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Antibacterial Screening and Molecular Docking of 2-Chloro/ Nitrophenyl Benzimidazole Derivatives

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Abstract

The multidrug-resistant (MDR) bacteria have increased at an alarming rate and caused serious health problems throughout the world. The lack of newly introduced antibiotics prompts researchers to design and develop efficient antimicrobials to combat this issue. Application of benzimidazole as a precursor in synthesis is one of many approaches to the discovery of new antibacterial compounds. Fifteen benzimidazole derivatives bearing chlorophenyl and nitrophenyl groups were screened using 96-well plate microdilution against eight bacteria strains; Bacillus cereus (ATCC 11778), Streptococcus pyogenes (ATCC 19615), Staphylococcus aureus (ATCC 25923) and Micrococcus luteus (IIUM), Escherichia coli (ATCC 25922), Pseudomonas aeruginosa (ATCC 27853), Klebsiella pneumonia (ATCC 700603) and Salmonella typhimurium (IMR S 974/05 B). Norfloxacin was used as a positive control, incorporated with resazurin dye to indicate bacterial growth. All compounds showed inhibition against Gram-positive and Gram-negative bacteria albeit with low activity. Molecular docking of selected

compounds was also conducted to analyse their interactions with the protein targets of E.coli (PDB ID:4KFG) and S.aureus (PDB ID:4URM). Most of the synthesised compounds showed better binding affinities than norfloxacin. The solubility of the compounds in the in vitro analysis may contribute to the low antimicrobial activity results.

Author keywords

96-well plate microdilution; antibacterial; Benzimidazole; Resazurin dye

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