

Table SI02. Expected values <math>\langle D_k \rangle</math> of molecular descriptors for assay conditions

TARGET_CHEMBLID	$\langle \text{LOGP} \rangle$	$\langle \text{PSA} \rangle$	nj	NAME
CHEMBL217	4.16	54.74	11887	Dopamine D2 receptor
CHEMBL339	3.78	48.43	7186	Dopamine D2 receptor
CHEMBL234	4.14	54.48	6844	Dopamine D3 receptor
CHEMBL338	3.95	35.64	5753	Dopamine transporter
CHEMBL238	3.81	36.99	5153	Dopamine transporter
CHEMBL219	3.83	43.39	3487	Dopamine D4 receptor
CHEMBL2056	3.68	57.18	2995	Dopamine D1 receptor
CHEMBL265	3.72	42.60	1705	Dopamine D1 receptor
CHEMBL2094252	4.55	32.09	1141	Monoamine transporters; serotonin & dopamine
CHEMBL2093868	3.65	41.60	1112	Dopamine receptor
CHEMBL3138	4.36	51.63	917	Dopamine D3 receptor
CHEMBL3998	2.52	56.11	681	Dopamine D2 receptor
CHEMBL2095169	4.74	57.80	630	Dopamine receptors; D2 & D3
CHEMBL1850	3.93	37.96	568	Dopamine D5 receptor
CHEMBL2095175	3.99	36.17	551	Monoamine transporters ; Norepinephrine & dopamine
CHEMBL2095201	4.11	31.75	408	Monoamine transporters ; serotonin & dopamine
CHEMBL2967	3.67	41.53	368	Dopamine D1 receptor
CHEMBL5067	4.58	51.66	352	Dopamine D1 receptor
CHEMBL2095396	3.81	36.64	340	Dopamine receptors; D2 & D4
CHEMBL4702	2.12	54.21	280	Dopamine beta-hydroxylase
CHEMBL2096910	4.00	36.74	258	Dopamine receptors; D1 & D2
CHEMBL2096970	1.53	61.70	254	Dopamine receptor
CHEMBL3427	4.06	41.39	241	Dopamine D2 receptor
CHEMBL2097165	4.56	51.03	205	Dopamine receptors; D3 & D4 Monoamine transporters;
CHEMBL2096990	4.53	23.67	205	Norepinephrine & dopamine
CHEMBL3361	3.93	43.25	202	Dopamine D4 receptor
CHEMBL2111341	4.54	56.44	191	Dopamine D1 and D2 receptor
CHEMBL2799	3.69	37.77	171	Dopamine transporter
CHEMBL2111342	4.41	40.74	162	Dopamine receptor D2 and D3 Dopamine D2 receptor/
CHEMBL2097175	4.02	54.86	132	Serotonin 2 (5-HT2) receptor
CHEMBL3102	2.46	69.28	130	Dopamine beta-hydroxylase Dopamine D2 receptor and serotonin 2a
CHEMBL2111468	3.95	50.69	107	receptor
CHEMBL2109245	3.96	77.09	105	Dopamine D2 receptor/Serotonin 2 (5-HT2)
CHEMBL2368	3.71	75.86	87	receptor
CHEMBL2096905	3.59	42.09	80	Dopamine D1 receptor
				Dopamine receptor

CHEMBL2703	2.03	81.58	75	Dopamine D2 receptor
CHEMBL2111406	3.64	46.49	59	Dopamine D2 receptor and Serotonin 2a receptor
CHEMBL2111359	4.33	45.34	59	Dopamine receptor
CHEMBL2992	2.38	61.13	57	Dopamine beta-hydroxylase
CHEMBL3071	3.62	47.25	37	Dopamine D1 receptor
CHEMBL2281	4.33	41.28	30	Dopamine D5 receptor
CHEMBL5032	4.47	33.99	28	Dopamine transporter
CHEMBL5456	3.90	34.40	26	Dopamine D2 receptor
CHEMBL2986	2.13	65.98	17	Dopamine transporter
CHEMBL2304406	4.13	32.35	16	Dopamine D3 receptor
CHEMBL2111460	3.39	65.11	9	Dopamine D2 receptor and serotonin 1a receptor
CHEMBL3038478	3.93	49.64	1	Dopamine receptor D2L /neurotensin receptor NTS1
c2 = ORGANISM	<LOGP>	<PSA>	nj	
Homo sapiens	4.02	50.08	33240	
Rattus norvegicus	3.91	42.33	19265	
Bos taurus	2.55	53.42	1600	
Mus musculus	3.94	47.27	613	
Sus scrofa	4.58	51.66	352	
Carassius auratus	3.71	75.86	87	
Canis lupus familiaris	2.03	81.58	75	
Chlorocebus aethiops	3.99	33.62	42	
Macaca fascicularis	4.47	33.99	28	
c3 = ASSAY				
ORGANISM	<LOGP>	<PSA>	nj	
Mus musculus	3.63	61.58	232	
Homo sapiens	4.03	51.11	21699	
Rattus norvegicus	3.94	43.62	7342	
MD	3.87	45.21	24204	
Cricetulus griseus	3.40	25.89	82	
Carassius auratus	3.71	75.86	87	
Canis lupus familiaris	3.38	46.67	50	
Bos taurus	3.26	41.80	429	
Sus scrofa	4.39	48.18	443	
Felis catus	3.59	30.21	3	
Cavia porcellus	3.64	37.65	136	
Cercopithecidae	3.97	46.92	322	
Spodoptera frugiperda	3.09	43.58	14	
Macaca fascicularis	4.47	33.99	28	
monkey	3.75	30.13	36	
Chlorocebus aethiops	3.72	39.71	14	

Cyprinus carpio	2.35	72.59	54
Oryctolagus cuniculus	4.01	54.76	53
Mustela putorius furo	2.29	55.99	10
Papio hamadryas	2.88	34.80	5
Macaca nemestrina	3.46	61.80	9
Ovis aries	2.94	152.87	49
Rattus rattus	4.24	23.47	1

c4 = CELL_CHEMBL_ID	<LOGP>	<PSA>	nj	CELL_NAME
CHEMBL3307715	3.96	43.95	4835	HEK293
CHEMBL3308072	4.17	50.68	6846	CHO
CHEMBL3307512	4.05	41.52	1079	CHO-K1
CHEMBL3307551	4.33	26.90	4	SK-N-MC
CHEMBL3308860	4.81	46.21	227	Sf9
CHEMBL3308345	4.70	49.92	122	C6
CHEMBL3307648	4.78	18.38	29	COS-7
CHEMBL3307655	4.08	45.54	15	LLC-PK1
CHEMBL3307716	3.83	11.91	3	NIH3T3
CHEMBL3308370	3.06	74.79	4	MDCK
CHEMBL3308376	4.25	77.75	7	HeLa
CHEMBL3308783	4.01	34.60	11	SCH

c5 = ASSAY_TYPE	<LOGP>	<PSA>	nj	DETAILS
B	3.99	46.41	46964	Binding (B)
F	3.62	53.60	8336	Functional (F)
U	3.27	54.48	2	Other

c6 = CONFIDENCE SCORE	<LOGP>	<PSA>	nj	DESCRIPTION
9	3.98	50.34	28648	Direct single protein target assigned Multiple direct protein targets may be assigned
5	4.14	42.14	2539	assigned
8	3.84	45.17	20645	Homologous single protein target assigned Multiple homologous protein targets may be assigned
4	4.01	42.00	3469	assigned
7	3.93	49.64	1	Direct protein complex subunits assigned

c7 = CURATED_BY	<LOGP>	<PSA>	nj
Expert	3.97	43.75	24129
Autocuration	3.90	50.97	28000
Intermediate	4.01	45.59	3173

c0 = ACTIVITY(UNITS)	<LOGP>	<PSA>	nj
Ki(nM)	4.12	47.07	28030
IC50(nM)	3.79	44.31	10740
Ratio	4.27	40.10	3034
Inhibition(%)	3.67	46.45	2877

EC50(nM)	3.44	57.44	1595
Potency(nM)	2.97	67.04	1267
Activity(%)	3.84	55.83	1127
Selectivity ratio	4.01	42.21	577
Selectivity	4.59	42.40	569
ED50(mg.kg-1)	3.10	64.01	561
Ratio Ki	4.59	47.62	540
Emax(%)	4.69	61.92	440
Efficacy(%)	3.25	51.47	362
Intrinsic activity(%)	3.53	49.87	325
ED50(umol.kg-1)	4.29	28.41	285
Kd(nM)	3.45	75.92	242
Kb(nM)	4.34	66.16	108
DA release(%)	2.50	15.21	95
K0.5(nM)	3.25	51.37	92
Control(%)	3.73	54.01	91
AC50(nM)	3.12	94.24	82
Log potency ratio	3.07	39.59	75
pKD	5.20	26.95	68
Potency ratio	4.06	33.39	68
IA(%)	3.10	76.01	66
pKb	4.80	66.93	65
Hill coefficient	2.65	36.67	59
Change(%)	3.13	30.80	55
K bind(uM)	3.11	44.64	54
pKa	4.54	50.64	53
Increase(%)	-2.22	109.24	52
Log 1/C	5.88	19.79	50
Binding(%)	2.99	39.40	48
Ki 0.5(nM)	4.58	5.82	47
Log Ki(nM)	4.43	37.95	46
Activity	3.49	40.32	45
nH	3.88	26.01	44
Discrimination ratio	3.36	23.79	43
logKi	4.03	60.83	40
Selectivity Index	4.77	44.88	39
RH(%)	-1.35	110.94	38
RL(%)	-1.35	111.35	37
K 0.5(nM)	2.59	44.89	34
EDmin(mg kg-1)	3.38	38.10	33
ID50(mg.kg-1)	4.21	31.28	33
KL(nM)	1.03	69.62	33
Displacement(%)	3.55	45.81	32

Enhancement(%)	-0.97	120.61	31
Intrinsic activity	3.54	40.77	31
Log Ki(D4)	3.59	27.54	29
Max effect(%)	3.93	42.46	27
Kis(uM)	2.17	51.42	25
Uptake/Binding ratio	2.98	36.63	25
pKi ratio	3.78	39.32	24
INH(uM)	4.64	22.48	23
K inact(min-1)	1.96	31.17	23
Stimulation(%)	3.66	56.78	23
FC	4.27	55.04	22
Binding affinity(nM)	3.81	37.31	21
IC50(ug.mL-1)	2.26	73.14	21
Ki ratio	3.95	41.06	21
Ratio IC50	3.92	14.84	21
Agonist(%)	3.22	37.08	20
EC50	4.91	51.55	20
Turnover	5.00	19.98	20
Affinity(%)	2.94	58.46	18
Total turnings	3.94	40.85	18
Intrinsic activity(nM)	2.31	55.87	17
DOPA accumulation	3.55	28.19	16
Uptake ratio	4.27	9.82	16
%max(%)	5.72	86.81	15
Accumulation	4.99	13.80	15
Duration(hr)	4.10	39.56	15
Km(nM)	0.88	80.60	15
Max intensity(turns min-1)	4.10	39.56	15
Imax(%)	4.33	56.66	14
Log IC50(uM)	3.11	24.73	14
log(activity)	4.75	81.25	14
pD2	4.90	60.78	14
ED20(nM kg-1)	5.15	70.15	12
K 0.5(uM)	2.38	45.68	12
RH/RL	-0.80	118.46	12
Activity(nM)	3.66	56.65	11
K bind(nM)	2.44	78.57	11
k cat(s-1)	1.55	47.18	11
Log 1/Kd	2.28	60.06	11
Low(%)	3.48	52.59	11
Specific binding(%)	3.74	30.90	11
ED50(nM)	1.90	83.43	10

KH(nM)	-1.46	95.64	10
Ratio EC50	6.47	69.59	10
Effect(%)	3.58	47.19	9
PRL(ng ml-1)	3.93	32.08	9
Ratio(nM)	4.65	65.04	9
Activity(pmol)	3.47	195.74	8
D-2(%)	3.17	50.21	8
EI	3.02	24.57	8
Potency(%)	2.12	55.84	8
Bmax(fmol/mg)	3.83	58.79	7
D2 duration(min)	3.77	128.44	7
Bmax(fM (mg of protein)-1)	5.58	51.84	6
Concentration(ng g-1)	4.29	23.47	6
Delta pKi	6.93	68.36	6
High(%)	3.25	53.75	6
ED50(uM)	1.44	66.48	5
Ki(/nM)	4.08	56.23	5
Log 1/KL	2.67	46.48	5
Log Ki(uM)	2.67	65.49	5
pKH	4.70	108.31	5
pKL	4.70	108.31	5
Total binding inhibited(%)	2.64	56.86	5
Activity(nmol)	1.28	51.85	4
Activity(uM)	3.27	44.37	4
Agonist effect(%)	2.93	31.13	4
Dopamine level(ng mg-1)	2.41	3.24	4
IC5(nM)	3.16	38.50	4
Bmax(pM (mg of protein)-1)	2.90	55.82	3
E(%)	3.24	54.52	3
ID50(uM)	3.59	30.21	3
Max stimulation(%)	5.73	39.88	3
Binding affinity	4.91	20.31	2
Intinsic activity(%)	3.39	17.97	2
k cat(min-1)	1.81	47.26	2
Ki	4.93	58.59	2
p[A]50	3.69	115.10	2
p[A50]	2.46	57.36	2
pK1	3.02	46.06	2
pKa(nM)	1.74	38.75	2
T1/2(hr)	7.86	97.32	2
IC50	2.82	52.49	1

INH(10^{-5} M)	3.61	26.02	1
Ka(nM)	6.36	111.95	1
KH(%)	-0.72	95.74	1
KiH(nM)	0.77	66.48	1
KiL(nM)	0.77	66.48	1
Log Ki	3.49	157.54	1
Partition ratio	2.54	20.23	1
pRatio	3.91	20.20	1
Ratio pKi	3.83	94.51	1
Response(%)	4.09	3.24	1
Vmax(pM min ⁻¹ mg ⁻¹)	-0.45	60.69	1
Vmax(pmol/min)	3.40	3.24	1
