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Synthesis and Molecular Docking of Isonicotinohydrazide Derivatives as Anti-Tuberculosis Candidates

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Abstract : Tuberculosis (TB) is a chronic disease as a result of Mycobacterium tuberculosis. It can affect all age groups, and hence, is a global health problem that causes the death of millions of people every year. One of the drugs used in tuberculosis treatment is isonicotinohydrazide. In this study, N'-benzoylisonicotinohydrazide derivative compounds (a-l) were prepared using acylation reactions between isonicotinohydrazide and benzoyl chloride derivatives, through the reflux method. Molecular docking studies suggested that all of the compounds had better interaction with Mycobacterium tuberculosis enoyl-acyl carrier protein reductase (InhA) than isonicotinohydrazide. It can be concluded that N'-benzoylisonicotinohydrazide derivatives (a-l) could be used as anti-tuberculosis candidates. From the docking results revealed that all of the compounds interact well with InhA, with compound g (N'-(3-nitrobenzoyl)isonicotinohydrazide) exhibiting the best interaction.

Keywords : anti-tuberculosis , docking, InhA, N'-benzoylisonicotinohydrazide, synthesis
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