ORIGINAL RESEARCH ARTICLES

COMPUTATIONAL DESIGN AND SYNTHESIS OF BIOLOGICALLY RELEVANT ANTIMICROBIAL AGENTS OF INDOLE BENZIMIDAZOLE DERIVATIVES

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(Received 16 May 2025) (Accepted 09 October 2025)

ABSTRACT

Drug design and development play a crucial role in the development of novel pharmacologically active compounds based on the knowledge of biological targets. *In silico* molecular modelling, ADME property prediction and molecular docking of proposed substituted indole-linked benzimidazole derivatives were carried out using computational software such as ACD Labs Chemsketch 2020, Molinspiration software, PreADMET software and Schrodinger Maestro 12.8. The derivatives were docked on DNA gyrase subunit B (PDB ID: 3U2K) and lanosterol 14α-demethylase (PDB ID: 5TZ1). The derivatives were docked on DNA gyrase subunit B (PDB ID: 3U2K) and lanosterol 14α-demethylase (PDB ID: 5TZ1). The derivatives with higher docking scores and favourable drug-likeness properties were selected for wet lab synthesis. Derivatives were synthesised from indole aldehyde and O-phenylenediamine as key reagents. Mass spectroscopy, ^{1}H NMR, ^{13}C NMR, and TLC's melting point and purity of synthetic compounds confirmed by TLC defined by IR. The minimum inhibitory concentration (MIC) and zone of inhibition by tube macro dilution and cup plate technique, respectively, define the therapeutic potency as antibacterial drugs. All the synthesized derivatives showed good to moderate activity towards gram-positive and gram-negative bacteria as well as the fungal strain. Among them, 2-(5-methyl-1*H*-indol-3-yl)-1*H*-benzimidazole has shown potent activity with a higher MIC and inhibition zone. These findings may be useful for further investigation in the future.