

NOVEL β -LACTAMS AND THIAZOLIDINONE DERIVATIVES FROM 1,4-DIHYDROQUINOXALINE SCHIFF'S BASE: SYNTHESIS, ANTIMICROBIAL ACTIVITY AND MOLECULAR DOCKING STUDIES

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Abstract. A series of novel isolated β -lactams **3a-c** and thiazolidinone derivatives **4a-c** were successfully synthesized from reactions of new Schiff's bases **2a-c** with chloroacetyl chloride and thioglycolic acid. The chemical structures of the new compounds were confirmed through different spectroscopic techniques including IR, ¹H and ¹³C NMR, mass spectrometry and elemental analysis. The antimicrobial activity of the obtained compounds was assessed *in vitro* against gram-positive *Staphylococcus aureus* and gram-negative *Escherichia coli* bacteria and *Aspergillus flavus* and *Candida albicans* fungi. All compounds exhibited good to excellent antimicrobial activity against the tested strains. Furthermore, a molecular docking study was carried out for the synthesized compounds and the results indicated that compounds **3b** and **4b** display comparable binding affinity scores as that of glutamate. These two compounds are promising candidates as antibacterial and antifungal agents that would deserve further investigations.

Keywords: heterocycle, β -lactam, quinoxaline, antimicrobial activity, molecular docking.

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