Supporting Information

New Insights into the Binding Mode of Melanin Concentrating Hormone receptor-1 Antagonists: Homology Modeling and Explicit Membrane Molecular Dynamics Simulation Study

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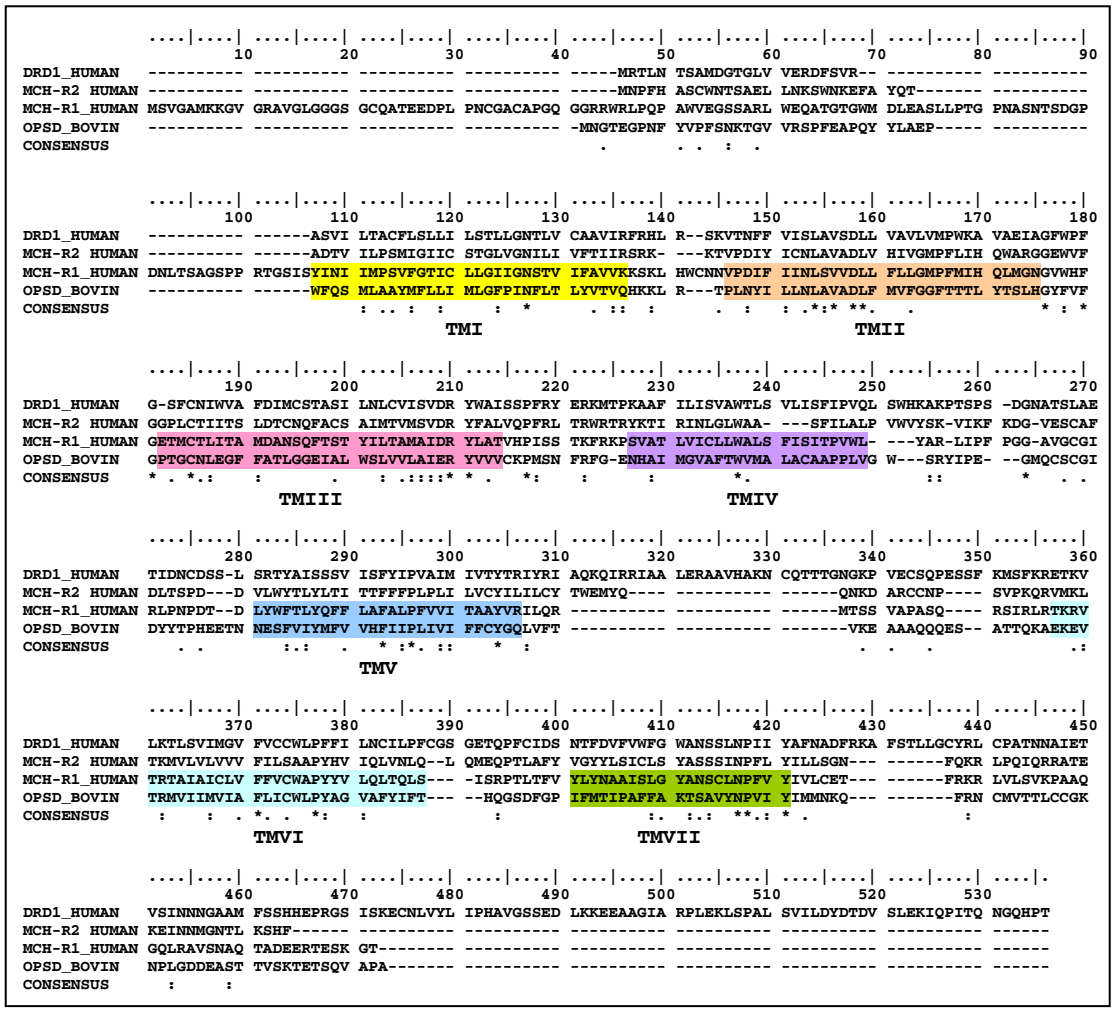
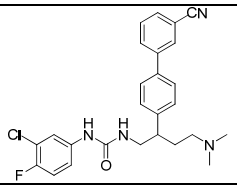
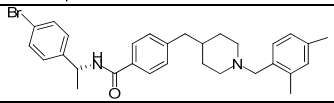
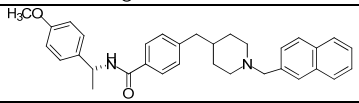
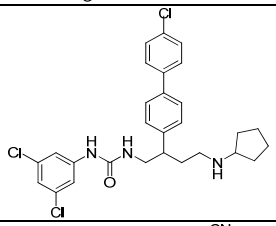
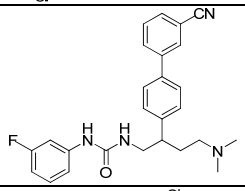
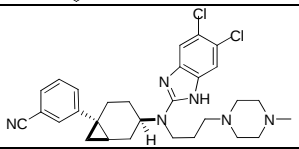
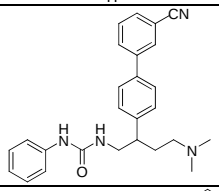
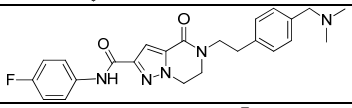
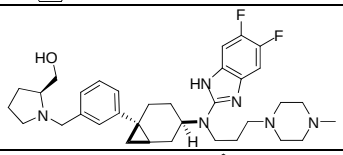
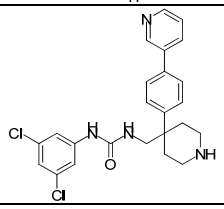
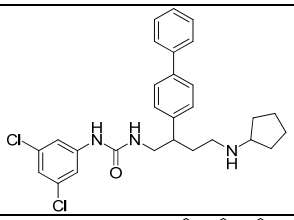
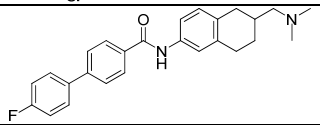
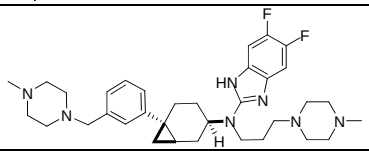
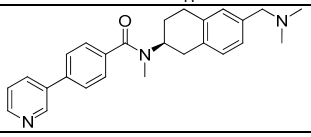
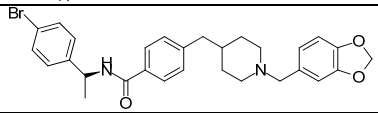
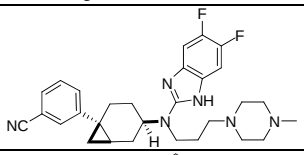
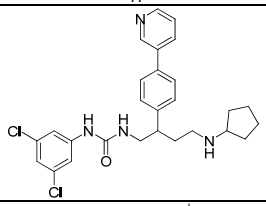
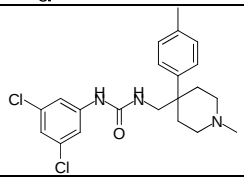


Figure S1: Multiple sequence alignment of the MCH-R1 receptor with bovine rhodopsin (1U19) and other class A GPCRs, MCH-R2 and human dopamine receptor D1.

Table S1: Compounds used for the docking validation.

Compound	Structure	P IC_{50}	Best Score	Average Score
1		9.01	71.23	70.09
2		6.98	53.44	47.13
3		7.4	53.79	46.54
4		6.55	56.99	55.57
5		8.92	67.44	65.87
6		8.66	70.61	67.88
7		8.59	68.5	67.91
8		7.09	63.06	60.17
9		5.52	47.74	39.32
10		7.41	53.9	45.84

11		7.3	71.6	64.26
12		6.85	54.02	51.09
13		6.49	68.48	64.65
14		6.05	57.09	55.02
15		5.89	45.49	41.18
16		7.68	65.13	56.14
17		7.62	69.8	65.87
18		6.52	38.26	29.15
Correlation			**0.6958**	**0.6982**