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Synthesis, antimycobacterial evaluation and molecular modeling studies of coumarin based pyrrole derivatives

Mymoona Akhter

3-Point pharmacophore based virtual screening of three different databases resulted in identification of novel hits asantimycobacterial agents. Herein this paper we present novel coumarin bearing pyrrole derivatives and their potential as antimycobacterial agents. The synthesis of all the title compounds was carried on CEM-Discover microwave reactor and purity was determined by HPLC. The structure of all the derivatives is established on the basis of IR, ^{1}H NMR, ^{13}C NMR and mass spectral data. The compounds were tested against *Mycobacterium tuberculosis* H37Rv (ATCC#27294) and resistant strain (INH, RIF and FQ resistant strains) by microplatealamarblue assay method by Division of Microbiology and Infectious Diseases, NIAID, National Institutes of Health, Bethesda (USA). The binding mode of compounds has been established by docking studies on receptor InhA (PDB id: 2H7M). The MIC of compound was found in the range of 145-6 µg/ml. Compound 4t has an MIC of 6.25 µg/ml and is also active against two resistant strains (RIF-R and FQ-R) with an MIC of 9.45 and 12.20 µg/ml (IC50 of 6.85 and 9.55 µg/ml) respectively. Other compounds have also showed moderate to good activity. The compounds were also found nontoxic when screened for their cytotoxicity.

mymoonaakhter@gmail.com