Abstract

Isoniazid is a first line tuberculosis drug used to treat tuberculosis. This prodrug is activated by Mycobacterial catalase-peroxidase and Ser315Thr mutation is found to affect the activation process. Docking studies were performed in order to find the effect of mutation on isoniazid binding to the active site. It is found that Ser315Thr mutation significantly affects the isoniazid binding to the active site. The change in isoniazid binding pattern is mainly responsible for the isoniazid resistance *Mycobacterium tuberculosis.* In order to find alternative to isoniazid certain imidazole derivatives are chosen for docking analysis and among them 4-nitro-1H-imidazole-5-carbohydrazide shows very good result.