D1 antagonist

Crystal structure of human D1 was downloaded from PDB (PDB id: 4IAR, 2.7 Å resolutions). 7.5 Å area around bound ligand ergotamine (anti-migraine drug) was selected. Self-docking revealed rmsd of 1.4 Å. HYDE analyses also showed good affinity

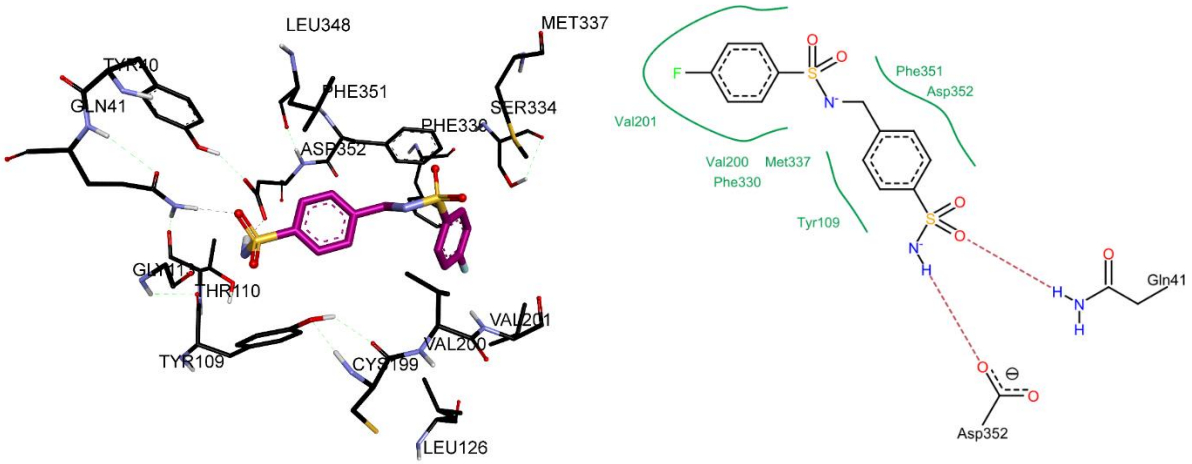

Figure S1. Docked conformation of 4-FBS against D1 receptor

Figure S1 shows docked conformation of compound 4-FBS against D1 receptor. All compounds were found to bind in the same region as that of co-crystallized ligand, ergotamine. The terminal sulfonamide group was found to make hydrogen bonds with Asp353 and Gln41 via sulfonamide nitrogen and oxygen atoms respectively.

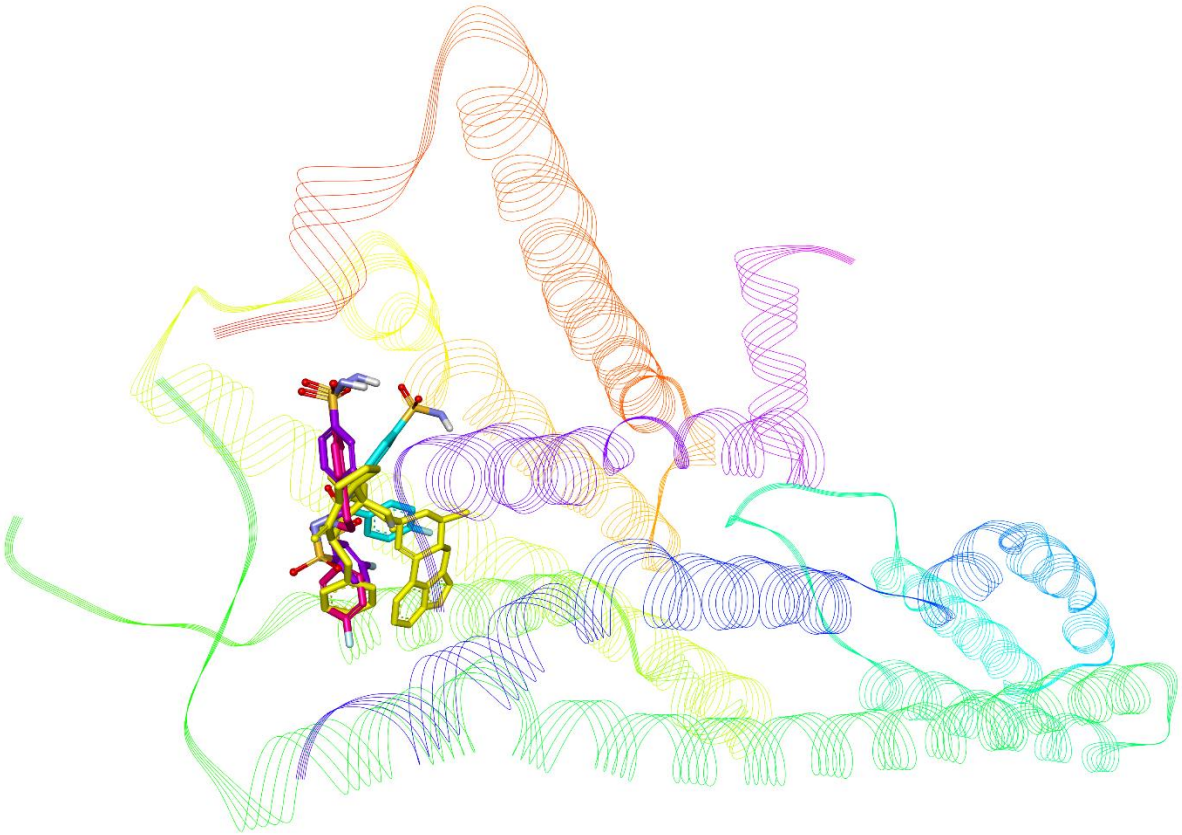

Figure S2. Overlap of docked conformations of 4-FBS with co-crystallized anti-migraine drug ergotamine (yellow).

Table S1. Predicted binding free energy (ΔG, kJ/mol) for all docked compounds 4-FBS

Compound	Binding Energy (kJ/mol)
4-FBS	-16