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Design, synthesis, and *in silico* studies of ofloxacin carboxamide analogs as new potential anti-tubercular agents

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ABSTRACT The investigation was initiated to synthesize a new chemical entity as a hit for virulent pathogens like *Mycobacterium tuberculosis*. The present scheme was designed to obtain amide pharmacophore derivatives of ofloxacin, which acts as a cell wall permeability enhancement for the selected pharmacophore. The designed schemes utilized ofloxacin as a hydrophobic scaffold and different amino acids like Phenylalanine, Methionine, Arginine, Threonine, Tryptophan, Norleucine, Histidine, Alanine, Cysteine, Valine, Aspartic acid, Glutamic acid and Glycine were used as pharmacophores. Autodock vina software was used for docking studies. Thirteen compounds were synthesized and screened for antimycobacterial activity. The synthetic scheme involved two step procedures starting from ofloxacin, which was first converted to its acid chloride. Subsequent reaction of the acid chloride with various amino acids led to the formation of amide-linked ofloxacin derivatives **1-13**. Microplate Alamar Blue assay method was used to test the antimycobacterial activity of compounds against MTB. *M. tuberculosis*, H37 RV is the Standard strain used for the Anti-TB test. The final concentrations of the drugs were tested from 100 to 0.80 µg/mL. All compounds exhibited activity at the concentration of 1.6 µg/mL and 0.8 µg/mL. All compounds exhibited antimycobacterial activity. Overall amino acids combined with ofloxacin were more active against *M. tuberculosis* than standard drugs. All compounds showed good binding affinity values and are therapeutically potential antitubercular agents.

KEYWORDS Ofloxacin carboxamide, Antimycobacterial activity, *In silico* studies, Autodock vina.

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