Facile Synthesis of Functionalized Phenoxy Quinolines: Antibacterial Activities against ESBL Producing *Escherichia coli* and MRSA, Docking Studies, and Structural Features Determination through Computational Approach

ABSTRACT

The synthesis of new 6-Bromoquinolin-4-ol derivatives (3a–3h) by Chan–Lam coupling utilizing different types of solvents (protic, aprotic, and mixed solvents) and bases was studied in the present manuscript. Furthermore, their potential against ESBL producing *Escherichia coli* (ESBL *E. coli*) and methicillin-resistant *Staphylococcus aureus* (MRSA) were investigated. Commercially available 6-bromoquinolin-4-ol (3a) was reacted with different types of aryl boronic acids along with $Cu(OAc)_2$ via Chan–Lam coupling methodology utilizing the protic and aprotic and mixed solvents. The molecules (3a–3h) exhibited very good yields with methanol, moderate yields with DMF, and low yields with ethanol solvents, while the mixed solvent CH_3OH/H_2O (8:1) gave more excellent results as compared to the other solvents. The in vitro antiseptic values against ESBL *E. coli* and MRSA were calculated at five different deliberations (10, 20, 30, 40, 50 mg/well) by agar well diffusion method. The molecule 3e depicted highest antibacterial activity while compounds 3b and 3d showed low antibacterial activity. Additionally, MIC and MBC standards were calculated against the established bacteria by broth dilution method. Furthermore, a molecular docking investigation of the derivatives (3a–3h) were performed. Compound (3e) was highly active and depicted the least binding energy of −5.4. Moreover, to investigate the essential structural and physical properties, the density functional theory (DFT) findings of the synthesized molecules were accomplished by using the basic set PBE0-D3BJ/def2-TZVP/SMD water level of the theory. The synthesized compounds showed an energy gap from 4.93 to 5.07 eV.