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Synthesis, computational docking, and biological evaluation of new pyrazine-2-carboxamide derivatives as antitubercular agents

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ABSTRACT The main objective of this study was to design and synthesize new pyrazine-2-carboxamide derivatives as potential anti-tubercular agents. These derivatives were synthesized through nucleophilic acyl substitution reaction between (pyrazine-2-carbonyl)valinoyl chloride and various substitutes of aromatic amines. Antitubercular potential was checked through *in vitro* and computational docking. Biological screening against *Mycobacterium tuberculosis* H37Rv revealed promising inhibitory activity, with several compounds showing significant potency. Among them, **JS-2** (*N*-(1-((4-fluorophenyl)amino)-3-methyl-1-oxobutan-2-yl)pyrazine-2-carboxamide) and **JS-4** (*N*-(1-((2,4-dimethoxyphenyl)amino)-3-methyl-1-oxobutan-2-yl)pyrazine-2-carboxamide) demonstrated the highest activity. Computational studies support these findings, as **JS-2** and **JS-4** showing strong binding affinities and multiple hydrogen-bonding interactions because of fluorine and methoxy functional groups. This study suggests that the synthesized pyrazine-2-carboxamide derivatives are strong candidates for the treatment of tuberculosis, justifying further pharmacological and preclinical studies.

KEY WORDS Pyrazine-2-carboxamide, Antitubercular activity, Docking, *Mycobacterium Tuberculosis*, Microplate alamar blue assay method

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