Supplementary Table S4. 364 Predicted interactions and experimental validation.

Predicted interactions between activators and targets						
No.	**Drug Name**	**No. Predicted Targets**	**Target Name**	**Gene Name**	**Confidence Score**	**Experimental Validation, Ki (nM)**
1	**Acetylcholine**	1	Muscarinic acetylcholine receptor M5	CHRM5	0.8279	800
2	**Amiodarone**	1	Beta-2 adrenergic receptor	ADRB2	0.6398	n.a.
			Beta-3 adrenergic receptor	ADRB3	0.6155	n.a.
3	**Cabergoline**	6	5-hydroxytryptamine receptor 6	HTR6	0.8499	n.a.
			Beta-3 adrenergic receptor	ADRB3	0.8131	n.a.
			5-hydroxytryptamine receptor 1E	HTR1E	0.7972	n.a.
			5-hydroxytryptamine receptor 3A	HTR3A	0.755	n.a.
			5-hydroxytryptamine receptor 1F	HTR1F	0.6822	n.a.
			Muscarinic acetylcholine receptor M1	CHRM1	0.616	n.a.
4	**Citalopram**	24	5-hydroxytryptamine receptor 2A	HTR2A	0.831	n.a.
			Alpha-1D adrenergic receptor	ADRA1D	0.8283	n.a.
			Alpha-1B adrenergic receptor	ADRA1B	0.8265	n.a.
			Muscarinic acetylcholine receptor M2	CHRM2	0.8162	n.a.
			Muscarinic acetylcholine receptor M3	CHRM3	0.8002	n.a.
			D(2) dopamine receptor	DRD2	0.7851	n.a.
			Muscarinic acetylcholine receptor M5	CHRM5	0.7558	n.a.
			Alpha-2A adrenergic receptor	ADRA2A	0.7488	n.a.
			Muscarinic acetylcholine receptor M4	CHRM4	0.7466	n.a.
			Sodium-dependent noradrenaline transporter	SLC6A2	0.7355	n.a.
			Sodium-dependent dopamine transporter	SLC6A3	0.7271	n.a.
			Alpha-2C adrenergic receptor	ADRA2C	0.7199	n.a.
			D(1A) dopamine receptor	DRD1	0.7155	n.a.
			Alpha-2B adrenergic receptor	ADRA2B	0.7071	n.a.
			D(4) dopamine receptor	DRD4	0.6847	n.a.
			5-hydroxytryptamine receptor 1A	HTR1A	0.6829	n.a.
			D(3) dopamine receptor	DRD3	0.6721	n.a.
			D(1B) dopamine receptor	DRD5	0.6638	n.a.
			5-hydroxytryptamine receptor 7	HTR7	0.6596	n.a.
			5-hydroxytryptamine receptor 6	HTR6	0.6445	n.a.
			5-hydroxytryptamine receptor 3A	HTR3A	0.6193	n.a.
			5-hydroxytryptamine receptor 1B	HTR1B	0.616	n.a.
			5-hydroxytryptamine receptor 2B	HTR2B	0.6148	n.a.
			5-hydroxytryptamine receptor 1D	HTR1D	0.6139	n.a.
5	**Chlorpromazine**	14	Muscarinic acetylcholine receptor M2	CHRM2	0.9115	150
			Muscarinic acetylcholine receptor M5	CHRM5	0.8418	42
			5-hydroxytryptamine receptor 1B	HTR1B	0.8376	1489
			5-hydroxytryptamine receptor 3A	HTR3A	0.8355	776
			Muscarinic acetylcholine receptor M4	CHRM4	0.8275	n.a.
			5-hydroxytryptamine receptor 1D	HTR1D	0.8053	452
			5-hydroxytryptamine receptor 1E	HTR1E	0.7314	344
			Sodium-dependent serotonin transporter	SLC6A4	0.6925	n.a.
			Beta-1 adrenergic receptor	ADRB1	0.6684	n.a.
			Beta-3 adrenergic receptor	ADRB3	0.641	n.a.
			Histamine H2 receptor	HRH2	0.6398	172
			Beta-2 adrenergic receptor	ADRB2	0.6382	n.a.
			Sodium-dependent noradrenaline transporter	SLC6A2	0.6358	n.a.
			Sodium-dependent dopamine transporter	SLC6A3	0.6344	n.a.
6	**Clonidine**	1	5-hydroxytryptamine receptor 2B	HTR2B	0.6078	n.a.
7	**Copper**	8	Progesterone receptor	PGR	0.7289	n.a.
			Triosephosphate isomerase	TPI1	0.6895	n.a.
			Plasma kallikrein	KLKB1	0.6581	n.a.
			Desmoplakin	DSP	0.6578	n.a.
			Estrogen receptor	ESR1	0.6329	n.a.
			Phosphoserine phosphatase	PSPH	0.6248	n.a.
			Protein S100-A9	S100A9	0.6066	n.a.
			Glyceraldehyde-3-phosphate dehydrogenase, testis-specific	GAPDHS	0.6051	n.a.
8	**Dasatinib**	2	Platelet-derived growth factor receptor alpha	PDGFRA	0.6393	0.47
			Fibroblast growth factor receptor 2	FGFR2	0.6121	1400
9	**Diazoxide**	1	Carbonic anhydrase 4	CA4	0.6209	n.a.
10	**Doxazosin**	3	Alpha-2A adrenergic receptor	ADRA2A	0.6978	n.a.
			Alpha-2B adrenergic receptor	ADRA2B	0.6642	n.a.
			Alpha-2C adrenergic receptor	ADRA2C	0.6474	n.a.
11	**Dronedarone**	7	Beta-2 adrenergic receptor	ADRB2	0.7452	n.a.
			Voltage-dependent T-type calcium channel subunit alpha-1H	CACNA1H	0.7078	n.a.
			Beta-3 adrenergic receptor	ADRB3	0.69	n.a.

			Voltage-dependent T-type calcium channel subunit alpha-1I	CACNA1I	0.6553	n.a.
			D(1B) dopamine receptor	DRD5	0.6428	n.a.
			5-hydroxytryptamine receptor 1B	HTR1B	0.6116	n.a.
			5-hydroxytryptamine receptor 1D	HTR1D	0.6006	n.a.
12	**Felodipine**	3	Voltage-dependent L-type calcium channel subunit alpha-1F	CACNA1F	0.644	n.a.
			Voltage-dependent L-type calcium channel subunit beta-1	CACNB1	0.6013	n.a.
			Voltage-dependent P/Q-type calcium channel subunit alpha-1A	CACNA1A	0.6004	n.a.
13	**Fluoxetine**	5	5-hydroxytryptamine receptor 2A	HTR2A	0.7219	147.9
			Sodium-dependent noradrenaline transporter	SLC6A2	0.7109	n.a.
			Alpha-2A adrenergic receptor	ADRA2A	0.616	n.a.
			Sodium-dependent dopamine transporter	SLC6A3	0.6147	n.a.
			5-hydroxytryptamine receptor 3A	HTR3A	0.6017	n.a.
14	**Fluphenazine**	10	D(1B) dopamine receptor	DRD5	0.7277	12
			5-hydroxytryptamine receptor 2B	HTR2B	0.6877	n.a.
			D(3) dopamine receptor	DRD3	0.6526	0.11
			5-hydroxytryptamine receptor 7	HTR7	0.6422	7.94
			D(4) dopamine receptor	DRD4	0.6339	50
			5-hydroxytryptamine receptor 1A	HTR1A	0.6335	145
			Sodium-dependent noradrenaline transporter	SLC6A2	0.6223	n.a.
			5-hydroxytryptamine receptor 3A	HTR3A	0.6077	n.a.
			Alpha-2B adrenergic receptor	ADRA2B	0.6064	82
			Sodium-dependent serotonin transporter	SLC6A4	0.6062	n.a.
15	**Fluspirilene**	3	D(1A) dopamine receptor	DRD1	0.6867	450
			D(3) dopamine receptor	DRD3	0.6085	0.4
			5-hydroxytryptamine receptor 1A	HTR1A	0.604	56
16	**Genistein**	1	Estrogen-related receptor gamma	ESRRG	0.6159	n.a.
17	**Imatinib**	1	Receptor-type tyrosine-protein kinase FLT3	FLT3	0.6206	6300
18	**Isradipine**	4	Voltage-dependent L-type calcium channel subunit alpha-1F	CACNA1F	0.6565	n.a.
			Voltage-dependent L-type calcium channel subunit beta-1	CACNB1	0.6187	n.a.
			Voltage-dependent L-type calcium channel subunit beta-4	CACNB4	0.6092	n.a.
			Voltage-dependent L-type calcium channel subunit beta-3	CACNB3	0.6023	n.a.
19	**Ivermectin**	16	Gamma-aminobutyric acid receptor subunit gamma-2	GABRG2	0.7215	n.a.
			Gamma-aminobutyric acid receptor subunit alpha-1	GABRA1	0.7192	n.a.
			Gamma-aminobutyric acid receptor subunit alpha-3	GABRA3	0.6978	n.a.
			Gamma-aminobutyric acid receptor subunit beta-2	GABRB2	0.6843	n.a.
			Gamma-aminobutyric acid receptor subunit beta-1	GABRB1	0.6817	n.a.
			Gamma-aminobutyric acid receptor subunit alpha-5	GABRA5	0.6755	n.a.
			Gamma-aminobutyric acid receptor subunit delta	GABRD	0.668	n.a.
			Gamma-aminobutyric acid receptor subunit alpha-4	GABRA4	0.6602	n.a.
			Gamma-aminobutyric acid receptor subunit theta	GABRQ	0.6591	n.a.
			Gamma-aminobutyric acid receptor subunit alpha-2	GABRA2	0.6584	n.a.
			Gamma-aminobutyric acid receptor subunit alpha-6	GABRA6	0.6575	n.a.
			Gamma-aminobutyric acid receptor subunit gamma-1	GABRG1	0.6476	n.a.
			Gamma-aminobutyric acid receptor subunit pi	GABRP	0.6402	n.a.
			Glycine receptor subunit alpha-1	GLRA1	0.6401	n.a.
			Gamma-aminobutyric acid receptor subunit gamma-3	GABRG3	0.6314	n.a.
			Gamma-aminobutyric acid receptor subunit epsilon	GABRE	0.6189	n.a.
20	**Ketanserin**	1	5-hydroxytryptamine receptor 2C	HTR2C	0.6015	n.a.
21	**Lacidipine**	3	Voltage-dependent T-type calcium channel subunit alpha-1H	CACNA1H	0.6523	n.a.
			Voltage-dependent T-type calcium channel subunit alpha-1I	CACNA1I	0.6283	n.a.

			Voltage-dependent T-type calcium channel subunit alpha-1G	CACNA1G	0.6049	n.a.
22	**Lamotrigine**	29	Alpha-1B adrenergic receptor	ADRA1B	0.9845	n.a.
			Alpha-1D adrenergic receptor	ADRA1D	0.9675	n.a.
			Alpha-2B adrenergic receptor	ADRA2B	0.9361	n.a.
			Alpha-2C adrenergic receptor	ADRA2C	0.9097	n.a.
			5-hydroxytryptamine receptor 2C	HTR2C	0.9066	n.a.
			5-hydroxytryptamine receptor 2B	HTR2B	0.8793	n.a.
			Sodium-dependent noradrenaline transporter	SLC6A2	0.828	n.a.
			5-hydroxytryptamine receptor 6	HTR6	0.8206	n.a.
			D(4) dopamine receptor	DRD4	0.7965	n.a.
			5-hydroxytryptamine receptor 7	HTR7	0.7951	n.a.
			Gamma-aminobutyric acid receptor subunit rho-1	GABRR1	0.7867	n.a.
			D(3) dopamine receptor	DRD3	0.7861	n.a.
			Sodium-dependent serotonin transporter	SLC6A4	0.7755	n.a.
			Gamma-aminobutyric acid receptor subunit rho-2	GABRR2	0.7751	n.a.
			Sodium-dependent dopamine transporter	SLC6A3	0.7684	n.a.
			Gamma-aminobutyric acid receptor subunit rho-3	GABRR3	0.7582	n.a.
			Beta-3 adrenergic receptor	ADRB3	0.7536	n.a.
			Histamine H4 receptor	HRH4	0.7178	n.a.
			Glycine receptor subunit alpha-1	GLRA1	0.7084	n.a.
			Histamine H2 receptor	HRH2	0.7004	n.a.
			5-hydroxytryptamine receptor 1D	HTR1D	0.6976	n.a.
			Sigma non-opioid intracellular receptor 1	SIGMAR1	0.6881	n.a.
			Potassium voltage-gated channel subfamily A member 1	KCNA1	0.6844	n.a.
			Beta-2 adrenergic receptor	ADRB2	0.6746	n.a.
			5-hydroxytryptamine receptor 1E	HTR1E	0.6427	n.a.
			5-hydroxytryptamine receptor 1B	HTR1B	0.6394	n.a.
			5-hydroxytryptamine receptor 1A	HTR1A	0.6387	n.a.
			Translocator protein	TSPO	0.6287	n.a.
			5-hydroxytryptamine receptor 5A	HTR5A	0.6077	n.a.
23	**Maprotiline**	14	5-hydroxytryptamine receptor 1A	HTR1A	0.8676	n.a.
			D(1A) dopamine receptor	DRD1	0.8489	402
			5-hydroxytryptamine receptor 2B	HTR2B	0.8308	n.a.
			D(3) dopamine receptor	DRD3	0.8063	504
			Sodium-dependent serotonin transporter	SLC6A4	0.8046	n.a.
			5-hydroxytryptamine receptor 6	HTR6	0.8039	n.a.
			D(1B) dopamine receptor	DRD5	0.7922	429
			5-hydroxytryptamine receptor 1D	HTR1D	0.7913	n.a.
			D(4) dopamine receptor	DRD4	0.791	n.a.
			5-hydroxytryptamine receptor 3A	HTR3A	0.7621	n.a.
			5-hydroxytryptamine receptor 1B	HTR1B	0.7484	n.a.
			Sodium-dependent dopamine transporter	SLC6A3	0.7274	n.a.
			5-hydroxytryptamine receptor 1E	HTR1E	0.7229	n.a.
			Histamine H4 receptor	HRH4	0.6462	n.a.
24	**Memantine**	7	Glutamate receptor ionotropic, NMDA 2D	GRIN2D	0.7144	n.a.
			D(3) dopamine receptor	DRD3	0.6879	n.a.
			Glutamate receptor ionotropic, NMDA 3B	GRIN3B	0.6488	n.a.
			Glutamate receptor ionotropic, NMDA 2C	GRIN2C	0.64	n.a.
			Muscarinic acetylcholine receptor M1	CHRM1	0.619	n.a.
			5-hydroxytryptamine receptor 2A	HTR2A	0.6094	n.a.
			D(1A) dopamine receptor	DRD1	0.6082	n.a.
25	**Minoxidil**	1	Prostaglandin G/H synthase 2	PTGS2	0.7051	n.a.
26	**Nicardipine**	17	Voltage-dependent L-type calcium channel subunit alpha-1S	CACNA1S	0.7513	n.a.
			Voltage-dependent T-type calcium channel subunit alpha-1H	CACNA1H	0.7357	n.a.
			D(2) dopamine receptor	DRD2	0.7162	n.a.
			Alpha-2B adrenergic receptor	ADRA2B	0.6993	n.a.
			Alpha-2C adrenergic receptor	ADRA2C	0.6899	n.a.
			D(1A) dopamine receptor	DRD1	0.6834	n.a.
			Potassium voltage-gated channel subfamily H member 2	KCNH2	0.6751	n.a.
			Histamine H1 receptor	HRH1	0.6717	n.a.
			Alpha-2A adrenergic receptor	ADRA2A	0.658	n.a.
			Voltage-dependent L-type calcium channel subunit alpha-1F	CACNA1F	0.636	n.a.
			D(4) dopamine receptor	DRD4	0.6341	n.a.
			5-hydroxytryptamine receptor 2A	HTR2A	0.6286	n.a.
			5-hydroxytryptamine receptor 6	HTR6	0.6283	n.a.

			D(1B) dopamine receptor	DRD5	0.6242	n.a.
			5-hydroxytryptamine receptor 7	HTR7	0.6187	n.a.
			Beta-2 adrenergic receptor	ADRB2	0.6109	n.a.
			5-hydroxytryptamine receptor 2C	HTR2C	0.6104	n.a.
27	**Nifedipine**	6	Voltage-dependent L-type calcium channel subunit beta-1	CACNB1	0.6818	n.a.
			Voltage-dependent L-type calcium channel subunit alpha-1F	CACNA1F	0.6683	n.a.
			Voltage-dependent T-type calcium channel subunit alpha-1G	CACNA1G	0.6479	n.a.
			Voltage-dependent T-type calcium channel subunit alpha-1I	CACNA1I	0.617	n.a.
			Voltage-dependent L-type calcium channel subunit beta-3	CACNB3	0.6112	n.a.
			Voltage-dependent L-type calcium channel subunit beta-4	CACNB4	0.6051	n.a.
28	**Nilvadipine**	6	Voltage-dependent L-type calcium channel subunit beta-1	CACNB1	0.6781	n.a.
			Voltage-dependent L-type calcium channel subunit alpha-1F	CACNA1F	0.6658	n.a.
			Voltage-dependent L-type calcium channel subunit beta-3	CACNB3	0.6356	n.a.
			Voltage-dependent T-type calcium channel subunit alpha-1H	CACNA1H	0.6129	n.a.
			Voltage-dependent L-type calcium channel subunit beta-4	CACNB4	0.6108	n.a.
			Voltage-dependent N-type calcium channel subunit alpha-1B	CACNA1B	0.6094	n.a.
29	**Nitrendipine**	2	Voltage-dependent L-type calcium channel subunit alpha-1F	CACNA1F	0.6687	n.a.
			Voltage-dependent L-type calcium channel subunit beta-1	CACNB1	0.6672	n.a.
30	**Nortriptyline**	14	D(1A) dopamine receptor	DRD1	0.8884	n.a.
			Sodium-dependent dopamine transporter	SLC6A3	0.8835	n.a.
			5-hydroxytryptamine receptor 7	HTR7	0.8492	n.a.
			D(3) dopamine receptor	DRD3	0.8351	n.a.
			D(1B) dopamine receptor	DRD5	0.83	n.a.
			D(4) dopamine receptor	DRD4	0.7977	n.a.
			5-hydroxytryptamine receptor 1B	HTR1B	0.7894	n.a.
			5-hydroxytryptamine receptor 2B	HTR2B	0.7665	n.a.
			5-hydroxytryptamine receptor 3A	HTR3A	0.759	n.a.
			5-hydroxytryptamine receptor 1D	HTR1D	0.7504	n.a.
			Histamine H4 receptor	HRH4	0.7092	6918
			Histamine H2 receptor	HRH2	0.7008	645
			5-hydroxytryptamine receptor 1E	HTR1E	0.699	n.a.
			5-hydroxytryptamine receptor 1F	HTR1F	0.6695	n.a.
31	**Olanzapine**	12	Alpha-1D adrenergic receptor	ADRA1D	0.9374	n.a.
			Gamma-aminobutyric acid receptor subunit rho-2	GABRR2	0.7549	n.a.
			Gamma-aminobutyric acid receptor subunit rho-1	GABRR1	0.7432	n.a.
			Gamma-aminobutyric acid receptor subunit rho-3	GABRR3	0.7071	n.a.
			Calmodulin	CALM1	0.6882	n.a.
			Translocator protein	TSPO	0.6871	n.a.
			Potassium voltage-gated channel subfamily A member 1	KCNA1	0.6802	n.a.
			Sodium-dependent serotonin transporter	SLC6A4	0.6781	n.a.
			Sodium-dependent noradrenaline transporter	SLC6A2	0.6748	n.a.
			Sodium-dependent dopamine transporter	SLC6A3	0.6649	n.a.
			5-hydroxytryptamine receptor 3B	HTR3B	0.6325	n.a.
			5-hydroxytryptamine receptor 1F	HTR1F	0.6298	310
32	**Paroxetine**	9	5-hydroxytryptamine receptor 2C	HTR2C	0.7465	n.a.
			Histamine H1 receptor	HRH1	0.704	n.a.
			D(2) dopamine receptor	DRD2	0.7031	n.a.
			Sodium-dependent dopamine transporter	SLC6A3	0.6657	n.a.
			5-hydroxytryptamine receptor 7	HTR7	0.6652	n.a.
			5-hydroxytryptamine receptor 2B	HTR2B	0.6502	n.a.
			Alpha-1A adrenergic receptor	ADRA1A	0.6402	n.a.
			5-hydroxytryptamine receptor 1A	HTR1A	0.6191	n.a.
			Alpha-2A adrenergic receptor	ADRA2A	0.6092	n.a.
33	**Pimozide**	7	D(1A) dopamine receptor	DRD1	0.7343	4100
			D(1B) dopamine receptor	DRD5	0.6578	n.a.
			D(4) dopamine receptor	DRD4	0.6457	1.8
			Alpha-2C adrenergic receptor	ADRA2C	0.6434	376.5

			5-hydroxytryptamine receptor 2C	HTR2C	0.6197	874
			Alpha-2B adrenergic receptor	ADRA2B	0.6089	821
			5-hydroxytryptamine receptor 1A	HTR1A	0.6044	88
34	**Ponatinib**	1	Platelet-derived growth factor receptor beta	PDGFRB	0.7043	n.a.
35	**Prazosin**	4	Alpha-2C adrenergic receptor	ADRA2C	0.8713	10.7
			Beta-1 adrenergic receptor	ADRB1	0.7357	n.a.
			Beta-2 adrenergic receptor	ADRB2	0.6915	n.a.
			5-hydroxytryptamine receptor 2A	HTR2A	0.6402	400.76
36	**Regorafenib**	2	Receptor-type tyrosine-protein kinase FLT3	FLT3	0.6484	n.a.
			Fibroblast growth factor receptor 3	FGFR3	0.6372	n.a.
37	**Rilmenidipine**	3	Alpha-2B adrenergic receptor	ADRA2B	0.7527	n.a.
			Alpha-2C adrenergic receptor	ADRA2C	0.7383	n.a.
			Alpha-1A adrenergic receptor	ADRA1A	0.6467	n.a.
38	**Sertindole**	23	Alpha-2A adrenergic receptor	ADRA2A	0.8811	640
			Alpha-2C adrenergic receptor	ADRA2C	0.8499	450
			D(3) dopamine receptor	DRD3	0.8265	2.5
			D(1A) dopamine receptor	DRD1	0.8248	12
			Alpha-2B adrenergic receptor	ADRA2B	0.8143	450
			5-hydroxytryptamine receptor 2B	HTR2B	0.7972	n.a.
			D(1B) dopamine receptor	DRD5	0.7929	n.a.
			5-hydroxytryptamine receptor 7	HTR7	0.7782	28
			D(4) dopamine receptor	DRD4	0.7722	9
			5-hydroxytryptamine receptor 1A	HTR1A	0.7715	280
			Histamine H1 receptor	HRH1	0.7125	130
			5-hydroxytryptamine receptor 1B	HTR1B	0.7029	60
			5-hydroxytryptamine receptor 1D	HTR1D	0.6851	20
			Sodium-dependent serotonin transporter	SLC6A4	0.6791	n.a.
			5-hydroxytryptamine receptor 3A	HTR3A	0.6655	3180
			Muscarinic acetylcholine receptor M3	CHRM3	0.6543	2692
			Muscarinic acetylcholine receptor M1	CHRM1	0.6471	631
			Muscarinic acetylcholine receptor M5	CHRM5	0.6463	n.a.
			Sodium-dependent noradrenaline transporter	SLC6A2	0.6412	n.a.
			5-hydroxytryptamine receptor 1E	HTR1E	0.6407	430
			Muscarinic acetylcholine receptor M2	CHRM2	0.6353	n.a.
			Muscarinic acetylcholine receptor M4	CHRM4	0.6234	n.a.
			Beta-1 adrenergic receptor	ADRB1	0.6164	5000
39	**Sorafenib**	2	Platelet-derived growth factor receptor alpha	PDGFRA	0.6289	62
			Fibroblast growth factor receptor 3	FGFR3	0.6166	4200
40	**Spironolactone**	1	Estrogen receptor	ESR1	0.6151	n.a.
41	**Taurine**	14	Gamma-aminobutyric acid receptor subunit rho-1	GABRR1	0.7582	n.a.
			Gamma-aminobutyric acid receptor subunit rho-2	GABRR2	0.6823	n.a.
			Gamma-aminobutyric acid receptor subunit rho-3	GABRR3	0.6789	n.a.
			Neuronal acetylcholine receptor subunit alpha-7	CHRNA7	0.674	n.a.
			Glutamate receptor ionotropic, NMDA 3A	GRIN3A	0.6705	n.a.
			Glutamate receptor 2	GRIA2	0.6659	n.a.
			Translocator protein	TSPO	0.6574	n.a.
			Glutamate receptor ionotropic, NMDA 2A	GRIN2A	0.6562	n.a.
			Glutamate receptor ionotropic, kainate 2	GRIK2	0.655	n.a.
			Glutamate receptor ionotropic, NMDA 3B	GRIN3B	0.6546	n.a.
			Neuronal acetylcholine receptor subunit alpha-4	CHRNA4	0.6454	n.a.
			Glutamate receptor ionotropic, NMDA 2C	GRIN2C	0.6297	n.a.
			Glutamate receptor ionotropic, NMDA 2D	GRIN2D	0.6281	n.a.
			Glutamate receptor ionotropic, NMDA 1	GRIN1	0.6172	n.a.
42	**Thalidomide**	1	Prostaglandin G/H synthase 1	PTGS1	0.6197	n.a.
43	**Triflupromazine**	20	Muscarinic acetylcholine receptor M3	CHRM3	0.8613	n.a.
			Muscarinic acetylcholine receptor M4	CHRM4	0.8321	n.a.
			Muscarinic acetylcholine receptor M5	CHRM5	0.8211	n.a.
			D(1B) dopamine receptor	DRD5	0.7602	n.a.
			5-hydroxytryptamine receptor 2A	HTR2A	0.7556	n.a.
			D(4) dopamine receptor	DRD4	0.7379	n.a.
			5-hydroxytryptamine receptor 2C	HTR2C	0.736	n.a.
			D(3) dopamine receptor	DRD3	0.7345	n.a.
			Histamine H1 receptor	HRH1	0.7118	n.a.
			5-hydroxytryptamine receptor 1A	HTR1A	0.7051	n.a.
			Alpha-1A adrenergic receptor	ADRA1A	0.6867	n.a.
			Alpha-1D adrenergic receptor	ADRA1D	0.6791	n.a.
			Alpha-1B adrenergic receptor	ADRA1B	0.6768	n.a.
			5-hydroxytryptamine receptor 7	HTR7	0.6683	n.a.
			Alpha-2B adrenergic receptor	ADRA2B	0.6637	n.a.

			Alpha-2A adrenergic receptor	ADRA2A	0.6522	n.a.
			5-hydroxytryptamine receptor 1D	HTR1D	0.6486	n.a.
			5-hydroxytryptamine receptor 3A	HTR3A	0.6451	n.a.
			Alpha-2C adrenergic receptor	ADRA2C	0.6402	n.a.
			5-hydroxytryptamine receptor 1B	HTR1B	0.6057	n.a.
44	**Verapamil**	14	Voltage-dependent T-type calcium channel subunit alpha-1H	CACNA1H	0.825	n.a.
			Sodium-dependent dopamine transporter	SLC6A3	0.7956	n.a.
			Alpha-2A adrenergic receptor	ADRA2A	0.7544	n.a.
			Sodium-dependent noradrenaline transporter	SLC6A2	0.7425	n.a.
			Alpha-2C adrenergic receptor	ADRA2C	0.7335	n.a.
			Alpha-2B adrenergic receptor	ADRA2B	0.6913	n.a.
			Voltage-dependent calcium channel subunit alpha-2/delta-1	CACNA2D1	0.6581	n.a.
			5-hydroxytryptamine receptor 2C	HTR2C	0.6489	n.a.
			5-hydroxytryptamine receptor 2A	HTR2A	0.6419	140
			Histamine H1 receptor	HRH1	0.6348	n.a.
			Muscarinic acetylcholine receptor M2	CHRM2	0.6258	n.a.
			D(1B) dopamine receptor	DRD5	0.6246	n.a.
			D(2) dopamine receptor	DRD2	0.6136	n.a.
			Muscarinic acetylcholine receptor M3	CHRM3	0.6052	n.a.
			Plasminogen	PLG	0.7173	n.a.
45	**Zinc**	3	Progesterone receptor	PGR	0.6077	n.a.
			Apolipoprotein D	APOD	0.6007	n.a.

Predicted interactions between inhibitors and targets

No.	Drug Name	No. Predicted Targets	Target Name	Gene Name	Confidence Score	Ki (nM)
			5-hydroxytryptamine receptor 1D	HTR1D	0.7201	4,070
			5-hydroxytryptamine receptor 2C	HTR2C	0.6593	574
			Alpha-2B adrenergic receptor	ADRA2B	0.6491	n.a.
1	**Propranolol**	7	Alpha-2A adrenergic receptor	ADRA2A	0.6468	n.a.
			Alpha-2C adrenergic receptor	ADRA2C	0.6301	n.a.
			5-hydroxytryptamine receptor 2B	HTR2B	0.6262	n.a.
			Alpha-1B adrenergic receptor	ADRA1B	0.6034	n.a.
2	**Esmolol**	1	Beta-2 adrenergic receptor	ADRB2	0.7053	n.a.
			Breakpoint cluster region protein	BCR	0.6543	n.a.
3	**Fostamatinib**	4	Mitogen-activated protein kinase 11	MAPK11	0.6298	n.a.
			Fibroblast growth factor receptor 4	FGFR4	0.6267	350
			Histamine H1 receptor	HRH1	0.6243	n.a.
4	**Atropine**	1	Neuronal acetylcholine receptor subunit alpha-7	CHRNA7	0.6356	n.a.

Predicted interactions between dual-modulators and targets

No.	Drug Name	No. Predicted Targets	Target Name	Gene Name	Confidence Score	Ki (nM)
1	**Dexmedetomidine**	2	Alpha-2B adrenergic receptor	ADRA2B	0.7197	2.04
			Alpha-2C adrenergic receptor	ADRA2C	0.7018	2.51
2	**Nimodipine**	1	Voltage-dependent T-type calcium channel subunit alpha-1H	CACNA1H	0.6462	n.a.
			Alpha-1D adrenergic receptor	ADRA1D	0.9429	n.a.
			5-hydroxytryptamine receptor 2C	HTR2C	0.7665	46
			D(1B) dopamine receptor	DRD5	0.7547	216
			D(3) dopamine receptor	DRD3	0.7203	1.5
			5-hydroxytryptamine receptor 1A	HTR1A	0.7135	108
			Alpha-2C adrenergic receptor	ADRA2C	0.7115	52.48
3	**Thioridazine**	14	D(4) dopamine receptor	DRD4	0.7015	1.5
			Alpha-2B adrenergic receptor	ADRA2B	0.6908	341.3
			5-hydroxytryptamine receptor 7	HTR7	0.68	99
			Histamine H1 receptor	HRH1	0.6722	16
			Alpha-2A adrenergic receptor	ADRA2A	0.6601	134
			5-hydroxytryptamine receptor 2B	HTR2B	0.6421	n.a.
			Muscarinic acetylcholine receptor M1	CHRM1	0.6273	2.7
			5-hydroxytryptamine receptor 6	HTR6	0.6162	6.3
			Alpha-1B adrenergic receptor	ADRA1B	0.8257	n.a.
			Alpha-1D adrenergic receptor	ADRA1D	0.7834	n.a.
4	**Trifluoperazine**	10	5-hydroxytryptamine receptor 2A	HTR2A	0.7411	5.4
			D(1A) dopamine receptor	DRD1	0.7057	740
			Alpha-2C adrenergic receptor	ADRA2C	0.6919	n.a.

	Alpha-2A adrenergic receptor	ADRA2A	0.6858	n.a.
	Alpha-2B adrenergic receptor	ADRA2B	0.6696	n.a.
	D(1B) dopamine receptor	DRD5	0.6469	n.a.
	D(4) dopamine receptor	DRD4	0.6094	326
	D(3) dopamine receptor	DRD3	0.6003	4.2