SUPPLEMENTARY INFORMATION

Synthesis, Structural Characterization and Computational Studies of Novel Co(II) and Zn(II) Fluoroquinoline Complexes for antibacterial and antioxidant Activities

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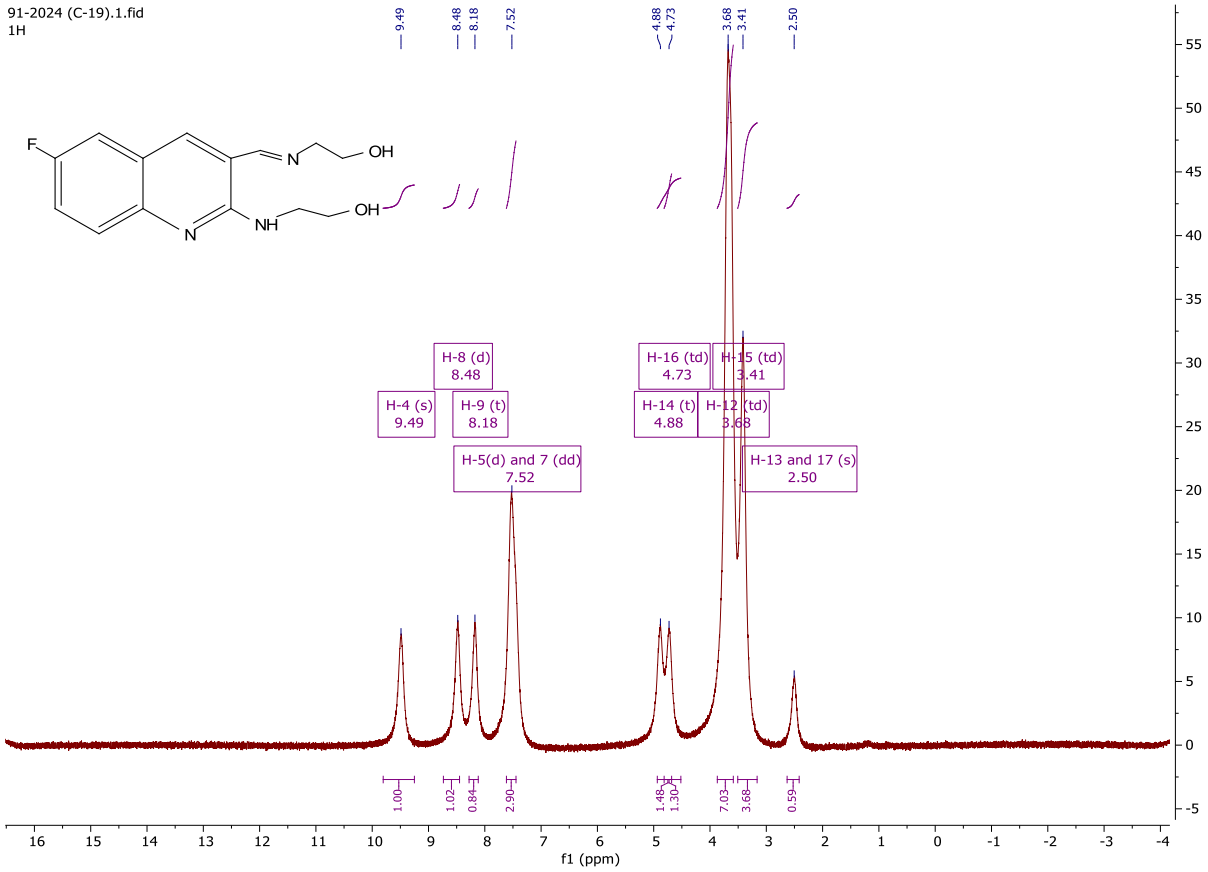

Figure S1. ^{1}HNMR spectrum of (**H_2L**), (*E*)-2-(((6-fluoro-2-((2-hydroxyethyl)amino)quinolin-3-yl)methylene)amino)ethanol

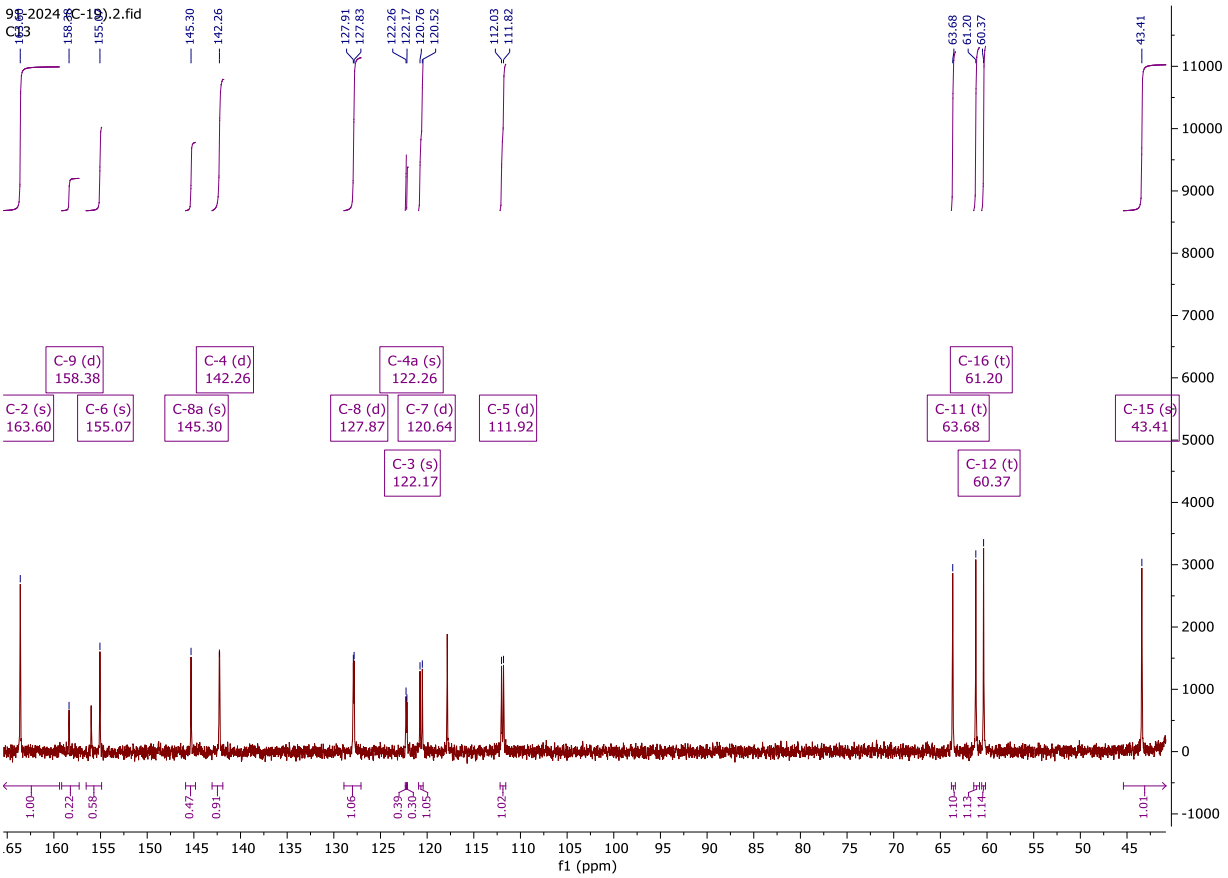

Figure S2. ^{13}CNMR C) DEPT-135 spectrum of (**H_2L**), (*E*)-2-(((6-fluoro-2-((2-hydroxyethyl)amino)quinolin-3-yl)methylene)amino)ethanol

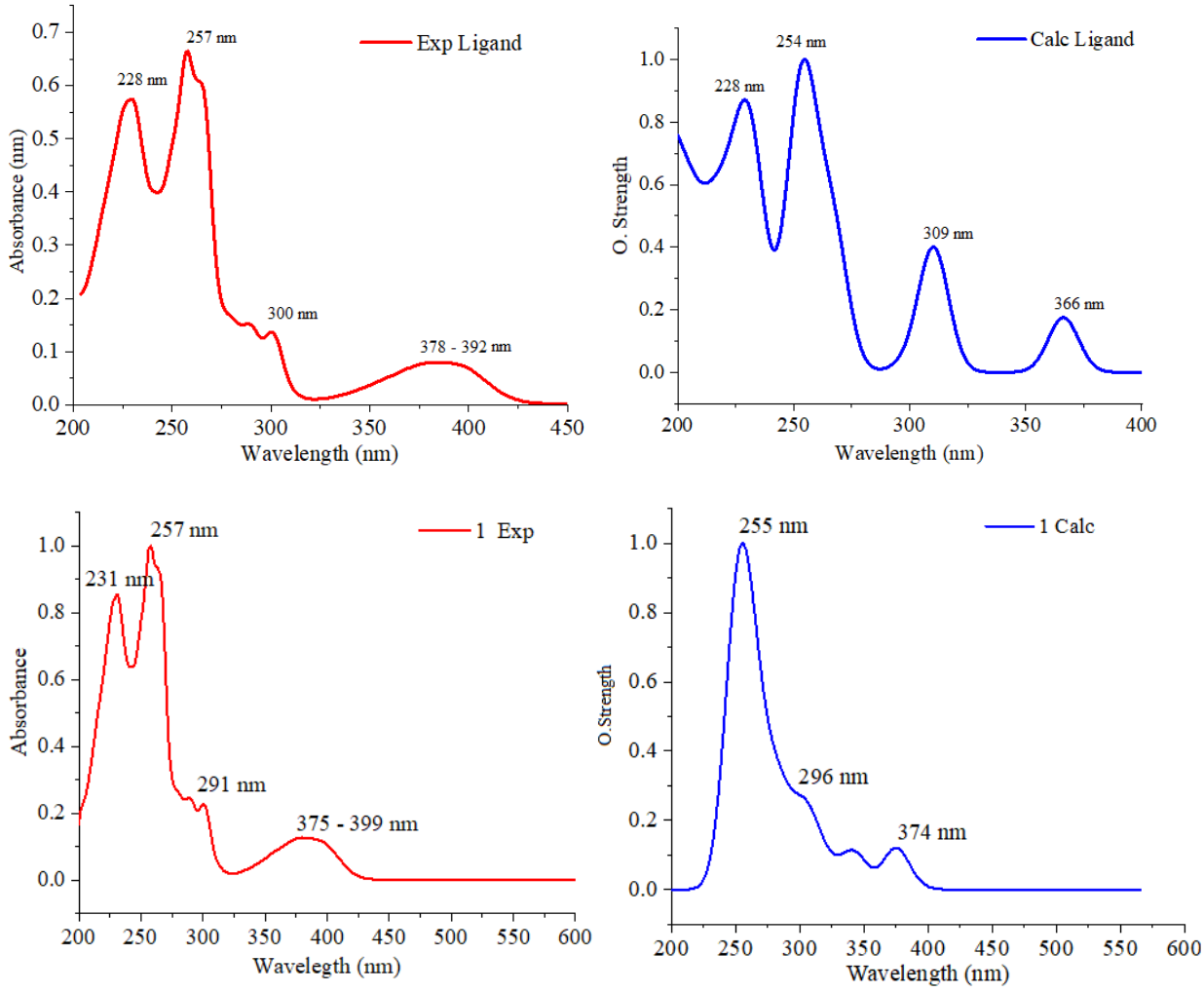

Figure S3. Comparison of the experimental absorption wavelengths with the corresponding TD-B3LYP-GD3/6–311++G (d,p)/LanL2DZ/IEF-PCM/methanol calculated results of the ligand (H_2L) and the Zn(II) (**1**) complexes. The calculated were red shifted by 20 nm comparison with the experimental results.

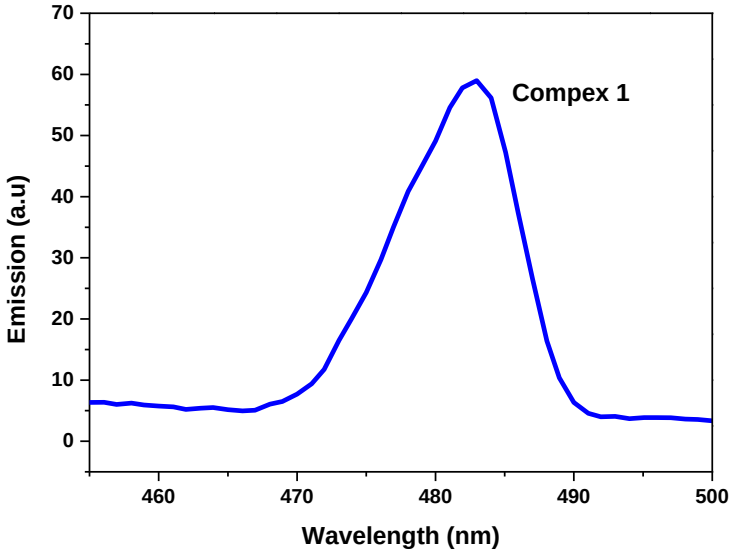

Figure S4. Fluorescence spectra of complex **1**

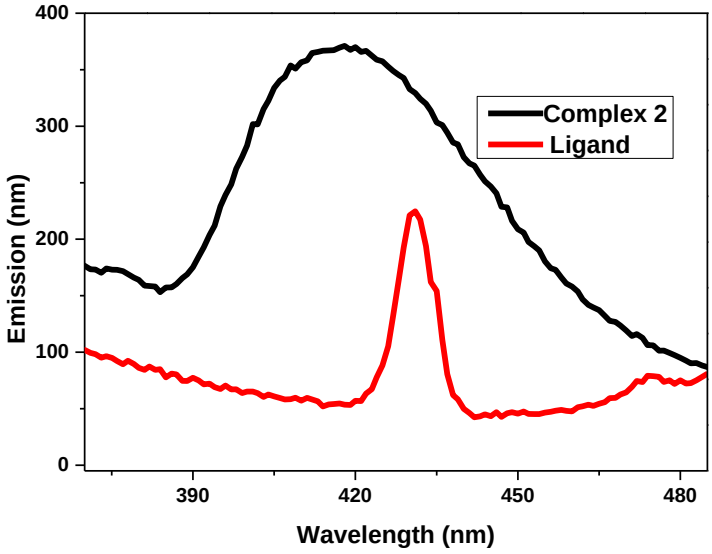

Figure S5. Emission spectra of complex ligand and complex **2**

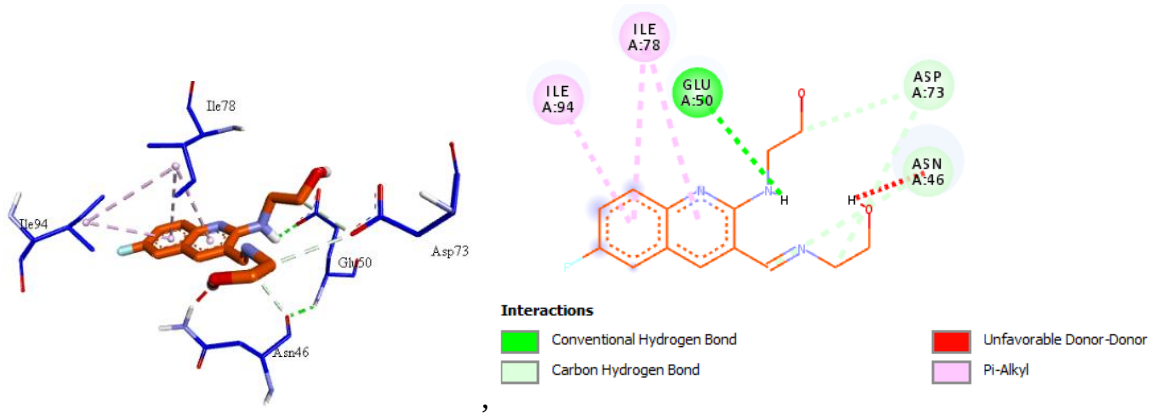

Figure S6. The 3D and 2D binding interactions of ligand against *E. coli DNA gyrase B (PDB ID:*

6F86).

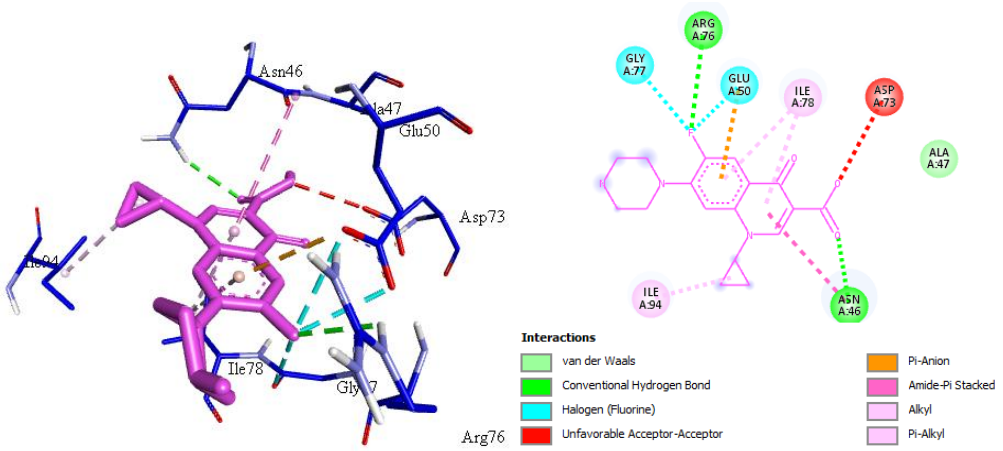

Figure S7. The 3D and 2D binding interactions of ciprofloxacin against *E. coli* DNA gyrase B (PDB ID: 6F86).

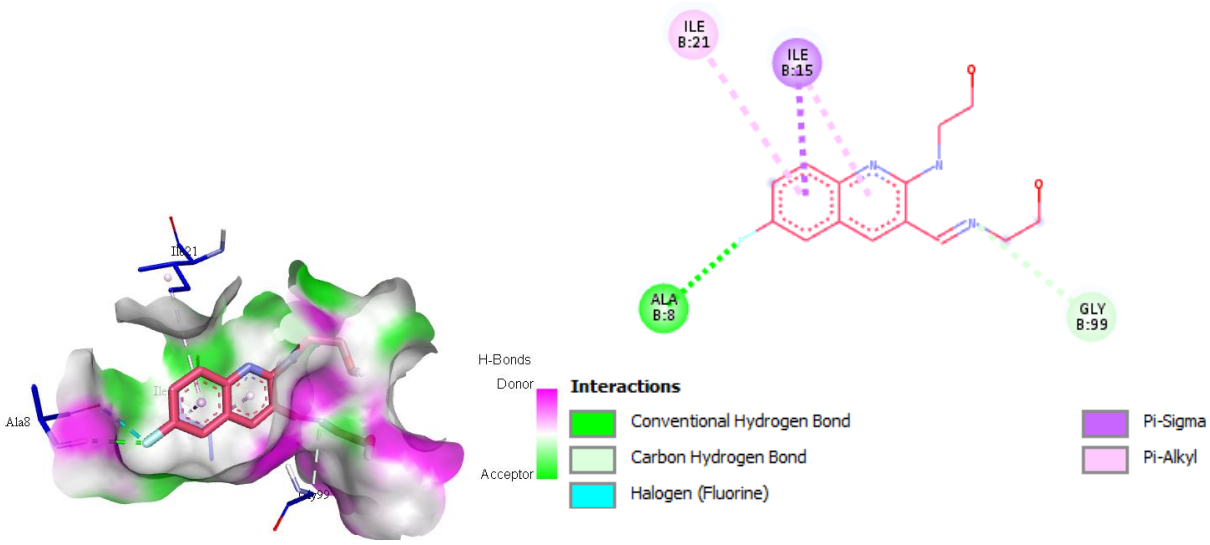

Figure S8. The 3D and 2D binding interactions of Ligand against *E.coli against dihydrofolate reductase B (7r6g) (PDB ID 5fsa)*

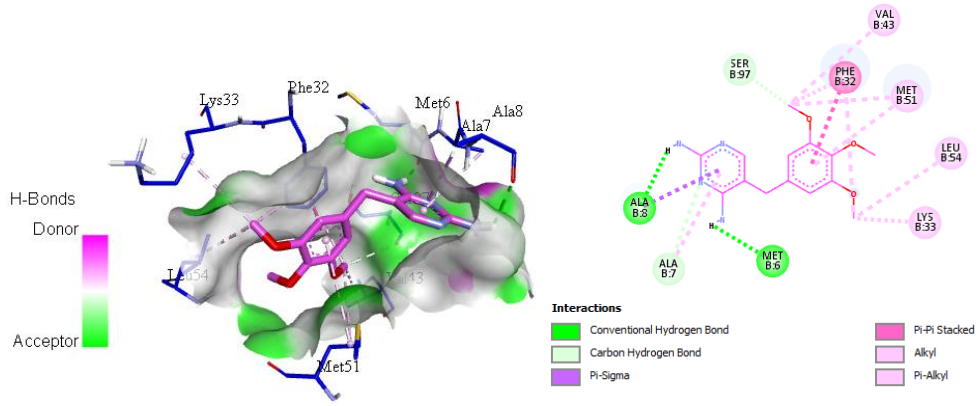

Figure S9.The 3D and 2D binding interactions of Trimethoprim against *E.coli against dihydrofolate reductase B (7r6g) (PDB ID 5fsa)*

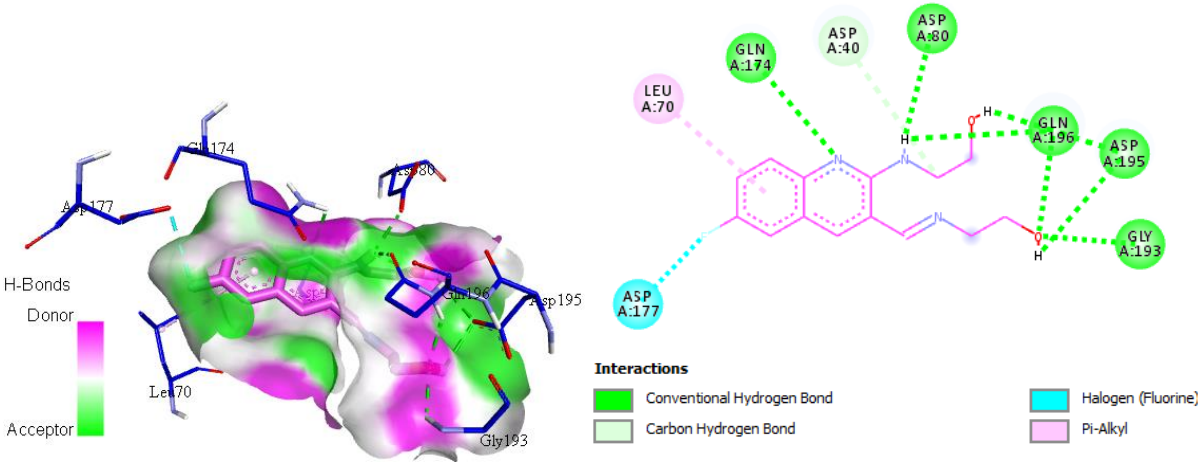

Figure S10. The 3D and 2D binding interactions of ligand against *Staphylococcus aureus tyrosyl-*

tRNA synthetase.

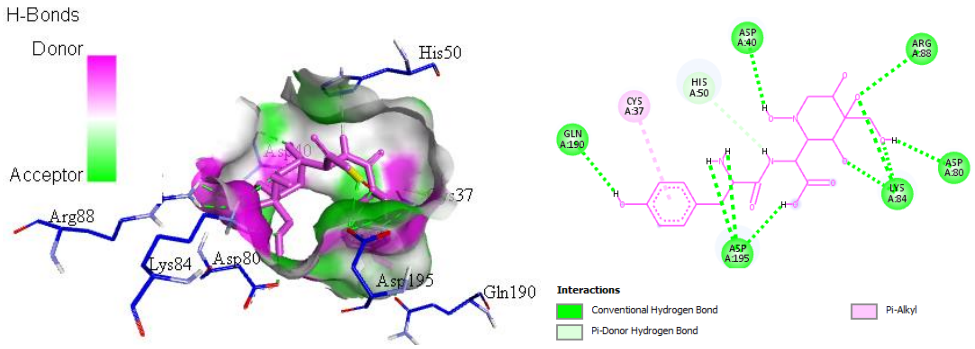

Figure S11. The 3D and 2D binding interactions of [2-amino-3-(4-hydroxy-phenyl)-propionylamino]-(1,3,4,5-tetrahydroxy-4-hydroxymethyl-piperidin-2-yl)- acetic acid (SB-239629) against *Staphylococcus aureus tyrosyl-tRNA synthetase*

Table S1. Mean inhibition zone of complexes (**1 – 2**) in mm (mean ± SD).

Bacterial strains	**Conc. (µg/mL)**	**Compounds**			
		1	**2**	**H_2L**	**Ciprofloxacin**
E.coli	100	18.33 ± 0.62	13.17 ± 0.36	11.21± 0.11	20.00 ± 0.76
	200	19.84 ± 0.81	14.57 ± 0.90	11.32 ± 0.13	22.22 ± 0.66
P. aeruginosa	100	15.75 ± 0.38	12.49 ± 0.44	9.57 ± 0.75	18.71 ± 0.90
	200	17.45 ± 0.46	13.55 ± 0.73	10.40 ± 0.66	19.38 ± 0.49
S. aureus	100	17.55 ± 0.69	16.17 ± 0.97	NA	19.09 ± 0.55
	200	18.41 ± 0.55	19.98 ± 0.85	NA	20.90 ± 0.67
S. pyogenesis	100	13.67 ±	9.40 ± 0.68	9.77 ± 0.33	18.00 ± 0.63
	200	14.82 ± 0.58	10.81 ± 0.91	10.21 ± 0.92	19.07 ± 0.83

Table S2. Percentage radical scavenging activity and IC_{50} of the compounds (mean ± SD).

(µg/mL)	Ligand(**H_2L**)	**Complex 1**	**Complex 2**	**A/A**
150	67.98 ±0.42	84.25±.50	74.67±0.62	88.81±0.45
135	64.61±0.53	80.7±0.56	74.28±0.5	86.43±0.52
120	63.19±0.46	79.59±0.78	73.61±0.46	85.45±0.56
105	60.81± 0.52	76.89±0.47	70.70±0.42	81.76±0.74
90	58.31±0.46	75.82±0.36	69.82±0.46	79.67±0.83
75	57.65±0.37	70.54±0.40	68.53±0.57	75.55±0.49
60	56.45±0.55	69.72±0.33	67.38±0.45	70.9±0.81
45	53.10±0.44	68.05±0.80	67.08±0.64	57.60±0.73
30	48.60±0.50	60.58±0.71	56.71±0.50	50.70±0.59
15	47.71±0.47	45.97±0.65	44.83±0.60	49.76±0.60
1	46.59±0.52	39.55±0.62	34.44±0.53	48.55±0.61
IC_{50}(µg/mL)	27.5	6.96	15.02	4.69

Table S3. The minimum binding energy and interacting amino acids in the molecular docking of complexes and ligands and against *E. coli dihydrofolate reductase* B (PDB ID: 7r6g)

Compounds	**Binding energy (kcal/mol)**	**H-bond**	**Hydrophobic/ Pi –sigma/ anion**
Complex 1	-9.9	Ala-8, Ser-97, Tyr-103	Ile-21, Glu-28, Phe-32, Met-51, Gly-52
Complex 2	-8.0	Trp-23, Gln-29	Ile-21, Phe-32, Met-51
Ligand	-7.1	Ala-8, Gly-99	Ile-15, Ile-21
Trimethoprim	-7.3	Ala-8, Met-6, Ala-7, Ser-97	Phe-32, Lys-33, Val-43, Met-51, Leu-54,