



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; ^1H 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, 118.75, 120.97, 122.46, 123.08, 127.52, 140.98, 152.14, 156.51; MS: m/z [M+H]⁺ calculated for $\text{C}_{24}\text{H}_{31}\text{ClN}_4\text{O}$ 427.22592, found 427.22408.

SUMMARY RESULTS OF MD SIMULATIONS

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

Residue	Leu 94	Trp 100	Asp 114	Cys 118	Ile 184	Phe 382	Trp 389	Phe 390	Tyr 408	Thr 412	Tyr 416
5e		54	81	68	27		76	65	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			96	84	42	22	30
5j	36	94	82	73			95	53	31	25	
5l		22	82	64	26		95	75	34	37	
5m		75	81	73			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 interaction observed to occur. Interacting residues in OBS are shaded in grey colour; residues found in EBP are white.