Supplementary information on molecular docking analysis of the synthesized compounds

Table **1**. Molecular docking value of **4**-**17** against *S. aureus* DNA gyraseB

Compounds	Affinity (kcal/mol)	H-bond	Receptor interactions
4	-4.8	Ser-438, Asp-437	Arg-1122, Glu-435, Phe-1123, Gly-436, Asp-508
5	-5.1	Arg-1122, Ser-438	Glu-435, Phe-1123, Asp-508, Asp-512, Lys-460, Ile-516, Gly-459
6	-5.2	Arg-1122, Ser-438	Glu-435, Phe-1123, Asp-512, Lys-460, Ile-516
7	-5.4	Arg-1122, Ser-438	Glu-435, Phe-1123, Asp-512, Asp-437, Gly-459, Gly-436, Lys-460
8	-5.4	Arg-1122	Glu-435, Phe-1123, Asp-508, Asp-510, Gly-459
11	-6.7	Arg-1122, Ser-438, Gly-459	Arg-458, Asp-437, Glu-435, Asp-508, Phe-1123, Gly-436, Leu-457
14	-5.2	Ser-438	Arg-1122, Glu-435, Phe-1123, Gly-436, Asp-437, Asp-508
15	-5.3	Arg-1122, Ser-438	Glu-435, Phe-1123, Gly-459, Ile-516, Lys-460, Asp-512, His-1081
16	-5.2	Arg-1122, Ser-438	Glu-435, Phe-1123, Asp-512, Lys-460, Ile-516, Gly-459
17	-5.4	Arg-1122, Ser-438	Glu-435, Phe-1123, Asp-508, His-1081, Asp-512, Lys-460, Ile-516, Gly-459
Ciprofloxacin	-6.5	Arg-1122, Ser-438	Glu-435, Asp-512, Arg-1033, His-1081, Asp-508, Phe-1123, Gly-436, Ala-439

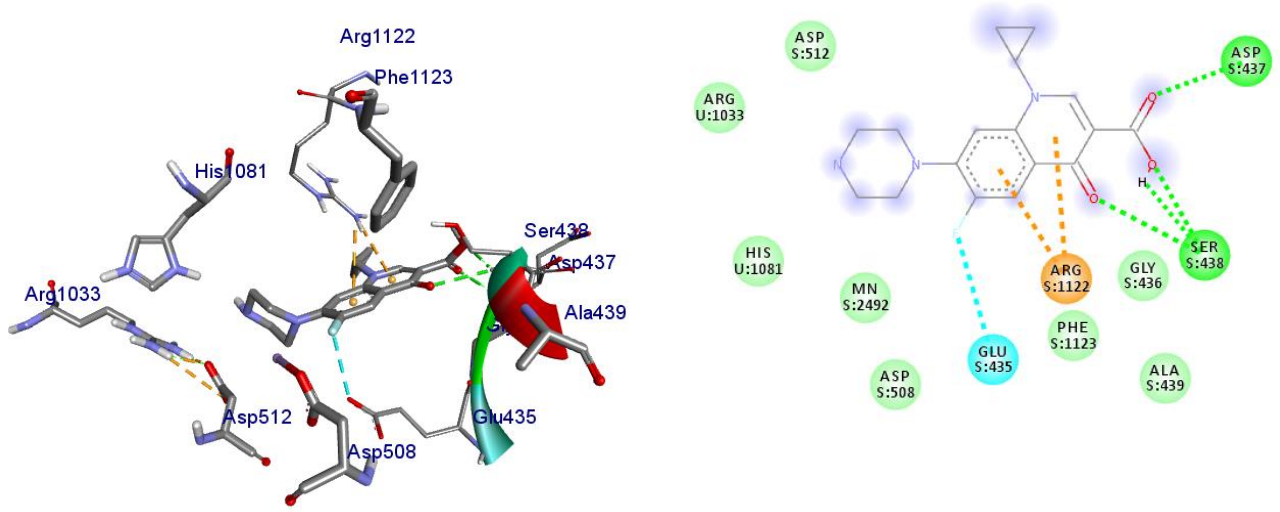


Fig 1. The binding interactions of Ciprofloxin against *S. aureus* DNA gyrase (PDB ID: 2XCT).

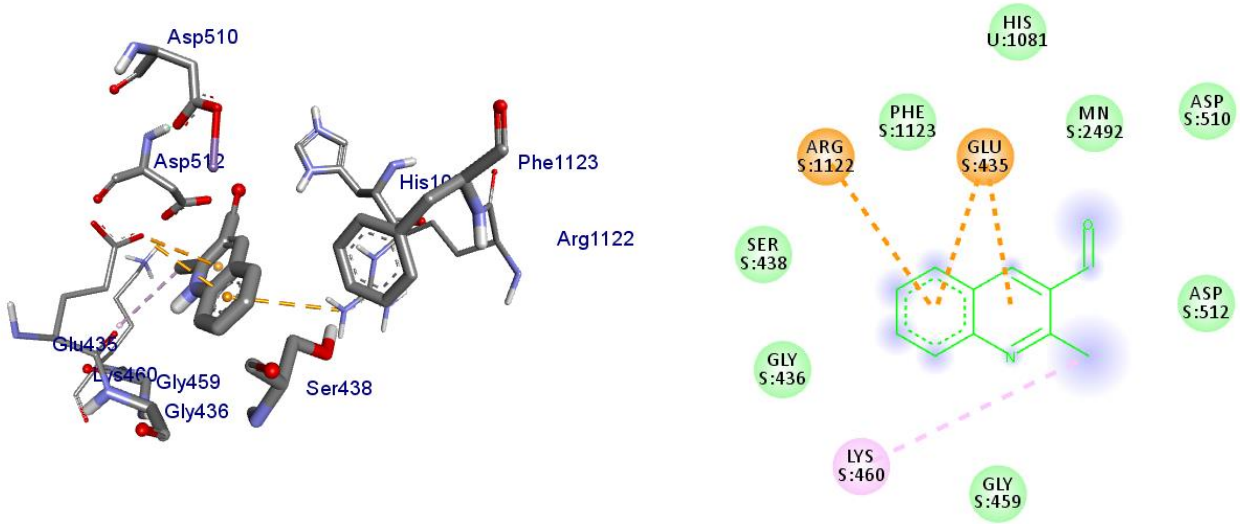


Fig 2. The binding interactions of compound **4** against *S. aureus* DNA gyrase (PDB ID: 2XCT).

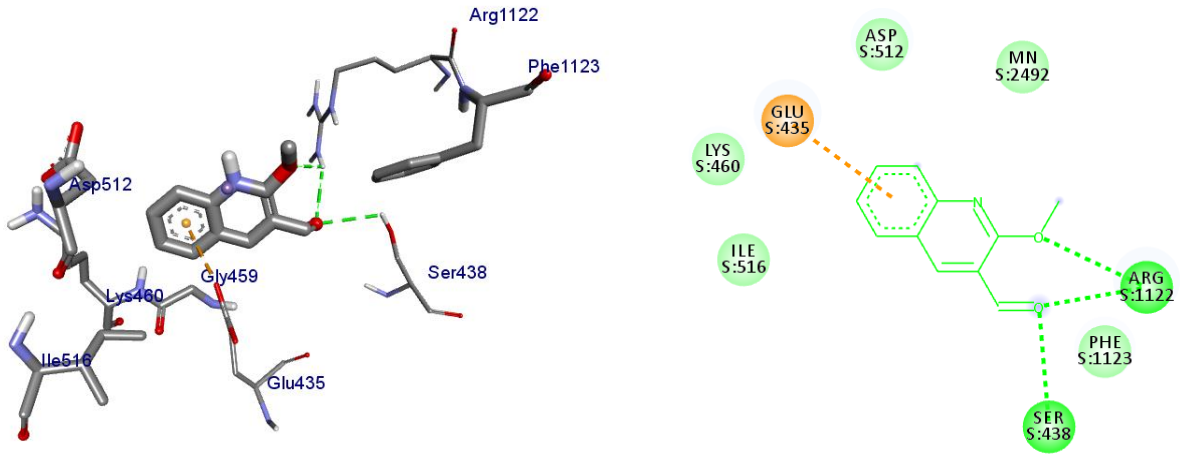


Fig 3. The binding interactions of compound 5 against *S. aureus* DNA gyrase (PDB ID: 2XCT).

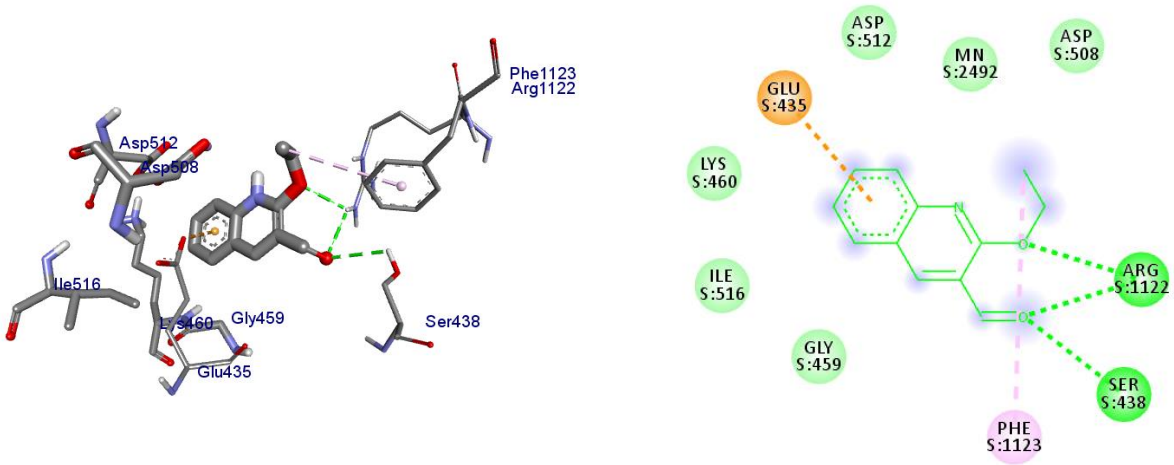


Fig 4. The binding interactions of compound 6 against *S. aureus* DNA gyrase (PDB ID: 2XCT).

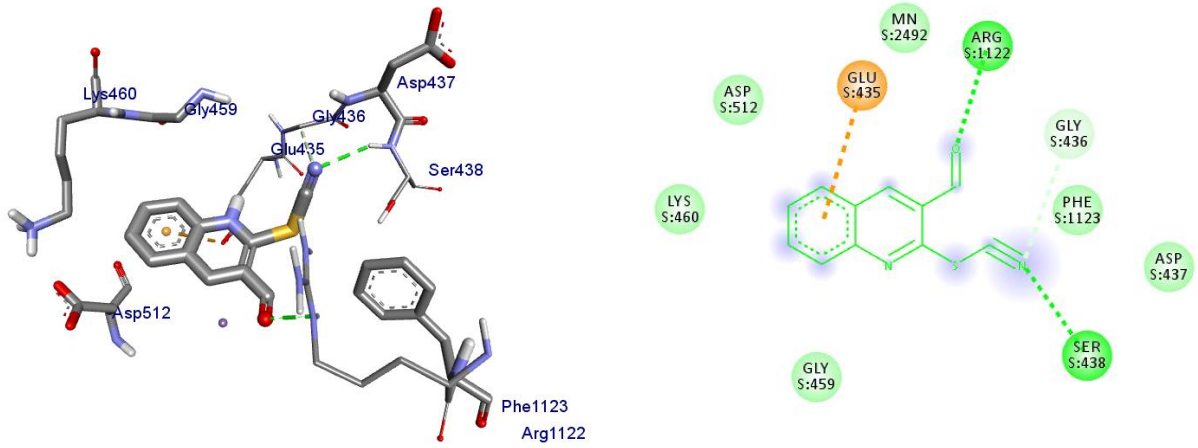


Fig 5. The binding interactions of compound 7 against *S. aureus* DNA gyrase (PDB ID: 2XCT).

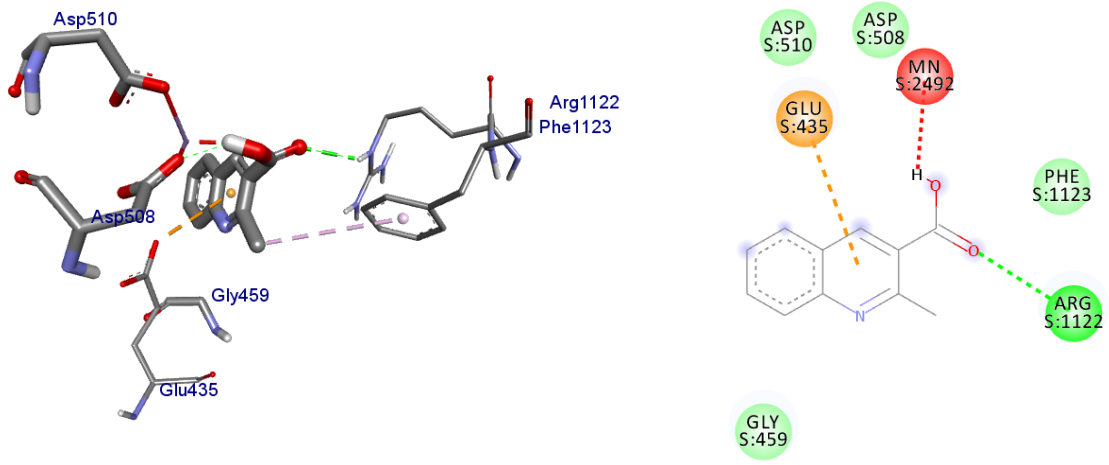


Fig 6. The binding interactions of compound **8** against *S. aureus* DNA gyrase (PDB ID: 2XCT).

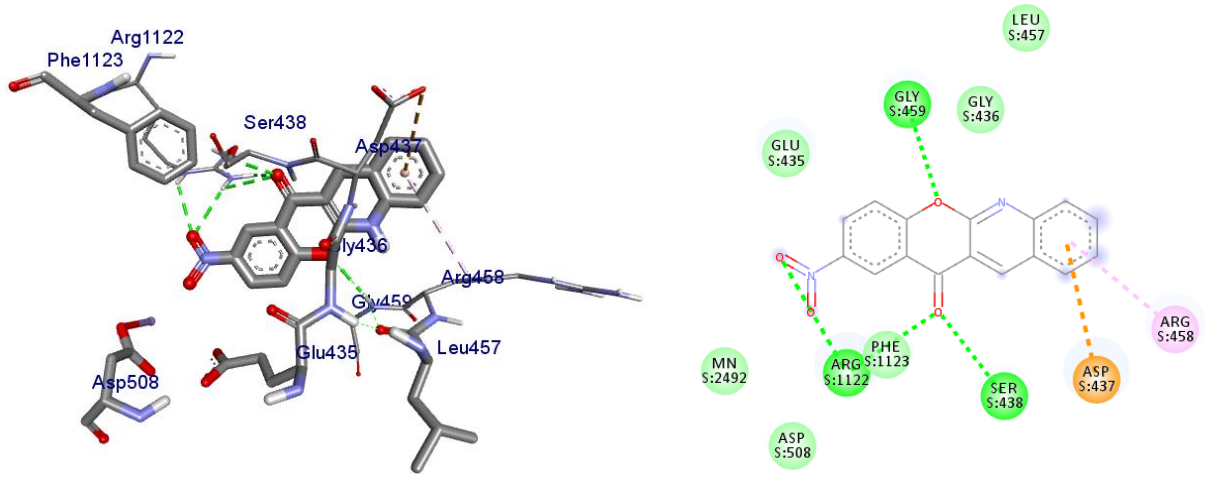


Fig 7. The binding interactions of compound **11** against *S. aureus* DNA gyrase (PDB ID: 2XCT).

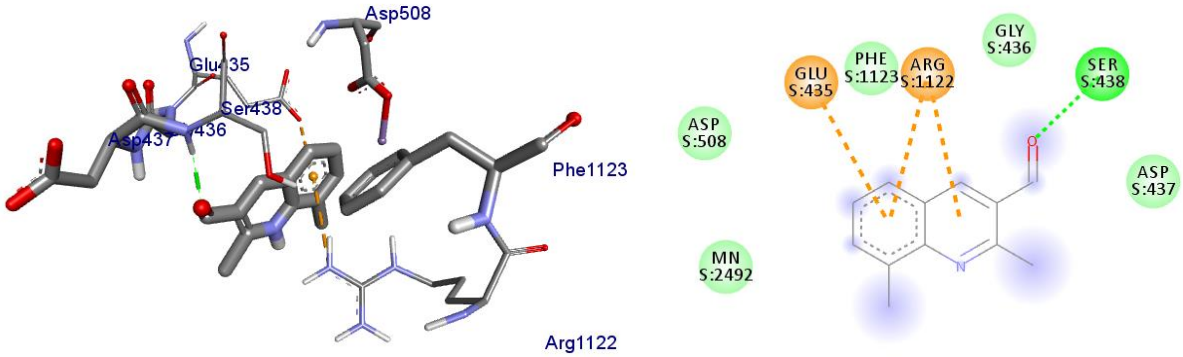


Fig 8. The binding interactions of compound **14** against *S. aureus* DNA gyrase (PDB ID: 2XCT).

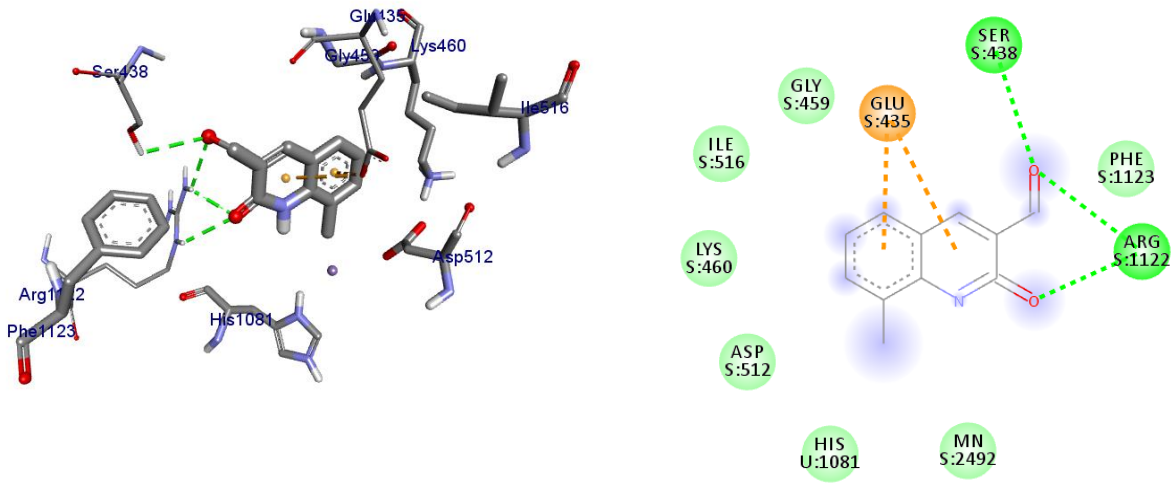


Fig 9. The binding interactions of compound **15** against *S. aureus* DNA gyrase (PDB ID: 2XCT).

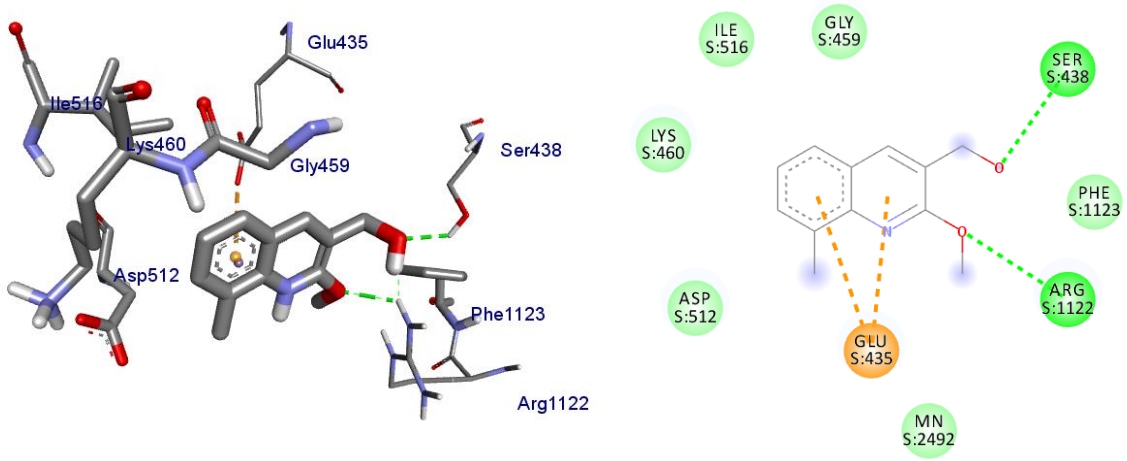


Fig 10. The binding interactions of compound **16** against *S. aureus* DNA gyrase (PDB ID: 2XCT).

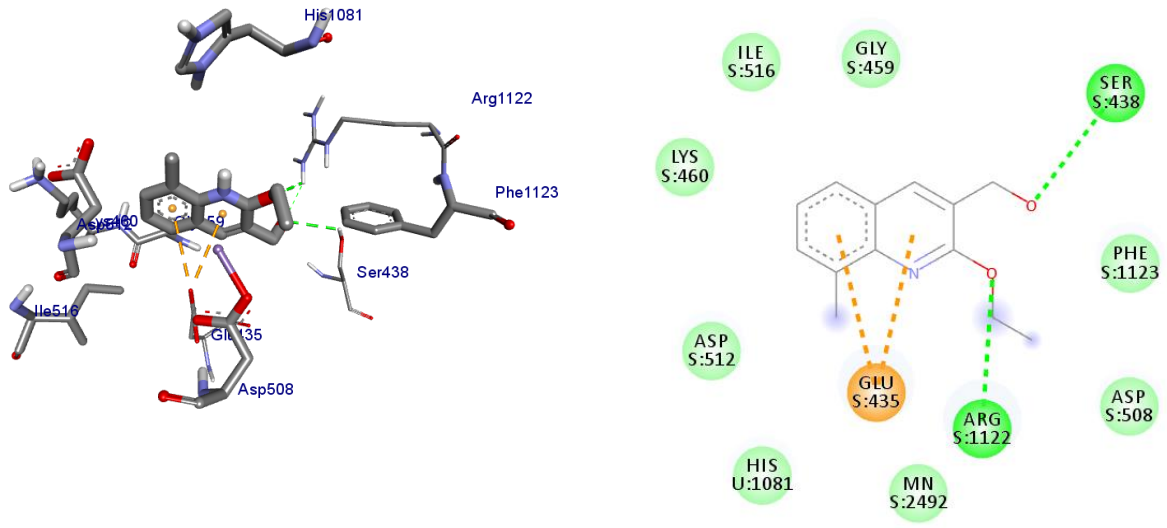


Fig 11. The binding interactions of compound 17 against *S. aureus* DNA gyrase (PDB ID: 2XCT).

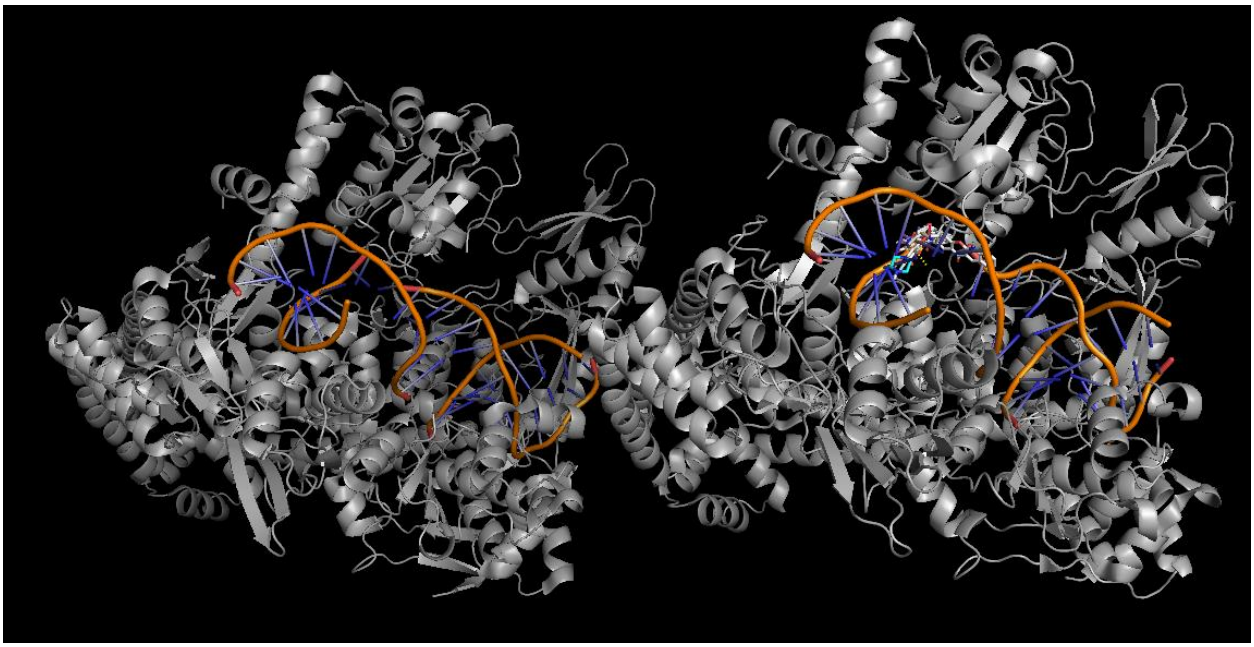


Fig 12. The binding interactions of all compounds **(4-17)** and Ciprofloxacin against *S. aureus* DNA gyrase (PDB ID: 2XCT).

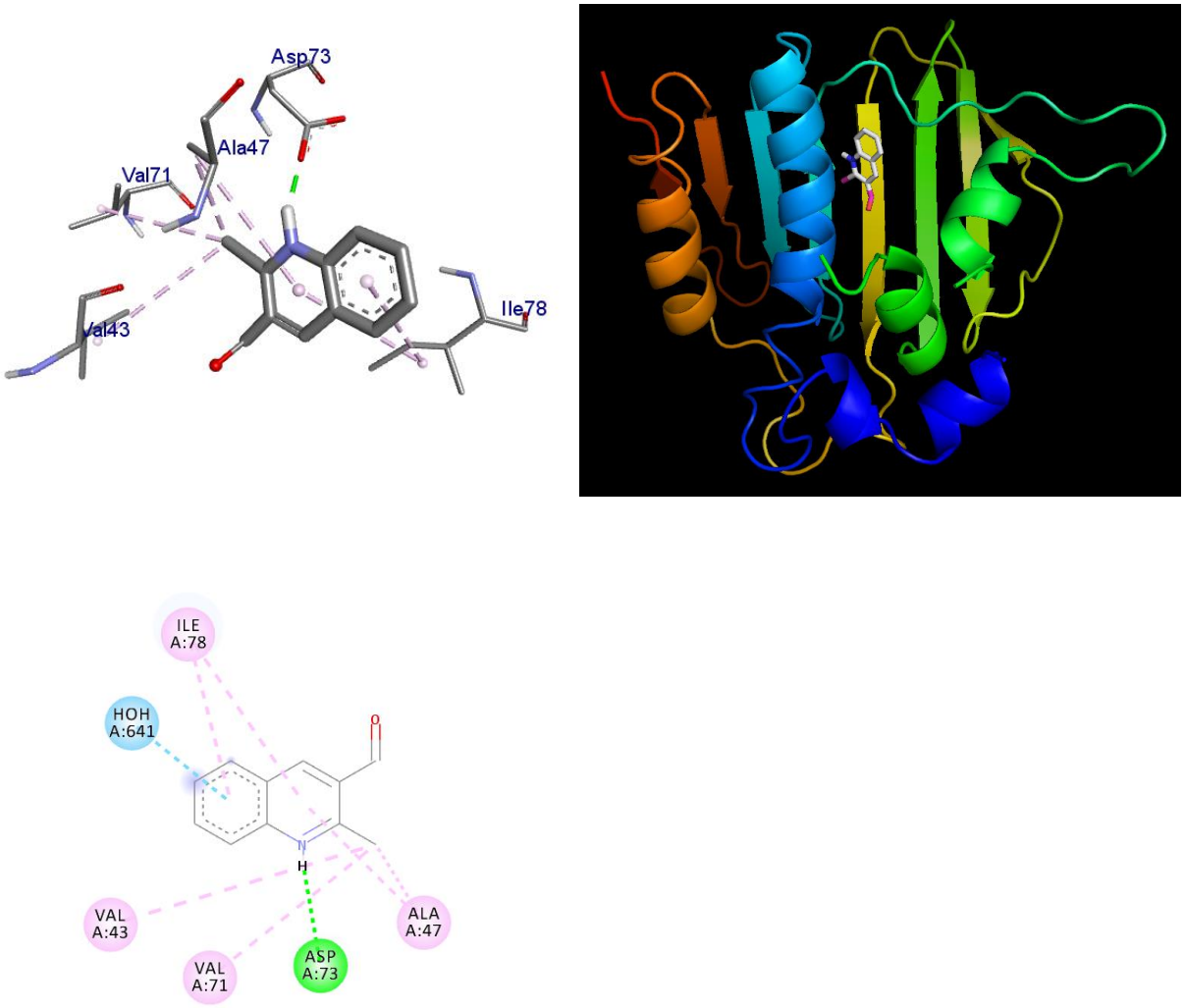
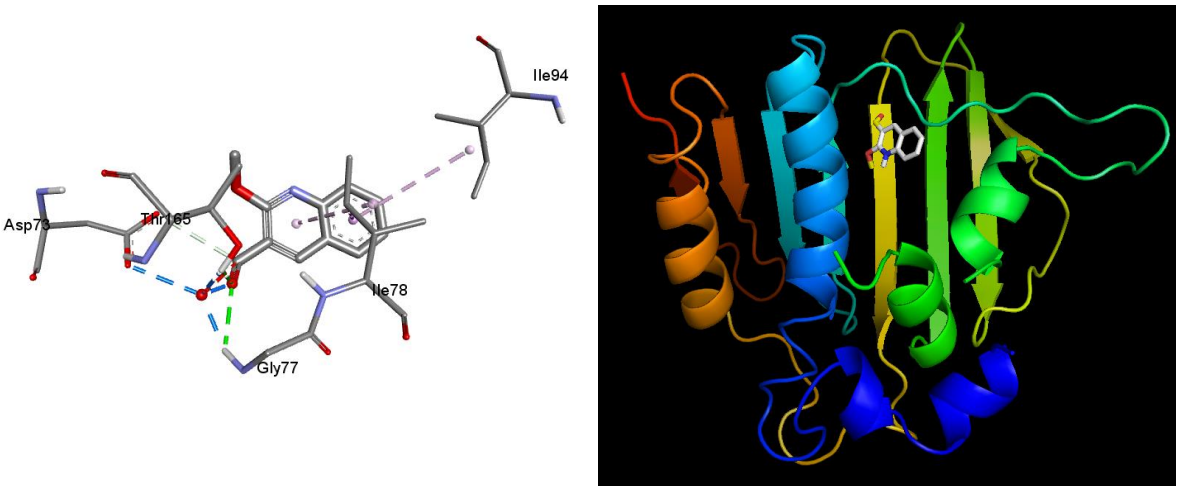


Fig 13. The binding interactions of compound **4** against *E.coli* DNA gyraseB (PDB ID: 6F86).



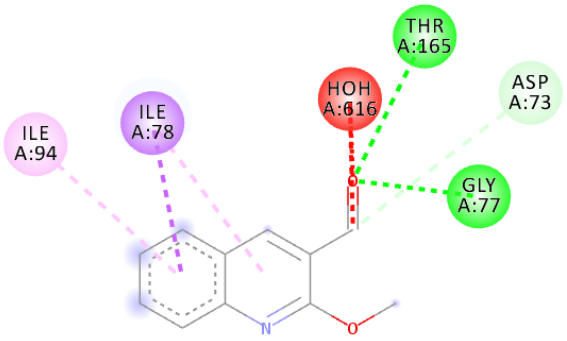
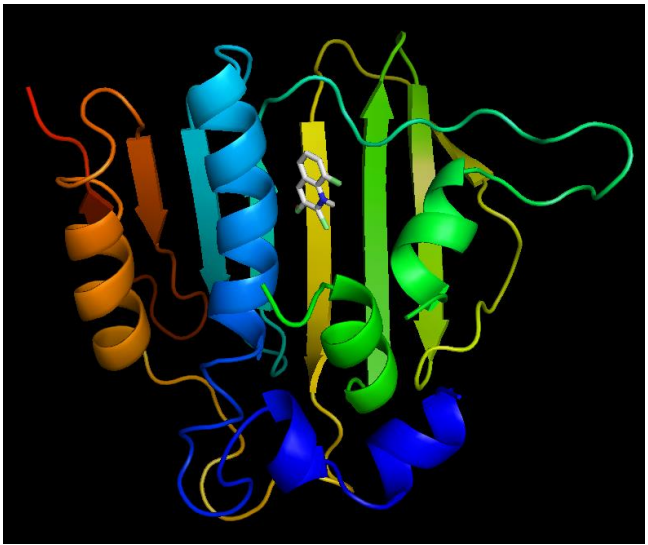


Fig 14. The binding interactions of compound 5 against *E.coli* DNA gyraseB (PDB ID: 6F86)



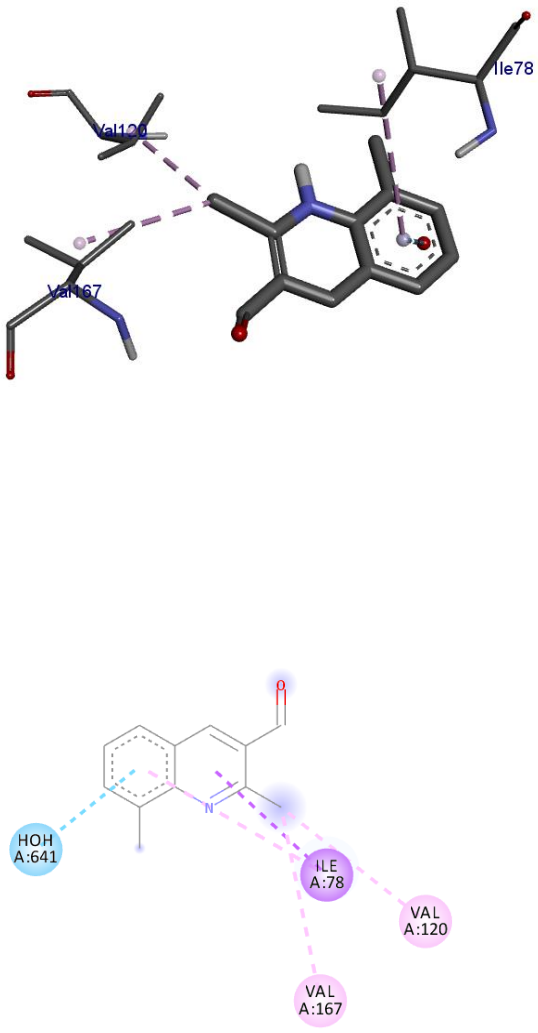


Fig 15. The binding interactions of compound **14** against *E.coli* DNA gyraseB (PDB ID: 6F86) .

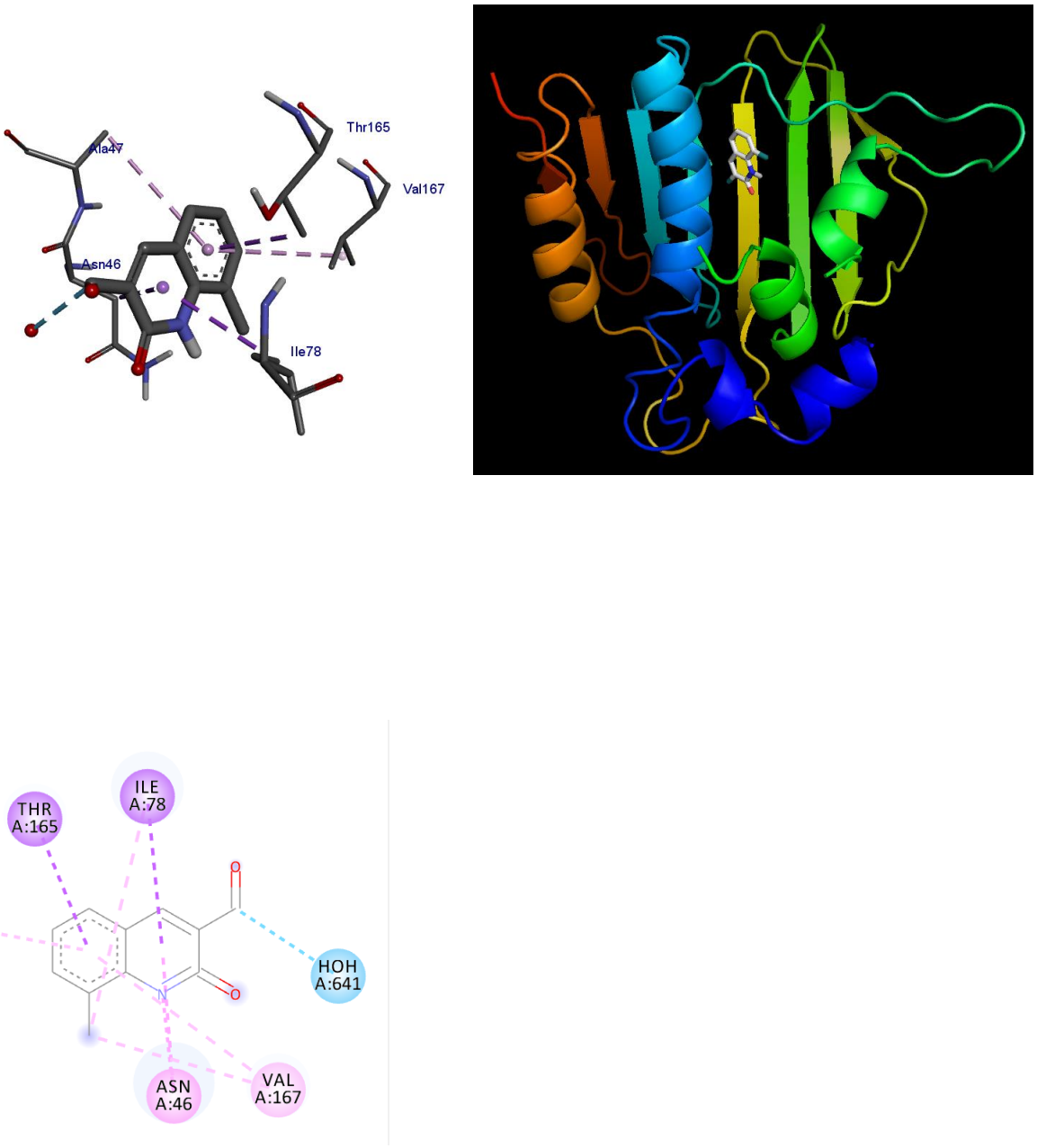


Fig 16. The binding interactions of compound **15** against *E.coli* DNA gyraseB (PDB ID: 6F86)

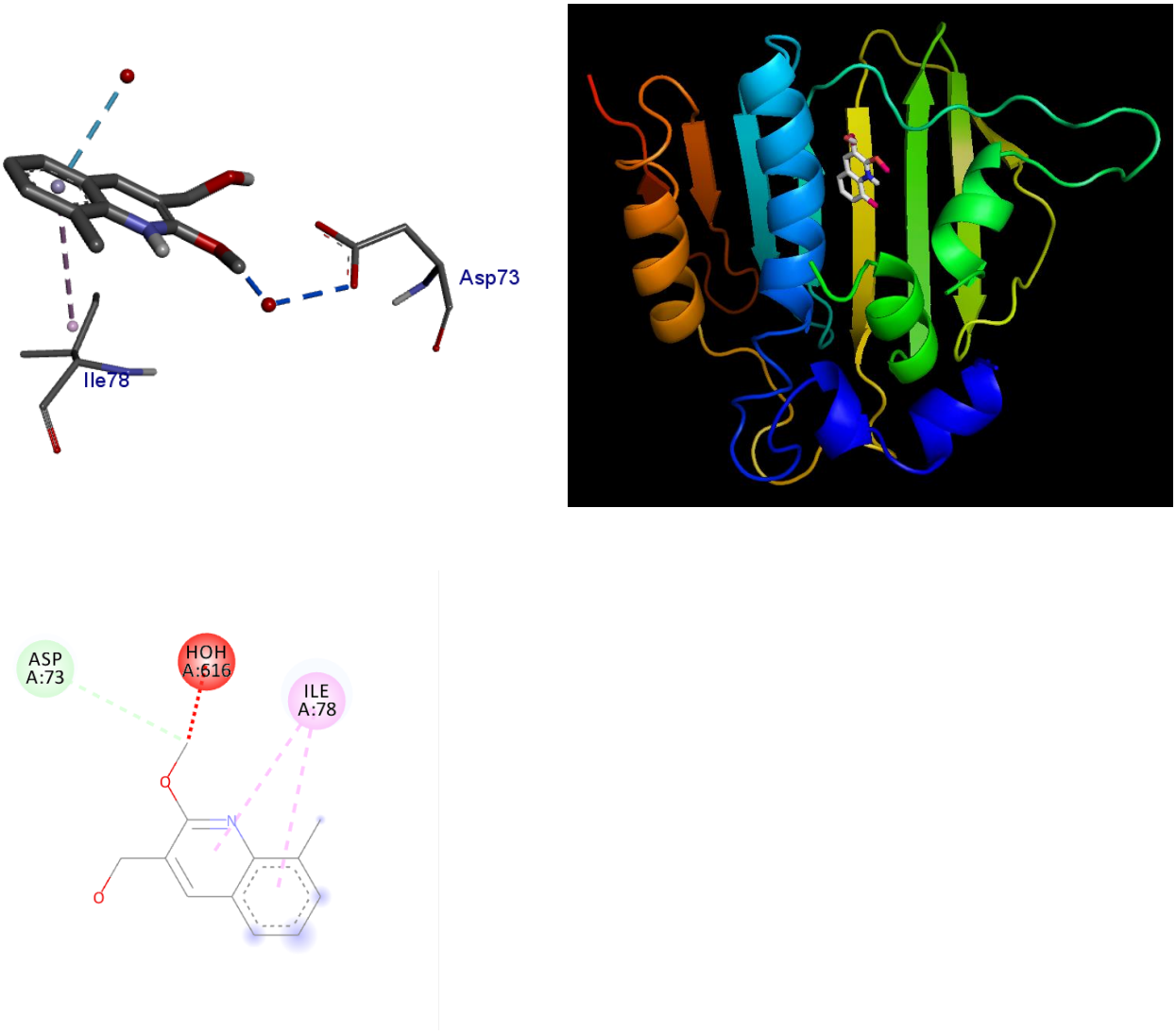


Fig 17. The binding interactions of compound **16** against *E.coli* DNA gyraseB (PDB ID: 6F86)