

Correction: Homology Modeling of Dopamine D₂ and D₃ Receptors: Molecular Dynamics Refinement and Docking Evaluation

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There were errors in Tables 3 and 4. The correct tables can be found here:

Table 3. Ligand protein-interaction of D₂-preferring receptor agonists docked with AD4.2.

Ligands	hD ₂ Hydrogen bonds-polar contacts	hD ₂ Hydrophobic contacts	hD ₃ Hydrogen_bonds polar contacts	hD ₃ Hydrophobic contacts
Dopamine	Asp_110, Thr 115, Ser 192, Ser 196.	Ile 183, Phe 345, His 349.	Asp_114, Ser 194	Val 111, His 393, Phe 389, Phe 390.
α-7-OH-DPAT	Asp_110, Ser 192, Ser 196, Thr 115.	Ile 183, Phe 345, His 349.	Asp_114, Ser 194, Ser 193.	Val 111, Phe 110, Ile 184, Phe 390.
α-7-OH-PDAT	Asp_110, Val 111 (C=O of peptide bond), Thr 115, Ser 192.	Val 111, Val 107, Ile 183, Trp 342, Phe 345, His 349.	Asp_114, Val 190 (C=O of peptide bond), Ser 193.	Val 111, Phe 110, Ile 184, Phe 390.
Pranipexole	Asp_110, Thr 115, Ser 192, Ser 196.	Val 111, Trp 342, Phe 345, Thr 369.	Asp_114, Val 190 (C=O of peptide bond), Ser 194.	Phe 110, Val 111, Phe 390, His 393.
Ropipexole	Asp_110, Ser 192.	Val 189, Trp 342, Phe 345, His 349, Tyr 373.	Asp_114, Ser 193.	Val 111, Phe 110, Val 115, Phe 390, His 393.
Rotigotine	Asp_110, Ser 192.	Val 107, Phe 108, Phe 345, Phe 346, His 349.	Asp_114	Phe 110, Val 111, Val 115, Ile 184, Phe 390, His 393.
Quinpirole	Asp_110, Ser 192.	Val 111, Ile 183, Trp 342, Phe 345, Thr 369, Tyr 373.	Asp_114	Val 115, Trp 386, Phe 389, Gly 415, Tyr 416.
PD128907	Asp_110, Ser 192.	Val 111, Ile 183, Phe 188, Trp 342, Phe 345, Phe 346, Thr 369, Tyr 373.	Asp_114	Val 111, Phe 389, His 393.
cis-8-OH-PBR1	Asp_110, Ser 192, Ser 196, Thr 115.	Val 111, Ile 183, Trp 342, Phe 346, Tyr 373, Thr 369.	*ND	*ND

*ND = Not Determined

Residues involved in H-Bonds are underlined.

Table 4. Virtual Screening. Top scored compound ZINC4525456.

	hD ₂	hD ₃
Vina (Kcal/mol)	-8.7	-8.1
AD4.2 (Kcal/mol)	-8.8	-7.98
Exp. Ki (nM)	4.78	270
H-bonds and Polar contacts	Asp_110, Thr 115, Ser 196, Ser 182,	Ser 197, Ser 193, Thr 119
Hydrophobic interactions	Val 111, Ile 183, Phe 345, Phe 346, His 349, Tyr 365, Pro 362, Thr 369.	Leu 94, Val 91, Val 111, Ile 184, Val 115, Phe 198, Phe 389, Phe 390, His 393, Thr 412, Tyr 416.

Residues involved in H-bonds are underlined.

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