1	-2.3	6	=	1.4
Candidate-010	Candidates	Opioid Receptor	=	12.3	7.5	61.1	5.3	80.0	-55.4	2	=	3.0
Candidate-011	Candidates	Dopaminergic GPCR	=	7.6	11.1	145.7	6.4	35.1	-19.9	3	=	4.6
Candidate-012	Candidates	Peptide GPCR	=	4.6	6.5	141.4	4.6	62.9	-53.7	2	=	4.2
Candidate-013	Candidates	Enzyme	=	22.9	0.0	0.0	0.0	22.9	22.9	1	=	0.0
Candidate-014	Candidates	Opioid Receptor	=	88.0	0.0	0.0	0.0	88.0	88.0	1	=	16.7
Candidate-015	Candidates	Nicotinic Receptor	=	4.4	4.8	109.0	2.8	16.3	-7.5	3	=	4.7
Candidate-016	Candidates	Gaba Receptors	=	26.2	10.7	40.8	3.6	34.4	18.0	9	=	11.9
Candidate-017	Candidates	Enzyme	=	0.0	0.0	0.0	0.0	0.0	0.0	1	=	0.0
Candidate-018	Candidates	Cannabinoids	=	2.3	3.5	155.2	1.4	6.0	-1.5	6	=	1.0
Candidate-019	Candidates	Peptide GPCR	=	8.5	7.8	91.9	3.0	15.6	1.4	7	=	15.0
Candidate-020	Candidates	Glutamate receptors	=	1.6	0.0	0.0	0.0	1.6	1.6	1	=	0.0
Candidate-021	Candidates	Enzyme	=	2.9	3.7	124.9	1.8	8.8	-2.9	4	=	0.6
Candidate-022	Candidates	Enzyme	=	4.2	3.3	78.1	1.7	9.5	-1.1	4	=	25.5
Candidate-023	Candidates	Nicotinic Receptor	=	1.9	3.3	173.2	1.9	10.1	-6.3	3	=	2.7
Candidate-024	Candidates	Calcium Channels	=	20.0	0.0	0.0	0.0	20.0	20.0	1	=	0.0
Candidate-025	Candidates	Reuptake Inhibitors	=	87.1	2.4	2.7	1.7	108.5	65.7	2	=	0.0
Candidate-026	Candidates	Serotonergic GPCR	=	12.8	5.8	45.3	2.6	20.0	5.5	5	=	3.6
Candidate-027	Candidates	Serotonergic GPCR	=	4.6	6.6	141.4	4.6	63.5	-54.2	2	=	4.9
Candidate-028	Candidates	Histaminergic GPCR	=	0.7	1.7	244.4	0.7	2.5	-1.1	6	=	13.1
Candidate-029	Candidates	Glutamate receptors	=	24.8	0.4	1.4	0.3	27.9	21.6	2	=	15.3

Pub-Name	Set	Target Mechanism	2D6 Inh (% @ 3uM) OP	2D6 Inh (% @ 3uM) Mean	2D6 Inh (% @ 3uM) SD	2D6 Inh (% @ 3uM) CV	2D6 Inh (% @ 3uM) SEM	2D6 Inh (% @ 3uM) Upp95	2D6 Inh (% @ 3uM) Low95	2D6 Inh (% @ 3uM) N	3A4 Inh (% @ 3uM) OP	3A4 Inh (% @ 3uM) Mean
Candidate-030	Candidates	Peptide GPCR	=	79.5	9.2	11.6	6.5	162.3	-3.3	2	=	13.5
Candidate-031	Candidates	Serotonergic GPCR	=	3.0	4.4	147.2	2.0	8.5	-2.5	5	=	16.9
Candidate-032	Candidates	Gaba Receptors	=	2.4	3.4	140.1	1.5	6.6	-1.8	5	=	27.6
Candidate-033	Candidates	Opioid Receptor	=	5.5	5.3	96.4	1.7	9.0	2.0	10	=	2.5
Candidate-034	Candidates	Reuptake Inhibitors	=	6.8	4.2	61.5	1.4	10.0	3.6	9	=	41.2
Candidate-035	Candidates	Calcium Channels	=	33.5	47.4	141.4	33.5	458.7	-391.8	2	=	1.0
Candidate-036	Candidates	Peptide GPCR	=	0.0	0.0	0.0	0.0	0.0	0.0	1	=	10.4
Candidate-037	Candidates	Gaba Receptors	=	0.4	0.8	200.0	0.4	1.7	-0.9	4	=	0.0
Candidate-038	Candidates	Serotonergic GPCR	=	5.2	0.0	0.0	0.0	5.2	5.2	1	=	12.2
Candidate-039	Candidates	Glutamate receptors	=	5.4	5.1	93.7	2.9	17.9	-7.2	3	=	11.9
Candidate-040	Candidates	Enzyme	=	0.0	0.0	0.0	0.0	0.0	0.0	1	=	0.0
Candidate-041	Candidates	Peptide GPCR	=	88.8	5.2	5.9	3.0	101.8	75.8	3	=	10.1
Candidate-042	Candidates	Serotonergic GPCR	=	37.3	15.6	41.9	5.5	50.6	24.0	8	=	3.8
Candidate-043	Candidates	Peptide GPCR	=	2.7	4.7	176.7	1.9	7.6	-2.3	6	=	4.3
Candidate-044	Candidates	Serotonergic GPCR	=	7.9	7.3	92.9	3.0	15.6	0.1	6	=	10.9
Candidate-045	Candidates	Cannabinoids	=	0.0	0.0	0.0	0.0	0.0	0.0	1	=	0.0
Candidate-046	Candidates	Serotonergic GPCR	=	10.6	0.0	0.0	0.0	10.6	10.6	1	=	2.3
Candidate-047	Candidates	Calcium Channels	=	20.0	28.3	141.4	20.0	274.0	-234.0	2	=	1.2
Candidate-048	Candidates	Dopaminergic GPCR	=	18.0	8.1	45.2	3.3	26.7	9.4	6	=	3.9
Candidate-049	Candidates	Serotonergic GPCR	=	11.5	0.7	6.0	0.5	17.7	5.3	2	=	9.4
Candidate-050	Candidates	Gaba Receptors	=	2.6	3.5	134.2	1.7	8.1	-3.0	4	=	9.6
Candidate-051	Candidates	Reuptake Inhibitors	=	6.4	6.7	106.0	2.7	13.5	-0.8	6	=	2.1
Candidate-052	Candidates	Enzyme	=	14.5	0.0	0.0	0.0	14.5	14.5	1	=	12.8
Candidate-053	Candidates	Nicotinic Receptor	=	0.0	0.0	0.0	0.0	0.0	0.0	1	=	4.8
Candidate-054	Candidates	Opioid Receptor	=	69.8	0.0	0.0	0.0	69.8	69.8	1	=	25.7
Candidate-055	Candidates	Enzyme	=	10.3	7.0	67.7	4.0	27.6	-7.0	3	=	0.0
Candidate-056	Candidates	Enzyme	=	26.8	22.5	84.1	11.3	62.9	-9.3	4	=	20.6
Candidate-057	Candidates	Dopaminergic GPCR								0		
Candidate-058	Candidates	Peptide GPCR										
Candidate-059	Candidates	Dopaminergic GPCR										
Candidate-060	Candidates	Serotonergic GPCR	=	4.4	4.3	97.4	1.7	8.9	-0.1	6	=	12.8
Candidate-061	Candidates	Histaminergic GPCR	=	3.8	6.5	173.2	3.8	19.9	-12.4	3	=	4.6
Candidate-062	Candidates	Dopaminergic GPCR	=	13.4	6.5	48.4	4.6	71.7	-44.9	2	=	15.8
Candidate-063	Candidates	Nicotinic Receptor	=	0.5	0.7	141.4	0.5	6.7	-5.7	2	=	0.0
Candidate-064	Candidates	Serotonergic GPCR	=	5.2	6.4	123.2	3.2	15.4	-5.0	4	=	0.0
Candidate-065	Candidates	Peptide GPCR	=	3.3	0.4	12.3	0.3	6.9	-0.3	2	=	13.3
Candidate-066	Candidates	Serotonergic GPCR	=	3.0	5.2	173.2	3.0	15.9	-9.9	3	=	8.2

Pub-Name	Set	Target Mechanism	2D6 Inh (% @ 3uM) OP	2D6 Inh (% @ 3uM) Mean	2D6 Inh (% @ 3uM) SD	2D6 Inh (% @ 3uM) CV	2D6 Inh (% @ 3uM) SEM	2D6 Inh (% @ 3uM) Upp95	2D6 Inh (% @ 3uM) Low95	2D6 Inh (% @ 3uM) N	3A4 Inh (% @ 3uM) OP	3A4 Inh (% @ 3uM) Mean
Candidate-067	Candidates	Dopaminergic GPCR	=	39.1	13.1	33.5	6.5	60.1	18.2	4	=	17.5
Candidate-068	Candidates	Serotonergic GPCR	=	2.3	3.2	141.4	2.3	31.0	-26.5	2	=	0.0
Candidate-069	Candidates	Reuptake Inhibitors	=	70.6	0.0	0.0	0.0	70.6	70.6	1	=	10.5
Candidate-070	Candidates	Dopaminergic GPCR	=	0.0	0.0	0.0	0.0	0.0	0.0	1	=	0.0
Candidate-071	Candidates	Reuptake Inhibitors	=	36.5	50.9	139.6	36.0	493.6	-420.7	2	=	0.0
Candidate-072	Candidates	Dopaminergic GPCR	=	54.3	8.9	16.5	5.2	76.4	32.1	3	=	0.0
Candidate-073	Candidates	Gaba Receptors	=	2.2	2.2	102.0	0.7	3.9	0.5	9	=	2.8
Candidate-074	Candidates	Peptide GPCR	=	0.0	0.0	0.0	0.0	0.0	0.0	1	=	0.0
Candidate-075	Candidates	Nicotinic Receptor	=	2.0	2.9	141.4	2.0	27.9	-23.9	2	=	0.8
Candidate-076	Candidates	Nicotinic Receptor	=	5.6	4.2	73.9	2.1	12.3	-1.0	4	=	7.8
Candidate-077	Candidates	Gaba Receptors	=	2.8	3.3	117.4	1.6	8.0	-2.4	4	=	0.4
Candidate-078	Candidates	Reuptake Inhibitors	=	11.6	11.9	102.4	4.5	22.4	0.8	7	=	8.8
Candidate-079	Candidates	Calcium Channels	=	0.0	0.0	0.0	0.0	0.0	0.0	1	=	10.3
Candidate-080	Candidates	Dopaminergic GPCR	=	42.3	0.0	0.0	0.0	42.3	42.3	1	=	0.0
Candidate-081	Candidates	Serotonergic GPCR	=	8.4	9.8	116.3	4.9	24.1	-7.2	4	=	10.2
Candidate-082	Candidates	Gaba Receptors	=	3.0	4.7	154.3	2.1	8.9	-2.8	5	=	2.3
Candidate-083	Candidates	Cannabinoids	=	2.4	3.4	141.4	2.4	32.9	-28.1	2	=	0.0
Candidate-084	Candidates	Gaba Receptors	=	5.3	8.2	155.6	2.9	12.3	-1.7	8	=	7.2
Candidate-085	Candidates	Reuptake Inhibitors										
Candidate-086	Candidates	Muscarinic Receptor	=	0.0	0.0	0.0	0.0	0.0	0.0	1	=	6.4
Candidate-087	Candidates	Cannabinoids	=	0.0	0.0	0.0	0.0	0.0	0.0	2	=	20.3
Candidate-088	Candidates	Dopaminergic GPCR	=	23.9	0.0	0.0	0.0	23.9	23.9	1	=	0.0
Candidate-089	Candidates	Enzyme	=	4.2	3.7	89.4	2.1	13.4	-5.1	3	=	1.2
Candidate-090	Candidates	Glutamate receptors	=	15.7	9.3	58.9	4.6	30.6	0.9	4	=	18.5
Candidate-091	Candidates	Gaba Receptors	=	1.2	1.7	138.7	0.8	3.9	-1.5	4	=	1.3
Candidate-092	Candidates	Reuptake Inhibitors	=	0.0	0.0	0.0	0.0	0.0	0.0	2	=	0.0
Candidate-093	Candidates	Muscarinic Receptor	=	17.2	0.0	0.0	0.0	17.2	17.2	1	=	0.0
Candidate-094	Candidates	Dopaminergic GPCR	=	9.1	10.0	109.7	5.8	33.9	-15.7	3	=	10.9
Candidate-095	Candidates	Gaba Receptors	=	4.0	4.7	116.8	2.3	11.5	-3.5	4	=	1.9
Candidate-096	Candidates	Serotonergic GPCR										
Candidate-097	Candidates	Reuptake Inhibitors	=	93.7	1.7	1.8	0.7	95.4	91.9	6	=	2.0
Candidate-098	Candidates	Enzyme	=	9.9	9.8	98.5	4.4	22.1	-2.3	5	=	13.3
Candidate-099	Candidates	Peptide GPCR	=	56.4	8.6	15.2	6.1	133.4	-20.6	2	=	5.3
Candidate-100	Candidates	Enzyme	=	0.0	0.0	0.0	0.0	0.0	0.0	1	=	0.0
Candidate-101	Candidates	Dopaminergic GPCR	=	0.5	0.9	173.2	0.5	2.8	-1.7	3	=	6.2
Candidate-102	Candidates	Serotonergic GPCR	=	8.0	4.9	61.0	2.8	20.1	-4.1	3	=	8.9
Candidate-103	Candidates	Dopaminergic GPCR	=	87.8	0.0	0.0	0.0	87.8	87.8	1	=	0.0

Pub-Name	Set	Target Mechanism	2D6 Inh (% @ 3uM) OP	2D6 Inh (% @ 3uM) Mean	2D6 Inh (% @ 3uM) SD	2D6 Inh (% @ 3uM) CV	2D6 Inh (% @ 3uM) SEM	2D6 Inh (% @ 3uM) Upp95	2D6 Inh (% @ 3uM) Low95	2D6 Inh (% @ 3uM) N	3A4 Inh (% @ 3uM) OP	3A4 Inh (% @ 3uM) Mean
Candidate-104	Candidates	Peptide GPCR	=	19.8	11.1	56.1	6.4	47.4	-7.8	3	=	16.9
Candidate-105	Candidates	Gaba Receptors	=	2.6	4.6	173.2	2.6	14.0	-8.7	3	=	0.1
Candidate-106	Candidates	Peptide GPCR	=	20.8	0.0	0.0	0.0	20.8	20.8	1	=	64.0
Candidate-107	Candidates	Calcium Channels	=	0.0	0.0	0.0	0.0	0.0	0.0	1	=	0.0
Candidate-108	Candidates	Nicotinic Receptor	=	4.5	5.3	117.9	2.7	13.1	-4.0	4	=	26.5

Pub-Name	Set	Target Mechanism	3A4 Inh (% @ 3uM) SD	3A4 Inh (% @ 3uM) CV	3A4 Inh (% @ 3uM) SEM	3A4 Inh (% @ 3uM) Upp95	3A4 Inh (% @ 3uM) Low95	3A4 Inh (% @ 3uM) TotCnt	3A4 Inh (% @ 3uM) N	Dof Inh (% @ 10uM) Mean	Dof Inh (% @ 10uM) SD	Dof Inh (% @ 10uM) CV	Dof Inh (% @ 10uM) SEM
Acamprosate	Drugs	Glutamate receptors	2.9	176.7	1.5	6.3	-3.0	4	4	-2.8	3.7	-130.1	0.9
Alprazolam	Drugs	Gaba Receptors	0.0	0.0	0.0	6.0	6.0	1	1	-5.5	1.2	-21.8	0.6
Amfebutamone	Drugs	Dopaminergic GPCR	0.3	200.0	0.2	0.7	-0.4	4	4	-0.9	5.2	-606.1	1.6
Amisulpride	Drugs	Dopaminergic GPCR	1.6	173.2	0.9	4.9	-3.0	3	3	15.2	2.6	17.2	0.8
Amphetamine	Drugs	Reuptake Inhibitors											
Aniracetam	Drugs		4.5	141.4	3.2	43.2	-36.9	2	2	3.3	6.1	182.2	2.1
Apomorphine	Drugs	Dopaminergic GPCR	4.9	98.3	1.8	9.4	0.5	7	7	21.8	7.0	32.0	1.4
Aprepitant	Drugs		24.0	61.6	9.8	64.4	13.5	6	6	12.1	10.6	87.5	2.8
Aripiprazole	Drugs	Dopaminergic GPCR	0.0	0.0	0.0	0.0	0.0	7	7	86.3	7.0	8.1	1.5
Atomoxetine	Drugs	Reuptake Inhibitors	4.0	173.2	2.3	12.3	-7.7	4	3	63.2	12.6	20.0	3.2
Bromazepam	Drugs	Gaba Receptors	0.0	0.0	0.0	0.0	0.0	1	1	5.3	7.3	139.6	3.7
Bromocriptine	Drugs	Dopaminergic GPCR	7.5	8.9	4.3	102.8	65.5	3	3	19.0	9.2	48.3	2.8
Brotizolam	Drugs	Gaba Receptors	2.7	68.7	1.5	10.5	-2.7	3	3	2.0	4.9	238.9	1.4
Budipine	Drugs	Calcium Channels											
Buprenorphine	Drugs	Opioid Receptor											
Buspirone	Drugs	Serotonergic GPCR	12.3	194.4	5.0	19.4	-6.7	6	6	27.4	7.3	26.7	1.8
Cabergoline	Drugs	Dopaminergic GPCR	4.7	159.6	2.1	8.7	-2.9	5	5	31.2	14.7	47.3	3.3
Caffeine	Drugs	Serotonergic GPCR	14.5	141.4	10.3	140.4	-119.9	2	2				
Carbamazepine	Drugs	Reuptake Inhibitors	15.9	139.2	6.5	28.3	-5.4	8	6	-0.3	5.8	-2205.2	1.2
Carisoprodol	Drugs		0.0	0.0	0.0	0.0	0.0	1	1	6.9	3.9	56.1	1.9
Chlorpromazine	Drugs	Dopaminergic GPCR	6.4	51.7	3.2	22.5	2.1	4	4				
Citalopram	Drugs	Serotonergic GPCR	3.9	102.7	2.2	13.3	-5.8	4	3	41.0	19.5	47.6	5.2
Clomipramine	Drugs	Serotonergic GPCR	10.0	99.4	4.5	22.6	-2.5	5	5	70.1	15.6	22.2	4.5
Clonazepam	Drugs	Gaba Receptors	0.0	0.0	0.0	0.0	0.0	1	1	-4.2	1.9	-46.3	0.7
Clozapine	Drugs	Serotonergic GPCR	4.9	136.9	1.6	7.4	-0.2	9	9	49.9	12.0	24.1	2.3
Cyclobenzaprine	Drugs		0.0	0.0	0.0	18.5	18.5	1	1				
Dexmethylphenidate	Drugs	Dopaminergic GPCR											
Dextropropoxyphene	Drugs	Opioid Receptor	0.0	0.0	0.0	36.8	36.8	1	1	0.7	3.1	429.4	1.6
Diazepam	Drugs	Gaba Receptors	0.0	0.0	0.0	0.0	0.0	1	1				
Donepezil	Drugs	Enzyme	5.2	158.8	2.3	9.9	-3.3	5	5	72.6	12.8	17.6	3.7
Dronabinol	Drugs	Cannabinoids											
Duloxetine	Drugs	Serotonergic GPCR	11.4	95.1	5.1	26.2	-2.3	5	5	61.6	31.7	51.4	11.2
Eletriptan	Drugs	Serotonergic GPCR	11.3	68.3	5.1	30.8	2.4	5	5	53.9	10.0	18.6	2.9
Escitalopram	Drugs	Serotonergic GPCR	2.6	200.0	1.3	5.5	-2.9	4	4	57.2	7.6	13.2	1.9
Eszopiclone	Drugs	Gaba Receptors											
Ethosuximide	Drugs	Calcium Channels	9.2	141.4	4.1	18.0	-5.0	5	5				
Felbamate	Drugs	Gaba Receptors	9.9	173.2	5.7	30.2	-18.8	4	3	-2.3	6.1	-271.5	1.6

Pub-Name	Set	Target Mechanism	3A4 Inh (% @ 3uM) SD	3A4 Inh (% @ 3uM) CV	3A4 Inh (% @ 3uM) SEM	3A4 Inh (% @ 3uM) Upp95	3A4 Inh (% @ 3uM) Low95	3A4 Inh (% @ 3uM) TotCnt	3A4 Inh (% @ 3uM) N	Dof Inh (% @ 10uM) Mean	Dof Inh (% @ 10uM) SD	Dof Inh (% @ 10uM) CV	Dof Inh (% @ 10uM) SEM
Fentanyl	Drugs	Opioid Receptor											
Flumazenil	Drugs	Gaba Receptors	11.5	200.0	5.8	24.2	-12.7	4	4	2.7	13.4	505.2	3.9
Fluoxetine	Drugs	Serotonergic GPCR	7.7	-831.9	2.4	4.2	-6.1	10	10	58.2	11.5	19.7	2.3
Fluvoxamine	Drugs	Serotonergic GPCR	1.8	110.7	0.7	3.5	-0.3	6	6	29.4	13.0	44.3	2.7
Gabapentin	Drugs	Calcium Channels	8.5	160.2	3.0	12.6	-1.9	8	8	-0.2	7.7	-4216.9	1.7
Galantamine	Drugs	Enzyme	24.8	106.8	17.6	246.2	-199.7	2	2	2.0	5.3	271.1	1.9
Haloperidol	Drugs	Dopaminergic GPCR	0.0	0.0	0.0	0.0	0.0	2	2				
Hydrocodone	Drugs	Opioid Receptor	0.0	0.0	0.0	0.0	0.0	1	1	12.0	3.3	27.8	1.9
Indeloxazine	Drugs	Reuptake Inhibitors	2.6	141.4	1.8	24.9	-21.3	2	2	-2.5	5.2	-208.4	1.8
Lamotrigine	Drugs	Reuptake Inhibitors	2.4	88.1	0.9	4.9	0.5	7	7	-3.1	3.5	-116.0	0.9
Levetiracetam	Drugs	Calcium Channels	1.0	113.5	0.4	2.1	-0.4	5	5	-3.2	6.0	-186.7	1.7
Levomethadyl Acetate	Drugs	Opioid Receptor											
Lofexidine	Drugs		0.5	141.4	0.4	5.0	-4.3	2	2	26.0	8.1	31.3	3.1
Lorazepam	Drugs	Gaba Receptors	0.0	0.0	0.0	0.0	0.0	2	2	2.7	7.1	263.5	2.5
Meprobamate	Drugs												
Methylphenidate	Drugs	Dopaminergic GPCR	0.0	0.0	0.0	0.0	0.0	2	2	7.6	8.8	115.2	3.1
Metoclopramide	Drugs												
Midazolam	Drugs	Gaba Receptors	34.7	-64.6	5.3	-42.6	-64.8	44	43				
Milnacipran	Drugs	Serotonergic GPCR											
Minaprine	Drugs	Enzyme	2.2	67.8	1.5	22.5	-16.2	2	2	13.4	11.0	82.3	4.2
Mirtazapine	Drugs		0.7	138.2	0.3	1.5	-0.4	5	5	21.2	30.6	144.3	7.2
Moclobemide	Drugs	Enzyme	9.4	152.4	5.4	29.6	-17.2	3	3	-2.4	6.6	-280.6	2.0
Modafinil	Drugs	Dopaminergic GPCR	0.0	0.0	0.0	0.0	0.0	1	1	-5.8	2.1	-37.1	0.8
Morphine	Drugs	Opioid Receptor											
Nalmefene	Drugs	Opioid Receptor	0.6	141.4	0.4	5.5	-4.7	2	2	16.5	4.1	24.9	1.5
Naltrexone	Drugs	Opioid Receptor	2.8	195.6	1.1	4.3	-1.5	6	6	3.3	7.4	221.9	1.8
Nemonapride	Drugs	Dopaminergic GPCR	11.0	82.4	6.3	40.6	-13.9	3	3	76.0	11.4	14.9	3.6
Nicergoline	Drugs												
Nicotrol	Drugs	Nicotinic Receptor	5.3	148.8	2.4	10.2	-3.1	5	5	-1.6	4.9	-305.2	1.2
Nimodipine	Drugs	Calcium Channels	17.4	56.3	6.6	46.6	15.1	7	7	8.1	5.8	71.4	1.4
Nortriptyline	Drugs		0.0	0.0	0.0	0.0	0.0	1	1				
Olanzapine	Drugs	Dopaminergic GPCR	7.1	108.4	2.9	14.1	-1.0	6	6	35.9	14.5	40.4	3.4
Oxcarbazepine	Drugs	Reuptake Inhibitors	9.7	141.4	6.8	93.8	-80.1	2	2	9.5	11.1	116.6	4.2
Oxycodone	Drugs	Opioid Receptor	0.0	0.0	0.0	0.0	0.0	1	1	7.0	2.4	34.4	1.2
Paliperidone	Drugs	Dopaminergic GPCR	0.0	0.0	0.0	0.0	0.0	2	2	78.3	4.9	6.2	1.8
Paroxetine	Drugs	Serotonergic GPCR	5.5	117.9	2.8	13.5	-4.1	4	4	64.6	16.8	26.1	4.3
Pergolide	Drugs	Dopaminergic GPCR	3.9	163.8	2.3	12.2	-7.4	3	3	75.6	4.1	5.4	1.2

Pub-Name	Set	Target Mechanism	3A4 Inh (% @ 3uM) SD	3A4 Inh (% @ 3uM) CV	3A4 Inh (% @ 3uM) SEM	3A4 Inh (% @ 3uM) Upp95	3A4 Inh (% @ 3uM) Low95	3A4 Inh (% @ 3uM) TotCnt	3A4 Inh (% @ 3uM) N	Dof Inh (% @ 10uM) Mean	Dof Inh (% @ 10uM) SD	Dof Inh (% @ 10uM) CV	Dof Inh (% @ 10uM) SEM
Perospirone	Drugs	Dopaminergic GPCR	3.2	9.8	2.3	61.2	3.9	2	2	81.5	5.0	6.1	2.0
phenytoin	Drugs	Reuptake Inhibitors	10.0	146.9	3.3	14.5	-0.9	9	9	1.1	12.9	1216.3	3.0
Piracetam	Drugs		0.8	141.4	0.5	7.5	-6.4	3	2	1.8	4.8	265.9	1.4
Pramipexole	Drugs	Dopaminergic GPCR	0.0	0.0	0.0	0.0	0.0	4	4	-1.5	8.0	-548.9	2.1
Pregabalin	Drugs	Calcium Channels	2.4	141.4	1.7	23.7	-20.3	2	2	-4.2	5.7	-134.9	1.6
Propofol	Drugs		2.8	200.0	1.4	5.8	-3.0	4	4	1.0	5.7	585.8	1.5
Propoxyphene	Drugs												
Quazepam	Drugs	Gaba Receptors											
Quetiapine	Drugs	Serotonergic GPCR	8.6	149.2	3.9	16.6	-5.0	5	5	15.4	8.3	53.7	2.1
Ramelteon	Drugs	Melatonin Receptor	5.3	189.1	2.3	9.4	-3.8	5	5	-1.4	6.9	-503.0	2.0
Rasagiline	Drugs	Enzyme	0.0	0.0	0.0	2.7	2.7	1	1	-6.2	7.3	-118.2	3.6
Reboxetine	Drugs	Reuptake Inhibitors	5.4	76.3	3.1	20.4	-6.3	3	3	6.0	7.3	121.8	2.6
Remifentanyl	Drugs	Opioid Receptor											
Riluzole	Drugs	Reuptake Inhibitors	1.7	200.0	0.9	3.6	-1.9	4	4	-4.6	4.3	-93.9	1.4
Rimonabant	Drugs	Cannabinoids	0.0	0.0	0.0	0.0	0.0	3	3	28.7	13.3	46.6	4.0
Risperidone	Drugs	Dopaminergic GPCR	7.5	65.3	2.5	17.2	5.7	9	9	75.0	7.2	9.7	1.2
Rivastigmine	Drugs	Enzyme	2.5	89.1	1.2	6.7	-1.2	4	4	1.8	6.3	353.2	1.6
Ropinirole	Drugs	Dopaminergic GPCR	1.1	200.0	0.6	2.3	-1.2	4	4	44.8	5.2	11.6	1.3
Ropivacaine	Drugs		4.9	200.0	2.5	10.3	-5.4	4	4	11.8	12.2	104.1	3.1
Selegiline	Drugs	Enzyme											
Sertindole	Drugs	Serotonergic GPCR	6.6	126.5	4.7	64.6	-54.1	2	2	102.7	3.5	3.4	1.2
Sertraline	Drugs	Serotonergic GPCR	12.4	120.5	4.4	20.9	-0.2	8	8	64.0	14.6	22.9	3.7
Sinequan	Drugs	Serotonergic GPCR	5.9	117.5	3.0	14.6	-4.4	4	4	41.7	12.3	29.4	3.7
Sulpiride	Drugs	Dopaminergic GPCR	0.0	0.0	0.0	1.0	1.0	1	1				
Tacrine	Drugs	Enzyme	4.7	175.4	1.7	6.6	-1.3	9	8	54.6	5.9	10.8	1.4
Talipexole	Drugs	Dopaminergic GPCR	5.0	125.5	2.5	12.0	-4.0	4	4	2.5	5.8	229.4	1.6
Terguride	Drugs	Dopaminergic GPCR											
Thiopental	Drugs	Gaba Receptors											
Tiagabine	Drugs	Gaba Receptors	7.9	185.3	3.5	14.1	-5.6	5	5	19.0	39.2	206.2	10.1
Tianeptine	Drugs	Reuptake Inhibitors	0.0	0.0	0.0	0.0	0.0	3	3	-1.4	8.6	-609.8	2.5
Topiramate	Drugs	Enzyme	0.0	0.0	0.0	0.0	0.0	3	3	1.8	2.6	143.2	0.8
Tramadol	Drugs	Reuptake Inhibitors	0.6	12.8	0.4	10.2	-0.7	2	2	-0.7	7.0	-1071.0	2.5
Trazodone	Drugs	Serotonergic GPCR											
Tropisetron	Drugs	Serotonergic GPCR	1.4	20.3	1.0	19.8	-5.8	2	2	57.6	5.2	9.1	2.0
Valproic Acid	Drugs		0.0	0.0	0.0	0.0	0.0	5	3	-3.8	5.8	-152.0	1.3
Varenicline	Drugs	Nicotinic Receptor	11.2	212.1	4.6	17.1	-6.6	7	6	-0.4	4.9	-1139.1	1.2
Venlafaxine	Drugs	Serotonergic GPCR	6.2	144.2	2.5	10.9	-2.3	6	6	-3.4	4.2	-123.1	1.1

Pub-Name	Set	Target Mechanism	3A4 Inh (% @ 3uM) SD	3A4 Inh (% @ 3uM) CV	3A4 Inh (% @ 3uM) SEM	3A4 Inh (% @ 3uM) Upp95	3A4 Inh (% @ 3uM) Low95	3A4 Inh (% @ 3uM) TotCnt	3A4 Inh (% @ 3uM) N	Dof Inh (% @ 10uM) Mean	Dof Inh (% @ 10uM) SD	Dof Inh (% @ 10uM) CV	Dof Inh (% @ 10uM) SEM
Verapamil	Drugs	Calcium Channels	16.5	86.5	2.8	24.9	13.2	35	35	76.4	2.7	3.5	1.3
Vigabatrin	Drugs	Gaba Receptors	0.0	0.0	0.0	0.0	0.0	2	2	-2.3	6.2	-272.7	2.2
Vinpocetine	Drugs		4.0	79.0	2.0	11.4	-1.3	4	4	99.4	3.6	3.6	0.9
Zaleplon	Drugs	Gaba Receptors	0.0	0.0	0.0	4.0	4.0	1	1	-4.8	2.1	-44.3	0.7
Ziprasidone	Drugs	Dopaminergic GPCR	14.2	79.9	5.0	29.8	5.7	8	8	78.0	27.0	34.6	8.1
Zolpidem	Drugs	Gaba Receptors	0.0	0.0	0.0	6.1	6.1	1	1	0.0	2.5	12672.0	0.9
Zonisamide	Drugs	Enzyme	2.7	144.9	1.1	4.7	-1.0	6	6	-1.0	4.7	-460.9	1.1
Zotepine	Drugs	Serotonergic GPCR	14.1	151.6	8.1	44.2	-25.7	3	3	81.7	11.8	14.5	3.4
Candidate-001	Candidates	Glutamate receptors	0.0	0.0	0.0	10.4	10.4	1	1				
Candidate-002	Candidates	Reuptake Inhibitors	5.0	155.4	2.2	9.4	-3.0	5	5	24.2	11.6	48.0	2.6
Candidate-003	Candidates	Reuptake Inhibitors	5.2	93.8	3.0	18.4	-7.4	3	3	67.1	6.8	10.2	2.4
Candidate-004	Candidates	Serotonergic GPCR											
Candidate-005	Candidates	Enzyme	0.0	0.0	0.0	1.3	1.3	1	1				
Candidate-006	Candidates	Peptide GPCR											
Candidate-007	Candidates	Enzyme	1.9	99.1	0.9	4.9	-1.1	4	4	4.6	8.3	178.4	2.1
Candidate-008	Candidates	Calcium Channels	0.0	0.0	0.0	0.0	0.0	1	1	14.9	7.1	47.8	3.6
Candidate-009	Candidates	Nicotinic Receptor	2.3	158.0	0.9	3.8	-1.0	6	6	0.7	8.4	1248.3	2.2
Candidate-010	Candidates	Opioid Receptor	4.2	141.4	3.0	40.6	-34.7	2	2	44.9	10.2	22.7	3.9
Candidate-011	Candidates	Dopaminergic GPCR	4.0	86.6	2.3	14.6	-5.3	3	3	80.5	7.6	9.4	2.7
Candidate-012	Candidates	Peptide GPCR	4.2	100.9	3.0	42.2	-33.8	2	2	24.1	3.7	15.4	1.9
Candidate-013	Candidates	Enzyme	0.0	0.0	0.0	0.0	0.0	1	1				
Candidate-014	Candidates	Opioid Receptor	0.0	0.0	0.0	16.7	16.7	1	1	24.3	11.1	45.9	6.4
Candidate-015	Candidates	Nicotinic Receptor	2.7	57.1	1.5	11.3	-2.0	3	3	27.4	7.7	28.0	2.2
Candidate-016	Candidates	Gaba Receptors	7.6	63.9	2.5	17.7	6.0	9	9	8.8	11.5	130.5	3.1
Candidate-017	Candidates	Enzyme	0.0	0.0	0.0	0.0	0.0	1	1	43.8	2.6	6.0	1.3
Candidate-018	Candidates	Cannabinoids	2.4	244.9	1.0	3.6	-1.6	6	6	22.1	10.2	46.4	2.3
Candidate-019	Candidates	Peptide GPCR	9.1	60.8	3.5	23.3	6.7	7	7				
Candidate-020	Candidates	Glutamate receptors	0.0	0.0	0.0	0.0	0.0	1	1	79.8	4.9	6.2	2.5
Candidate-021	Candidates	Enzyme	1.2	200.0	0.6	2.5	-1.3	5	4	4.4	13.2	297.8	3.0
Candidate-022	Candidates	Enzyme	7.5	29.4	3.7	37.4	13.5	4	4	61.2	3.5	5.7	1.2
Candidate-023	Candidates	Nicotinic Receptor	1.4	52.2	0.8	6.1	-0.8	3	3	3.8	7.8	202.4	2.2
Candidate-024	Candidates	Calcium Channels	0.0	0.0	0.0	0.0	0.0	1	1	-1.1	6.0	-527.2	3.4
Candidate-025	Candidates	Reuptake Inhibitors	0.0	0.0	0.0	0.0	0.0	2	2	63.7	2.0	3.2	1.0
Candidate-026	Candidates	Serotonergic GPCR	5.4	149.1	2.4	10.3	-3.1	5	5	67.3	16.5	24.5	4.8
Candidate-027	Candidates	Serotonergic GPCR	6.9	141.4	4.9	67.0	-57.2	2	2	31.5	1.6	5.2	0.8
Candidate-028	Candidates	Histaminergic GPCR	24.3	184.6	9.9	38.9	-12.6	6	6	7.2	5.8	80.6	2.0
Candidate-029	Candidates	Glutamate receptors	11.0	71.9	7.8	113.7	-83.2	3	2				



Pub-Name	Set	Target Mechanism	3A4 Inh (% @ 3uM) SD	3A4 Inh (% @ 3uM) CV	3A4 Inh (% @ 3uM) SEM	3A4 Inh (% @ 3uM) Upp95	3A4 Inh (% @ 3uM) Low95	3A4 Inh (% @ 3uM) TotCnt	3A4 Inh (% @ 3uM) N	Dof Inh (% @ 10uM) Mean	Dof Inh (% @ 10uM) SD	Dof Inh (% @ 10uM) CV	Dof Inh (% @ 10uM) SEM
Candidate-030	Candidates	Peptide GPCR	9.1	67.4	6.5	95.6	-68.5	2	2				
Candidate-031	Candidates	Serotonergic GPCR	10.8	64.1	4.9	30.5	3.3	5	5	4.4	4.6	104.7	1.0
Candidate-032	Candidates	Gaba Receptors	16.2	58.6	7.2	47.8	7.3	5	5	-4.0	9.9	-247.1	3.7
Candidate-033	Candidates	Opioid Receptor	3.3	130.6	1.0	4.7	0.3	10	10	72.3	9.5	13.2	1.6
Candidate-034	Candidates	Reuptake Inhibitors	8.3	20.1	2.9	48.2	34.1	9	8	67.9	9.5	14.0	2.9
Candidate-035	Candidates	Calcium Channels	1.3	141.4	1.0	13.0	-11.1	2	2	9.4	10.9	115.7	4.1
Candidate-036	Candidates	Peptide GPCR	0.0	0.0	0.0	10.4	10.4	1	1				
Candidate-037	Candidates	Gaba Receptors	0.0	0.0	0.0	0.0	0.0	4	4	6.6	10.4	158.4	2.7
Candidate-038	Candidates	Serotonergic GPCR	0.0	0.0	0.0	12.2	12.2	1	1				
Candidate-039	Candidates	Glutamate receptors	6.1	51.5	3.5	27.2	-3.3	3	3	83.3	6.2	7.4	1.8
Candidate-040	Candidates	Enzyme	0.0	0.0	0.0	0.0	0.0	1	1				
Candidate-041	Candidates	Peptide GPCR	8.7	86.8	5.0	31.8	-11.6	3	3	58.2	2.9	5.1	1.5
Candidate-042	Candidates	Serotonergic GPCR	5.0	129.8	1.8	8.1	-0.4	8	8	46.0	4.6	10.1	1.6
Candidate-043	Candidates	Peptide GPCR	7.8	180.8	3.2	12.7	-4.0	8	6	24.9	8.8	35.1	4.4
Candidate-044	Candidates	Serotonergic GPCR	9.0	82.2	3.7	20.4	1.4	6	6	39.1	12.0	30.6	3.0
Candidate-045	Candidates	Cannabinoids	0.0	0.0	0.0	0.0	0.0	1	1	19.4	4.9	25.1	2.8
Candidate-046	Candidates	Serotonergic GPCR	0.0	0.0	0.0	2.3	2.3	1	1				
Candidate-047	Candidates	Calcium Channels	1.2	99.2	0.8	11.6	-9.3	2	2	-4.7	2.9	-61.7	1.4
Candidate-048	Candidates	Dopaminergic GPCR	3.8	97.2	1.6	8.0	-0.1	6	6	94.9	2.3	2.4	0.8
Candidate-049	Candidates	Serotonergic GPCR	12.9	137.5	9.1	125.3	-106.6	2	2	80.5	9.3	11.6	3.8
Candidate-050	Candidates	Gaba Receptors	12.1	126.3	6.0	28.9	-9.8	4	4	14.9	12.1	80.9	3.6
Candidate-051	Candidates	Reuptake Inhibitors	5.1	244.9	2.1	7.6	-3.4	6	6	10.2	6.7	65.3	2.4
Candidate-052	Candidates	Enzyme	0.0	0.0	0.0	12.8	12.8	1	1	6.1	4.9	80.7	2.5
Candidate-053	Candidates	Nicotinic Receptor	0.0	0.0	0.0	4.8	4.8	1	1	9.0	5.5	61.5	2.8
Candidate-054	Candidates	Opioid Receptor	0.0	0.0	0.0	25.7	25.7	1	1	74.6	10.1	13.5	5.0
Candidate-055	Candidates	Enzyme	0.0	0.0	0.0	0.0	0.0	3	3	98.6	2.2	2.2	0.7
Candidate-056	Candidates	Enzyme	23.3	112.9	11.7	57.9	-16.7	4	4	30.3	20.5	67.6	6.2
Candidate-057	Candidates	Dopaminergic GPCR						3	0	-1.7	9.1	-544.7	2.9
Candidate-058	Candidates	Peptide GPCR											
Candidate-059	Candidates	Dopaminergic GPCR											
Candidate-060	Candidates	Serotonergic GPCR	7.9	61.5	3.2	21.2	4.4	6	6	70.6	11.9	16.8	3.1
Candidate-061	Candidates	Histaminergic GPCR	7.9	173.2	4.6	24.2	-15.1	3	3	3.2	3.1	96.5	0.9
Candidate-062	Candidates	Dopaminergic GPCR	15.8	100.3	11.2	158.1	-126.5	2	2	59.0	1.5	2.5	0.7
Candidate-063	Candidates	Nicotinic Receptor	0.0	0.0	0.0	0.0	0.0	2	2	3.7	7.4	197.5	2.6
Candidate-064	Candidates	Serotonergic GPCR	0.0	0.0	0.0	0.0	0.0	4	4	19.4	6.7	34.6	1.9
Candidate-065	Candidates	Peptide GPCR	0.4	3.2	0.3	17.1	9.5	2	2	-2.5	7.5	-300.5	4.3
Candidate-066	Candidates	Serotonergic GPCR	2.4	28.6	1.4	14.1	2.4	3	3	26.3	3.8	14.5	1.9

Pub-Name	Set	Target Mechanism	3A4 Inh (% @ 3uM) SD	3A4 Inh (% @ 3uM) CV	3A4 Inh (% @ 3uM) SEM	3A4 Inh (% @ 3uM) Upp95	3A4 Inh (% @ 3uM) Low95	3A4 Inh (% @ 3uM) TotCnt	3A4 Inh (% @ 3uM) N	Dof Inh (% @ 10uM) Mean	Dof Inh (% @ 10uM) SD	Dof Inh (% @ 10uM) CV	Dof Inh (% @ 10uM) SEM
Candidate-067	Candidates	Dopaminergic GPCR	7.8	44.8	3.9	30.0	4.9	4	4	36.6	37.9	103.6	13.4
Candidate-068	Candidates	Serotonergic GPCR	0.0	0.0	0.0	0.0	0.0	2	2	8.2	12.2	148.7	4.6
Candidate-069	Candidates	Reuptake Inhibitors	0.0	0.0	0.0	10.5	10.5	1	1				
Candidate-070	Candidates	Dopaminergic GPCR	0.0	0.0	0.0	0.0	0.0	1	1	4.2	3.8	89.9	2.7
Candidate-071	Candidates	Reuptake Inhibitors	0.0	0.0	0.0	0.0	0.0	2	2	27.7	7.1	25.7	2.5
Candidate-072	Candidates	Dopaminergic GPCR	0.0	0.0	0.0	0.0	0.0	3	3	97.0	2.9	2.9	0.9
Candidate-073	Candidates	Gaba Receptors	3.4	119.9	1.1	5.4	0.2	9	9	-4.3	7.6	-175.2	1.9
Candidate-074	Candidates	Peptide GPCR	0.0	0.0	0.0	0.0	0.0	1	1				
Candidate-075	Candidates	Nicotinic Receptor	1.1	141.4	0.8	10.8	-9.2	2	2	13.3	10.5	79.1	3.7
Candidate-076	Candidates	Nicotinic Receptor	9.4	120.3	4.7	23.0	-7.3	4	4	3.9	11.7	302.9	2.6
Candidate-077	Candidates	Gaba Receptors	0.9	200.0	0.4	1.8	-1.0	4	4	-3.9	10.6	-269.3	2.8
Candidate-078	Candidates	Reuptake Inhibitors	12.6	143.2	4.8	20.2	-2.6	7	7	8.8	5.0	57.0	1.3
Candidate-079	Candidates	Calcium Channels	0.0	0.0	0.0	10.3	10.3	1	1	16.6	11.0	66.5	7.8
Candidate-080	Candidates	Dopaminergic GPCR	0.0	0.0	0.0	0.0	0.0	1	1				
Candidate-081	Candidates	Serotonergic GPCR	19.2	189.3	9.6	40.9	-20.6	4	4	38.8	6.8	17.4	2.4
Candidate-082	Candidates	Gaba Receptors	3.4	144.7	1.5	6.6	-1.9	5	5	-0.3	5.7	-1733.0	1.3
Candidate-083	Candidates	Cannabinoids	0.0	0.0	0.0	0.0	0.0	2	2	13.0	11.1	85.6	5.6
Candidate-084	Candidates	Gaba Receptors	10.5	145.3	3.7	16.1	-1.7	8	8	19.5	12.4	63.6	3.6
Candidate-085	Candidates	Reuptake Inhibitors											
Candidate-086	Candidates	Muscarinic Receptor	0.0	0.0	0.0	6.4	6.4	2	1	24.4	6.2	25.4	3.1
Candidate-087	Candidates	Cannabinoids	22.0	108.3	15.5	217.5	-177.0	2	2	-6.8	6.6	-97.2	2.5
Candidate-088	Candidates	Dopaminergic GPCR	0.0	0.0	0.0	0.0	0.0	1	1				
Candidate-089	Candidates	Enzyme	2.0	173.2	1.2	6.3	-3.9	3	3	-0.8	6.3	-802.7	1.9
Candidate-090	Candidates	Glutamate receptors	16.0	86.6	9.3	58.3	-21.3	5	3	-5.2	5.4	-103.0	1.9
Candidate-091	Candidates	Gaba Receptors	2.5	200.0	1.3	5.3	-2.8	4	4	36.2	8.3	23.0	2.4
Candidate-092	Candidates	Reuptake Inhibitors	0.0	0.0	0.0	0.0	0.0	2	2	28.0	5.2	18.6	2.6
Candidate-093	Candidates	Muscarinic Receptor	0.0	0.0	0.0	0.0	0.0	1	1	23.0	2.3	10.0	1.2
Candidate-094	Candidates	Dopaminergic GPCR	7.4	68.0	4.3	29.2	-7.5	3	3	94.3	5.3	5.7	1.7
Candidate-095	Candidates	Gaba Receptors	2.7	147.5	1.4	6.2	-2.5	4	4	0.1	12.3	13720.6	3.9
Candidate-096	Candidates	Serotonergic GPCR											
Candidate-097	Candidates	Reuptake Inhibitors	3.5	177.0	1.4	5.8	-1.8	6	6	44.2	8.4	18.9	2.1
Candidate-098	Candidates	Enzyme	10.4	77.9	4.6	26.3	0.3	5	5	43.1	20.1	46.6	5.2
Candidate-099	Candidates	Peptide GPCR	3.2	59.9	2.2	33.6	-23.1	3	2	71.5	14.5	20.2	4.4
Candidate-100	Candidates	Enzyme	0.0	0.0	0.0	0.0	0.0	1	1	18.3	5.3	29.1	2.7
Candidate-101	Candidates	Dopaminergic GPCR	6.3	101.6	3.6	21.8	-9.4	3	3	62.0	7.6	12.2	3.8
Candidate-102	Candidates	Serotonergic GPCR	5.2	58.7	3.0	21.8	-4.1	3	3	87.7	9.5	10.9	2.8
Candidate-103	Candidates	Dopaminergic GPCR	0.0	0.0	0.0	0.0	0.0	1	1	86.8	2.7	3.1	1.4

Pub-Name	Set	Target Mechanism	3A4 Inh (% @ 3uM) SD	3A4 Inh (% @ 3uM) CV	3A4 Inh (% @ 3uM) SEM	3A4 Inh (% @ 3uM) Upp95	3A4 Inh (% @ 3uM) Low95	3A4 Inh (% @ 3uM) TotCnt	3A4 Inh (% @ 3uM) N	Dof Inh (% @ 10uM) Mean	Dof Inh (% @ 10uM) SD	Dof Inh (% @ 10uM) CV	Dof Inh (% @ 10uM) SEM
Candidate-104	Candidates	Peptide GPCR	1.0	6.0	0.6	19.4	14.4	3	3	19.6	1.8	9.4	0.9
Candidate-105	Candidates	Gaba Receptors	0.1	173.2	0.1	0.4	-0.2	3	3	6.2	11.6	187.8	3.5
Candidate-106	Candidates	Peptide GPCR	0.0	0.0	0.0	64.0	64.0	1	1	6.2	5.5	87.8	2.7
Candidate-107	Candidates	Calcium Channels	0.0	0.0	0.0	0.0	0.0	1	1	-5.2	2.3	-43.2	1.3
Candidate-108	Candidates	Nicotinic Receptor	11.4	43.0	5.7	44.8	8.3	4	4	1.7	7.7	443.5	2.4

Pub-Name	Set	Target Mechanism	Dof Inh (% @ 10uM) Upp95	Dof Inh (% @ 10uM) Low95	Dof Inh (% @ 10uM) N	THLE IC50 OP	THLE IC50 Mean	THLE IC50 SD	THLE IC50 CV	THLE IC50 SEM	THLE IC50 Upp95	THLE IC50 Low95	THLE IC50 N
Acamprosate	Drugs	Glutamate receptors	-0.9	-4.8	16	>	300.0		0.0		300.0	300.0	1
Alprazolam	Drugs	Gaba Receptors	-3.6	-7.4	4								
Amfebutamone	Drugs	Dopaminergic GPCR	2.6	-4.3	10	>	300.0	0.0	0.0		300.0	300.0	8
Amisulpride	Drugs	Dopaminergic GPCR	16.8	13.6	12	>	300.0	0.0	0.0		300.0	300.0	4
Amphetamine	Drugs	Reuptake Inhibitors											
Aniracetam	Drugs		8.5	-1.8	8	>	289.3	12.4	5.2	10.5	320.3	261.3	5
Apomorphine	Drugs	Dopaminergic GPCR	24.8	18.8	24	=	77.6	4.0	3.8	3.8	87.2	69.0	7
Aprepitant	Drugs		18.1	6.2	14	=	33.6	4.3	7.1	3.6	44.3	25.5	6
Aripiprazole	Drugs	Dopaminergic GPCR	89.6	83.1	21	=	29.1	8.8	11.0	5.5	47.6	17.8	6
Atomoxetine	Drugs	Reuptake Inhibitors	69.8	56.5	16	=	182.6	23.2	5.1	20.1	237.8	140.2	8
Bromazepam	Drugs	Gaba Receptors	17.0	-6.5	4								
Bromocriptine	Drugs	Dopaminergic GPCR	19.0	19.0	11	>	83.9	168.5	35.4	63.1	689.2	10.2	5
Brotizolam	Drugs	Gaba Receptors	5.0	-0.9	12	=	71.3	21.5	13.7	14.0	123.5	41.1	5
Budipine	Drugs	Calcium Channels											
Buprenorphine	Drugs	Opioid Receptor											
Buspirone	Drugs	Serotonergic GPCR	31.2	23.5	16	>	300.0	0.0	0.0		300.0	300.0	8
Cabergoline	Drugs	Dopaminergic GPCR	38.1	24.3	20	>	300.0	0.0	0.0		300.0	300.0	6
Caffeine	Drugs	Serotonergic GPCR				>	300.0		0.0		300.0	300.0	1
Carbamazepine	Drugs	Reuptake Inhibitors	2.3	-2.9	22	>	300.0	0.0	0.0		300.0	300.0	7
Carisoprodol	Drugs		13.1	0.7	4	>	300.0		0.0		300.0	300.0	1
Chlorpromazine	Drugs	Dopaminergic GPCR				=	26.6		0.0		26.6	26.6	1
Citalopram	Drugs	Serotonergic GPCR	52.0	30.1	14	>	272.3	35.8	7.2	26.4	350.3	211.7	6
Clomipramine	Drugs	Serotonergic GPCR	79.5	60.6	12	=	57.9	1.7	3.4	1.5	62.0	54.0	6
Clonazepam	Drugs	Gaba Receptors	-2.5	-5.8	8								
Clozapine	Drugs	Serotonergic GPCR	54.8	45.1	27	=	148.0	10.1	3.3	9.7	172.1	127.3	9
Cyclobenzaprine	Drugs												
Dexmethylphenidate	Drugs	Dopaminergic GPCR											
Dextropropoxyphene	Drugs	Opioid Receptor	5.7	-4.3	4	=	52.9		0.0		52.9	52.9	1
Diazepam	Drugs	Gaba Receptors											
Donepezil	Drugs	Enzyme	80.3	64.9	12	>	300.0	0.0	0.0		300.0	300.0	6
Dronabinol	Drugs	Cannabinoids											
Duloxetine	Drugs	Serotonergic GPCR	88.5	34.7	8	=	33.5	5.1	9.7	4.8	49.8	22.5	5
Eletriptan	Drugs	Serotonergic GPCR	60.0	47.8	12	>	285.8	17.0	4.1	13.9	321.1	254.4	7
Escitalopram	Drugs	Serotonergic GPCR	61.2	53.2	16	>	288.3	13.6	4.3	11.4	319.7	260.1	6
Eszopiclone	Drugs	Gaba Receptors											
Ethosuximide	Drugs	Calcium Channels				>	300.0	0.0	0.0		300.0	300.0	4
Felbamate	Drugs	Gaba Receptors	1.1	-5.6	15	>	300.0	0.0	0.0		300.0	300.0	5

Pub-Name	Set	Target Mechanism	Dof Inh (% @ 10uM) Upp95	Dof Inh (% @ 10uM) Low95	Dof Inh (% @ 10uM) N	THLE IC50 OP	THLE IC50 Mean	THLE IC50 SD	THLE IC50 CV	THLE IC50 SEM	THLE IC50 Upp95	THLE IC50 Low95	THLE IC50 N
Fentanyl	Drugs	Opioid Receptor											
Flumazenil	Drugs	Gaba Receptors	10.8	-5.5	12	>	300.0	0.0	0.0		300.0	300.0	6
Fluoxetine	Drugs	Serotonergic GPCR	63.1	53.4	25	=	82.3	20.2	6.2	17.4	134.0	50.6	9
Fluvoxamine	Drugs	Serotonergic GPCR	35.1	23.7	23	>	142.4	18.7	6.0	19.6	198.3	102.3	7
Gabapentin	Drugs	Calcium Channels	3.4	-3.8	20	>	300.0	0.0	0.0		300.0	300.0	7
Galantamine	Drugs	Enzyme	6.5	-2.6	8	>	300.0		0.0		300.0	300.0	1
Haloperidol	Drugs	Dopaminergic GPCR											
Hydrocodone	Drugs	Opioid Receptor	20.3	3.7	3								
Indeloxazine	Drugs	Reuptake Inhibitors	1.9	-6.9	8								
Lamotrigine	Drugs	Reuptake Inhibitors	-1.2	-4.9	16	>	277.0	29.6	5.5	22.1	335.4	228.8	7
Levetiracetam	Drugs	Calcium Channels	0.3	-6.7	13	>	300.0	0.0	0.0		300.0	300.0	6
Levomethadyl Acetate	Drugs	Opioid Receptor											
Lofexidine	Drugs		33.3	18.6	7	>	300.0	0.0	0.0		300.0	300.0	4
Lorazepam	Drugs	Gaba Receptors	8.7	-3.3	8								
Meprobamate	Drugs												
Methylphenidate	Drugs	Dopaminergic GPCR	15.0	0.2	8	>	300.0		0.0		300.0	300.0	1
Metoclopramide	Drugs					>	300.0	0.0	0.0		300.0	300.0	2
Midazolam	Drugs	Gaba Receptors											
Milnacipran	Drugs	Serotonergic GPCR											
Minaprine	Drugs	Enzyme	23.4	3.4	7	>	300.0	0.0	0.0		300.0	300.0	5
Mirtazapine	Drugs		36.3	6.1	18	>	299.1	1.0	1.2	0.9	301.5	296.8	6
Moclobemide	Drugs	Enzyme	-2.4	-2.4	11	>	300.0	0.0	0.0		300.0	300.0	5
Modafinil	Drugs	Dopaminergic GPCR	-4.0	-7.6	8								
Morphine	Drugs	Opioid Receptor											
Nalmefene	Drugs	Opioid Receptor	20.0	13.0	8	>	300.0	0.0	0.0		300.0	300.0	4
Naltrexone	Drugs	Opioid Receptor	7.2	-0.5	16	>	300.0	0.0	0.0		300.0	300.0	8
Nemonapride	Drugs	Dopaminergic GPCR	83.5	68.4	10	=	69.3	13.6	14.8	11.5	118.0	40.7	4
Nicergoline	Drugs												
Nicotrol	Drugs	Nicotinic Receptor	1.0	-4.2	16	>	300.0	0.0	0.0		300.0	300.0	5
Nimodipine	Drugs	Calcium Channels	11.2	5.1	16	=	103.1	11.6	4.8	9.1	127.6	83.3	8
Nortriptyline	Drugs												
Olanzapine	Drugs	Dopaminergic GPCR	43.1	28.7	18	>	296.1	4.4	2.4	3.9	306.4	286.1	6
Oxcarbazepine	Drugs	Reuptake Inhibitors	19.5	-0.5	7	>	300.0	0.0	0.0		300.0	300.0	3
Oxycodone	Drugs	Opioid Receptor	10.9	3.2	4								
Paliperidone	Drugs	Dopaminergic GPCR	82.8	73.9	7	>	209.5	36.8	8.4	32.3	312.8	140.3	6
Paroxetine	Drugs	Serotonergic GPCR	73.7	55.5	15	=	28.2	2.5	4.3	2.4	34.7	22.9	8
Pergolide	Drugs	Dopaminergic GPCR	78.1	73.2	12	>	300.0	0.0	0.0		300.0	300.0	4

Pub-Name	Set	Target Mechanism	Dof Inh (% @ 10uM) Upp95	Dof Inh (% @ 10uM) Low95	Dof Inh (% @ 10uM) N	THLE IC50 OP	THLE IC50 Mean	THLE IC50 SD	THLE IC50 CV	THLE IC50 SEM	THLE IC50 Upp95	THLE IC50 Low95	THLE IC50 N
Perospirone	Drugs	Dopaminergic GPCR	86.8	76.2	6	=	52.4	5.0	10.3	4.1	67.2	40.8	4
phenytoin	Drugs	Reuptake Inhibitors	7.3	-5.2	19	>	300.0	0.0	0.0		300.0	300.0	8
Piracetam	Drugs		4.7	-1.1	12	>	300.0	0.0	0.0		300.0	300.0	6
Pramipexole	Drugs	Dopaminergic GPCR	2.9	-5.8	15	>	300.0	0.0	0.0		300.0	300.0	6
Pregabalin	Drugs	Calcium Channels	-0.8	-7.6	12								
Propofol	Drugs		4.1	-2.1	15	>	300.0	0.0	0.0		300.0	300.0	8
Propoxyphene	Drugs												
Quazepam	Drugs	Gaba Receptors											
Quetiapine	Drugs	Serotonergic GPCR	19.9	10.9	15	>	215.4	66.2	9.2	42.6	346.4	133.9	7
Ramelteon	Drugs	Melatonin Receptor	2.8	-5.5	12	>	300.0	0.0	0.0		300.0	300.0	6
Rasagiline	Drugs	Enzyme	5.5	-17.8	4	>	300.0	0.0	0.0		300.0	300.0	3
Reboxetine	Drugs	Reuptake Inhibitors	12.1	-0.2	8	=	245.5		0.0		245.5	245.5	1
Remifentanil	Drugs	Opioid Receptor											
Riluzole	Drugs	Reuptake Inhibitors	-1.3	-7.9	9	=	90.8	9.0	3.9	7.7	110.3	74.7	9
Rimonabant	Drugs	Cannabinoids	28.7	28.7	11	=	61.4	3.4	5.9	2.9	70.0	53.9	5
Risperidone	Drugs	Dopaminergic GPCR	77.5	72.4	35	>	238.3	158.9	10.2	54.8	404.6	140.4	9
Rivastigmine	Drugs	Enzyme	5.1	-1.5	16	>	300.0	0.0	0.0		300.0	300.0	6
Ropinirole	Drugs	Dopaminergic GPCR	47.5	42.0	16	>	300.0	0.0	0.0		300.0	300.0	6
Ropivacaine	Drugs		18.2	5.3	16	>	300.0	0.0	0.0		300.0	300.0	5
Selegiline	Drugs	Enzyme											
Sertindole	Drugs	Serotonergic GPCR	105.6	99.7	8								
Sertraline	Drugs	Serotonergic GPCR	71.7	56.3	16	=	27.8	1.8	3.2	1.9	32.6	23.7	9
Sinequan	Drugs	Serotonergic GPCR	41.7	41.7	11	>	184.6	29.0	7.9	27.3	271.3	125.6	6
Sulpiride	Drugs	Dopaminergic GPCR											
Tacrine	Drugs	Enzyme	57.4	51.7	19	>	202.3	19.1	0.6	11.7	228.5	179.2	56
Talipexole	Drugs	Dopaminergic GPCR	5.8	-0.7	14	>	300.0	0.0	0.0		300.0	300.0	5
Terguride	Drugs	Dopaminergic GPCR											
Thiopental	Drugs	Gaba Receptors											
Tiagabine	Drugs	Gaba Receptors	40.3	-2.2	15	>	300.0	0.0	0.0		300.0	300.0	5
Tianeptine	Drugs	Reuptake Inhibitors	3.8	-6.6	12								
Topiramate	Drugs	Enzyme	1.8	1.8	11	>	300.0	0.0	0.0		300.0	300.0	8
Tramadol	Drugs	Reuptake Inhibitors	5.3	-6.6	8	>	300.0	0.0	0.0		300.0	300.0	4
Trazodone	Drugs	Serotonergic GPCR											
Tropisetron	Drugs	Serotonergic GPCR	62.4	52.9	7	>	293.7	7.4	5.3	6.2	314.3	274.4	4
Valproic Acid	Drugs		-1.0	-6.6	19	>	300.0	0.0	0.0		300.0	300.0	9
Varenicline	Drugs	Nicotinic Receptor	2.1	-3.0	16	>	300.0	0.0	0.0		300.0	300.0	6
Venlafaxine	Drugs	Serotonergic GPCR	-1.2	-5.7	16	>	291.2	10.0	3.7	8.6	314.6	269.7	6

Pub-Name	Set	Target Mechanism	Dof Inh (% @ 10uM) Upp95	Dof Inh (% @ 10uM) Low95	Dof Inh (% @ 10uM) N	THLE IC50 OP	THLE IC50 Mean	THLE IC50 SD	THLE IC50 CV	THLE IC50 SEM	THLE IC50 Upp95	THLE IC50 Low95	THLE IC50 N
Verapamil	Drugs	Calcium Channels	80.7	72.1	4	>	222.3	63.2	26.7	46.6	547.1	90.3	3
Vigabatrin	Drugs	Gaba Receptors	3.0	-7.5	8	>	300.0	0.0	0.0		300.0	300.0	4
Vinpocetine	Drugs		101.4	97.5	15	>	237.5	40.3	10.3	32.9	350.0	161.1	5
Zaleplon	Drugs	Gaba Receptors	-3.0	-6.5	8								
Ziprasidone	Drugs	Dopaminergic GPCR	78.0	78.0	11	>	300.0		0.0		300.0	300.0	1
Zolpidem	Drugs	Gaba Receptors	2.1	-2.1	8								
Zonisamide	Drugs	Enzyme	1.3	-3.3	19	>	300.0	0.0	0.0		300.0	300.0	8
Zotepine	Drugs	Serotonergic GPCR	88.9	74.5	12	=	29.8	6.2	15.2	5.2	52.3	17.0	4
Candidate-001	Candidates	Glutamate receptors				>	300.0	0.0	0.0		300.0	300.0	5
Candidate-002	Candidates	Reuptake Inhibitors	29.6	18.7	20	=	55.6	6.9	4.4	5.0	68.2	45.3	9
Candidate-003	Candidates	Reuptake Inhibitors	72.9	61.3	8	=	55.1	10.2	5.4	7.9	76.6	39.6	9
Candidate-004	Candidates	Serotonergic GPCR											
Candidate-005	Candidates	Enzyme				>	240.7	35.5	6.4	28.5	319.7	181.2	7
Candidate-006	Candidates	Peptide GPCR				>	300.0	0.0	0.0		300.0	300.0	6
Candidate-007	Candidates	Enzyme	9.1	0.2	15	>	253.9	45.8	6.1	30.5	338.7	190.2	8
Candidate-008	Candidates	Calcium Channels	26.2	3.5	4	>	300.0	0.0	0.0		300.0	300.0	5
Candidate-009	Candidates	Nicotinic Receptor	5.2	-3.9	15	>	300.0	0.0	0.0		300.0	300.0	8
Candidate-010	Candidates	Opioid Receptor	54.2	35.7	7								
Candidate-011	Candidates	Dopaminergic GPCR	86.9	74.1	8	>	300.0	0.0	0.0		300.0	300.0	7
Candidate-012	Candidates	Peptide GPCR	30.1	18.2	4	=	92.9	10.0	3.3	10.2	92.9	92.9	11
Candidate-013	Candidates	Enzyme				=	158.1	15.9	4.5	16.4	202.8	123.2	8
Candidate-014	Candidates	Opioid Receptor	51.9	-3.4	3	>	300.0	0.0	0.0		300.0	300.0	4
Candidate-015	Candidates	Nicotinic Receptor	32.1	22.8	12	>	300.0	0.0	0.0		300.0	300.0	5
Candidate-016	Candidates	Gaba Receptors	15.3	2.4	14	>	291.4	6.2	1.8	5.6	304.6	278.8	9
Candidate-017	Candidates	Enzyme	48.0	39.5	4								
Candidate-018	Candidates	Cannabinoids	26.9	17.3	20	=	61.5	7.0	4.2	5.9	76.6	49.4	9
Candidate-019	Candidates	Peptide GPCR				=	45.8	6.3	6.2	4.9	59.3	35.3	7
Candidate-020	Candidates	Glutamate receptors	87.7	71.9	4	=	197.1	19.4	7.9	18.6	256.7	151.4	5
Candidate-021	Candidates	Enzyme	10.8	-1.9	19	>	265.1	30.8	4.3	22.9	323.4	217.3	9
Candidate-022	Candidates	Enzyme	64.2	58.2	8	=	43.3	10.2	6.9	9.4	73.0	25.7	8
Candidate-023	Candidates	Nicotinic Receptor	8.6	-0.9	12	>	300.0	0.0	0.0		300.0	300.0	8
Candidate-024	Candidates	Calcium Channels	13.7	-16.0	3	>	300.0	0.0	0.0		300.0	300.0	5
Candidate-025	Candidates	Reuptake Inhibitors	67.0	60.5	4	=	29.9	8.1	6.5	6.0	47.6	18.8	9
Candidate-026	Candidates	Serotonergic GPCR	77.3	57.3	12	=	26.6	1.8	3.3	1.8	31.1	22.7	9
Candidate-027	Candidates	Serotonergic GPCR	34.2	28.9	4	>	244.4	25.0	3.6	20.8	292.1	204.5	10
Candidate-028	Candidates	Histaminergic GPCR	12.1	2.3	8	>	300.0	0.0	0.0		300.0	300.0	9
Candidate-029	Candidates	Glutamate receptors				>	300.0	0.0	0.0		300.0	300.0	7

Pub-Name	Set	Target Mechanism	Dof Inh (% @ 10uM) Upp95	Dof Inh (% @ 10uM) Low95	Dof Inh (% @ 10uM) N	THLE IC50 OP	THLE IC50 Mean	THLE IC50 SD	THLE IC50 CV	THLE IC50 SEM	THLE IC50 Upp95	THLE IC50 Low95	THLE IC50 N
Candidate-030	Candidates	Peptide GPCR				>	284.0	19.4	4.4	15.5	323.9	249.1	7
Candidate-031	Candidates	Serotonergic GPCR	6.6	2.2	20	>	300.0	0.0	0.0		300.0	300.0	5
Candidate-032	Candidates	Gaba Receptors	5.0	-13.0	7	>	300.0	0.0	0.0		300.0	300.0	8
Candidate-033	Candidates	Opioid Receptor	75.6	69.0	36	>	136.6	22.3	2.5	18.7	182.1	102.5	17
Candidate-034	Candidates	Reuptake Inhibitors	67.9	67.9	11	=	48.0	4.6	3.9	4.0	58.2	39.6	9
Candidate-035	Candidates	Calcium Channels	19.3	-0.5	7	>	300.0	0.0	0.0		300.0	300.0	5
Candidate-036	Candidates	Peptide GPCR				>	278.2	27.9	5.3	21.0	333.5	232.0	7
Candidate-037	Candidates	Gaba Receptors	12.3	0.9	15	>	298.0	2.2	1.2	2.0	302.8	293.3	8
Candidate-038	Candidates	Serotonergic GPCR				>	300.0	0.0	0.0		300.0	300.0	8
Candidate-039	Candidates	Glutamate receptors	87.0	79.5	12	=	31.6	2.6	4.1	2.6	38.7	25.9	8
Candidate-040	Candidates	Enzyme											
Candidate-041	Candidates	Peptide GPCR	62.9	53.5	4	>	80.4	18.0	5.9	20.5	144.6	44.7	9
Candidate-042	Candidates	Serotonergic GPCR	49.9	42.0	8	=	87.7	6.4	3.4	5.9	102.4	75.0	9
Candidate-043	Candidates	Peptide GPCR	39.0	10.9	4	>	300.0	0.0	0.0		300.0	300.0	8
Candidate-044	Candidates	Serotonergic GPCR	45.4	32.8	16	=	37.3	3.0	3.6	3.0	44.8	31.1	9
Candidate-045	Candidates	Cannabinoids	31.5	7.3	3	=	108.5	10.3	10.3	8.3	138.6	84.9	4
Candidate-046	Candidates	Serotonergic GPCR				=	42.7	3.0	0.9	3.3	50.2	36.3	31
Candidate-047	Candidates	Calcium Channels	-0.1	-9.3	4	>	300.0	0.0	0.0		300.0	300.0	7
Candidate-048	Candidates	Dopaminergic GPCR	96.9	92.9	8	=	64.6	10.3	8.0	11.5	102.7	40.6	6
Candidate-049	Candidates	Serotonergic GPCR	90.4	70.6	6	=	34.9	3.0	4.2	2.6	41.8	29.1	8
Candidate-050	Candidates	Gaba Receptors	14.9	14.9	11	>	167.7	19.7	4.9	19.6	222.1	126.6	8
Candidate-051	Candidates	Reuptake Inhibitors	15.8	4.5	8	=	36.1	4.0	5.6	3.7	46.2	28.2	7
Candidate-052	Candidates	Enzyme	14.0	-1.8	4	=	126.9	4.1	4.5	3.8	138.1	116.6	5
Candidate-053	Candidates	Nicotinic Receptor	17.8	0.2	4	>	300.0	0.0	0.0		300.0	300.0	7
Candidate-054	Candidates	Opioid Receptor	90.7	58.5	4	=	133.6	46.2	14.7	30.5	253.0	70.5	5
Candidate-055	Candidates	Enzyme	98.6	98.6	11	>	300.0	0.0	0.0		300.0	300.0	8
Candidate-056	Candidates	Enzyme	30.3	30.3	11	=	51.2	8.0	4.9	6.1	67.3	38.9	9
Candidate-057	Candidates	Dopaminergic GPCR	4.4	-7.7	10	>	289.1	13.0	2.6	10.7	314.8	265.5	9
Candidate-058	Candidates	Peptide GPCR				>	300.0	0.0	0.0		300.0	300.0	4
Candidate-059	Candidates	Dopaminergic GPCR				=	18.5		0.0		18.5	18.5	1
Candidate-060	Candidates	Serotonergic GPCR	77.0	64.1	15	>	300.0	0.0	0.0		300.0	300.0	7
Candidate-061	Candidates	Histaminergic GPCR	5.0	1.3	12	>	267.5	45.5	5.9	29.4	348.3	205.5	8
Candidate-062	Candidates	Dopaminergic GPCR	61.4	56.7	4	>	300.0		0.0		300.0	300.0	1
Candidate-063	Candidates	Nicotinic Receptor	10.0	-2.5	8	>	300.0	0.0	0.0		300.0	300.0	5
Candidate-064	Candidates	Serotonergic GPCR	23.5	15.3	12	=	48.3	10.1	6.5	6.6	67.0	34.9	8
Candidate-065	Candidates	Peptide GPCR	16.0	-21.0	3	=	48.4	16.8	9.8	10.5	81.5	28.8	7
Candidate-066	Candidates	Serotonergic GPCR	32.4	20.2	4	>	257.1	44.8	8.3	31.7	354.3	186.6	6



Pub-Name	Set	Target Mechanism	Dof Inh (% @ 10uM) Upp95	Dof Inh (% @ 10uM) Low95	Dof Inh (% @ 10uM) N	THLE IC50 OP	THLE IC50 Mean	THLE IC50 SD	THLE IC50 CV	THLE IC50 SEM	THLE IC50 Upp95	THLE IC50 Low95	THLE IC50 N
Candidate-067	Candidates	Dopaminergic GPCR	68.7	4.4	8	=	26.8	5.3	8.9	4.4	40.9	17.6	6
Candidate-068	Candidates	Serotonergic GPCR	19.3	-2.9	7	>	300.0	0.0	0.0		300.0	300.0	8
Candidate-069	Candidates	Reuptake Inhibitors				=	75.4	4.8	3.2	4.7	87.0	65.3	9
Candidate-070	Candidates	Dopaminergic GPCR	38.3	-29.8	2	>	300.0	0.0	0.0		300.0	300.0	5
Candidate-071	Candidates	Reuptake Inhibitors	33.8	21.7	8	>	239.3	133.5	10.7	54.1	411.7	139.1	8
Candidate-072	Candidates	Dopaminergic GPCR	97.0	97.0	11	>	300.0	0.0	0.0		300.0	300.0	9
Candidate-073	Candidates	Gaba Receptors	-0.3	-8.3	16	>	262.5	74.2	5.3	35.0	262.5	262.5	11
Candidate-074	Candidates	Peptide GPCR				>	247.7	29.0	4.3	22.8	306.0	200.5	9
Candidate-075	Candidates	Nicotinic Receptor	22.2	4.4	8	>	300.0	0.0	0.0		300.0	300.0	6
Candidate-076	Candidates	Nicotinic Receptor	9.4	-1.6	20	>	300.0	0.0	0.0		300.0	300.0	9
Candidate-077	Candidates	Gaba Receptors	2.0	-9.9	14	=	142.6	9.1	3.2	8.4	163.3	124.5	9
Candidate-078	Candidates	Reuptake Inhibitors	11.4	6.2	16	>	175.6	12.1	2.9	12.7	204.5	150.8	10
Candidate-079	Candidates	Calcium Channels	115.7	-82.5	2	>	300.0	0.0	0.0		300.0	300.0	5
Candidate-080	Candidates	Dopaminergic GPCR				=	54.6	5.4	3.9	5.5	68.8	43.3	9
Candidate-081	Candidates	Serotonergic GPCR	44.6	33.1	8	=	183.4	17.3	4.4	17.1	229.5	146.5	8
Candidate-082	Candidates	Gaba Receptors	2.3	-3.0	20	>	287.1	16.0	2.6	12.6	314.9	261.7	10
Candidate-083	Candidates	Cannabinoids	30.8	-4.8	4	=	82.6	9.8	4.3	8.6	105.1	65.0	9
Candidate-084	Candidates	Gaba Receptors	27.1	12.0	12	>	270.8	41.7	5.6	27.7	346.1	211.8	8
Candidate-085	Candidates	Reuptake Inhibitors				>	300.0	0.0	0.0	0.0	300.0	300.0	10
Candidate-086	Candidates	Muscarinic Receptor	34.3	14.5	4	>	225.7	20.0	7.4	18.5	283.8	179.5	5
Candidate-087	Candidates	Cannabinoids	-0.8	-12.8	7	>	284.3	19.0	4.3	15.3	323.4	250.0	7
Candidate-088	Candidates	Dopaminergic GPCR				>	300.0	0.0	0.0		300.0	300.0	4
Candidate-089	Candidates	Enzyme	-0.8	-0.8	11	>	300.0	0.0	0.0		300.0	300.0	7
Candidate-090	Candidates	Glutamate receptors	-0.7	-9.8	8	>	277.1	19.4	3.3	15.6	315.5	243.4	9
Candidate-091	Candidates	Gaba Receptors	41.2	31.1	12	=	175.4	17.6	4.0	16.6	217.9	141.1	9
Candidate-092	Candidates	Reuptake Inhibitors	36.4	19.7	4	>	121.3	23.0	5.4	22.6	186.0	79.1	9
Candidate-093	Candidates	Muscarinic Receptor	26.7	19.3	4	=	77.3	14.5	10.8	12.2	120.1	49.8	5
Candidate-094	Candidates	Dopaminergic GPCR	97.9	90.8	10	>	287.5	7.9	1.8	7.1	302.8	273.0	10
Candidate-095	Candidates	Gaba Receptors	8.3	-8.1	10	>	156.1	17.2	4.1	16.8	199.8	121.9	9
Candidate-096	Candidates	Serotonergic GPCR											
Candidate-097	Candidates	Reuptake Inhibitors	48.6	39.8	16	=	64.9	2.5	2.8	2.4	70.9	59.5	8
Candidate-098	Candidates	Enzyme	54.0	32.2	15	=	34.7	5.2	4.3	4.3	45.0	26.8	10
Candidate-099	Candidates	Peptide GPCR	71.5	71.5	11	>	150.2	27.4	6.1	23.0	216.8	104.0	8
Candidate-100	Candidates	Enzyme	26.8	9.8	4	=	117.9	47.0	21.0	35.0	304.8	45.6	4
Candidate-101	Candidates	Dopaminergic GPCR	74.1	49.8	4	=	41.8	6.7	13.4	5.8	65.2	26.8	4
Candidate-102	Candidates	Serotonergic GPCR	93.5	81.9	12	>	111.6	37.2	7.2	28.9	202.5	61.5	9
Candidate-103	Candidates	Dopaminergic GPCR	91.2	82.5	4	>	131.5	64.3	17.5	44.4	338.5	51.1	5

Pub-Name	Set	Target Mechanism	Dof Inh (% @ 10uM) Upp95	Dof Inh (% @ 10uM) Low95	Dof Inh (% @ 10uM) N	THLE IC50 OP	THLE IC50 Mean	THLE IC50 SD	THLE IC50 CV	THLE IC50 SEM	THLE IC50 Upp95	THLE IC50 Low95	THLE IC50 N
Candidate-104	Candidates	Peptide GPCR	22.5	16.6	4	>	173.9	31.4	4.7	25.4	236.3	128.0	10
Candidate-105	Candidates	Gaba Receptors	6.2	6.2	11	>	300.0	0.0	0.0	300.0	300.0	300.0	8
Candidate-106	Candidates	Peptide GPCR	15.0	-2.5	4	=	78.6	9.3	8.6	8.4	106.1	58.3	5
Candidate-107	Candidates	Calcium Channels	0.4	-10.8	3								
Candidate-108	Candidates	Nicotinic Receptor	6.8	-3.4	10	>	300.0	0.0	0.0		300.0	300.0	9