

Supplementary material:

Table 1: Amino acid sequence and MolDock scores were presented in Table. From table, it is clear that Ligand with pose Unknown 1 is said to be best fit into Cytochrome p450 3A4 leading to least MolDock score and re-rank scores.

S. NO	Ligand	Cavity Volume	Amino Acid Sequence Surrounding the Cavity	MolDock score	Rerank score	RMSD	HBond
1	Piperine-Fe conjugate 1	605.696 Proximity (A)-2.61	A ³ ; (A)- Ala(305,370) Phe(57,108,137,215,302,435); Arg (105,372) Thr (309); Ile (443, 301) Ser (119)	-132.788	-108.422	91.4833	- 7.41695
2	Piperine-Fe conjugate 2	59.904 Proximity(A)-2.61	A ³ ; Arg (162)	-127.055	-83.8605	91.487	-9.8363
3	Piperine-Fe conjugate 3	32.768 Proximity(A)-2.61	A ³ ; Phe (419)	-123.969	-90.9825	89.9825	-2.5
4	Piperine-Fe conjugate 4	31.744 Proximity(A)-2.61	A ³ ; Leu (133), Glu (294)	-117.297	-80.996	90.1965	-2.5
5	Piperine-Fe conjugate 5	27.648 Proximity(A)-2.65	A ³ ; Leu (351.499),Lys (453), Met (450)	119.177	-98.6817	90.0128	0