

Table S3. Summary of the molecular interactions of NPF, PFD, PGZ, and RGZ with FurAll by general molecular docking.

Ligands	Site interaction	Free Energy of Binding (Kcal/mol) AUTODOCK4	Free Energy of Binding (Kcal/mol) VINA	H bond classical and non-classical	Distance H-bond (Å)	Electrostatic	Hydrophobic
Naphthofluorescein (NPF)	Allosteric	-9.14 (0.00)	-10.9 (0.00)	Gly265 – O	2.4		Glu271
				Ans310 – H	2.1		Ala532
				Glu488 – O	2.3		Trp531 Pro266
Pirfenidone (PFD)	Allosteric	-6.28 (0.00)	-7.0 (0.00)	Ans310 – O	2.7	Glu271	Trp531
				Ala532 – O	3.4		Ala532
							Tyr313 Ile312
Pioglitazone (PGZ)	Allosteric	-8.20 (0.00)	-8.2 (0.00)	Ser311 – H	2.8	NA	Trp531
				Ile312 – O	2.0		
				Gln488 – O	2.6		
Rosiglitazone (RGZ)	Allosteric	-7.95 (0.00)	-7.3 (0.00)	Asn310 – O	2.1		Glu271
				Gly265 – O	2.4		Ala532
							Trp531 Pro266

NA= Not apply; Å = Ångstrom; NPF: Naphthofluorescein; PFD= Pirfenidone; PGZ: Pioglitazone; RGZ: Rosiglitazone.