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Synthesis, Characterization and Docking study of Fused Benzimidazole and Pyrazole Derivatives as Antitubercular Agents

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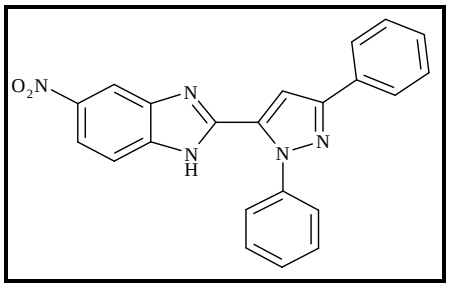
ABSTRACT

A series of fused benzimidazole with pyrazole derivatives (4A-D) were synthesized from 5-Nitro-1H-benzo[d]imidazol-2-yl)-3-phenylpropan-1-one on the basis of docking score which has been taken by Schrodinger. In docking study all the designed compounds were targeted with active site of M. Tuberculosis enoyl ACP reductase enzyme encoded with the gene InhA. (5 JFO), which is an important to mycobacteria for the synthesis of mycolic acid. Synthesized compounds were characterized by IR, H'NMR, Mass spectroscopy and evaluated for in-vitro anti-TB activity against Mycobacterium Tuberculosis H37Rv strain by Alamar-Blue assay. The results expressed as MIC (minimum inhibitory concentration) in mg mL^{-1}. Antitubercular assay has been carried out at Micropharm Diagnosis Center, Gandhi nagar. Among the four compounds 4A, 4C, 4D shown same docking and gliding score and activity at (MIC 6.25 mg mL^{-1}) followed by 4B(MIC 12.5 mg mL^{-1}).

Graphical Abstract



Pharmacophoric pattern required for Anti-tubercular activity

Keywords: Benzimidazole, Pyrazole, Alamar-blue assay, Antitubercular, MIC.