Abstract

Employing a molecular docking tool to find novel compounds to treat tuberculosis

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Tuberculosis is a matter of concern as quarter of the population in the world is affected with it. The disease is more dangerous in case of multi-drug resistant and extremely-drug resistant tuberculosis and when it is associated with HIV. Recently total drug resistance tuberculosis case was reported in India. The currently available treatment for tuberculosis includes vaccination and drugs. The drugs available for the treatment show toxic effects and poor patient compliance, which lead to development of resistant strains. This situation reflects serious concern and new molecules have to be discovered with good activity and less side effects. In literature we found that recently discovered some antibacterial agents show potent activity against tuberculosis strain. But main drawback of these compounds is monoamine oxidase enzyme inhibition in human which lead to serious side effects. We have rationally designed new molecules with main focus on reduction of toxic effects and good activity. The molecular modelling software is used to dock molecules inside active site of monoamine oxidase enzyme and molecules having the least or no interaction with enzyme have been selected for further development. The designed molecules show promising results.

Keywords: *Tuberculosis, Toxic effects, Resistance, Anti-TB activity, Docking study.*