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Design, Synthesis, Characterization, Molecular Docking, MM/GBSA and Biological Evaluation of Thiazolidinones Derivatives as Promising Antibacterial and Antifungal Agents

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In present study, a series of 24 thiazolidinone derivatives (**TH7-TH30**) was rationally designed as potential antibacterial and antifungal agents, of which twelve compounds (**TH7-TH18**) were successfully synthesized and fully characterized using IR, ^{1}H NMR, ^{13}C NMR, and HRMS techniques. The antimicrobial activity of the synthesized derivatives was evaluated by the tube dilution method, and minimum inhibitory concentrations (MICs) were determined against selected bacterial and fungal strains. To elucidate the molecular basis of activity, *in silico* studies were performed on all designed compounds using molecular docking with the Glide module of Schrödinger 9.6. Docking investigations targeted MurB (PDB ID: 7OSQ) and lanosterol 14-α demethylase (PDB ID: 5V5Z), key enzymes involved in bacterial cell wall synthesis and fungal sterol biosynthesis, respectively. Binding modes were further analyzed through superimposition with standard inhibitors, streptomycin for MurB and ketoconazole for lanosterol 14-α demethylase. The stability and binding free energies of the docked complexes were assessed using MM/GBSA calculations. Furthermore, ADMET properties of the designed derivatives were predicted using QikProp (v3.5) to evaluate drug-likeness, oral bioavailability and gut blood barrier permeability. Based on the combined experimental and computational findings, novel thiazolidinone derivatives emerge as promising lead structures for the further development of antibacterial and antifungal agents.

Keywords: Thiazolidinone derivatives, Molecular docking, ADMET analysis, MurB inhibitors, Lanosterol 14-α demethylase.