Supplementary Materials

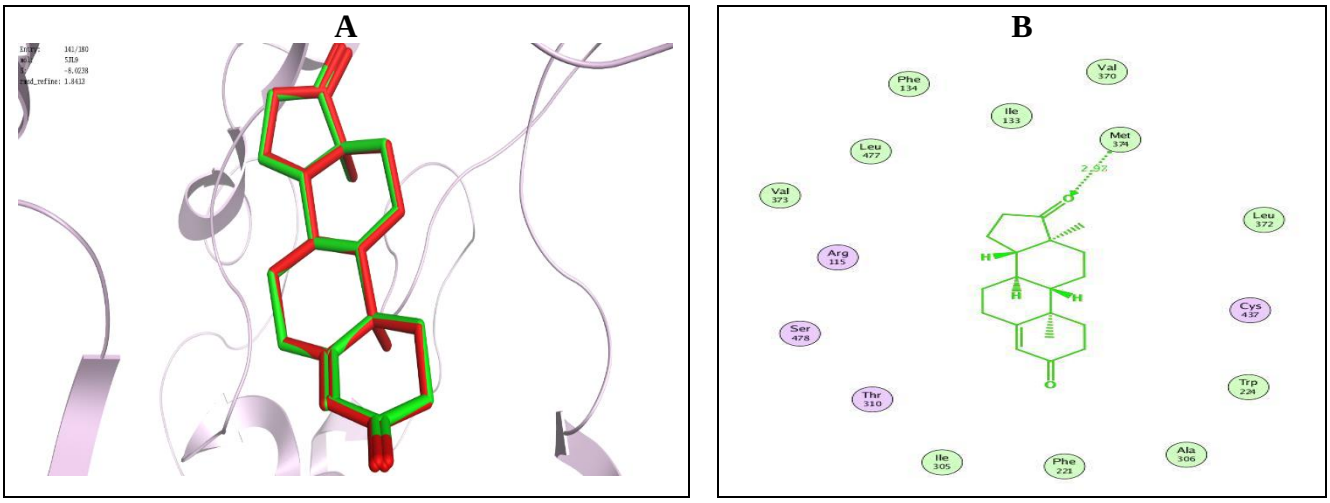

Figure S1: (**A**) 3D diagram and (**B**) 2D ovelay disclosing the superimposition of the native co-crystallized ligand (green), and the redocked co-crystallized ligand (Red) at aromatase enzyme with RMSD value of 1.84 Å for docking program validation.

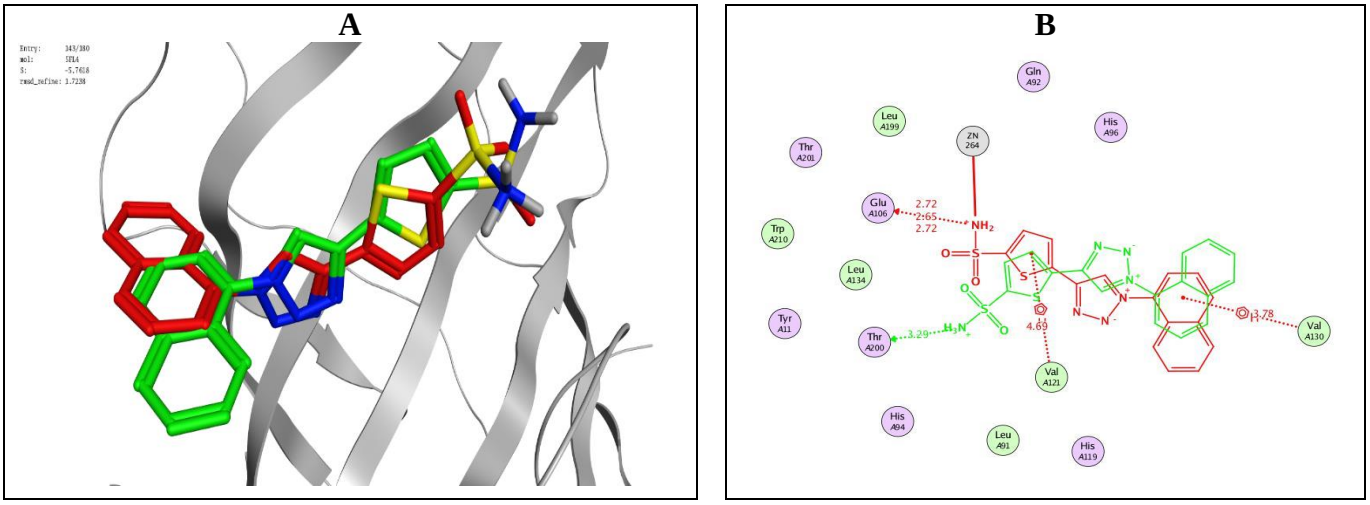

Figure S2: (**A**) 3D diagram and (**B**) 2D ovelay disclosing the superimposition of the native co-crystallized ligand (green), and the redocked co-crystallized ligand (Red) at **CA IV** with RMSD value of 1.72 Å for docking program validation.

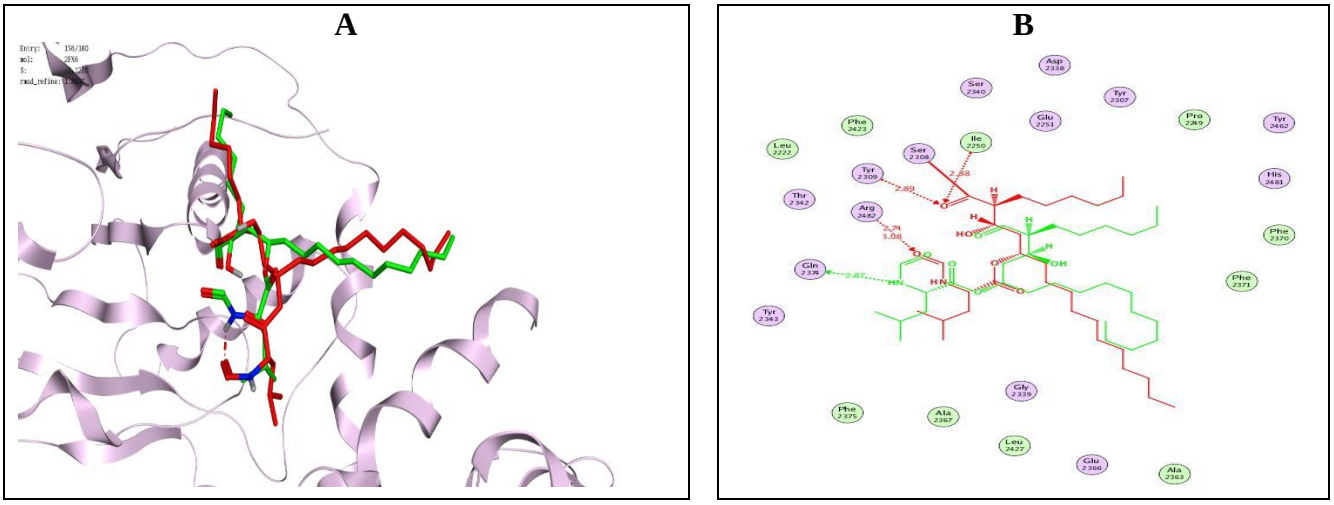

Figure S3: (**A**) 3D diagram and (**B**) 2D ovelay disclosing the superimposition of the native co-crystallized ligand (green), and the redocked co-crystallized ligand (Red) at **FAS** with RMSD value of 1.88 Å for docking program validation.

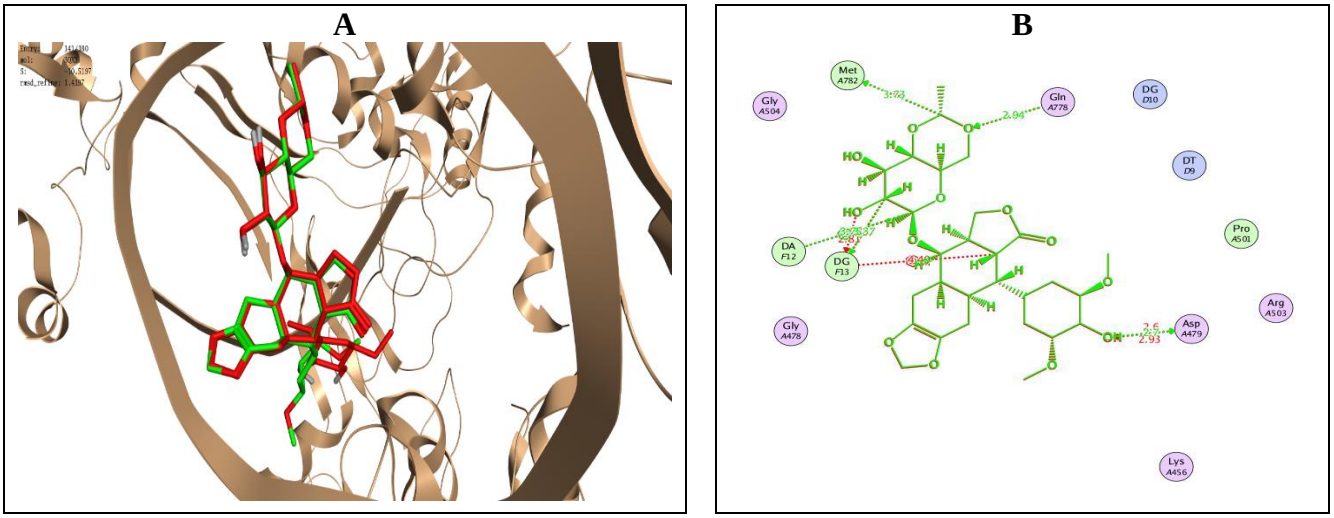

Figure S4: (**A**) 3D diagram and (**B**) 2D ovelay disclosing the superimposition of the native co-crystallized ligand (green), and the redocked co-crystallized ligand (Red) at **TOP II** with RMSD value of 1.42 Å for docking program validation.

Aromatase			
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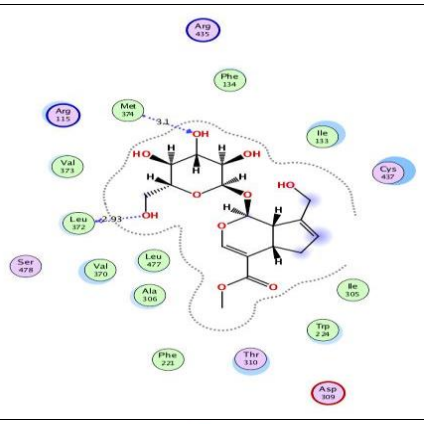
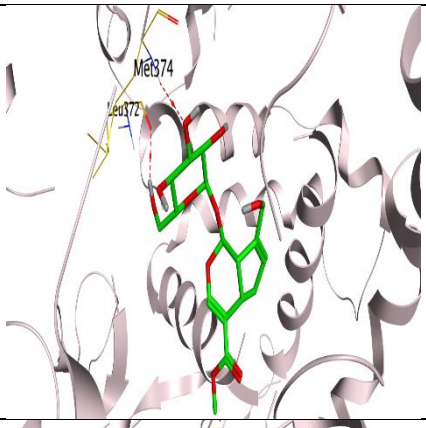
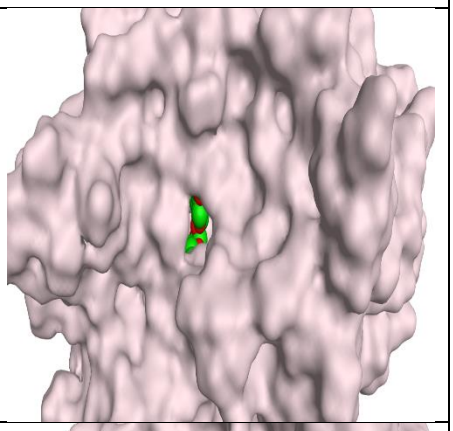
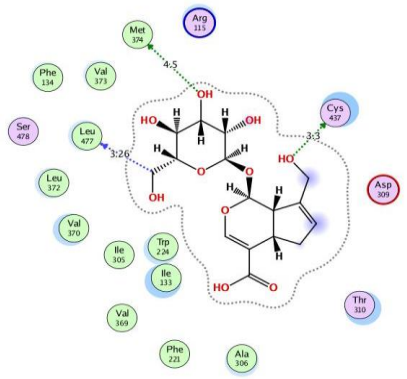
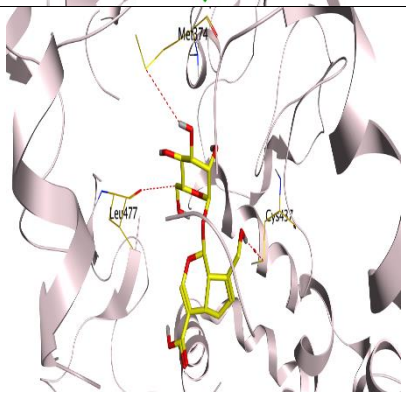
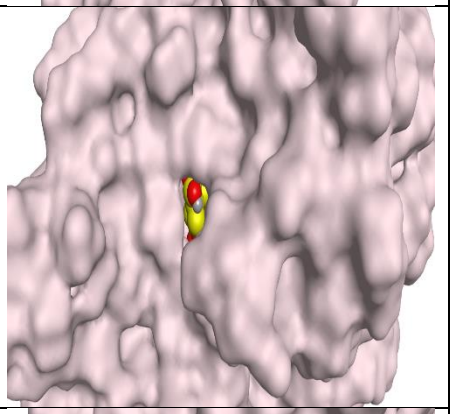
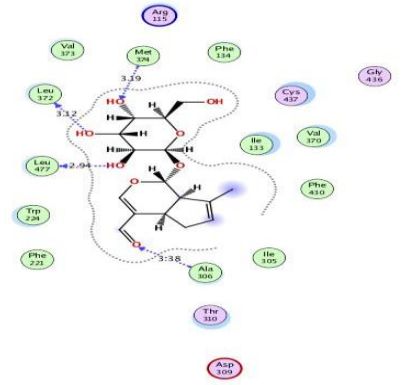
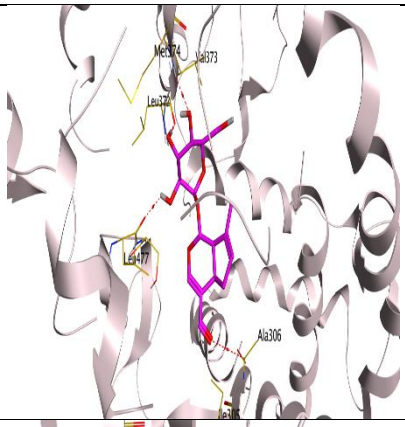
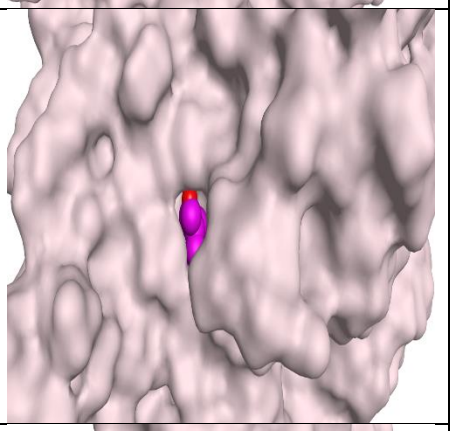
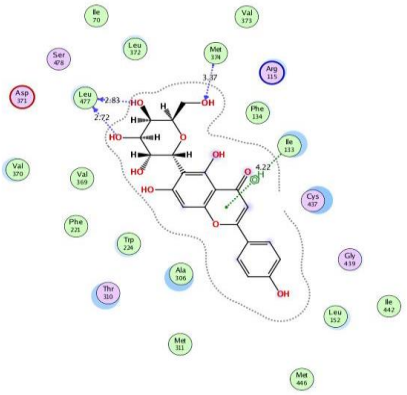
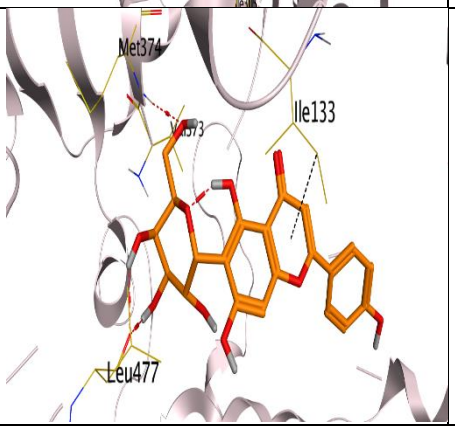
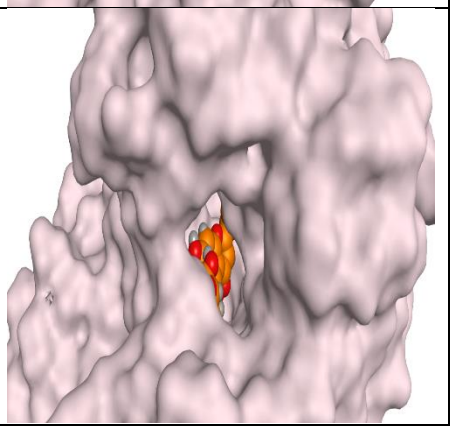
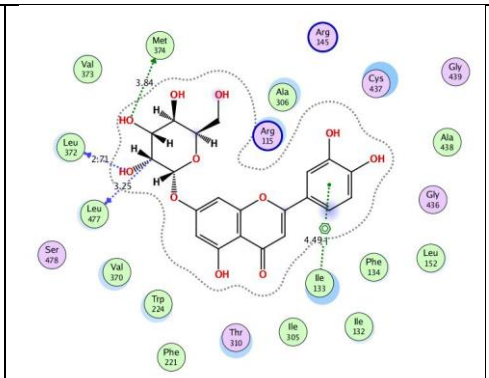
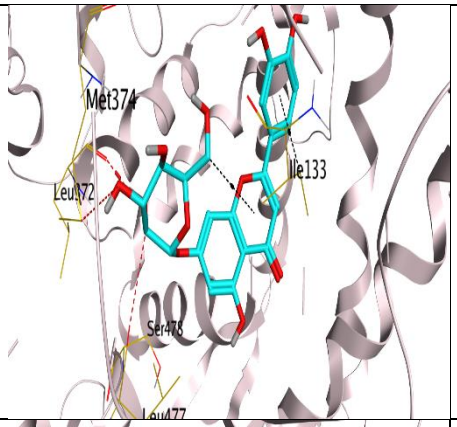
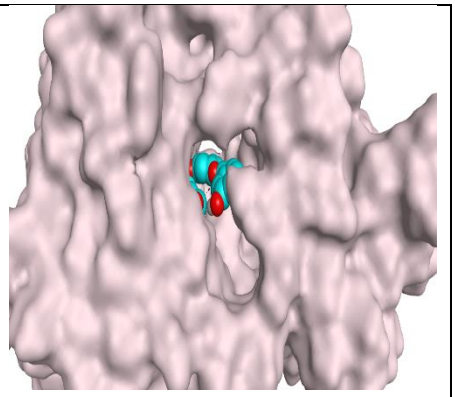
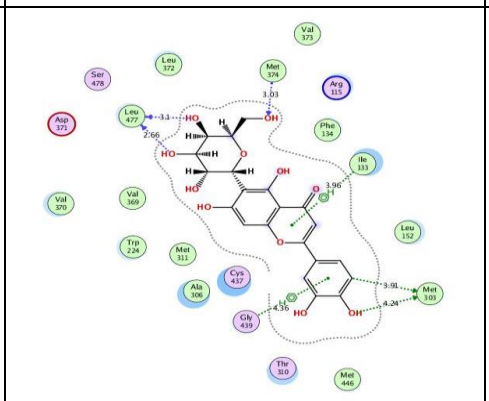
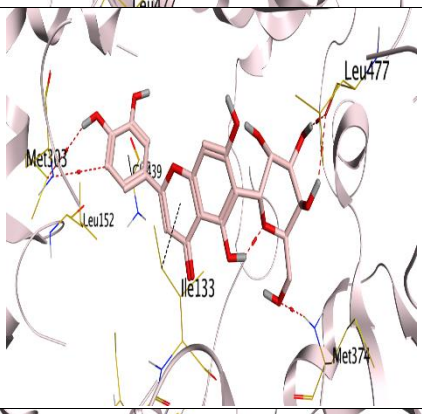
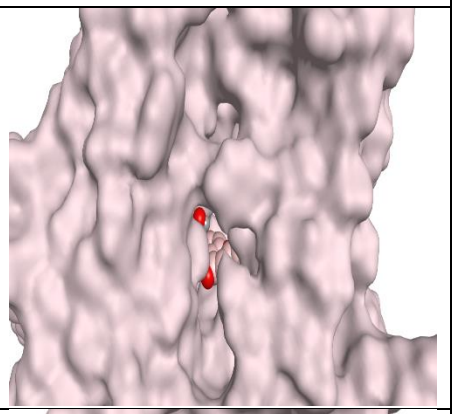
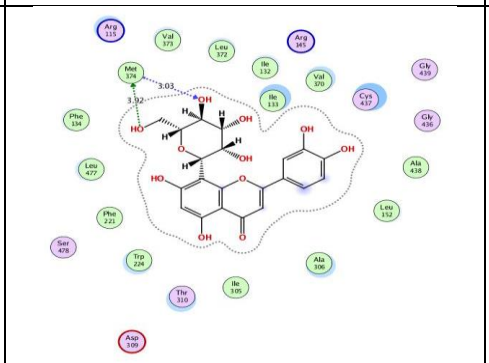
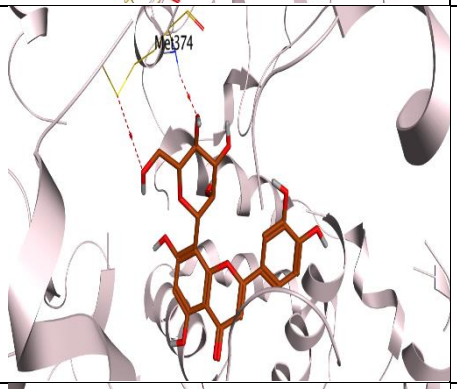
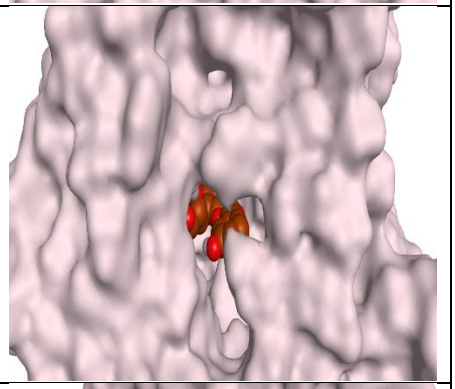
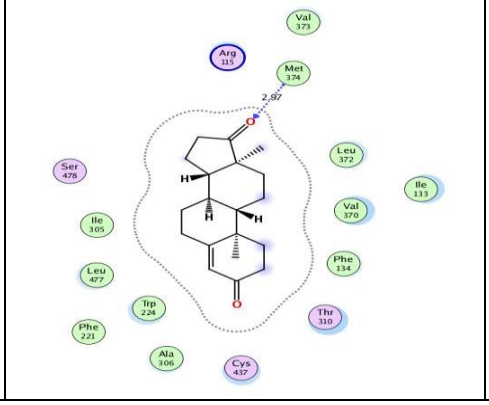
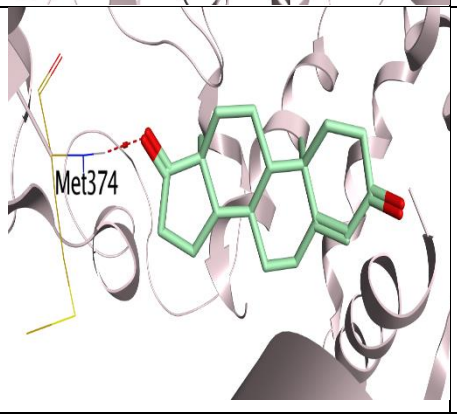
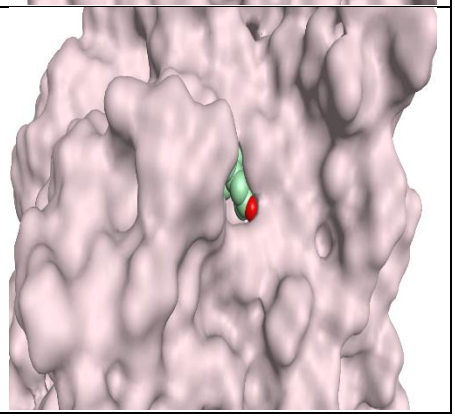
1			
2			
3			
4			

5			
6			
7			
Co-crystallized			

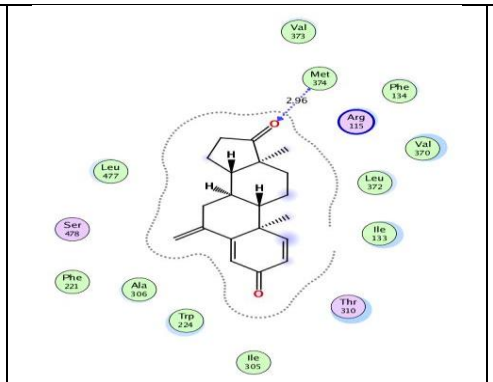
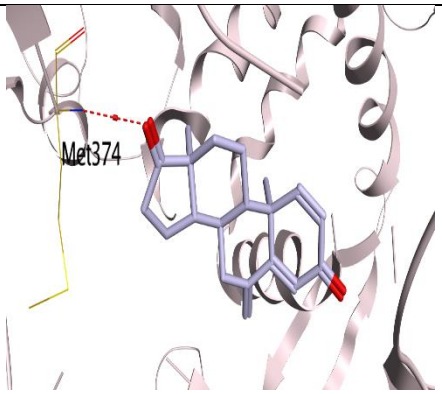
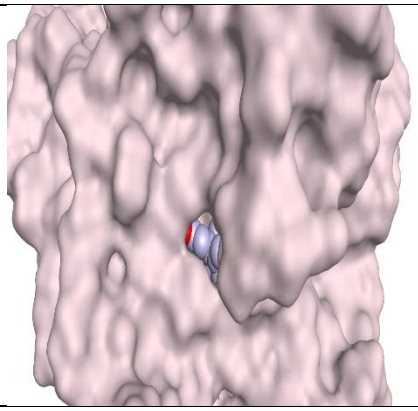
Reference			

Figure S5: the 2D, 3D, and 3D protein positioning of all investigated compound at the biological target, aromatase.

CA IX			
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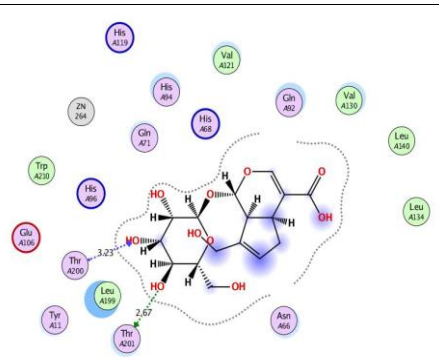
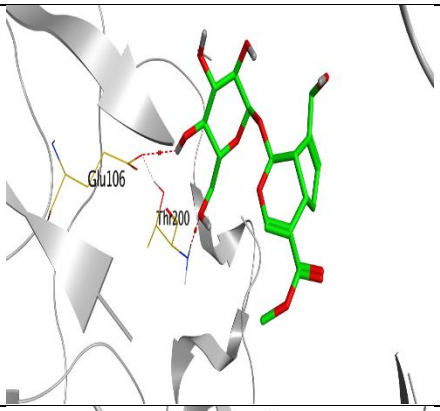
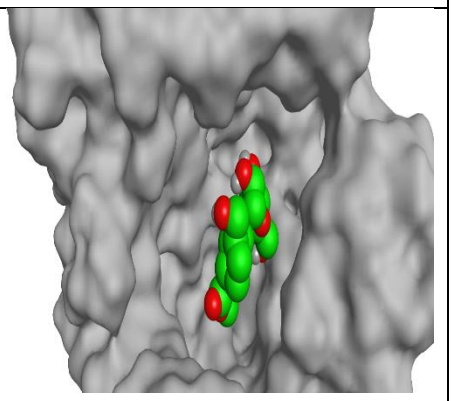
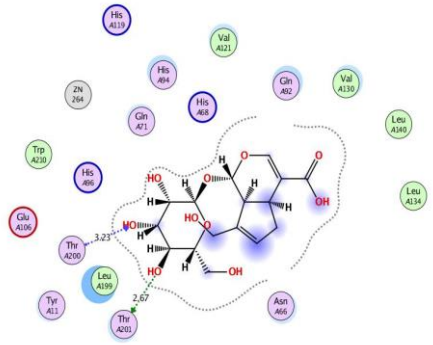
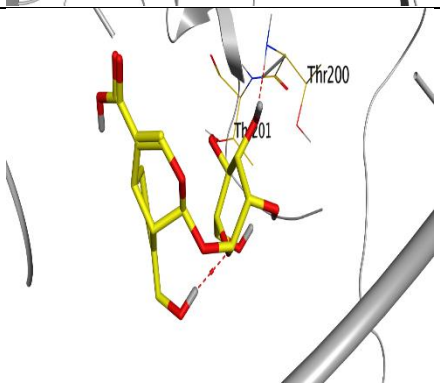
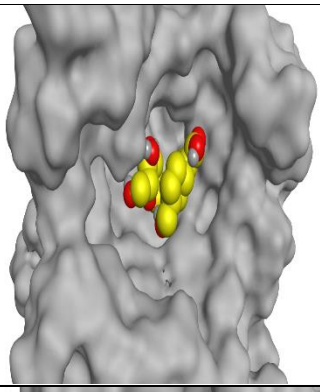
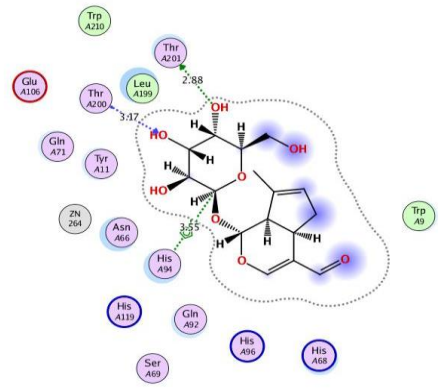
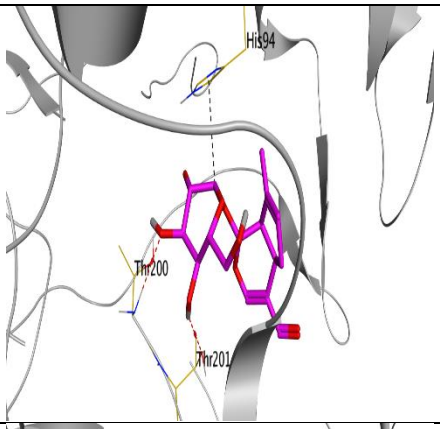
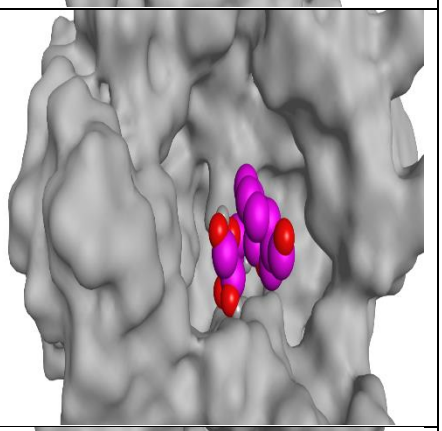
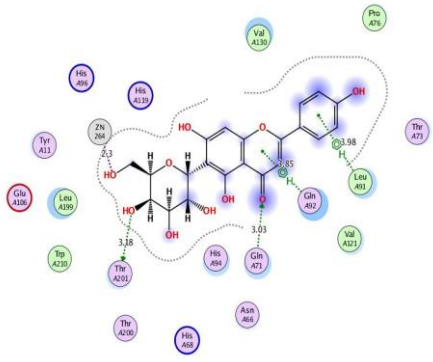
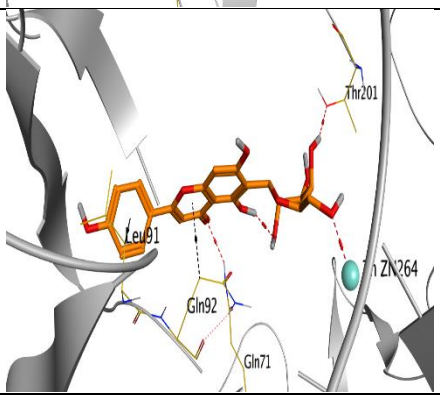
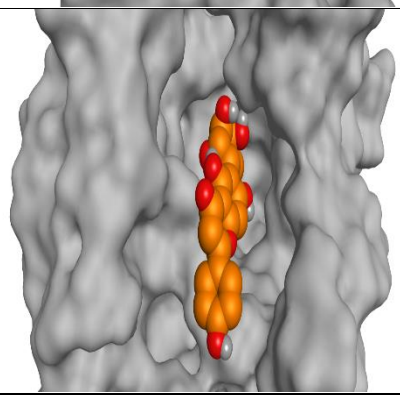
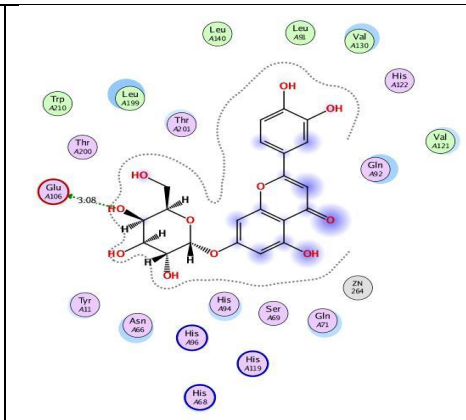
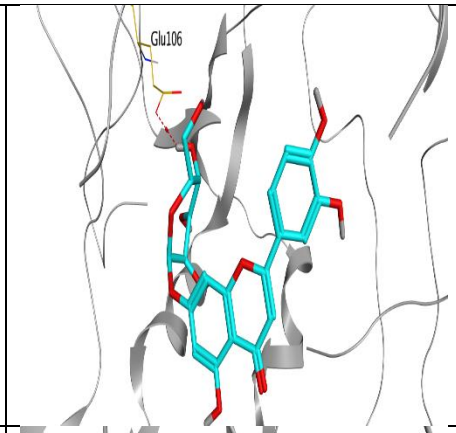
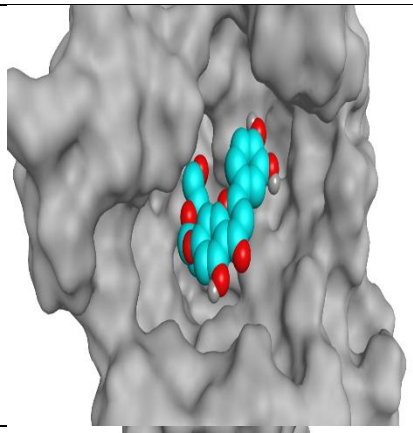
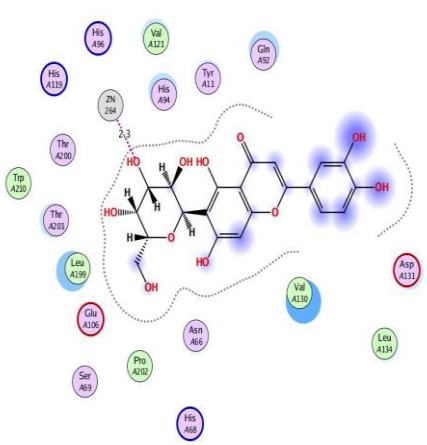
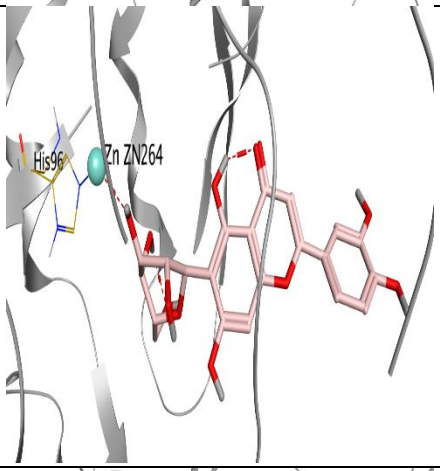
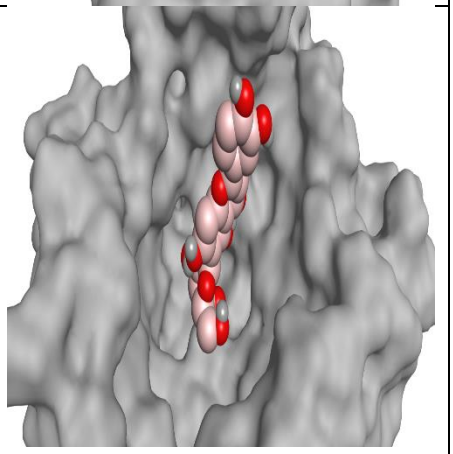
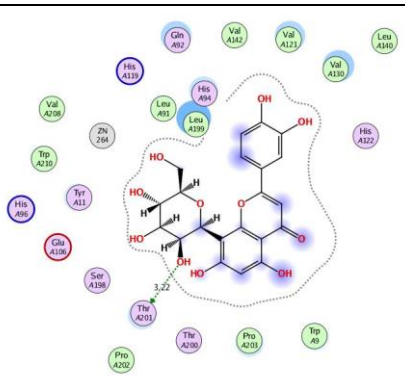
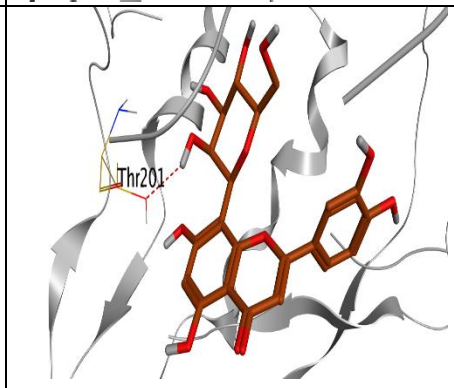
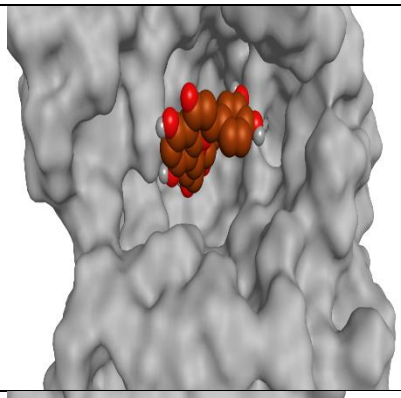
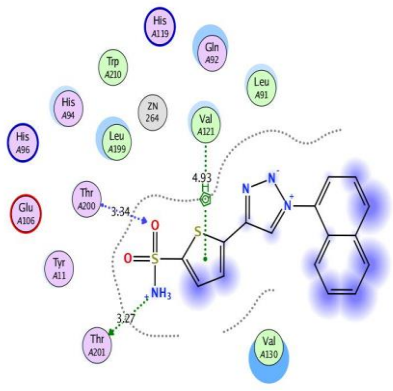
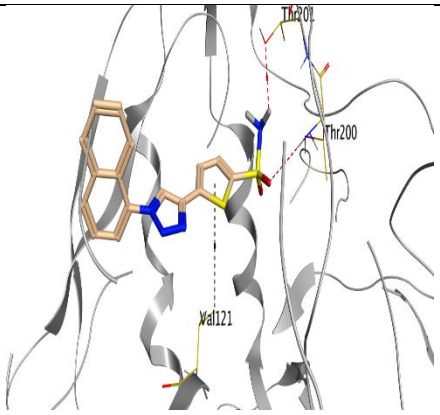
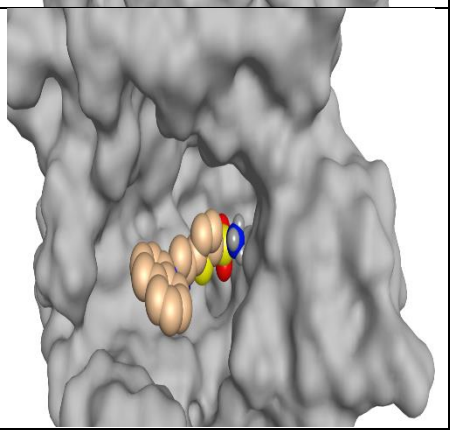
1			
2			
3			
4			

5			
6			
7			
Co-crystallized			

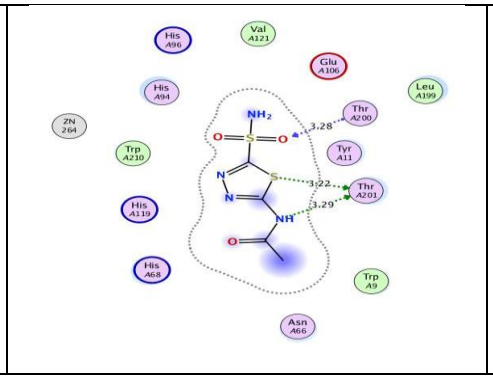
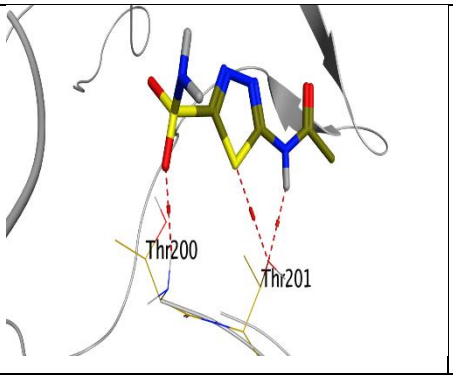
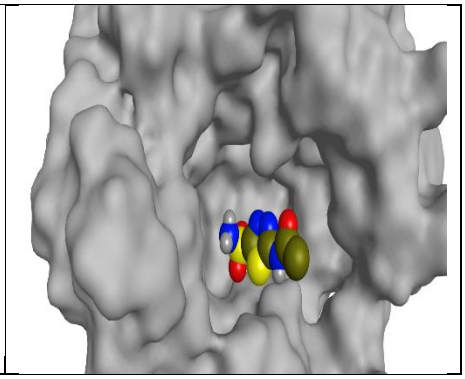
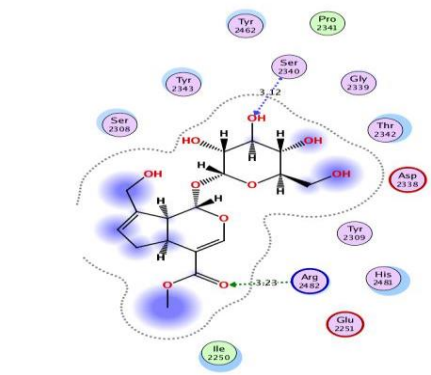
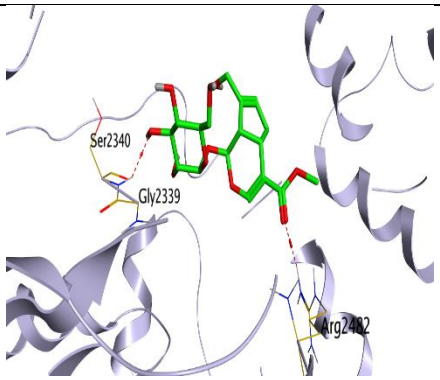
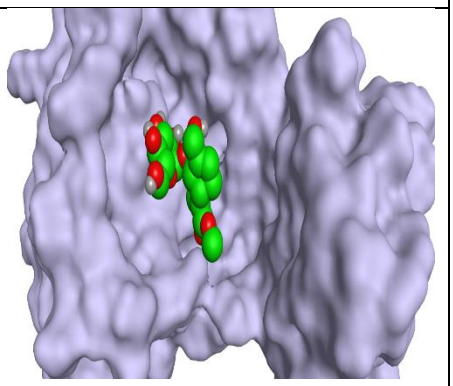
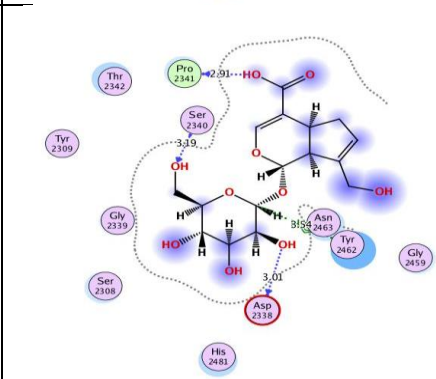
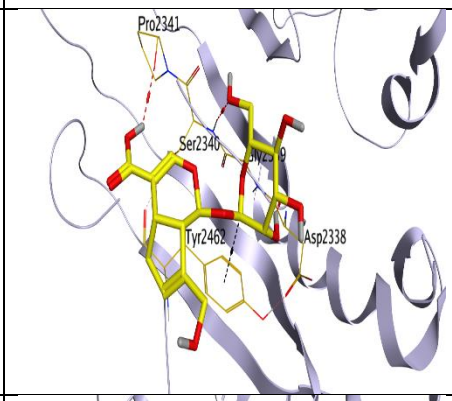
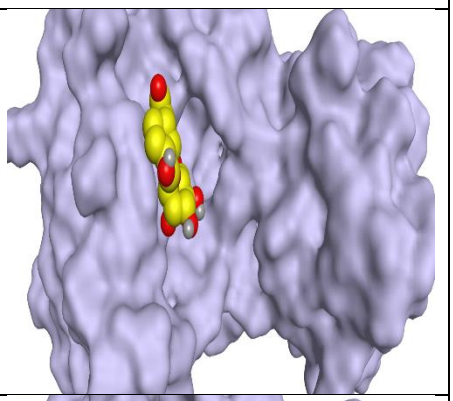
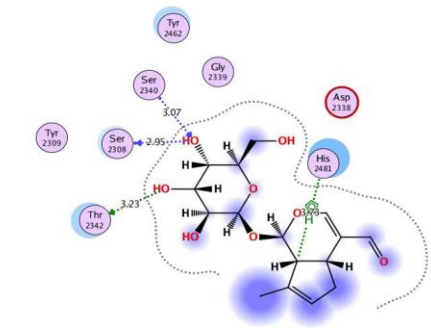
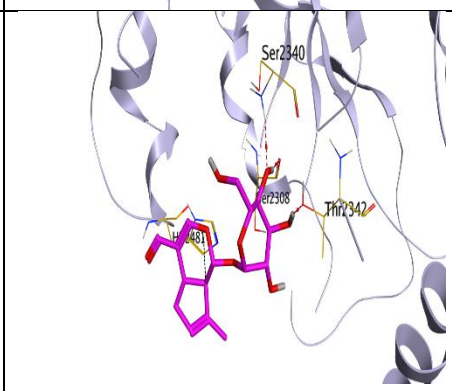
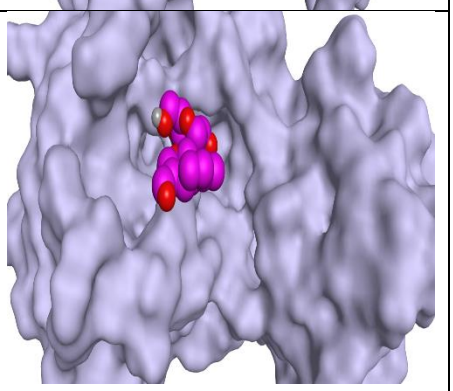
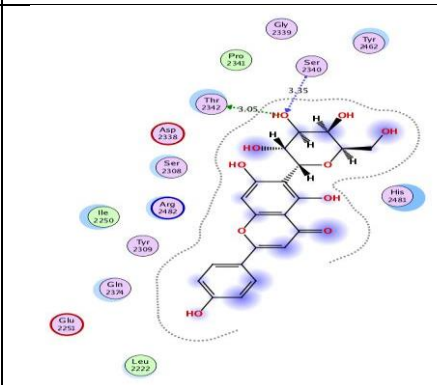
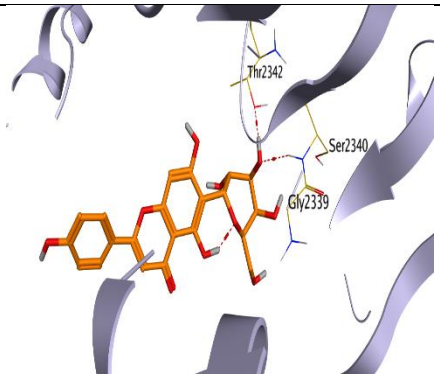
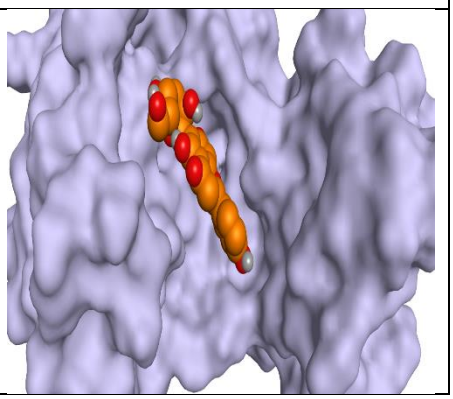
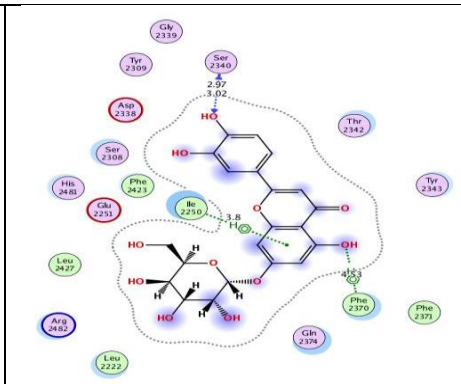
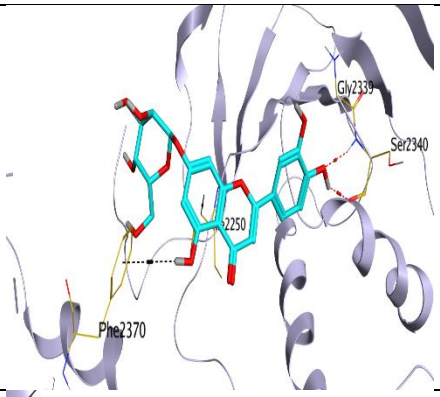
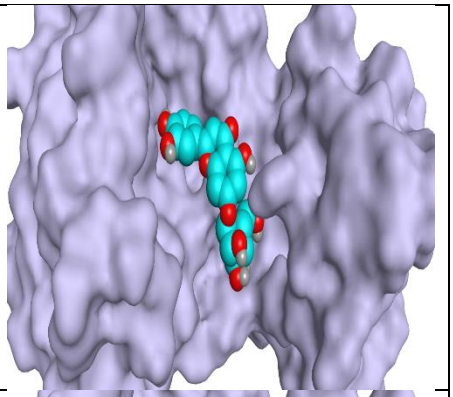
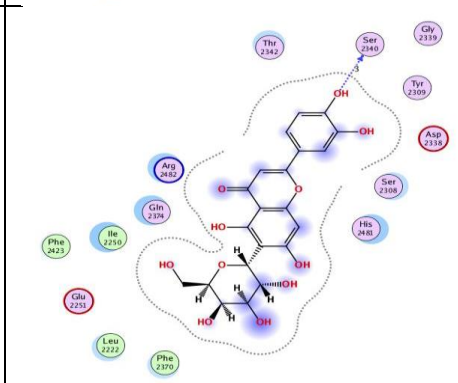
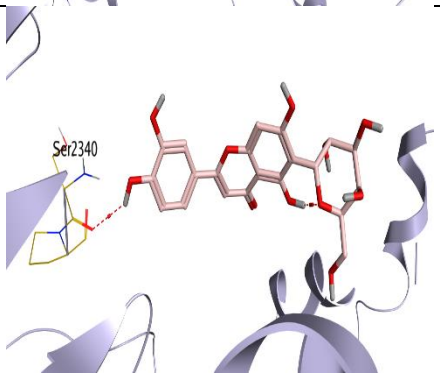
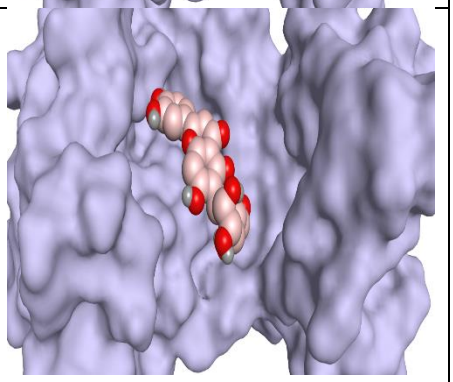
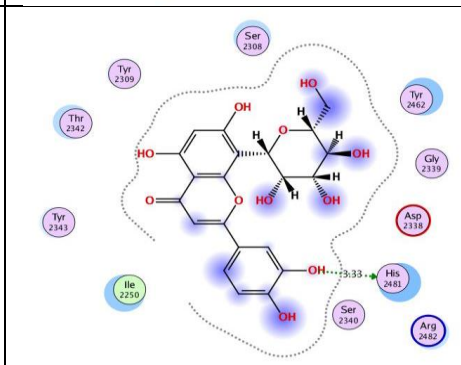
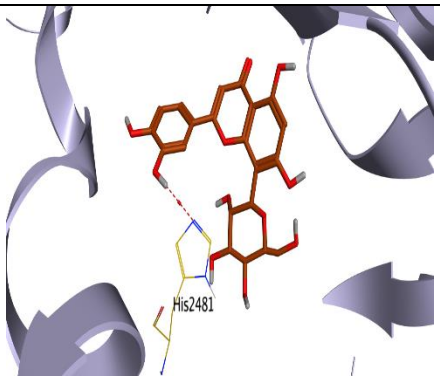
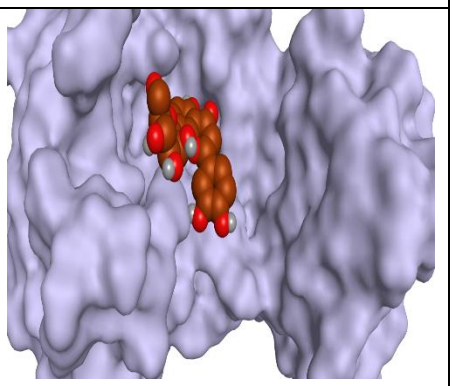
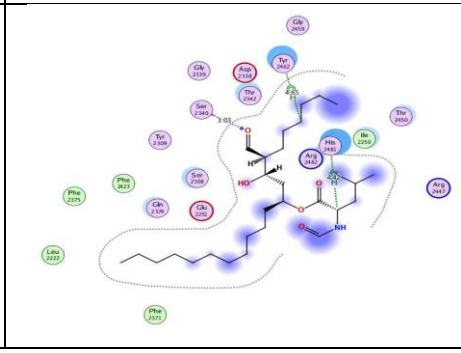
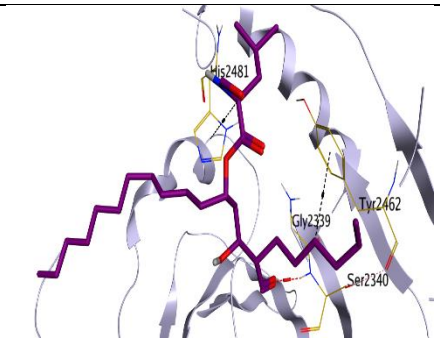
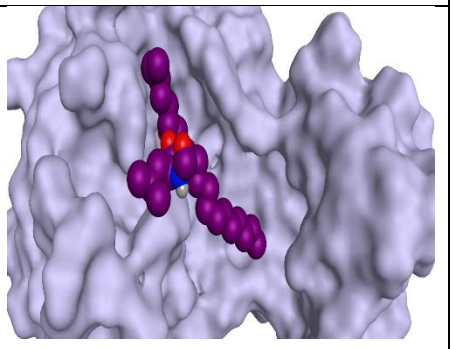
Reference			

Figure S6: the 2D, 3D, and 3D protein positioning of all investigated compound at the biological target, CA IX.

FAS			
Comp no.	**2D**	**3D**	**3D protein**
1			
2			
3			
4			

5			
6			
7			
Co-crystallized			

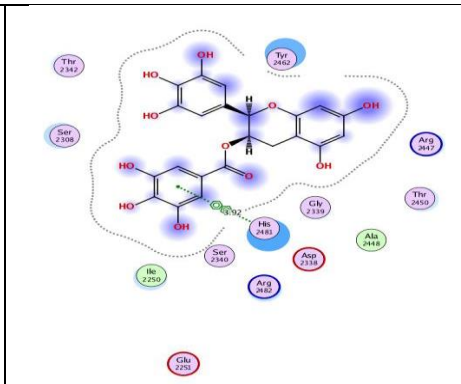
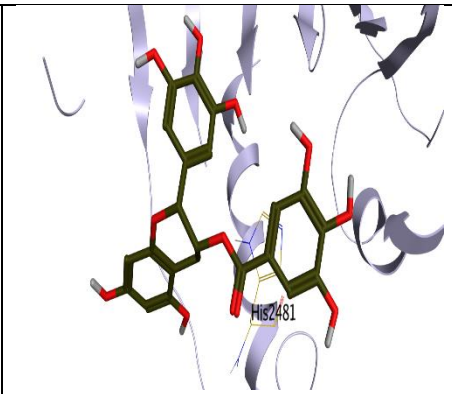
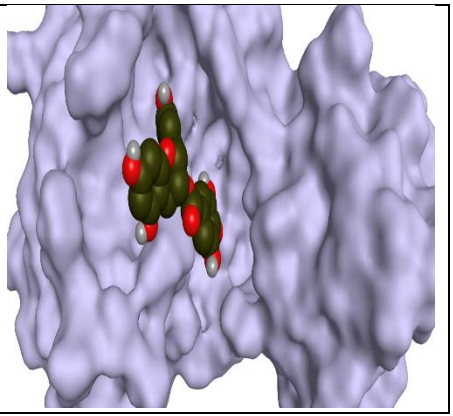
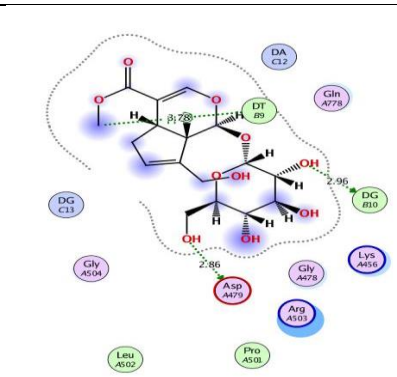
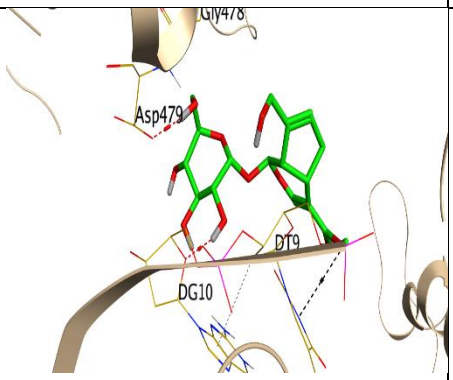
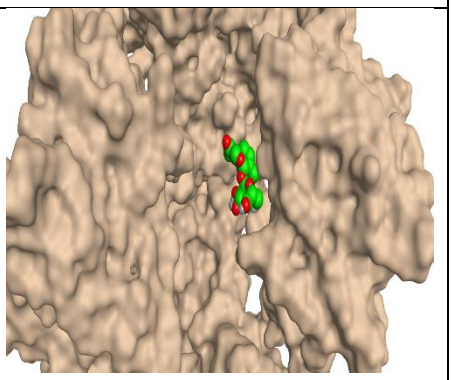
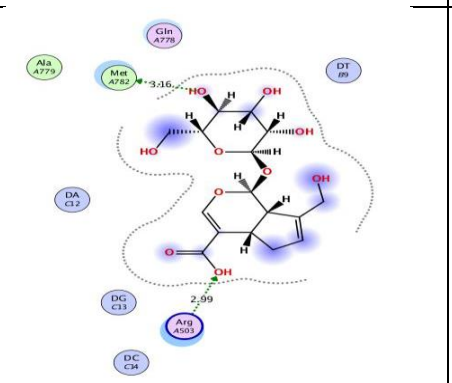
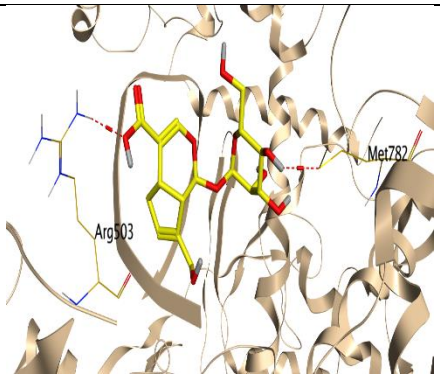
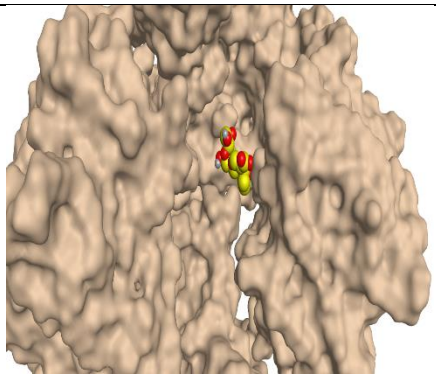
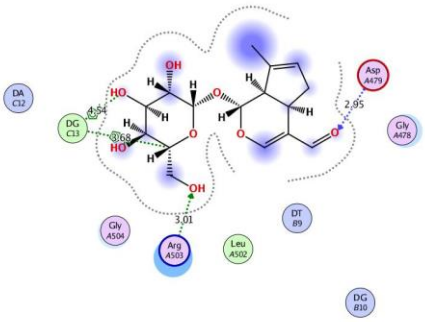
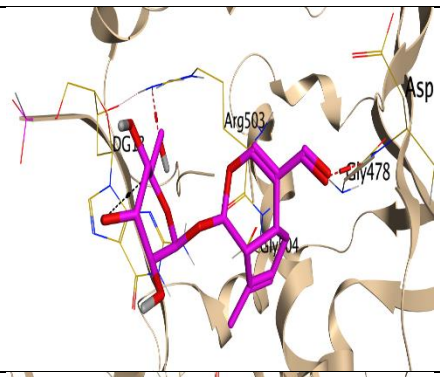
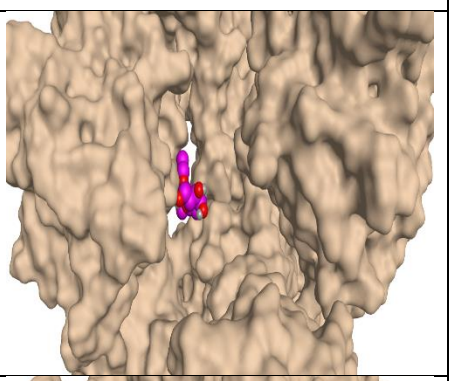
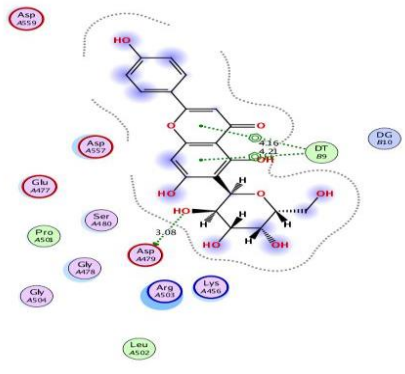
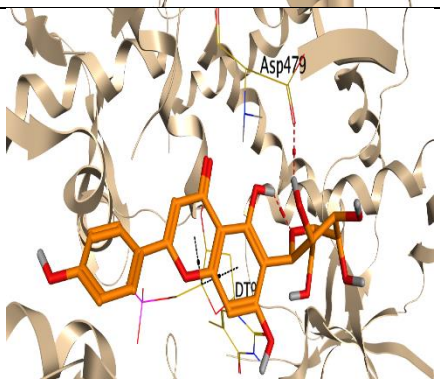
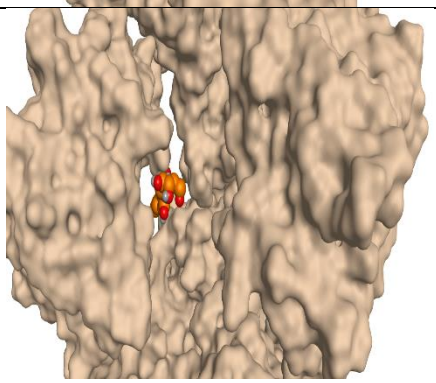
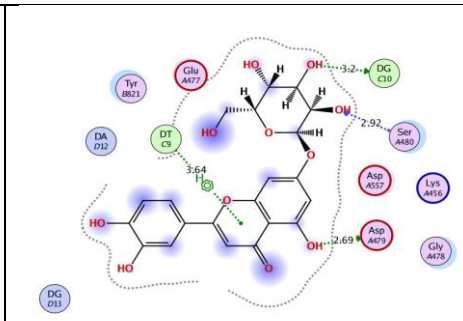
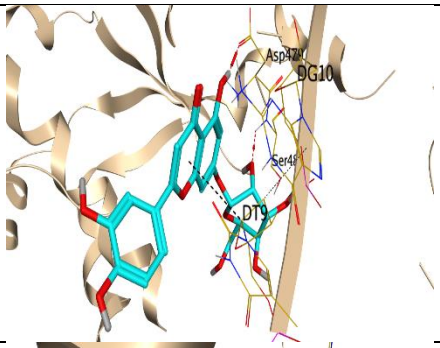
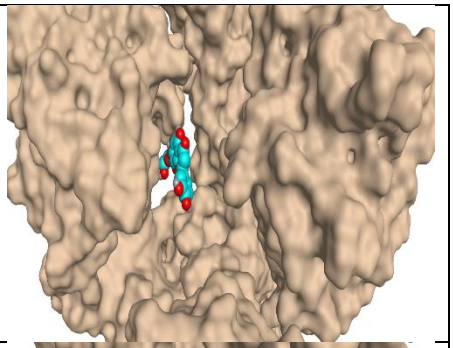
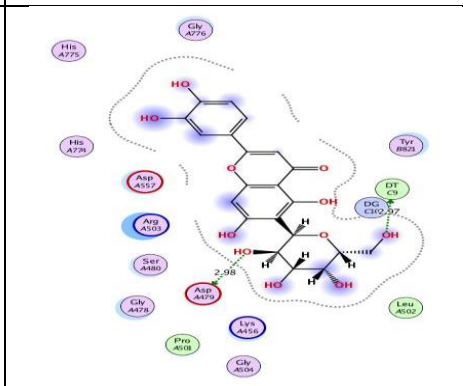
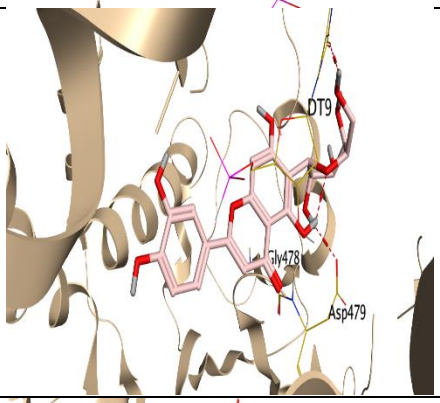
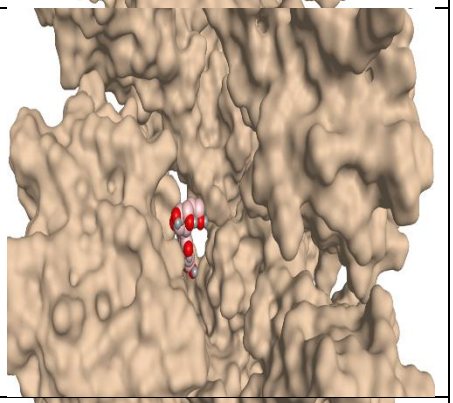
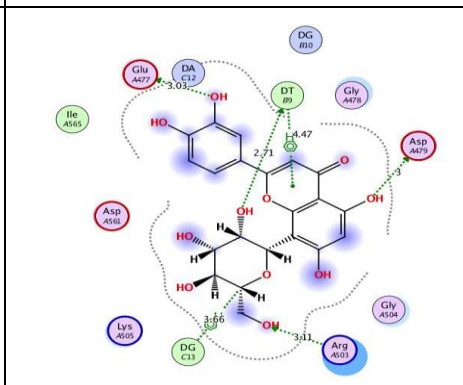
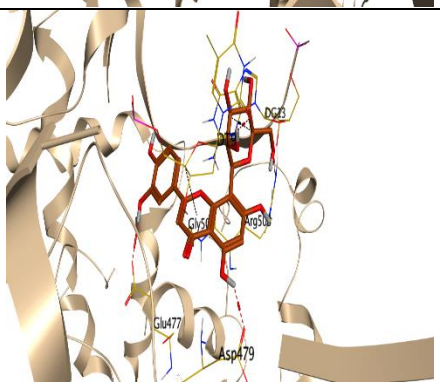
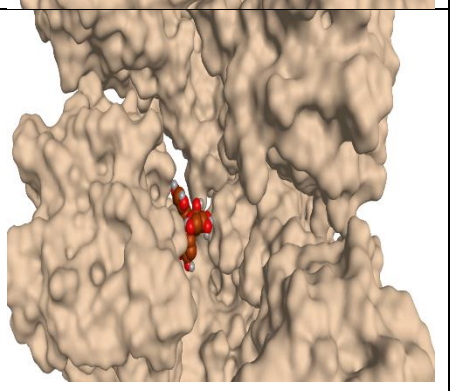
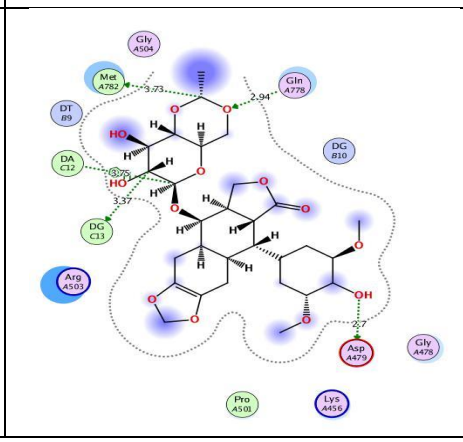
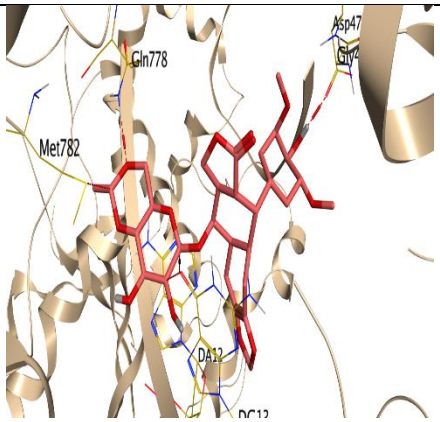
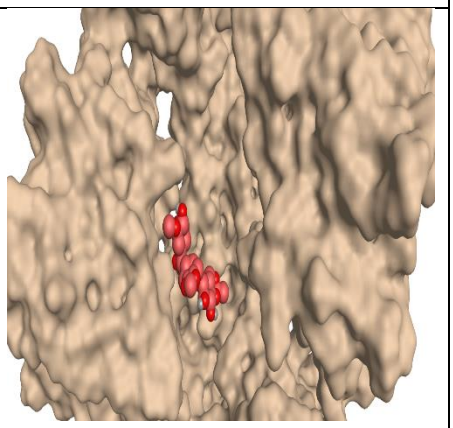
Reference			

Figure S7: the 2D, 3D, and 3D protein positioning of all investigated compound at the biological target, FAS.

TOP II			
Comp no.	**2D**	**3D**	**3D protein**
1			
2			
3			
4			

5			
6			
7			
Co-crystallized			

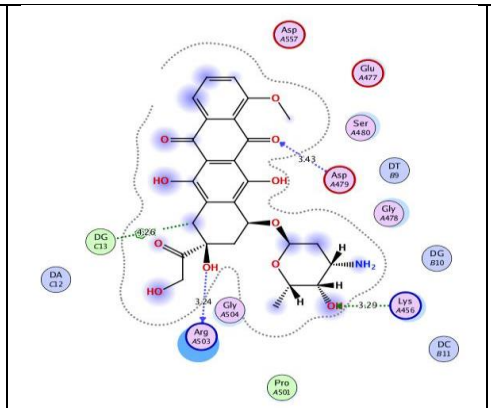
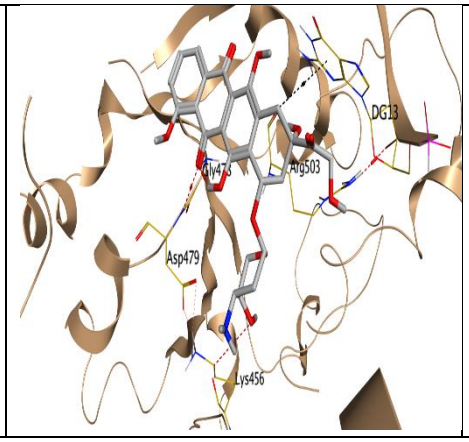
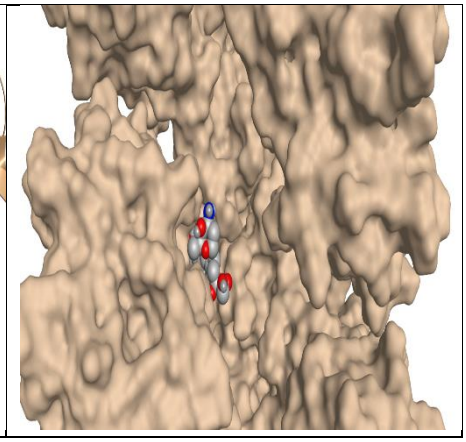
Reference			

Figure S8: the 2D, 3D, and 3D protein positioning of all investigated compound at the biological target, TOP II.