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ACCEPTED MANUSCRIPT

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*5-chloro-2-{6-[4-(2-methoxyphenyl)piperazin-1-yl]hexyl}-1H-benzo[d]imidazole (**5n**):*

Yield: 74%; oil; IR (ATR, cm^{-1}): 2825.8, 1500.6, 1451.2, 1241.8, 1027.6, 750.4; ^{1}H NMR (200 MHz, $CDCl_3$) δ: 1.30-1.46 (m, 6H, CH_2), 1.72-1.83 (m, 2H, CH_2), 2.34 (t, 2H, J=8.6 Hz, CH_2), 2.63 (s, 4H, piperazine), 2.86 (t, 2H, J=7.4 Hz, CH_2), 3.09 (s, 4H, piperazine), 3.84 (s, 3H, OCH_3), 6.84-7.06 (m, 4H, ArH), 7.12-7.18 (m, 1H, ArH), 7.38-7.48 (m, 2H, ArH); ^{13}C NMR (50 MHz, $CDCl_3$) δ: 26.27, 26.96, 27.91, 28.89, 29.09, 50.45, 53.27, 55.22, 58.42, 111.10, 111.[illegible], 120.97, 122.46, 123.08, 127.52, 140.98, 152.14, 156.51; MS: m/z [M+H]$^+$ calculated for $C_{24}H_{31}ClN_4O$ 427.22592, found 427.22408.

SUMMARY RESULTS OF MD SIMULATIONS

Table S1. D2DR-ligand key interactions observed in 100 ns long simulations.

Residue / Ligand	Leu 94	Trp 100	Asp 114	Cys 118	Ile 184	Phe 382	Trp [illegible]	[illegible]89	Phe 390	Tyr 408	Thr 412	Tyr 416
5e		54	81	68	27		76	6[illegible]	42	65	37	
5f	21	31	79	36	40		82	74	20	33	42	
5h		67	81	58			84	85	24	36		
5i	50	89	80	75			9[illegible]	84	42	22	30	
5j	36	94	82	73			[illegible]	53	31	25		
5l		22	82	6[illegible]	2[illegible]		95	75	34	37		
5m		75	[illegible]	[illegible]			78	50	49	63	40	
5n	32	42	80	32			82	68	35	28		32

D2DR-ligand interactions presented in more than 20% of MS simulation time are shown. Numbers provided in the table refers to the percentage of the total simulation time of the interaction observed to occur. Interacting residues in OBS are shaded in grey colour; residues found in EBP are white.