

Moving Beyond Rules: The Development of a Central Nervous System Multi-Parameter Optimization (CNS MPO) Approach to Enable Alignment of Drug-Like Properties

Travis T. Wager, *et. al*

Pub-Name	Set	Target Mechanism	MW	CLOGP	TPSA	CLOGD	HBD	PKA	T0_MW	T0_HBD	T0_CLOGP	T0_LOGD	T0_PSA	T0_BASIC1 PKA	CNS MPO
Acamprosate	Drugs	Glutamate receptors	181.2	-2.5	83.5	-6.1	2	1.0	1.00	0.50	1.00	1.00	1.00	1.00	5.5
Alprazolam	Drugs	Gaba Receptors	308.8	2.6	43.1	2.5	0	1.9	1.00	1.00	1.00	0.75	1.00	1.00	5.8
Amfebutamone	Drugs	Dopaminergic GPCR	239.7	3.2	29.1	3.3	1	7.2	1.00	0.83	0.89	0.37	0.46	1.00	4.5
Amisulpride	Drugs	Dopaminergic GPCR	369.5	1.8	101.7	-0.2	3	9.0	0.93	0.17	1.00	1.00	0.61	0.52	4.2
Amphetamine	Drugs	Reuptake Inhibitors	135.2	1.7	26.0	-0.6	2	9.9	1.00	0.50	1.00	1.00	0.30	0.03	3.8
Aniracetam	Drugs		219.2	0.7	46.6	0.3	0	1.0	1.00	1.00	1.00	1.00	1.00	1.00	6.0
Apomorphine	Drugs	Dopaminergic GPCR	267.3	2.5	43.7	2.5	2	7.9	1.00	0.50	1.00	0.75	1.00	1.00	5.2
Aprepitant	Drugs		534.4	4.6	83.2	4.1	2	4.0	0.00	0.50	0.20	0.00	1.00	1.00	2.7
Aripiprazole	Drugs	Dopaminergic GPCR	448.4	5.3	44.8	5.5	1	6.7	0.37	0.83	0.00	0.00	1.00	1.00	3.2
Atomoxetine	Drugs	Reuptake Inhibitors	255.4	3.9	21.3	0.7	1	10.1	1.00	0.83	0.53	1.00	0.06	0.00	3.4
Bromazepam	Drugs	Gaba Receptors	316.2	1.7	54.4	2.1	1	2.0	1.00	0.83	1.00	0.97	1.00	1.00	5.8
Bromocriptine	Drugs	Dopaminergic GPCR	654.6	6.6	118.2	5.1	3	6.7	0.00	0.17	0.00	0.00	0.06	1.00	1.2
Brotizolam	Drugs	Gaba Receptors	393.7	2.7	43.1	2.3	0	2.2	0.76	1.00	1.00	0.83	1.00	1.00	5.6
Budipine	Drugs	Calcium Channels	293.4	5.6	3.2	2.4	0	9.7	1.00	1.00	0.00	0.81	0.00	0.14	3.0
Buprenorphine	Drugs	Opioid Receptor	467.6	4.0	62.2	2.5	2	8.3	0.23	0.50	0.51	0.77	1.00	0.85	3.9
Buspirone	Drugs	Serotonergic GPCR	385.5	2.2	69.6	3.4	0	6.7	0.82	1.00	1.00	0.32	1.00	1.00	5.1
Cabergoline	Drugs	Dopaminergic GPCR	451.6	4.2	71.7	0.0	2	9.4	0.35	0.50	0.41	1.00	1.00	0.30	3.6
Caffeine	Drugs	Serotonergic GPCR	194.2	0.0	61.8	-0.1	0	1.0	1.00	1.00	1.00	1.00	1.00	1.00	6.0
Carbamazepine	Drugs	Reuptake Inhibitors	236.3	2.4	46.3	2.7	2	1.0	1.00	0.50	1.00	0.67	1.00	1.00	5.2
Carisoprodol	Drugs		260.3	2.3	90.7	2.2	3	1.0	1.00	0.17	1.00	0.93	0.98	1.00	5.1
Chlorpromazine	Drugs	Dopaminergic GPCR	318.9	5.3	6.5	2.9	0	9.4	1.00	1.00	0.00	0.57	0.00	0.30	2.9
Citalopram	Drugs	Serotonergic GPCR	324.4	3.1	36.3	0.4	0	9.6	1.00	1.00	0.93	1.00	0.81	0.22	5.0
Clomipramine	Drugs	Serotonergic GPCR	314.9	5.9	6.5	3.5	0	9.5	1.00	1.00	0.00	0.23	0.00	0.27	2.5
Clonazepam	Drugs	Gaba Receptors	315.7	2.4	84.6	2.3	1	1.6	1.00	0.83	1.00	0.83	1.00	1.00	5.7
Clozapine	Drugs	Serotonergic GPCR	326.8	3.7	30.9	3.4	1	7.1	1.00	0.83	0.64	0.33	0.54	1.00	4.3
Cyclobenzaprine	Drugs		275.4	5.1	3.2	3.3	0	9.2	1.00	1.00	0.00	0.37	0.00	0.43	2.8
Dexmethylphenidate	Drugs	Dopaminergic GPCR	233.3	2.6	38.3	-0.3	1	10.6	1.00	0.83	1.00	1.00	0.92	0.00	4.7
Dextropropoxyphene	Drugs	Opioid Receptor	339.5	5.2	29.5	3.7	0	9.2	1.00	1.00	0.00	0.17	0.48	0.41	3.1
Diazepam	Drugs	Gaba Receptors	284.7	3.0	32.7	3.0	0	3.4	1.00	1.00	1.00	0.52	0.63	1.00	5.2
Donepezil	Drugs	Enzyme	379.5	4.6	38.8	3.3	0	8.8	0.86	1.00	0.20	0.35	0.94	0.60	4.0
Dronabinol	Drugs	Cannabinoids	314.5	7.2	29.5	7.7	1	1.0	1.00	0.83	0.00	0.00	0.47	1.00	3.3

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Duloxetine	Drugs	Serotonergic GPCR	297.4	4.3	21.3	1.2	1	10.0	1.00	0.83	0.37	1.00	0.06	0.00	3.3
Eletriptan	Drugs	Serotonergic GPCR	382.5	3.4	53.2	0.3	1	10.4	0.84	0.83	0.82	1.00	1.00	0.00	4.5
Escitalopram	Drugs	Serotonergic GPCR	324.4	3.1	36.3	0.4	0	9.6	1.00	1.00	0.93	1.00	0.81	0.22	5.0
Eszopiclone	Drugs	Gaba Receptors	388.8	1.3	91.8	0.7	0	6.8	0.79	1.00	1.00	1.00	0.94	1.00	5.7
Ethosuximide	Drugs	Calcium Channels	141.2	0.4	46.2	0.4	1	1.0	1.00	0.83	1.00	1.00	1.00	1.00	5.8
Felbamate	Drugs	Gaba Receptors	238.2	0.5	104.6	1.2	4	1.0	1.00	0.00	1.00	1.00	0.51	1.00	4.5
Fentanyl	Drugs	Opioid Receptor	336.5	3.6	23.6	2.5	0	9.1	1.00	1.00	0.69	0.74	0.18	0.47	4.1
Flumazenil	Drugs	Gaba Receptors	303.3	1.3	64.4	0.9	0	1.1	1.00	1.00	1.00	1.00	1.00	1.00	6.0
Fluoxetine	Drugs	Serotonergic GPCR	309.3	4.6	21.3	1.6	1	10.1	1.00	0.83	0.22	1.00	0.06	0.00	3.1
Fluvoxamine	Drugs	Serotonergic GPCR	318.3	3.3	56.8	1.2	2	9.4	1.00	0.50	0.84	1.00	1.00	0.31	4.6
Gabapentin	Drugs	Calcium Channels	171.2	-0.7	63.3	-1.3	3	10.3	1.00	0.17	1.00	1.00	1.00	0.00	4.2
Galantamine	Drugs	Enzyme	287.4	1.0	41.9	1.1	1	7.9	1.00	0.83	1.00	1.00	1.00	1.00	5.8
Haloperidol	Drugs	Dopaminergic GPCR	375.9	3.8	40.5	2.1	1	8.3	0.89	0.83	0.58	0.98	1.00	0.88	5.1
Hydrocodone	Drugs	Opioid Receptor	299.4	1.1	38.8	0.7	0	8.5	1.00	1.00	1.00	1.00	0.94	0.74	5.7
Indeloxazine	Drugs	Reuptake Inhibitors	231.3	2.2	30.5	0.4	1	8.5	1.00	0.83	1.00	1.00	0.52	0.77	5.1
Lamotrigine	Drugs	Reuptake Inhibitors	256.1	2.5	90.7	-0.2	4	5.4	1.00	0.00	1.00	1.00	0.98	1.00	5.0
Levetiracetam	Drugs	Calcium Channels	170.2	-0.3	63.4	-0.7	2	1.0	1.00	0.50	1.00	1.00	1.00	1.00	5.5
Levomethadyl Acetate	Drugs	Opioid Receptor	353.5	4.6	29.5	3.5	0	9.4	1.00	1.00	0.21	0.26	0.48	0.30	3.2
Lofexidine	Drugs		259.1	3.5	33.6	1.7	1	9.8	1.00	0.83	0.77	1.00	0.68	0.10	4.4
Lorazepam	Drugs	Gaba Receptors	321.2	2.4	61.7	2.5	2	1.0	1.00	0.50	1.00	0.77	1.00	1.00	5.3
Meprobamate	Drugs		218.3	0.9	104.6	0.7	4	1.0	1.00	0.00	1.00	1.00	0.51	1.00	4.5
Methylphenidate	Drugs	Dopaminergic GPCR	233.3	2.6	38.3	-0.3	1	10.6	1.00	0.83	1.00	1.00	0.92	0.00	4.7
Metoclopramide	Drugs		299.8	2.2	67.6	0.0	3	9.7	1.00	0.17	1.00	1.00	1.00	0.18	4.3
Midazolam	Drugs	Gaba Receptors	325.8	3.4	30.2	3.9	0	5.6	1.00	1.00	0.79	0.04	0.51	1.00	4.3
Milnacipran	Drugs	Serotonergic GPCR	246.3	1.9	46.3	-1.5	2	10.4	1.00	0.50	1.00	1.00	1.00	0.00	4.5
Minaprine	Drugs	Enzyme	298.4	3.2	50.3	1.2	1	7.1	1.00	0.83	0.91	1.00	1.00	1.00	5.7
Mirtazapine	Drugs		265.4	2.8	19.4	2.1	0	8.1	1.00	1.00	1.00	0.95	0.00	0.95	4.9
Moclobemide	Drugs	Enzyme	268.7	2.2	41.6	0.7	1	6.9	1.00	0.83	1.00	1.00	1.00	1.00	5.8
Modafinil	Drugs	Dopaminergic GPCR	273.4	0.9	60.2	1.2	2	1.0	1.00	0.50	1.00	1.00	1.00	1.00	5.5
Morphine	Drugs	Opioid Receptor	285.3	0.6	52.9	-0.4	2	8.3	1.00	0.50	1.00	1.00	1.00	0.88	5.4
Nalmefene	Drugs	Opioid Receptor	339.4	2.6	52.9	2.1	2	7.7	1.00	0.50	1.00	0.96	1.00	1.00	5.5

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Naltrexone	Drugs	Opioid Receptor	341.4	0.4	70.0	1.4	2	7.5	1.00	0.50	1.00	1.00	1.00	1.00	5.5
Nemonapride	Drugs	Dopaminergic GPCR	387.9	4.2	53.6	2.0	2	8.4	0.80	0.50	0.40	0.99	1.00	0.82	4.5
Nicergoline	Drugs		484.4	4.1	56.6	3.8	0	7.8	0.11	1.00	0.46	0.10	1.00	1.00	3.7
Nicotrol	Drugs	Nicotinic Receptor	162.2	0.9	16.1	-0.5	0	8.0	1.00	1.00	1.00	1.00	0.00	1.00	5.0
Nimodipine	Drugs	Calcium Channels	418.4	4.0	117.0	3.9	1	2.8	0.58	0.83	0.50	0.08	0.10	1.00	3.1
Nortriptyline	Drugs		263.4	4.3	12.0	3.2	1	10.0	1.00	0.83	0.34	0.42	0.00	0.00	2.6
Olanzapine	Drugs	Dopaminergic GPCR	312.4	3.0	30.9	2.5	1	7.8	1.00	0.83	1.00	0.75	0.54	1.00	5.1
Oxcarbazepine	Drugs	Reuptake Inhibitors	252.3	1.2	63.4	1.3	2	1.0	1.00	0.50	1.00	1.00	1.00	1.00	5.5
Oxycodone	Drugs	Opioid Receptor	315.4	0.0	59.0	1.2	1	7.6	1.00	0.83	1.00	1.00	1.00	1.00	5.8
Paliperidone	Drugs	Dopaminergic GPCR	426.5	1.1	84.4	1.0	1	7.9	0.53	0.83	1.00	1.00	1.00	1.00	5.4
Paroxetine	Drugs	Serotonergic GPCR	329.4	4.2	39.7	1.2	1	10.3	1.00	0.83	0.38	1.00	0.99	0.00	4.2
Pergolide	Drugs	Dopaminergic GPCR	314.5	4.4	19.0	2.2	1	9.7	1.00	0.83	0.30	0.92	0.00	0.17	3.2
Perospirone	Drugs	Dopaminergic GPCR	426.6	3.8	56.8	2.4	0	8.4	0.52	1.00	0.62	0.82	1.00	0.80	4.8
phenytoin	Drugs	Reuptake Inhibitors	252.3	2.1	58.2	2.5	2	1.0	1.00	0.50	1.00	0.76	1.00	1.00	5.3
Piracetam	Drugs		142.2	-1.2	63.4	-1.6	2	1.0	1.00	0.50	1.00	1.00	1.00	1.00	5.5
Pramipexole	Drugs	Dopaminergic GPCR	211.3	1.2	50.9	-0.5	3	9.5	1.00	0.17	1.00	1.00	1.00	0.27	4.4
Pregabalin	Drugs	Calcium Channels	159.2	-0.9	63.3	-1.4	3	11.3	1.00	0.17	1.00	1.00	1.00	0.00	4.2
Propofol	Drugs		178.3	3.9	20.2	4.2	1	1.0	1.00	0.83	0.54	0.00	0.01	1.00	3.4
Propoxyphene	Drugs		339.5	5.2	29.5	3.7	0	9.2	1.00	1.00	0.00	0.17	0.48	0.41	3.1
Quazepam	Drugs	Gaba Receptors	386.8	3.2	15.6	4.1	0	1.0	0.81	1.00	0.90	0.00	0.00	1.00	3.7
Quetiapine	Drugs	Serotonergic GPCR	383.5	3.0	48.3	1.6	1	5.8	0.83	0.83	1.00	1.00	1.00	1.00	5.7
Ramelteon	Drugs	Melatonin Receptor	259.3	2.5	38.3	2.6	1	1.0	1.00	0.83	1.00	0.72	0.92	1.00	5.5
Rasagiline	Drugs	Enzyme	171.2	2.5	12.0	1.9	1	7.5	1.00	0.83	1.00	1.00	0.00	1.00	4.8
Reboxetine	Drugs	Reuptake Inhibitors	313.4	3.3	39.7	1.8	1	8.4	1.00	0.83	0.87	1.00	0.99	0.82	5.5
Remifentanyl	Drugs	Opioid Receptor	376.4	2.0	76.2	2.0	0	6.6	0.88	1.00	1.00	0.98	1.00	1.00	5.9
Riluzole	Drugs	Reuptake Inhibitors	234.2	3.2	48.1	2.8	2	3.6	1.00	0.50	0.88	0.58	1.00	1.00	5.0
Rimonabant	Drugs	Cannabinoids	463.8	6.5	50.2	6.0	1	3.2	0.26	0.83	0.00	0.00	1.00	1.00	3.1
Risperidone	Drugs	Dopaminergic GPCR	410.5	2.7	64.2	2.3	0	7.9	0.64	1.00	1.00	0.86	1.00	1.00	5.5
Rivastigmine	Drugs	Enzyme	250.3	2.1	32.8	0.9	0	8.6	1.00	1.00	1.00	1.00	0.64	0.69	5.3
Ropinirole	Drugs	Dopaminergic GPCR	260.4	2.8	32.3	1.2	1	9.5	1.00	0.83	1.00	1.00	0.62	0.28	4.7
Ropivacaine	Drugs		274.4	3.2	32.3	2.6	1	8.2	1.00	0.83	0.92	0.69	0.62	0.92	5.0

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Selegiline	Drugs	Enzyme	187.3	3.0	3.2	2.6	0	7.5	1.00	1.00	0.99	0.71	0.00	1.00	4.7
Sertindole	Drugs	Serotonergic GPCR	440.9	5.3	40.5	3.8	1	9.1	0.42	0.83	0.00	0.10	1.00	0.47	2.8
Sertraline	Drugs	Serotonergic GPCR	306.2	5.3	12.0	2.8	1	9.5	1.00	0.83	0.00	0.62	0.00	0.27	2.7
Sinequan	Drugs	Serotonergic GPCR	279.4	4.1	12.5	2.1	0	9.2	1.00	1.00	0.45	0.96	0.00	0.41	3.8
Sulpiride	Drugs	Dopaminergic GPCR	341.4	1.1	101.7	-1.4	3	9.0	1.00	0.17	1.00	1.00	0.61	0.52	4.3
Tacrine	Drugs	Enzyme	198.3	3.3	38.9	1.1	2	9.6	1.00	0.50	0.86	1.00	0.95	0.18	4.5
Talipexole	Drugs	Dopaminergic GPCR	209.3	1.1	42.2	1.0	2	7.2	1.00	0.50	1.00	1.00	1.00	1.00	5.5
Terguride	Drugs	Dopaminergic GPCR	340.5	2.8	51.4	1.4	2	9.8	1.00	0.50	1.00	1.00	1.00	0.11	4.6
Thiopental	Drugs	Gaba Receptors	242.3	1.8	58.5	-0.7	1	1.0	1.00	0.83	1.00	1.00	1.00	1.00	5.8
Tiagabine	Drugs	Gaba Receptors	375.5	2.8	40.5	3.2	1	9.4	0.89	0.83	1.00	0.42	1.00	0.31	4.4
Tianeptine	Drugs	Reuptake Inhibitors	437.0	1.5	86.7	0.4	2	7.5	0.45	0.50	1.00	1.00	1.00	1.00	5.0
Topiramate	Drugs	Enzyme	339.4	0.0	115.5	3.0	2	1.0	1.00	0.50	1.00	0.52	0.15	1.00	4.2
Tramadol	Drugs	Reuptake Inhibitors	263.4	3.1	32.7	0.5	1	9.6	1.00	0.83	0.95	1.00	0.64	0.20	4.6
Trazodone	Drugs	Serotonergic GPCR	371.9	3.9	45.8	1.6	0	6.7	0.92	1.00	0.58	1.00	1.00	1.00	5.5
Tropisetron	Drugs	Serotonergic GPCR	284.4	2.9	45.3	1.0	1	10.0	1.00	0.83	1.00	1.00	1.00	0.00	4.8
Valproic Acid	Drugs		144.2	2.8	37.3	0.2	1	1.0	1.00	0.83	1.00	1.00	0.87	1.00	5.7
Varenicline	Drugs	Nicotinic Receptor	211.3	0.9	37.8	-1.3	1	9.6	1.00	0.83	1.00	1.00	0.89	0.20	4.9
Venlafaxine	Drugs	Serotonergic GPCR	277.4	3.3	32.7	1.2	1	9.3	1.00	0.83	0.87	1.00	0.64	0.37	4.7
Verapamil	Drugs	Calcium Channels	454.6	4.5	64.0	2.3	0	9.0	0.32	1.00	0.27	0.84	1.00	0.52	3.9
Vigabatrin	Drugs	Gaba Receptors	129.2	-2.2	63.3	-2.6	3	10.6	1.00	0.17	1.00	1.00	1.00	0.00	4.2
Vinpocetine	Drugs		350.5	4.8	34.5	4.6	0	7.8	1.00	1.00	0.09	0.00	0.72	1.00	3.8
Zaleplon	Drugs	Gaba Receptors	305.3	1.4	74.3	0.9	0	1.0	1.00	1.00	1.00	1.00	1.00	1.00	6.0
Ziprasidone	Drugs	Dopaminergic GPCR	412.9	4.2	48.5	3.1	1	8.4	0.62	0.83	0.40	0.47	1.00	0.80	4.1
Zolpidem	Drugs	Gaba Receptors	307.4	3.0	37.6	2.9	0	6.6	1.00	1.00	0.99	0.57	0.88	1.00	5.4
Zonisamide	Drugs	Enzyme	212.2	-0.4	86.2	-0.1	2	1.0	1.00	0.50	1.00	1.00	1.00	1.00	5.5
Zotepine	Drugs	Serotonergic GPCR	331.9	5.1	12.5	5.2	0	8.7	1.00	1.00	0.00	0.00	0.00	0.64	2.6
Candidate-001	Candidates	Glutamate receptors	276.2	-0.5	112.1	0.3	2	6.9	1.00	0.50	1.00	1.00	0.26	1.00	4.8
Candidate-002	Candidates	Reuptake Inhibitors	255.3	3.7	21.3	1.7	1	9.1	1.00	0.83	0.67	1.00	0.06	0.46	4.0
Candidate-003	Candidates	Reuptake Inhibitors	326.2	5.5	21.3	2.7	1	10.1	1.00	0.83	0.00	0.67	0.06	0.00	2.6
Candidate-004	Candidates	Serotonergic GPCR	391.5	2.0	78.5	0.0	2	10.3	0.78	0.50	1.00	1.00	1.00	0.00	4.3
Candidate-005	Candidates	Enzyme	375.5	3.9	58.4	2.1	1	8.8	0.89	0.83	0.53	0.95	1.00	0.60	4.8

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Candidate-006	Candidates	Peptide GPCR	379.5	2.6	53.6	0.2	2	9.9	0.86	0.50	1.00	1.00	1.00	0.07	4.4
Candidate-007	Candidates	Enzyme	311.4	4.1	51.4	2.3	2	8.7	1.00	0.50	0.44	0.85	1.00	0.67	4.5
Candidate-008	Candidates	Calcium Channels	159.2	-0.8	63.3	-1.1	3	10.6	1.00	0.17	1.00	1.00	1.00	0.00	4.2
Candidate-009	Candidates	Nicotinic Receptor	269.1	1.0	34.0	-2.2	1	10.2	1.00	0.83	1.00	1.00	0.70	0.00	4.5
Candidate-010	Candidates	Opioid Receptor	372.5	4.7	49.4	2.3	1	9.4	0.91	0.83	0.16	0.84	1.00	0.32	4.1
Candidate-011	Candidates	Dopaminergic GPCR	436.5	3.7	87.2	3.1	1	6.6	0.45	0.83	0.66	0.45	1.00	1.00	4.4
Candidate-012	Candidates	Peptide GPCR	459.6	5.5	80.2	5.4	1	5.1	0.29	0.83	0.00	0.00	1.00	1.00	3.1
Candidate-013	Candidates	Enzyme	378.5	5.3	33.2	3.0	0	8.8	0.87	1.00	0.00	0.52	0.66	0.61	3.7
Candidate-014	Candidates	Opioid Receptor	396.5	3.3	45.9	1.8	0	9.9	0.74	1.00	0.84	1.00	1.00	0.07	4.6
Candidate-015	Candidates	Nicotinic Receptor	271.3	1.7	58.4	-0.9	1	9.1	1.00	0.83	1.00	1.00	1.00	0.45	5.3
Candidate-016	Candidates	Gaba Receptors	336.4	2.0	61.4	2.2	0	6.2	1.00	1.00	1.00	0.91	1.00	1.00	5.9
Candidate-017	Candidates	Enzyme	468.5	2.2	105.8	0.3	1	5.7	0.22	0.83	1.00	1.00	0.47	1.00	4.5
Candidate-018	Candidates	Cannabinoids	436.3	5.6	38.1	4.9	0	1.0	0.46	1.00	0.00	0.00	0.91	1.00	3.4
Candidate-019	Candidates	Peptide GPCR	392.9	6.0	80.7	6.3	2	4.0	0.77	0.50	0.00	0.00	1.00	1.00	3.3
Candidate-020	Candidates	Glutamate receptors	402.5	3.2	66.3	2.2	1	8.1	0.70	0.83	0.90	0.90	1.00	0.96	5.3
Candidate-021	Candidates	Enzyme	315.4	3.1	60.6	1.1	2	8.6	1.00	0.50	0.97	1.00	1.00	0.68	5.1
Candidate-022	Candidates	Enzyme	489.6	5.6	71.0	2.1	3	10.4	0.07	0.17	0.00	0.97	1.00	0.00	2.2
Candidate-023	Candidates	Nicotinic Receptor	227.2	2.6	12.0	-0.2	1	10.0	1.00	0.83	1.00	1.00	0.00	0.03	3.9
Candidate-024	Candidates	Calcium Channels	187.3	0.1	63.3	-0.3	3	11.2	1.00	0.17	1.00	1.00	1.00	0.00	4.2
Candidate-025	Candidates	Reuptake Inhibitors	319.8	4.5	21.3	1.5	1	10.3	1.00	0.83	0.24	1.00	0.06	0.00	3.1
Candidate-026	Candidates	Serotonergic GPCR	322.8	2.9	50.3	3.8	1	7.8	1.00	0.83	1.00	0.09	1.00	1.00	4.9
Candidate-027	Candidates	Serotonergic GPCR	447.6	4.1	57.9	1.5	0	8.7	0.37	1.00	0.46	1.00	1.00	0.65	4.5
Candidate-028	Candidates	Histaminergic GPCR	322.4	2.4	32.3	0.0	1	9.2	1.00	0.83	1.00	1.00	0.62	0.42	4.9
Candidate-029	Candidates	Glutamate receptors	327.4	1.8	63.9	0.8	3	8.2	1.00	0.17	1.00	1.00	1.00	0.90	5.1
Candidate-030	Candidates	Peptide GPCR	296.4	3.4	33.3	0.8	2	9.9	1.00	0.50	0.80	1.00	0.66	0.05	4.0
Candidate-031	Candidates	Serotonergic GPCR	383.5	1.9	69.6	2.0	0	6.7	0.83	1.00	1.00	1.00	1.00	1.00	5.8
Candidate-032	Candidates	Gaba Receptors	310.4	1.1	61.4	2.3	0	6.5	1.00	1.00	1.00	0.84	1.00	1.00	5.8
Candidate-033	Candidates	Opioid Receptor	426.6	3.1	69.6	0.8	2	10.3	0.52	0.50	0.95	1.00	1.00	0.00	4.0
Candidate-034	Candidates	Reuptake Inhibitors	308.4	3.5	41.1	3.3	1	7.1	1.00	0.83	0.75	0.83	1.00	1.00	5.4
Candidate-035	Candidates	Calcium Channels	185.3	-0.2	63.3	-0.9	3	10.3	1.00	0.17	1.00	1.00	1.00	0.00	4.2
Candidate-036	Candidates	Peptide GPCR	326.5	7.6	34.2	7.1	1	7.2	1.00	0.83	0.00	0.00	0.71	1.00	3.5

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Candidate-037	Candidates	Gaba Receptors	324.3	2.5	74.3	-2.8	2	12.4	1.00	0.50	1.00	1.00	1.00	0.00	4.5
Candidate-038	Candidates	Serotonergic GPCR	417.5	5.1	26.8	3.6	0	7.8	0.59	1.00	0.00	0.20	0.34	1.00	3.1
Candidate-039	Candidates	Glutamate receptors	462.9	5.6	51.0	4.0	0	8.5	0.26	1.00	0.00	0.00	1.00	0.77	3.0
Candidate-040	Candidates	Enzyme	395.5	-1.5	101.8	-0.7	1	7.9	0.75	0.83	1.00	1.00	0.61	1.00	5.2
Candidate-041	Candidates	Peptide GPCR	380.4	4.6	42.5	1.9	2	9.9	0.85	0.50	0.20	1.00	1.00	0.08	3.6
Candidate-042	Candidates	Serotonergic GPCR	304.8	2.9	50.3	2.8	1	7.4	1.00	0.83	1.00	0.60	1.00	1.00	5.4
Candidate-043	Candidates	Peptide GPCR	394.9	2.1	50.1	0.7	0	8.7	0.75	1.00	1.00	1.00	1.00	0.67	5.4
Candidate-044	Candidates	Serotonergic GPCR	355.4	3.3	37.4	2.5	1	8.2	1.00	0.83	0.84	0.77	0.87	0.92	5.2
Candidate-045	Candidates	Cannabinoids	510.4	4.1	102.0	2.7	3	7.0	0.00	0.17	0.46	0.26	0.60	1.00	2.5
Candidate-046	Candidates	Serotonergic GPCR	448.4	5.7	26.8	4.8	0	7.7	0.37	1.00	0.00	0.00	0.34	1.00	2.7
Candidate-047	Candidates	Calcium Channels	187.3	0.1	63.3	-0.2	3	10.3	1.00	0.17	1.00	1.00	1.00	0.00	4.2
Candidate-048	Candidates	Dopaminergic GPCR	430.5	5.2	57.7	4.8	1	7.1	0.50	0.83	0.00	0.00	1.00	1.00	3.3
Candidate-049	Candidates	Serotonergic GPCR	455.0	5.7	48.5	3.5	1	8.4	0.32	0.83	0.00	0.27	1.00	0.80	3.2
Candidate-050	Candidates	Gaba Receptors	373.4	2.5	83.2	-0.1	3	9.3	0.90	0.17	1.00	1.00	1.00	0.35	4.4
Candidate-051	Candidates	Reuptake Inhibitors	363.3	3.7	48.3	1.9	1	8.3	0.98	0.83	0.65	1.00	1.00	0.87	5.3
Candidate-052	Candidates	Enzyme	385.3	3.1	52.2	5.0	1	1.0	0.82	0.83	0.94	0.00	1.00	1.00	4.6
Candidate-053	Candidates	Nicotinic Receptor	227.2	2.6	12.0	-0.2	1	10.0	1.00	0.83	1.00	1.00	0.00	0.03	3.9
Candidate-054	Candidates	Opioid Receptor	319.5	6.4	3.2	5.3	0	8.6	1.00	1.00	0.00	0.00	0.00	0.72	2.7
Candidate-055	Candidates	Enzyme	388.5	5.1	34.5	2.6	0	8.8	0.80	1.00	0.00	0.69	0.72	0.61	3.8
Candidate-056	Candidates	Enzyme	392.5	3.8	52.8	3.5	0	4.3	0.77	1.00	0.58	0.24	1.00	1.00	4.6
Candidate-057	Candidates	Dopaminergic GPCR	391.5	4.3	39.5	4.7	0	7.3	0.78	1.00	0.36	0.00	0.98	1.00	4.1
Candidate-058	Candidates	Peptide GPCR	614.7	6.0	149.6	2.2	5	1.0	0.00	0.00	0.00	0.91	0.00	1.00	1.9
Candidate-059	Candidates	Dopaminergic GPCR	480.9	4.9	61.5	5.8	1	6.7	0.14	0.83	0.04	0.00	1.00	1.00	3.0
Candidate-060	Candidates	Serotonergic GPCR	464.6	5.3	45.0	1.5	0	9.7	0.25	1.00	0.00	1.00	1.00	0.18	3.4
Candidate-061	Candidates	Histaminergic GPCR	350.4	3.4	32.3	0.9	1	9.2	1.00	0.83	0.82	1.00	0.62	0.42	4.7
Candidate-062	Candidates	Dopaminergic GPCR	433.5	4.9	44.8	3.3	1	6.8	0.47	0.83	0.06	0.34	1.00	1.00	3.7
Candidate-063	Candidates	Nicotinic Receptor	288.3	1.7	50.8	-0.7	1	9.7	1.00	0.83	1.00	1.00	1.00	0.13	5.0
Candidate-064	Candidates	Serotonergic GPCR	275.7	3.7	21.3	1.4	1	9.0	1.00	0.83	0.63	1.00	0.06	0.49	4.0
Candidate-065	Candidates	Peptide GPCR	417.3	6.2	63.0	3.8	2	6.3	0.59	0.50	0.00	0.08	1.00	1.00	3.2
Candidate-066	Candidates	Serotonergic GPCR	436.6	3.3	59.9	2.2	1	7.8	0.45	0.83	0.84	0.91	1.00	1.00	5.0
Candidate-067	Candidates	Dopaminergic GPCR	463.5	5.4	69.7	4.3	2	6.8	0.26	0.50	0.00	0.00	1.00	1.00	2.8

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Candidate-068	Candidates	Serotonergic GPCR	469.0	6.2	48.5	4.8	1	8.4	0.22	0.83	0.00	0.00	1.00	0.80	2.8
Candidate-069	Candidates	Reuptake Inhibitors	300.2	5.1	21.3	3.4	1	9.0	1.00	0.83	0.00	0.33	0.06	0.48	2.7
Candidate-070	Candidates	Dopaminergic GPCR	221.3	1.3	42.2	1.1	2	7.0	1.00	0.50	1.00	1.00	1.00	1.00	5.5
Candidate-071	Candidates	Reuptake Inhibitors	376.9	1.7	41.4	-0.9	0	10.1	0.88	1.00	1.00	1.00	1.00	0.00	4.9
Candidate-072	Candidates	Dopaminergic GPCR	360.4	3.1	41.5	4.1	0	7.8	1.00	1.00	0.97	0.00	1.00	1.00	5.0
Candidate-073	Candidates	Gaba Receptors	323.3	2.2	84.1	4.1	2	1.0	1.00	0.50	1.00	0.00	1.00	1.00	4.5
Candidate-074	Candidates	Peptide GPCR	327.5	7.6	31.4	6.2	0	5.6	1.00	1.00	0.00	0.00	0.57	1.00	3.6
Candidate-075	Candidates	Nicotinic Receptor	271.3	1.7	58.4	-1.2	1	9.5	1.00	0.83	1.00	1.00	1.00	0.23	5.1
Candidate-076	Candidates	Nicotinic Receptor	258.3	1.6	45.4	0.4	0	8.9	1.00	1.00	1.00	1.00	1.00	0.57	5.6
Candidate-077	Candidates	Gaba Receptors	316.3	2.0	71.2	1.4	2	1.0	1.00	0.50	1.00	1.00	1.00	1.00	5.5
Candidate-078	Candidates	Reuptake Inhibitors	335.3	2.9	39.7	1.5	1	8.3	1.00	0.83	1.00	1.00	0.99	0.86	5.7
Candidate-079	Candidates	Calcium Channels	187.3	0.2	63.3	0.0	3	10.5	1.00	0.17	1.00	1.00	1.00	0.00	4.2
Candidate-080	Candidates	Dopaminergic GPCR	367.4	3.0	65.3	3.4	0	7.2	0.95	1.00	1.00	0.30	1.00	1.00	5.2
Candidate-081	Candidates	Serotonergic GPCR	382.5	2.8	39.7	2.3	0	7.2	0.84	1.00	1.00	0.86	0.98	1.00	5.7
Candidate-082	Candidates	Gaba Receptors	297.4	1.2	74.0	-1.9	3	9.6	1.00	0.17	1.00	1.00	1.00	0.21	4.4
Candidate-083	Candidates	Cannabinoids	452.3	5.8	47.4	5.1	0	1.0	0.34	1.00	0.00	0.00	1.00	1.00	3.3
Candidate-084	Candidates	Gaba Receptors	360.4	2.6	72.3	3.1	0	4.0	1.00	1.00	1.00	0.43	1.00	1.00	5.4
Candidate-085	Candidates	Reuptake Inhibitors	294.4	3.2	52.6	1.5	1	8.4	1.00	0.83	0.88	1.00	1.00	0.81	5.5
Candidate-086	Candidates	Muscarinic Receptor	270.3	2.5	34.1	3.9	0	5.5	1.00	1.00	1.00	0.07	0.70	1.00	4.8
Candidate-087	Candidates	Cannabinoids	496.4	4.3	101.4	2.2	3	5.7	0.03	0.17	0.37	0.90	0.62	1.00	3.1
Candidate-088	Candidates	Dopaminergic GPCR	357.8	3.5	44.8	2.3	1	5.8	1.00	0.83	0.75	0.86	1.00	1.00	5.4
Candidate-089	Candidates	Enzyme	271.4	2.2	60.2	0.3	3	9.4	1.00	0.17	1.00	1.00	1.00	0.33	4.5
Candidate-090	Candidates	Glutamate receptors	359.4	1.6	73.2	1.1	3	6.8	1.00	0.17	1.00	1.00	1.00	1.00	5.2
Candidate-091	Candidates	Gaba Receptors	330.4	2.5	71.2	2.0	2	1.0	1.00	0.50	1.00	1.00	1.00	1.00	5.5
Candidate-092	Candidates	Reuptake Inhibitors	360.3	3.1	50.2	0.6	1	8.1	1.00	0.83	0.95	1.00	1.00	0.97	5.7
Candidate-093	Candidates	Muscarinic Receptor	269.2	5.2	15.6	2.3	0	7.3	1.00	1.00	0.00	0.88	0.00	1.00	3.9
Candidate-094	Candidates	Dopaminergic GPCR	420.5	4.9	44.3	3.7	1	7.8	0.57	0.83	0.05	0.17	1.00	1.00	3.6
Candidate-095	Candidates	Gaba Receptors	321.3	2.9	68.5	0.9	1	2.1	1.00	0.83	1.00	1.00	1.00	1.00	5.8
Candidate-096	Candidates	Serotonergic GPCR	419.6	4.1	47.0	2.3	1	7.8	0.57	0.83	0.46	0.87	1.00	1.00	4.7
Candidate-097	Candidates	Reuptake Inhibitors	309.8	4.9	30.5	3.1	1	8.6	1.00	0.83	0.06	0.44	0.52	0.72	3.6
Candidate-098	Candidates	Enzyme	460.5	4.1	52.8	4.8	0	4.1	0.28	1.00	0.43	0.00	1.00	1.00	3.7

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Candidate-099	Candidates	Peptide GPCR	412.6	5.6	24.5	3.5	1	10.0	0.62	0.83	0.00	0.27	0.23	0.00	2.0
Candidate-100	Candidates	Enzyme	400.3	8.6	49.3	5.4	2	1.0	0.71	0.50	0.00	0.00	1.00	1.00	3.2
Candidate-101	Candidates	Dopaminergic GPCR	434.6	5.2	48.5	3.7	1	8.4	0.47	0.83	0.00	0.14	1.00	0.80	3.2
Candidate-102	Candidates	Serotonergic GPCR	450.6	4.1	69.9	3.7	0	8.0	0.35	1.00	0.48	0.16	1.00	1.00	4.0
Candidate-103	Candidates	Dopaminergic GPCR	329.5	6.4	3.2	5.0	0	8.4	1.00	1.00	0.00	0.00	0.00	0.83	2.8
Candidate-104	Candidates	Peptide GPCR	419.6	3.2	53.6	1.2	2	9.9	0.57	0.50	0.88	1.00	1.00	0.03	4.0
Candidate-105	Candidates	Gaba Receptors	298.3	2.4	71.2	1.5	2	1.3	1.00	0.50	1.00	1.00	1.00	1.00	5.5
Candidate-106	Candidates	Peptide GPCR	493.6	5.8	103.5	4.6	4	1.0	0.05	0.00	0.00	0.00	0.55	1.00	1.6
Candidate-107	Candidates	Calcium Channels	173.3	-0.3	63.3	-0.5	3	10.5	1.00	0.17	1.00	1.00	1.00	0.00	4.2
Candidate-108	Candidates	Nicotinic Receptor	209.2	2.5	12.0	0.2	1	10.1	1.00	0.83	1.00	1.00	0.00	0.00	3.8