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Docking and Dynamic Molecular Study of Isoniazid Derivatives as Anti-Tuberculosis Drug Candidate

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Abstract : In this research, we have designed four isoniazid derivatives i.e., isonicotinohydrazide (1-isonicotinoyl semicarbazide, 1-thiosemi isonicotinoyl carbazide, N '-(1,3-dimethyl-1 h-pyrazole-5-carbonyl) isonicotino hydrazide, and N '-(1,2,3- 4-thiadiazole-carbonyl) isonicotinohydrazide. The docking and molecular dynamic have performed to them in order to study its interaction with Mycobacterium tuberculosis Enoyl-Acyl Carrier Protein Reductase (InhA). Based on this research, all of the compounds were predicted to have a stable interaction with Mycobacterium tuberculosis Enoyl-Acyl Carrier Protein Reductase (INHA) receptor, so they could be used as an anti-tuberculosis drug candidate.

Keywords : anti-tuberculosis, docking, Inhibin alpha subunit, InhA, inhibition, synthesis, isonicotinohydrazide
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