

Supporting information

Article: Principal component analysis differentiates the receptor binding profiles of the antipsychotic drug candidates SLV310, SLV313, and SLV314 from current antipsychotic drugs.

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APPENDIX: Conditions of receptor binding assays (table 1). Contributions from the sixteen pharmacological assays to the three factors from the stepwise principal component analysis (table 2).

Table 1. Conditions of receptor binding assays.

Assay	Radioligand	Non Specific Binding	Incubation Conditions	Ref
D _{2s} ^a	[³ H] spiperone (0.3 nM)	(+)-butaclamol (10 µM)	60 min. / 22 °C	18
D ₃ ^a	[³ H] spiperone (0.3 nM)	(+)-butaclamol (10 µM)	60 min. / 22 °C	19
D _{4,4} ^a	[³ H] spiperone (0.3 nM)	(+)-butaclamol (10 µM)	60 min. / 22 °C	20
5-HT _{1A} ^a	[³ H] 8-OH-DPAT (0.3 nM)	8-OH-DPAT (10 µM)	60 min. / 22 °C	21
5-HT _{2A} ^a	[³ H] ketanserin (0.5 nM)	ketanserin (1 µM)	15 min. / 37 °C	22
5-HT _{2B} ^a	[³ H] LSD (1.2 nM) [¹²⁵ I] DOI (0.2 nM)	serotonin (1 µM) DOI (1 µM)	30 min. / 37 °C 15 min/37 °C	22, 23
5-HT _{2C} ^a	[³ H] mesulergine (0.7 nM)	mesulergine (1 µM)	30 min. / 37 °C	22
5-HT ₆ ^b	[³ H] LSD (2 nM)	serotonin (100 µM)	60 min. / 37 °C	24
5-HT ₇ ^a	[³ H] LSD (4 nM)	serotonin (10 µM)	120 min. / 22 °C	25
5-HT ₃ ^b	[³ H] BRL43694	MDL72222 (10 µM)	60 min. /22 °C	26
5-HT _{up} ^b	[³ H] paroxetine (0.1 nM)	imipramine (10 µM)	30 min/22 °C	27
M ₁ ^a	[³ H] pirenzepine (2 nM)	atropine (1 µM)	60 min. / 22 °C	28
M ₄ ^a	[³ H] 4-DAMP (0.2 nM)	atropine (1 µM)	60 min. / 22 °C	28
α ₁ (non-selective) ^c	[³ H] prazosin (0.25 nM)	prazosin (0.5 µM)	60 min. / 22 °C	29
α ₂ (non-selective) ^c	[³ H] RX 821002 (0.5 nM)	(-)-epinephrine (100 µM)	30 min. / 22 °C	30
H ₁ (central) ^d	[³ H] pyrilamine (0.5 nM)	triprolidine (100 µM)	10 min. / 22 °C	31

^a Receptor bindings assay in CHO cells, stably transfected with the appropriate human receptor. ^b Receptor bindings assay in HEK 293 cells, stably transfected with the appropriate human receptor. ^c Rat, cerebral cortex. ^d Guinea pig, cerebellum.

Table 2. Contributions from the sixteen pharmacological assays to the three factors from the stepwise principal component analysis.

Receptor Assay		Contribution factor 1	Contribution factor 2	Contribution factor 3
dopamine	D2s	1.90	-0.39	-0.53
	D3	1.95	-0.31	-1.01
	D4	1.03	-0.58	-0.94
serotonin	5-HT_{1A}	0.67	1.48	1.50
	5-HT_{2A}	-0.68	-0.55	0.33
	5-HT_{2B}	0.19	1.42	1.17
	5-HT_{2C}	-0.54	0.08	0.43
	5-HT₆	-1.00	1.01	-0.71
	5-HT₇	0.19	-1.68	1.83
	5-HT₃	-0.78	1.12	-0.10
muscarine	M1	-1.17	0.29	-0.98
	M4	-1.21	0.32	-0.93
adrenergic	α_1	-0.30	-1.01	-0.50
	α_2	-0.28	-1.71	0.39
histamine	H1	-0.96	-0.24	0.07
main contributions highlighted		positive	negative	