

Table S2. Bioactivity score of designed compounds

Product	GL	ICM	KI	NRL	PI	EI
8a	-0.01	-0.23	-0.15	-0.23	0.01	0.22
8b	-0.05	-0.29	-0.18	-0.25	-0.05	0.16

GL: GPCR ligand, ICM: Ion Channel Module, KI: Kinase Inhibitor, NRL: Nuclear Receptor ligand, PI: Protease inhibitor, EI: Enzyme inhibitor