

Table S2. Summary of the molecular interactions of 3DPP-D with FurAct and FurAll.

Ligands	Site interaction	Free Energy of Binding (Kcal/mol) and RMSD AUTODOCK4	Free Energy of Binding (Kcal/mol) and RMSD VINA	H bond classical and non-classical	Distance H-bond (Å)	Electrostatic	Hydrophobic
3-(3,5-Dichlorophenyl) pyridine-derived 3DPP-D	Active	-13.82 (0.98)	-10.2 (0.00)	Asp 233 – O	2.1	Pro 256 Asp 264 Glu 236 Asp 154	Trp 254 Ala 252 Met 226 Leu 240 Trp 291 Val 231 Gly 255
	Allosteric	NA (NA)	NA (NA)	NA	NA	NA	NA