

Supporting Information

Bio Spectra Analysis: Model Proteome Characterizations For Linking Molecular Structure and Biological Response

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S1 Title Page

S2 IC₅₀'s of Compounds **1-24** Residing in the Dopamine Cluster

S3 IC₅₀'s of Dopamine Agonists and Antagonists

S4 Table of 92 Bioassays

S5 Table of 92 Bioassays

IC₅₀'s of Compounds **1-24** Residing in the Dopamine Cluster

	5HT1A	5HT7	alpha-1	alpha-2	alpha-2A	D1	D2	D3	D4
Metoclopramide (1)	9130	34400	>10000	1520	5430	18800	260	141	1600
Molindone (2)	6540	1210	7340	5410	2950	5350	179	231	15300
Amisulpiride (3)	>10000	301	55700	429	1100	14000	32	19	3280
Bromocriptine (4)	142	552	100	272	250	3340	215	119	546
Co-dergocrine (5)	2.7	139	14	6.8	36	1290	26	108	330
Dihydroergocristine (6)	23	134	47	45	51	1230	86	45	257
Allyl norapomorphine (7)	267	599	9580	4040	2400	1050	131	11	3.9
Norapomorphine (8)	374	809	13300	1080	>10000	2300	10500	1600	63
Spiroxatrine (9)	4.8	105	153	550	>10000	>10000	28	14	30
WAY 100635 (10)	8.3	827	394	20200	>10000	>10000	2950	547	101
Yohimbine (11)	53	1830	1250	95	6600	7520	4430	10500	16200
Rauwolscine (12)	14	7960	3070	73	12	>10000	62	2340	11400
Urapidil (13)	56	255	600	4010	8080	>10000	5280	2000	176
5-Methyl Urapidil (14)	0.51	875	22	5830	5410	>10000	3530	848	96
CP-93,393 (15)	8.9	1510	6530	65	4	>10000	56	166	1750
RS-79,948 (16)	972	2470	3530	0.76	1.6	16700	1080	244	5610
Raclopride (17)	12300	>10000	61000	>10000	>10000	>10000	49	14	9330
Sulpiride (18)	>10000	7930	>10000	5167	6310	20700	133	270	639
Tiapride (19)	>10000	>10000	>10000	6190	11300	>10000	2470	989	7890
Levosulpiride (20)	>10000	>10000	>10000	14600	20300	40500	32	1230	1020
Dopamine (21)	3920	27100	>10000	917	5680	1660	5210	64	24
N-methyl Dopamine (22)	6710	>10000	>10000	125	3370	1810	35200	135	73
6,7-ADTN (23)	>10000	>10000	>10000	465	2000	1660	2440	21	353
Pramipexole (24)	3820	3180	>10000	>10000	17900	>10000	28300	54	111

IC50's of Dopamine Agonists and Antagonists

	AGONIST	D1	D2	D3	D4		Antagonist	D1	D2	D3	D4
4	Bromocriptine	3340	215	119	546	1	Metoclopramide	18800	260	141	1600
5	Co-dergocrine	1290	26	108	330	2	Molindone	5350	179	231	15300
6	Dihydroergocristine	1230	86	45	257	3	Amisulpride	14000	32	19	3280
7	N-allylnorapomorphine	1050	131	11	3.9	18	Sulpiride	20700	133	270	639
8	Norapomorphine	2300	10500	1600	63	19	Tiapride	> 10000	2470	989	7890
21	Dopamine	1660	5210	64	24	20	Levosulpiride	40500	32	1230	1020
22	N-methyldopamine	1810	35200	135	73	36	Thiothixene	89	1.3	12	499
23	6,7-ADTN	1660	2440	21	353	37	Fluphenazine	26	35	21	272
24	Pramipexole	> 10000	28300	54	111	38	Trifluoperazine	22	33	7	118
25	(+) 3-PPP	> 10000	> 10000	4030	1080	39	Thiethylperazine	58	15	11	583
26	(-) 3-PPP	12100	7240	679	959	40	Perphenazine	16	36	10	235
27	Dipropyldopamine	13700	6870	49	7.1	41	Acetophenazine	47	7.3	11	152
28	(+) 8-hydroxy-DPAT	> 10000	7760	883	8960	42	Eticlopride	> 10000	1.6	2.7	220
29	(+/-) 7-hydroxy-DPAT	5980	1130	8.4	267	43	Haloperidol	29	46	16	8.1
30	(+/-) 6,7-dihydroxy-DPAT	5850	2130	3.4	56	44	Bromperidol	24	9.1	24	6.7
31	Piribedil	> 10000	5510	767	400	45	Domperidone	1330	12	71	86
32	Ropinirole	> 10000	10200	754	1490	46	Droperidol	334	16	6.4	6.9
33	SKF 38,393	139	> 10000	20600	9330	47	Benperidol	548	1.8	5.3	7.7
34	SKF 77,434	26	5860	1180	449	48	Spiperone	884	2.6	3	3.8
35	SKF 82,958	19	7080	362	149	49	AMI-193	2000	21	22	5.6

Table of 92 Bioassays

Screen ID	Screen Desc
5ht1a	5-HT1A HUMAN
5ht1b	5-HT1B
5ht2a	5-HT2A HUMAN
5HT2C	5-HT2C HUMAN
5ht3	5-HT3 HUMAN
5ht4e	5-HT4e HUMAN
5ht6	5-HT6 HUMAN
5ht7	5-HT7 HUMAN
5HTtrans	5-HT TRANSPORTER HUMAN
A 1	ADENOSINE 1 HUMAN
A 2A	ADENOSINE 2A HUMAN
A CE	ANGIOTENSIN CONVERTING ENZYME HUMAN
A CHase	ACETYLCHOLINESTERASE HUMAN
alpha1	ADRENERGIC ALPHA 1 NON-SEL
alpha2	ADRENERGIC ALPHA 2 NON-SEL
A T1	ANGIOTENSIN 1 HUMAN
A T2	ANGIOTENSIN 2 HUMAN
A TPase	NA/K ATPASE ACTIVITY
B2	BRADYKININ2 HUMAN
beta1	ADRENERGIC BETA 1 HUMAN
beta2	ADRENERGIC BETA-2 HUMAN
Ca_channel_DHP	L-TYPE CALCIUM CHANNEL, DHP SITE
Ca_channel_VERA	CA CHANNEL L-SITE VERAPAMIL
CB1	CANNABINOID 1 HUMAN
CCKA	CHOLECYSTOKININ 1 HUMAN
CCR1	CCR1 HUMAN
Chol_trans	CHOLINE TRANSPORTER
Cl_channel	CL CHANNEL
COMT	CATECHOL-O-METHYL TRANSFERASE
not found	[avg(Primary_Value)', 'COX2']
cyp1a2	CYP1A2 HUMAN
cyp2b6	CYP2B6 HUMAN
cyp2c19	CYP2C19 HUMAN
cyp2c9	CYP2C9 HUMAN
cyp2d6	CYP2D6 HUMAN
cyp3a4	CYP3A4 HUMAN
D1	DOPAMINE D1 HUMAN
D2	DOPAMINE D2 HUMAN
D3	DOPAMINE D3 HUMAN
D4_4	DOPAMINE D4.4 HUMAN
delta	DELTA HUMAN
elastase	ELASTASE
ETB	ENDOTHELIN B HUMAN
GABA_A	GABA-A
GABA_A_BZD	GABA-A RECEPTOR BENZODIAZEPINE SITE CENTRAL
GABA_B	GABA-B
GABA_trans	GABA TRANSPORTER
GABA_transam	GABA TRANSAMINASE
Ghrelin	GHRELIN RECEPTOR HUMAN
glucocorticoid	GLUCOCORTICOID HUMAN
Glycine	GLYCINE STRYCHNINE-INSENSITIVE
H1	HISTAMINE 1 CENTRAL

Table of 92 Bioassays

Screen ID	Screen Desc
H1	HISTAMINE 1 CENTRAL
H2	HISTAMINE 2
HIV	HIV-1 PROTEASE
IR_1	IMIDAZOLINE 1
K_channel_ATP	K Channel (A TP)
K_channel_Ca	K CHANNEL CALCIUM DEPENDENT
K_channel_volt	K CHANNEL KV VOLTAGE GATED
Kainite	GLUTAMATE RECEPTOR KAINATE SITE
Kappa	KAPPA
M1	M1 HUMAN
M2	M2 HUMAN
M3	M3 HUMAN
MAO_a	MAO-A
MAO_b	MAO-B
MC1	MELANOCORTIN 1
MC4	MC4 HUMAN
ML1	MELANOTONIN 1
not found	[avg(Primary_Value) - 'ML2']
MMP_3	METALLOPROTEINASE 3 HUMAN
MMP_7	METALLOPROTEINASE 7 HUMAN
mu	MU HUMAN
Na_channel	NA CHANNEL SITE 2
nACHR_N	NICOTINIC ACHR NEURONAL ALPHA-BGT X-INSENSITIVE
NE_trans	NE TRANSPORTER BINDING
NK1	NEUROKININ 1 HUMAN
NMDA	GLUTAMATE RECEPTOR NMDA SITE
oxytocin	OXYTOCIN
p55fyn	P55FYN
PCP	PHENCYCLIDINE
PDE2	PHOSPHODIESTERASE II HUMAN
PDE3	PHOSPHODIESTERASE III HUMAN
PDE5	PHOSPHODIESTERASE V HUMAN
PDE6	PHOSPHODIESTERASE VI
phosphatase_1B	PHOSPHATASE 1B HUMAN
Ryanodine	RYANODINE RY3
sigma	SIGMA NON-SEL
Thy_R	THYROID HORMONE RECEPTOR
tryptase	TRYPTASE HUMAN
V1a	VASOPRESSIN 1A HUMAN
VIP1	VIP1 HUMAN
Y1	NEUROPEPTIDE Y1 HUMAN