

Novel Chitosan hybrid fluorinated Thiourea derivative as Dual promising Anti-Microbial and Biofilm Agents: Tailoring Molecular Interactions, *In-silico* Toxicity, and Docking Simulation

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Supplementary material

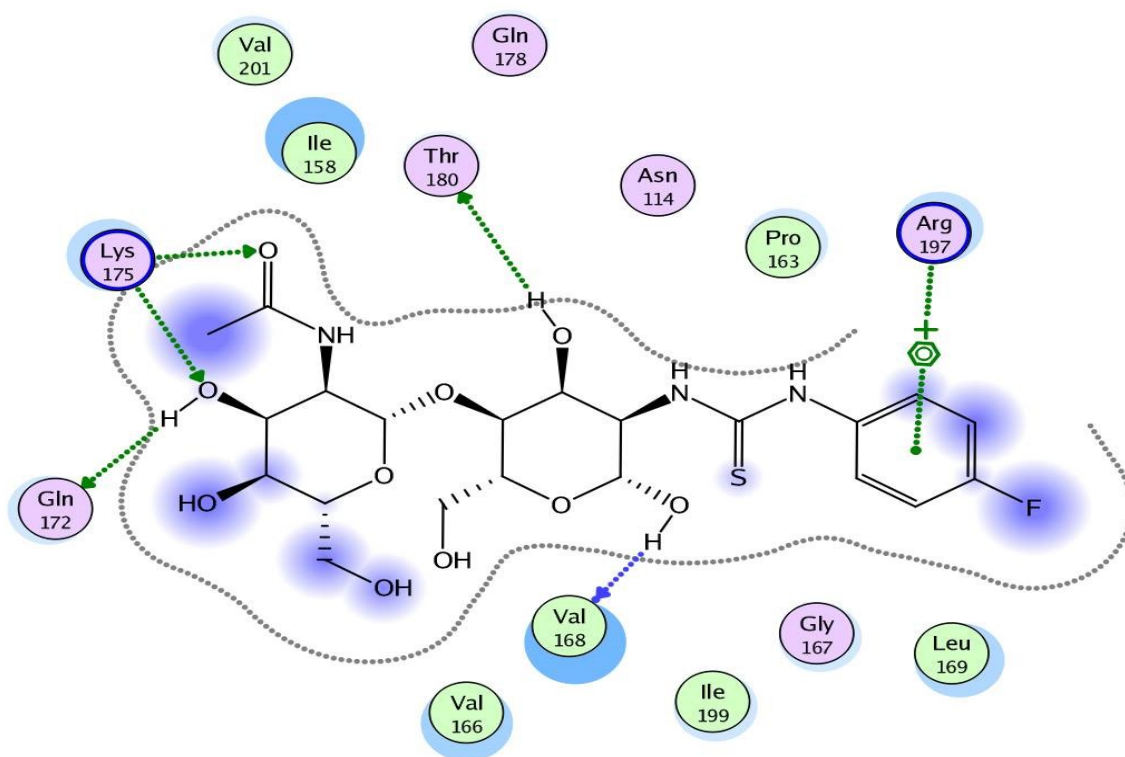


Figure (SI1): 2D docking conformation of **CHTUD1** inside the active site of Sortase A (**PDB:** 1T2P)

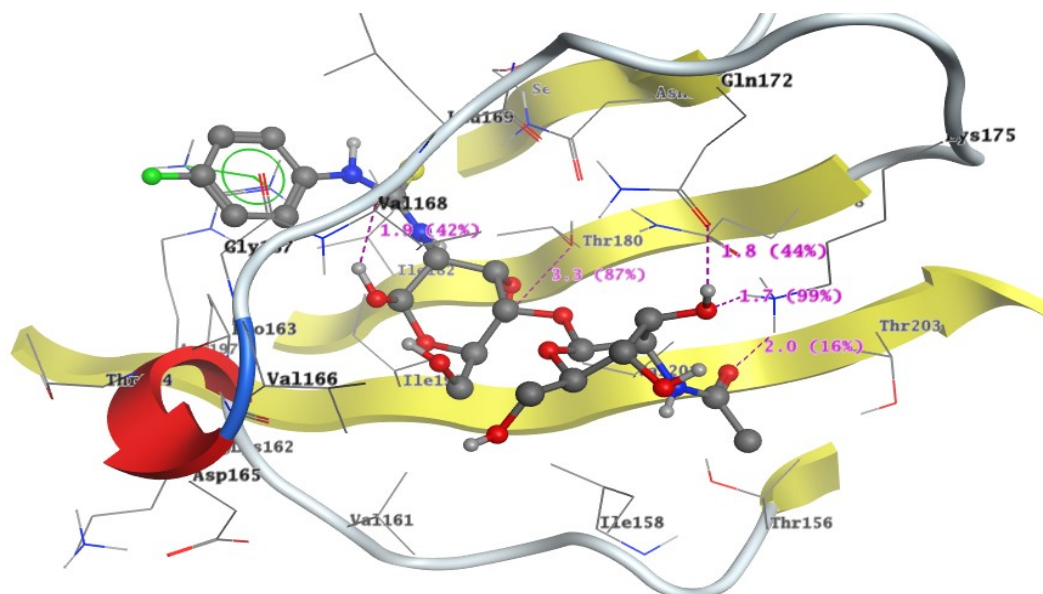


Figure (SI2): 3D docking conformation of **CHTUD1** inside the active site of Sortase A (PDB: 1T2P)

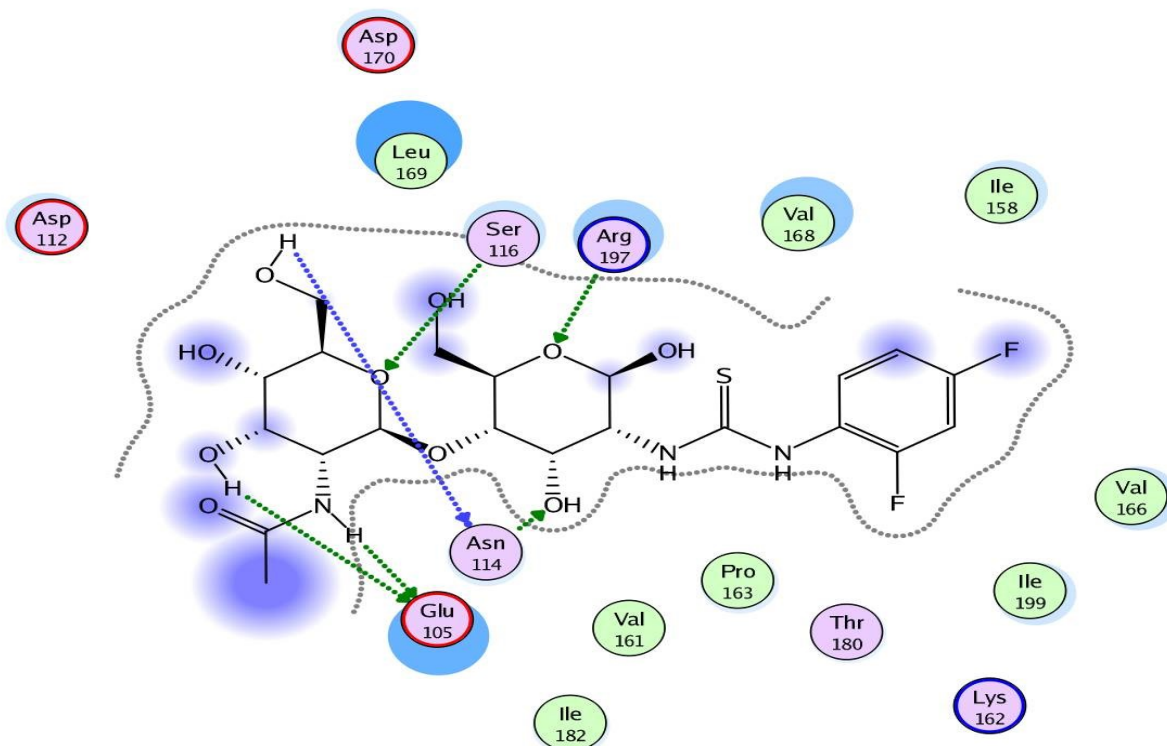


Figure (SI3): 2D docking conformation of **CHTUD2** inside the active site of Sortase A (PDB: 1T2P)

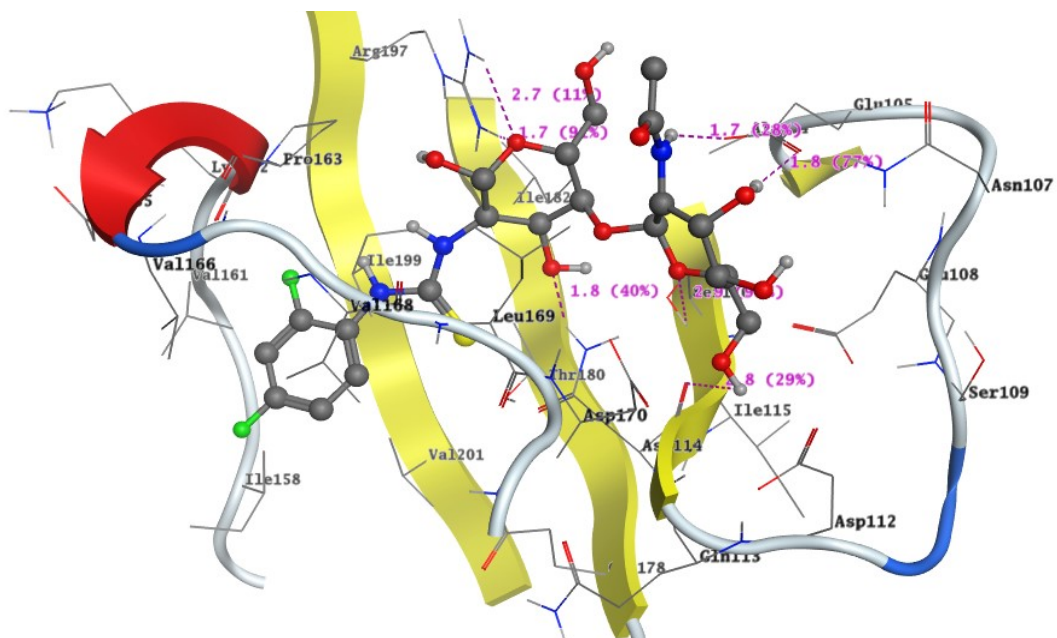


Figure (SI4): 3D docking conformation of CHTUD2 inside the active site of Sortase A (PDB: 1T2P)

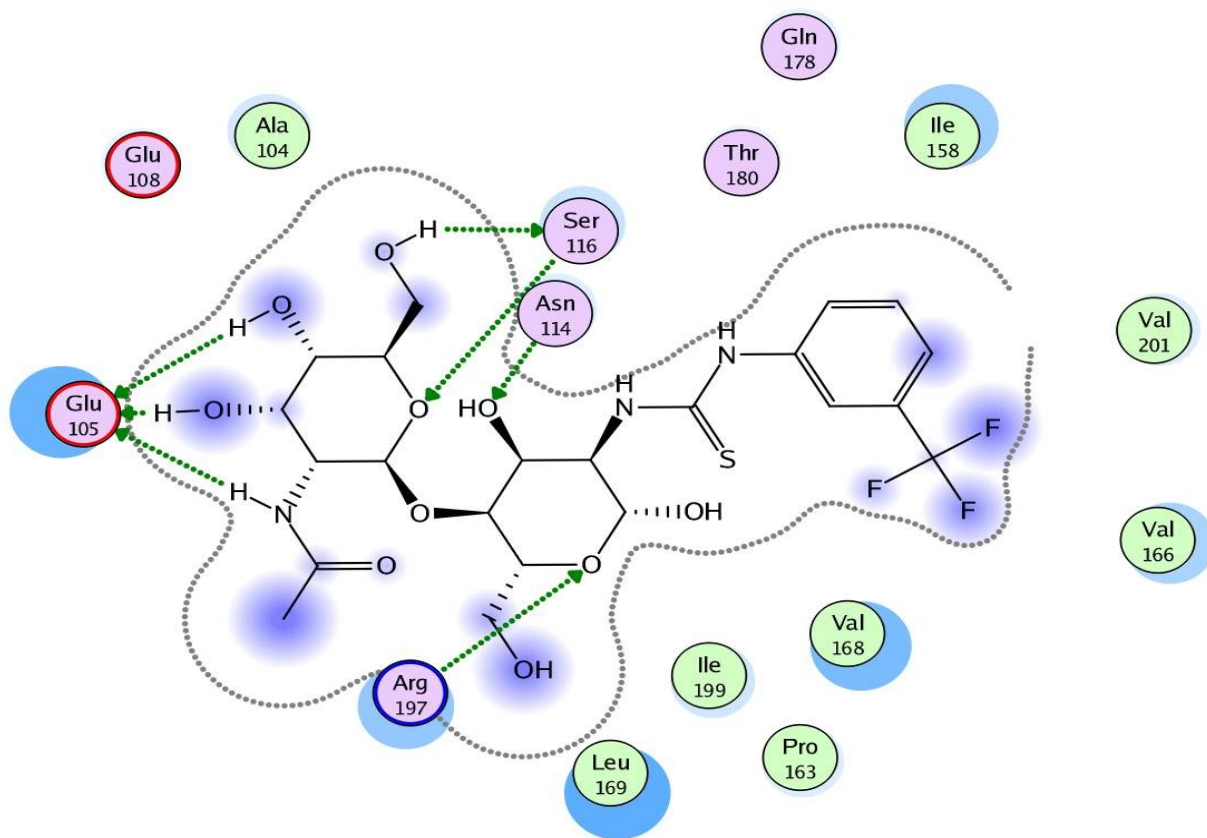


Figure (SI5): 2D docking conformation of **CHTUD3** inside the active site of Sortase A (**PDB: 1T2P**)

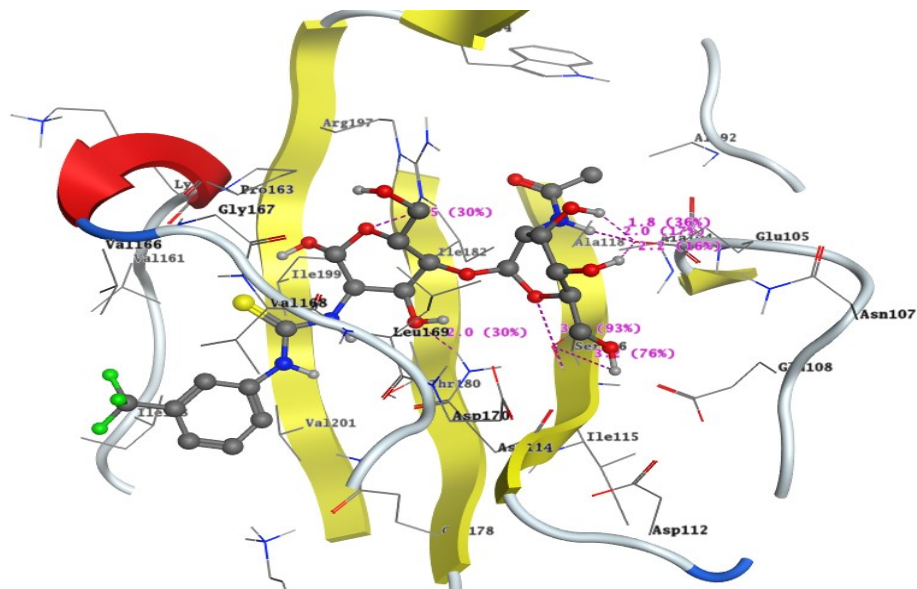


Figure (SI6): 3D docking conformation of **CHTUD3** inside the active site of Sortase A (**PDB: 1T2P**)

Docking process inside the active site of LpxC (**PDB: 4IS9**)

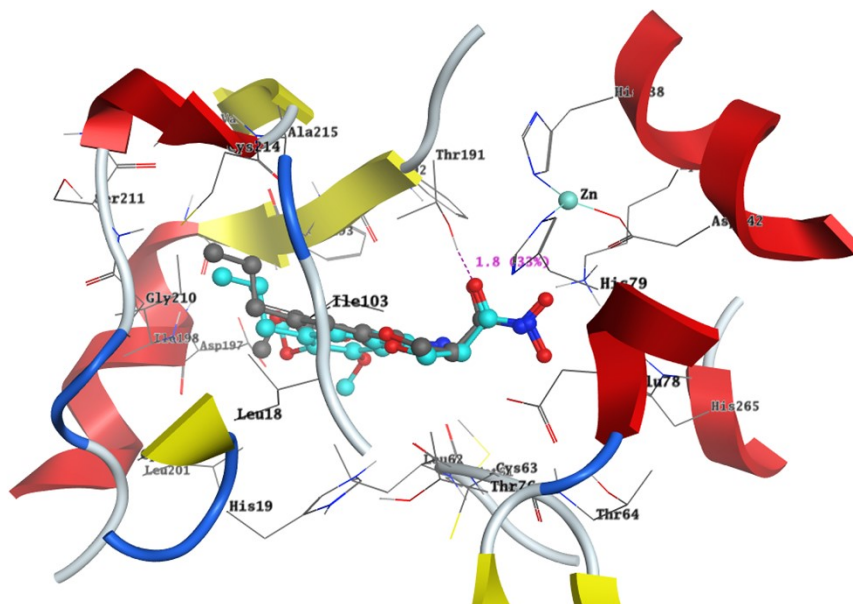


Figure (SI7): 3D docking conformation of superimposed structure of **co-crystallized ligand** inside the active site of LpxC (PDB: 4IS9)

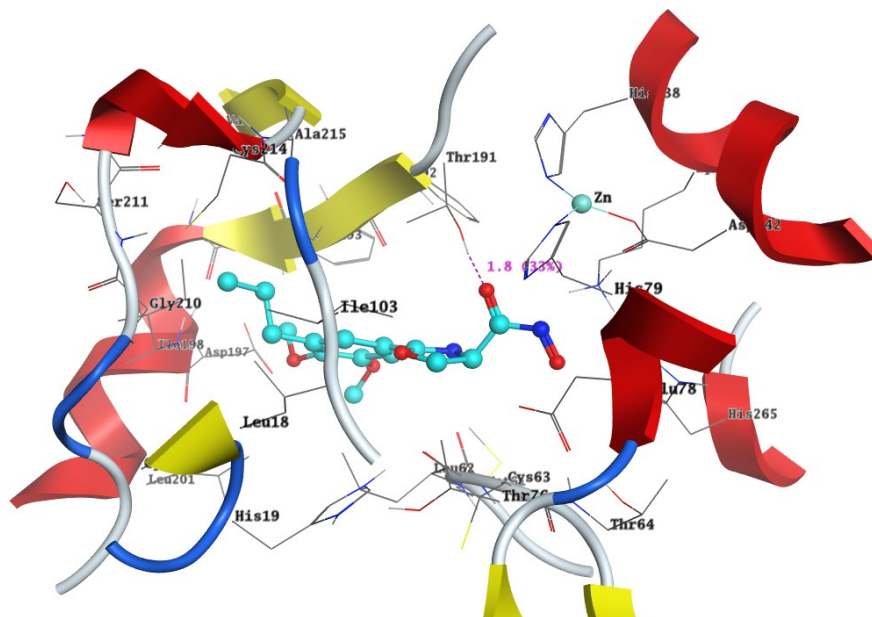


Figure (SI8): 2D docking conformation of **co-crystallized ligand** inside the active site of LpxC (PDB: 4IS9)

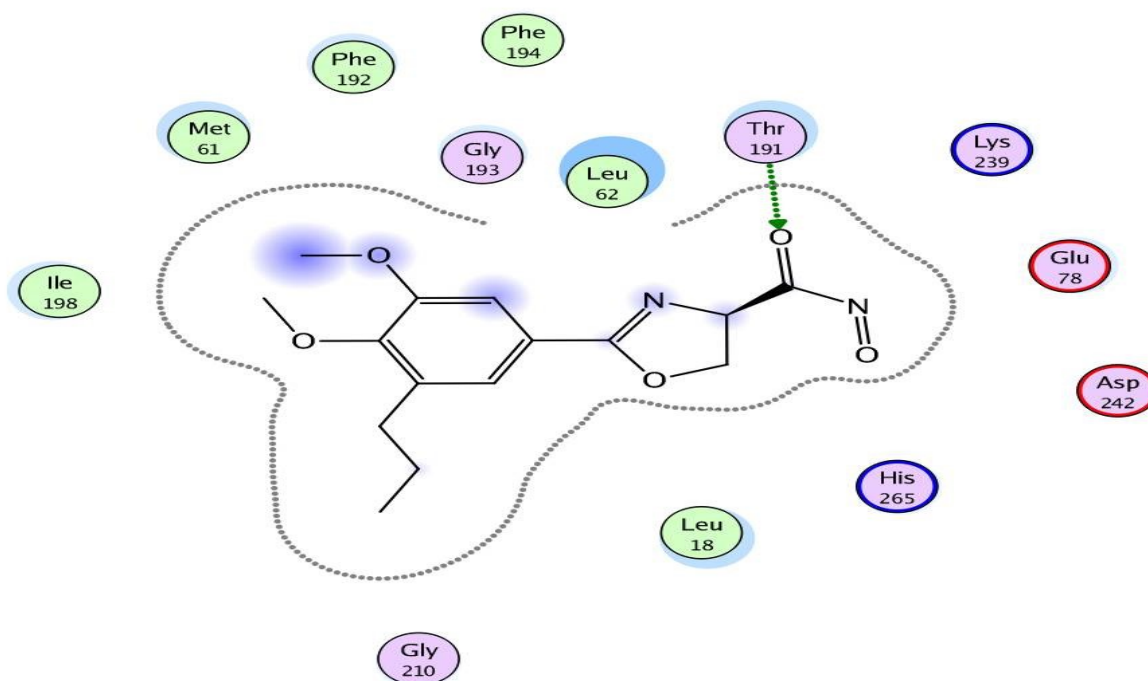


Figure (SI9): 3D docking conformation of **co-crystallized ligand** inside the active site of LpxC (PDB: 4IS9)

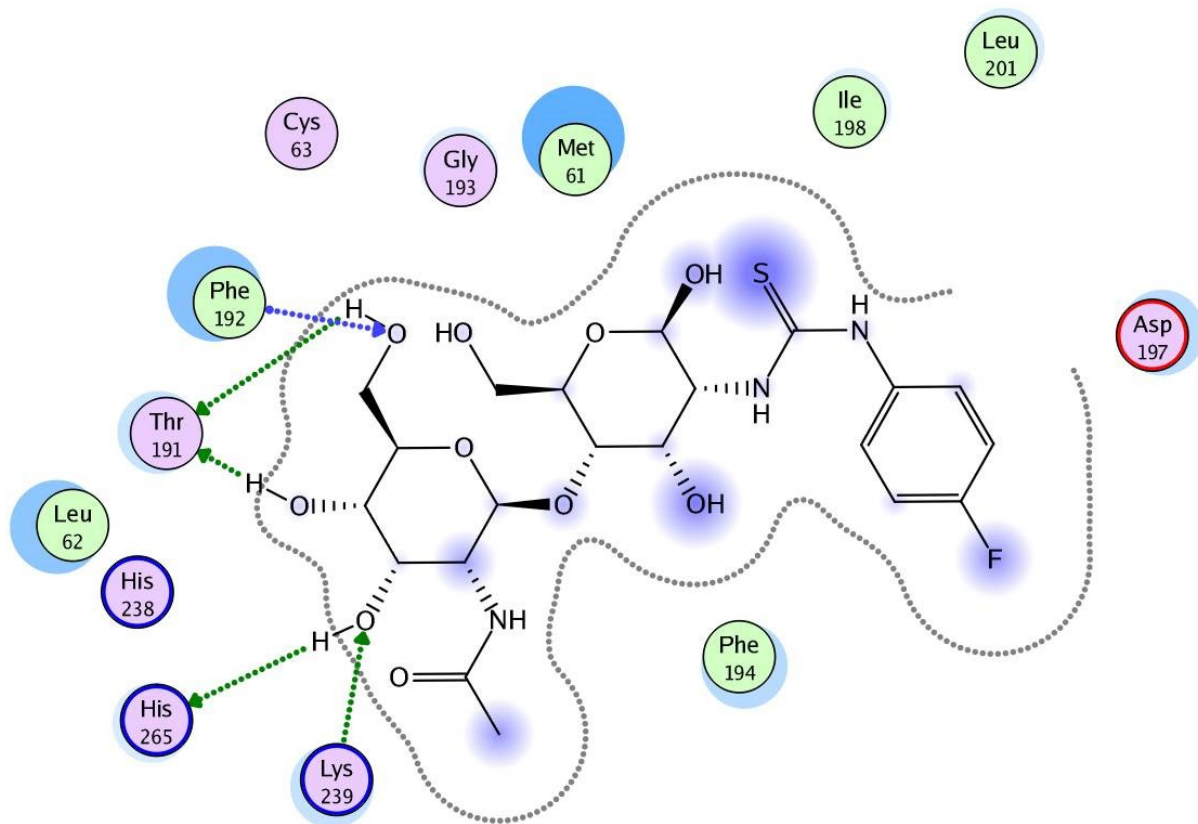


Figure (SI10): 2D docking conformation of **CHTUD1** inside the active site of **LpxC** (**PDB: 4IS9**)

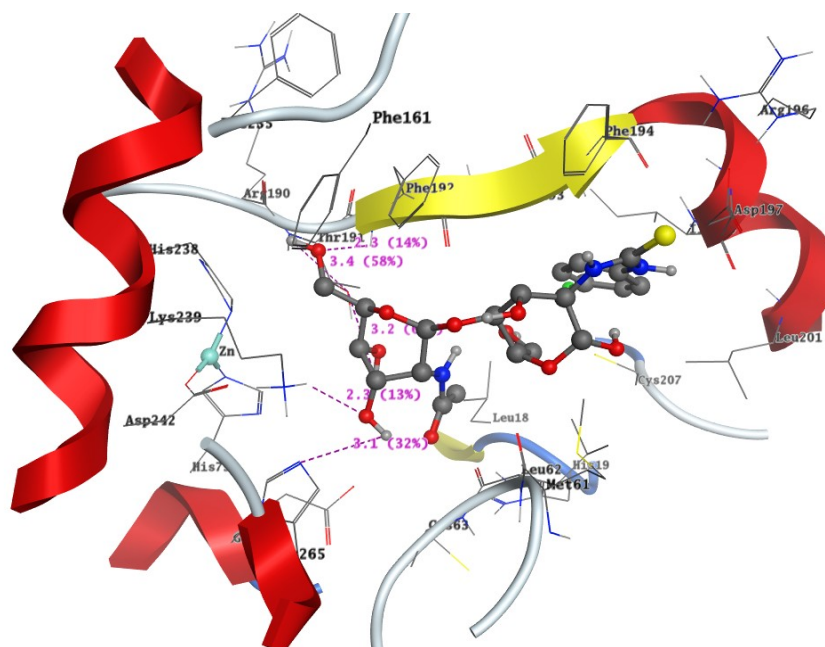


Figure (SI11): 3D docking conformation of **CHTUD1** inside the active site of LpxC (**PDB:** 4IS9)

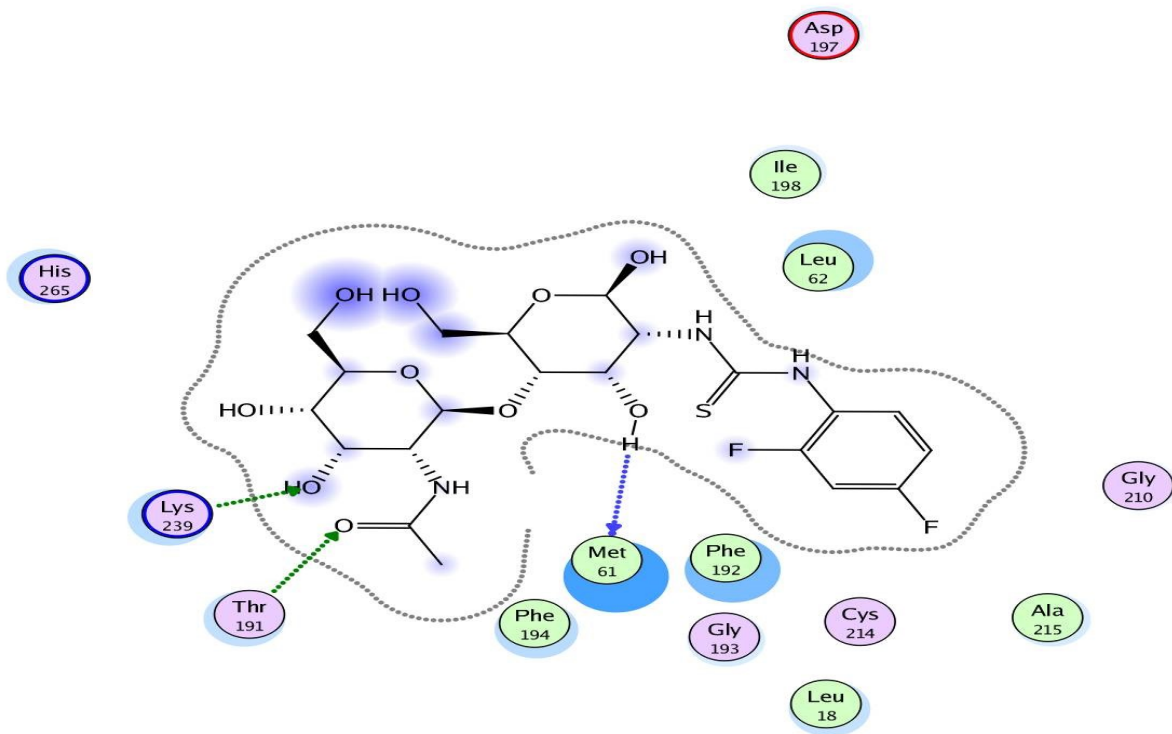


Figure (SI12): 2D docking conformation of **CHTUD2** inside the active site of LpxC (**PDB:** 4IS9)

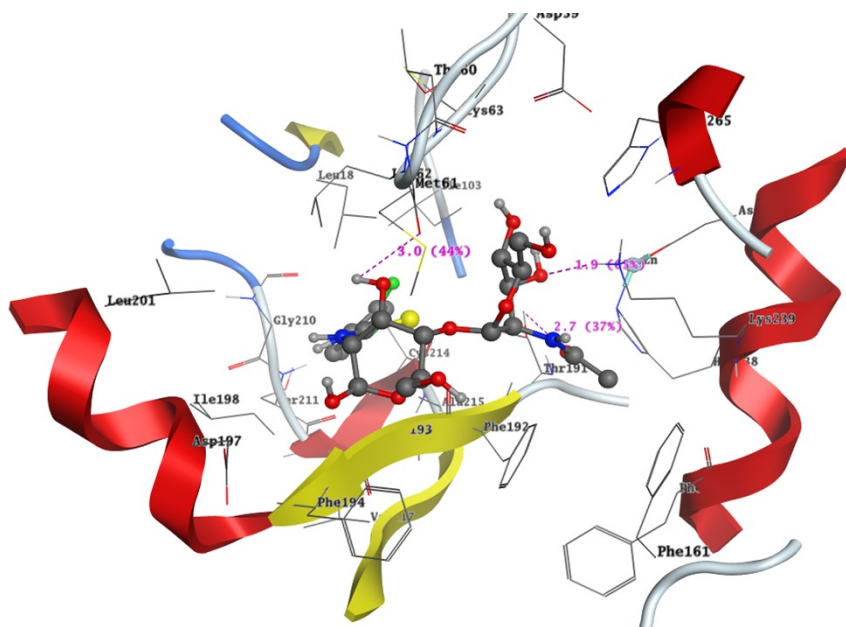


Figure (SI13): 3D docking conformation of **CHTUD2** inside the active site of LpxC (**PDB:** 4IS9)

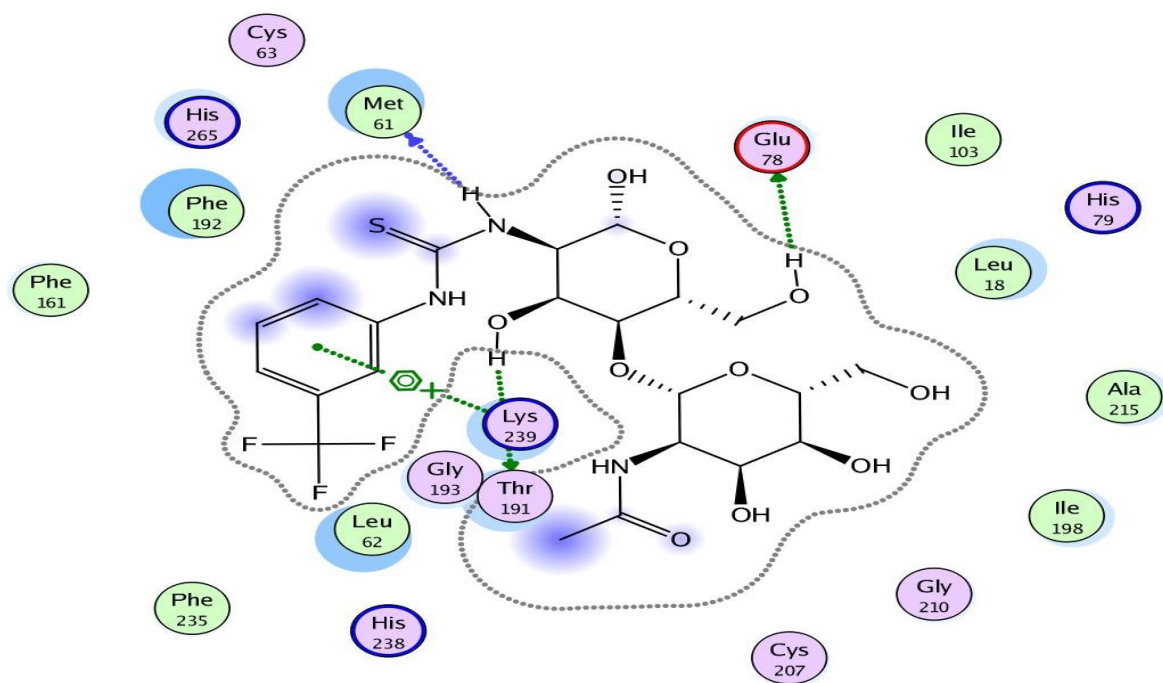


Figure (SI14): 2D docking conformation of **CHTUD3** inside the active site of LpxC (**PDB:** 4IS9)

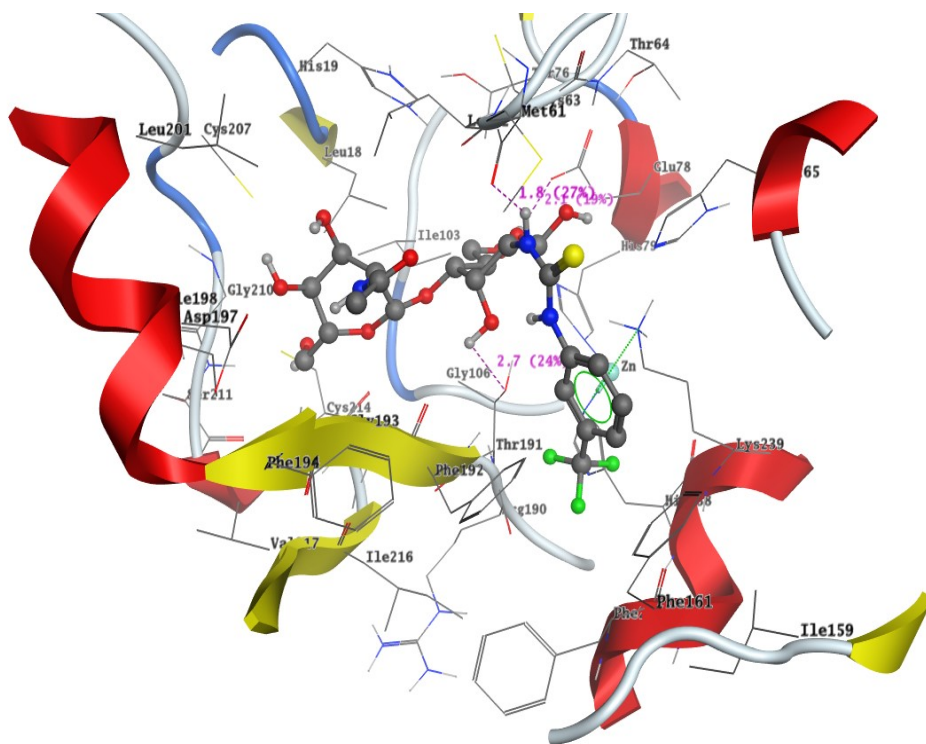


Figure (SI15): 3D docking conformation of **CHTUD3** inside the active site of LpxC (**PDB: 4IS9**)

Biofilm activity raw data

Anti Biofilm of Salmonella for sample N5	Replicate1 Ab	Replicate2 Ab	Replicate 3 Ab	Mean	Anti-Biofilm Activity %	SD
Blank (Media only)	0.012	0.008	0.005	0.008		0.004
Media+Organism(Cont.)	1.222	1.231	1.226	1.226	-	0.005
75% of MBC	0.091	0.085	0.082	0.086	93.06	0.005
50% of MBC	0.221	0.226	0.223	0.223	81.85	0.003
25% of MBC	0.314	0.315	0.318	0.316	74.31	0.002

Anti Biofilm of Salmonella for sample N7	Replicate1 Ab	Replicate2 Ab	Replicate 3 Ab	Mean	Anti-Biofilm Activity %	SD
Blank (Media only)	0.012	0.008	0.005	0.008		0.004
Media+Organism(Cont.)	1.222	1.231	1.226	1.226	-	0.005
75% of MBC	0.112	,116	0.119	0.077	93.80	0.005
50% of MBC	0.214	0.209	0.199	0.207	83.16	0.008
25% of MBC	0.289	0.291	0.295	0.292	76.27	0.003

Anti Biofilm of Salmonella for sample N6	Replicate1 Ab	Replicate2 Ab	Replicate 3 Ab	Mean	Anti-Biofilm Activity %	SD
Blank (Media only)	0.012	0.008	0.005	0.008		0.004
Media+Organism(Cont.)	1.222	1.231	1.226	1.226	-	0.005
75% of MBC	0.102	0.099	0.107	0.103	91.70	0.004
50% of MBC	0.273	0.278	0.277	0.276	77.55	0.003
25% of MBC	0.383	0.391	0.387	0.387	68.49	0.004

Anti Biofilm of Salmonella for sample CH	Replicate1 Ab	Replicate2 Ab	Replicate 3 Ab	Mean	Anti-Biofilm Activity %	SD
Blank (Media only)	0.012	0.008	0.005	0.008		0.004
Media+Organism(Cont.)	1.222	1.231	1.226	1.226	-	0.005
75% of MBC	0.116	0.118	0.122	0.119	90.39	0.003
50% of MBC	0.325	0.327	0.325	0.326	73.50	0.001
25% of MBC	0.603	0.598	0.594	0.598	51.24	0.005

Anti Biofilm of St. aureus for Sample N5	Replicate1 Ab	Replicate2 Ab	Replicate 3 Ab	Mean	Anti-Biofilm Activity %	SD
Blank (Media only)	0.01	0.007	0.002	0.006		0.004
Media+Organism(Cont.)	1.132	1.137	1.141	1.137	-	0.005
75% of MBC	0.044	0.042	0.041	0.042	96.36	0.002
50% of MBC	0.214	0.201	0.207	0.207	81.84	0.007
25% of MBC	0.313	0.311	0.308	0.311		0.003

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Anti Biofilm of St. aereus for Sample N7	Replicate 1 Ab	Replicate 2 Ab	Replicate 3 Ab	Mean	Anti-Biofilm Activity %	SD
Blank (Media only)	0.01	0.007	0.002	0.006		0.004
Media+Organism(Cont.)	1.132	1.137	1.141	1.137	-	0.005
75% of MBC	0.06	0.055	0.051	0.055	95.22	0.005
50% of MBC	0.214	0.201	0.207	0.207	82.04	0.007
25% of MBC	0.321	0.317	0.309	0.317	72.87	0.003

Anti Biofilm of St. aereus for Sample N6	Replicate 1 Ab	Replicate 2 Ab	Replicate 3 Ab	Mean	Anti-Biofilm Activity %	SD
Blank (Media only)	0.01	0.007	0.002	0.006		0.004
Media+Organism(Cont.)	1.132	1.137	1.141	1.137	-	0.005
75% of MBC	0.082	0.081	0.084	0.082	92.84	0.002
50% of MBC	0.312	0.305	0.301	0.306	73.15	0.006
25% of MBC	0.435	0.443	0.445	0.441	61.27	0.005

Anti Biofilm of St. aereus for Sample CH	Replicate 1 Ab	Replicate 2 Ab	Replicate 3 Ab	Mean	Anti-Biofilm Activity %	SD
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					y %	
Blank (Media only)	0.01	0.007	0.002	0.006		0.00 4
Media+Organism(Cont.)	1.132	1.137	1.141	1.137	-	0.00 5
75% of MBC	0.102	0.111	0.105	0.106	90.76	0.00 5
50% of MBC	0.345	0.354	0.348	0.349	69.37	0.00 5
25% of MBC	0.861	0.864	0.858	0.861	24.30	0.00 3