

S7 Table. Ligand enrichment (aLogAUC) by D₂R and 5-HT_{2A}R homology models without ECL2. Statistics are based on 50 homology models per template.

Template	aLogAUC					
	D ₂ R			5-HT _{2A} R		
	Median	Max	Ensemble ^a	Median	Max	Ensemble ^a
β₁AR	23.4	27.8	25.7	23.8	29.5	20.1
β₂AR	21.3	27.6	25.7	25.7	30.0	23.1
D₃R	24.9	30.7	27.0	21.9	29.4	22.2
D₄R	18.2	26.3	22.8	18.5	28.2	17.9
H₁R	19.2	23.7	21.6	21.3	29.7	24.2
M₁R	13.1	18.4	15.1	10.8	17.8	11.7
M₂R	14.0	19.3	16.2	10.1	16.8	8.9
M₃R	13.6	23.0	14.6	11.1	15.1	8.8
M₄R	14.2	19.8	17.8	11.3	16.3	12.6
5-HT_{1B}R	20.2	24.3	21.9	22.2	29.7	21.0
5-HT_{2B}R	20.0	26.0	24.1	25.6	32.7	26.1
5-HT_{2C}R	23.6	27.9	25.4	25.8	31.1	29.4
all aminergic	-	-	23.1	-	-	18.2
Rho	7.3	16.8	14.2	12.6	21.9	18.5
CXCR4	19.6	26.6	18.4	15.0	20.3	12.7
A_{2A}AR	11.0	17.9	11.2	15.8	24.4	18.3
CB1R	15.3	21.6	17.2	15.7	22.3	16.1

^aThe ensemble enrichment was calculated by identifying the best docking score of each docked compound among multiple homology models, leading to a single aLogAUC value for the set. The ensemble enrichment was calculated for each template (50 models) and all aminergic templates (600 models).