

Table S1: Ligands that were tested and replaced less than 50% of radioligand at 10 μ M in all targets.

ZINC ID	SMILES	A ₁ AR	A _{2A} AR	A ₃ AR	Model
06844430	<chem>CCOC(=O)c1cnc2nc(nn2c1[O-])NCc3cccc(c3)OC</chem>	3.4 \pm 3.4%	0%	11.1 \pm 3.8%	A
08653875	<chem>CCOC(=O)Cc1c(nc2cc([nH]n2c1=O)c3ccc(cc3)Cl)C</chem>	0%	2.1 \pm 2.1%	10.4 \pm 5.0%	A
05238266	<chem>C[C@@H](C(=O)OC(C)C)Sc1nc(c(c(n1)[O-])C#N)c2ccccc2</chem>	20.3 \pm 20.3%	7.6 \pm 4.3%	25.3 \pm 6.4%	A
18284742	<chem>CCOC(=O)Cc1c([nH]c2cc(nn2c1=O)c3ccc(cc3)C)C</chem>	8.9 \pm 5.5%	8.1 \pm 8.1%	20.7 \pm 7.3%	A
18156418	<chem>CCOc1cccc1CNc2nc3nc4c(c(n3n2)[O-])CCC4</chem>	10.9 \pm 10.9%	8.8 \pm 6.3%	26.8 \pm 8.1%	A
40488321	<chem>Cc1nc(nc(n1)Nc2[nH]c3ccccc3n2)c4ccccc4O</chem>	21 \pm 2%	37 \pm 4%	41 \pm 2%	B
08746576	<chem>Cn1cccc1C(=O)CSc2n[nH]c3n2c4ccccc4n3</chem>	28 \pm 6%**	20 \pm 4%	38 \pm 4%	B
20365432	<chem>C[C@@H](c1ccnc2n1nc(n2)NC=[N+](C)C)Oc3cccc(c3)OC</chem>	33 \pm 3%**	2 \pm 2%	19 \pm 5%	B
31875387	<chem>Cc1c(ccc(n1)C(=O)Nc2nc(cs2)c3ccc(cc3)F)C#N</chem>	11 \pm 1%**	1 \pm 1%	16 \pm 7%	B
54203984	<chem>Cc1cccc(n1)NC(=O)[C@H]2CCC[NH+](C2)CC(=O)N3CCNC3=O</chem>	3 \pm 3%	17 \pm 5%	28 \pm 2%	C
56482974	<chem>C[C@H](C(=O)Nc1ccc(c(c1)NC(=O)OC(C)(C)C)F)n2cc[nH+]c2</chem>	5 \pm 4%	45 \pm 5%	53 \pm 3%	C
47260884	<chem>Cc1cccc(n1)NC(=O)[C@H]2CCC[NH+](C2)CC(=O)NC3CCCC3</chem>	4 \pm 4%	48 \pm 3%	31 \pm 6%	C
31584575	<chem>CN(Cc1[nH]c(=O)c2ccccc2n1)C(=O)/C=C/c3cccc(c3)C#N</chem>	12 \pm 7%	12 \pm 6%	19 \pm 4%	C
43348592	<chem>c1ccc(cc1)Oc2ccccc2NC(=O)NC[C@@H](C(F)(F)F)O</chem>	3 \pm 2%	4 \pm 4%	23 \pm 6%	C
47260934	<chem>Cc1cccc(n1)NC(=O)[C@H]2CCC[NH+](C2)CC(=O)NCC(C)C</chem>	10 \pm 8%	53 \pm 3%	31 \pm 2%	C
47260835	<chem>CCNC(=O)NC(=O)C[NH+]1CCC[C@@H](C1)C(=O)Nc2cccc(n2)C</chem>	8 \pm 4%	14 \pm 3%	20 \pm 5%	C
08724684	<chem>Cc1cccc2c1nc([nH]c2=O)/C(=C/c3ccc(c(c3)O)OC)/Cl</chem>	10 \pm 5%	18 \pm 4%	46 \pm 5%	D
06647942	<chem>c1ccc2c(c1)c(=O)[nH]c(n2)CCC(=O)Nc3[nH]c4ccccc4n3</chem>	2 \pm 2%	15 \pm 4%	13 \pm 3%	D
04059122	<chem>c1ccc2c(c1)c(=O)cc(o2)C(=O)Nc3nc(cs3)c4cccn4</chem>	4 \pm 4%	27 \pm 6%	34 \pm 2%	D

**n=2