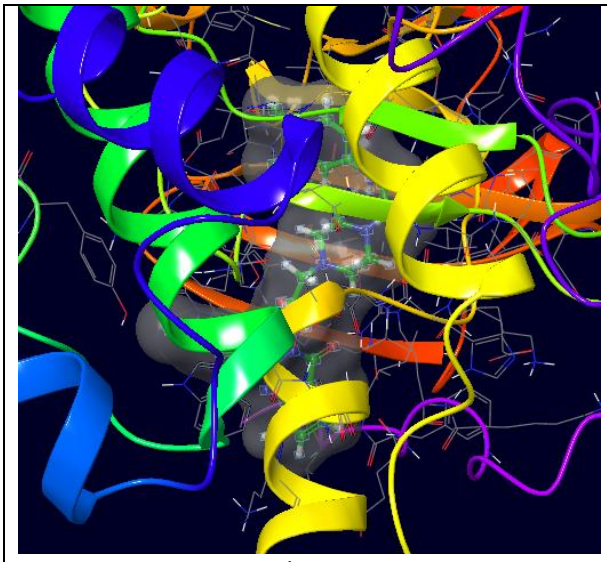
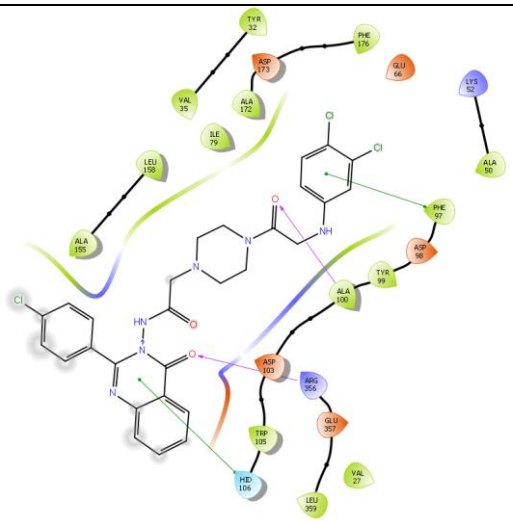
Additional File 3

Molecular docking results PDB ID: 5FGK			
Comp.	**Docking Score**	**Glide energy (kcal/mol)**	**Interacting residues**
5	-8.011	-64.796	Ala155, Leu158, Ile79, Ala172, Asp173, Phe176, VaL35, Tyr32, Glu66, Lys52, Ala50, Phe97, Asp98, Tyr99, Ala100, Asp103, Trp105, Hid106, Arg356, Glu357, Leu359, Val27
5XG	-8.72	-49.49	Ile79, Ala172, Asp173, Arg356, Phe 97, Ala 100, Val159, Glu101, Gly33
Raltitrexed (Tomudex)	-10.86	-54.30	Met174, Asp173, Phe176, Glu66A, Lys52, Leu70, Ile79
5-Fluorouracil	-5.753	-21.673	Leu158, Arg356, Ala100, Tyr99, Asp98, Phe97, Ile79, Ala50, Val35

Pictorial presentation of the active compounds in 3D and 2D view

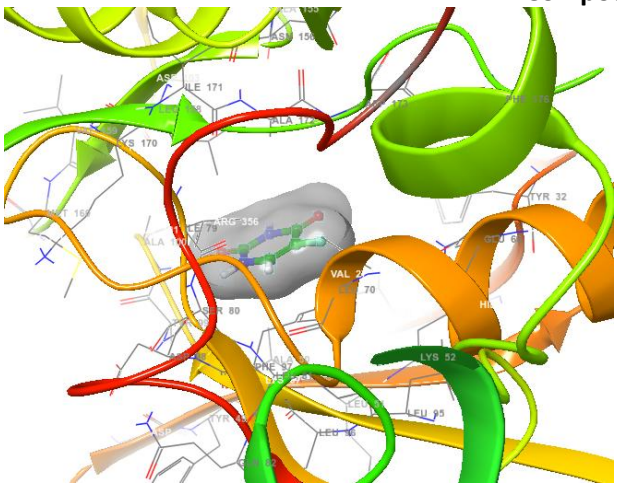


Pictorial presentation

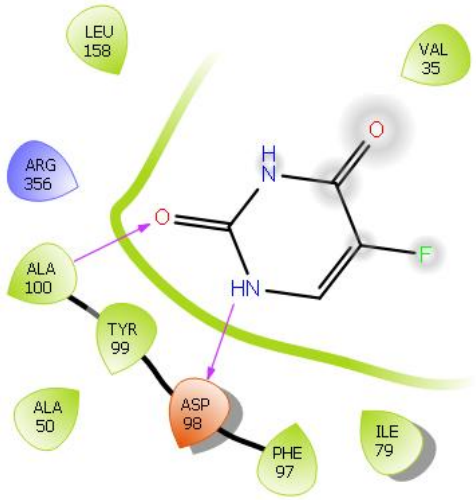


Ligand interaction diagram

Compound 5



Pictorial presentation

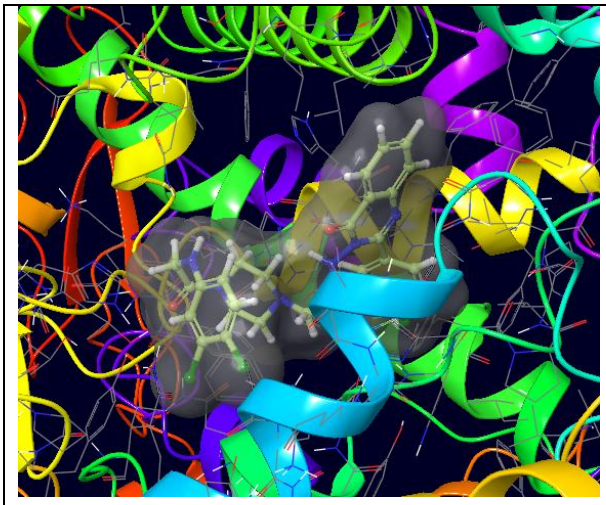


Ligand interaction diagram

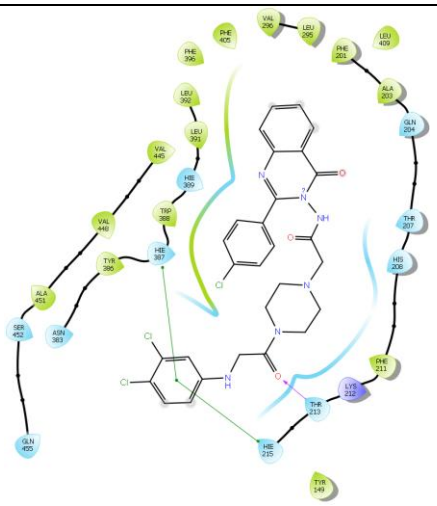
5-Fluorouracil

Molecular docking results PDB ID: 5JVY			
Comp.	**Docking Score**	**Glide energy (kcal/mol)**	**Interacting residues**
5	-11.054	-68.766	Gln455, Ser452, Ala451, Val448, Val445, Asn383, Tyr386, Hie387, Trp388, Hie389, Leu391, Leu392, Phe396, Phe405, Val296, Leu295, Phe201, Ala203, Gln204, Thr207, His208, Phe211, Lys212, Thr213, Hie215, Tyr149, Leu409
7	-11.284	-71.663	Phe405, Phe396, Leu392, Leu391, Hie389, Trp388, Hie387, Tyr386, Tyr149, Asn383, Leu409, Ala200, Phe201, Ala203, Gln204, Thr207, His208, Phe211, Lys212, Thr213, Asp214, Hie215, Val296, Leu295, Val292, Glu291, Gln290, Ile275, Arg223, Val448
COH	-8.93	-54.81	Glu291, Lys216, Arg223, Lys212, Gln290, His 215
Raltitrexed (Tomudex)	-10.83	-58.73	Glu291, Arg223, Lys212, Gln290, Thr238, Glu 209
5-Fluorouracil	-4.122	-26.585	Leu392, Leu391, Hie389, Trp388, Hie387, Tyr386, Thr207, Gln204, Ala203, Ala200

Pictorial presentation of the active compounds in 3D and 2D view

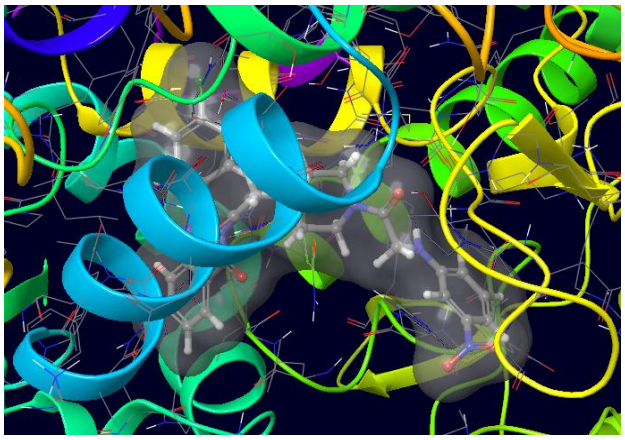


Pictorial presentation

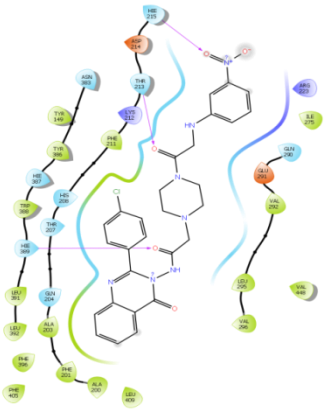


Ligand interaction diagram

Compound 5

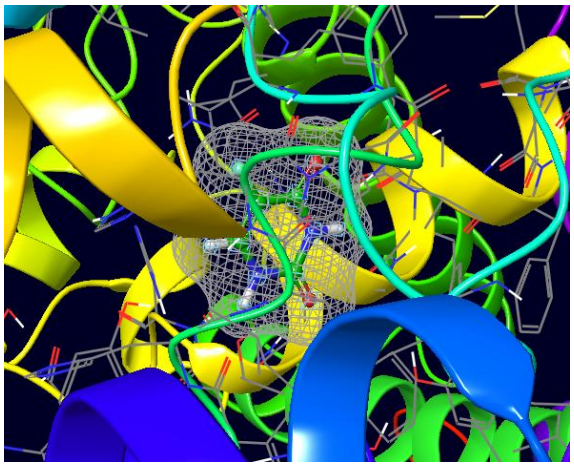


Pictorial presentation

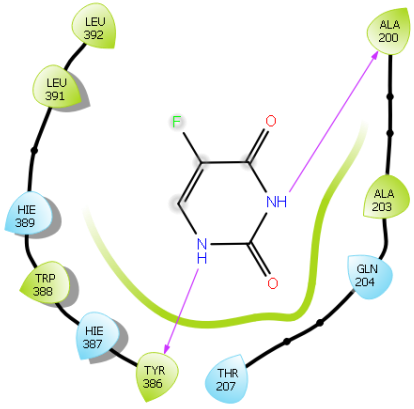


Ligand interaction diagram

Compound 7



Pictorial presentation



Ligand interaction diagram

5-Fluorouracil