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(57) Abstract :

ABSTRACT SUBSTITUTED BENZIMIDAZOLE COMPOUNDS AS THERAPEUTIC AGENTS AGAINST MYCOBACTERIUM TUBERCULOSIS The invention relates to substituted benzimidazole derivatives and their method of preparation for potential antitubercular applications. The method comprises synthesizing benzimidazole derivative of formula I through amine or aldehyde substitution, followed by purification and structural characterization. The compounds are evaluated using MABA assay, molecular docking, and molecular dynamic simulation to identify potent inhibitors of Mycobacterium tuberculosis KasA enzyme. Selected derivatives, particularly chloro-substituted compounds, exhibit strong binding affinity, stable protein-ligand interactions, and significant antimycobacterial activity, with MIC values comparable to rifampicin. The compounds demonstrate favorable safety profiles, making them suitable for further development as therapeutic agents against drug-resistant tuberculosis. Formula (I)

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