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DESIGNING, DOCKING AND TOXICITY STUDIES OF NOVEL HIV-1 PROTEASE INHIBITORS

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ABSTRACT

HIV virus causes Acquired immune deficiency syndrome (AIDS). HIV virus type-1 protease plays crucial role in the life cycle of the HIV viral particles. So this protein has been targeted as one of the antiretroviral treatment of AIDS, and HIV-1 Protease inhibitors as anti-HIV drugs. Due to the frequent development of drug resistance there is always a need to develop new drugs which are non toxic and efficient inhibitors. The present study aims to focus on designing of 10 non toxic, novel lead molecules which targets HIV 1 protease. And performing docking and toxicity studies to calculate their binding energies, and to predict their toxicity properties. Protein- ligand interactions were studied using HIV type 1 Protease protein, PDB ID - 1HXW extracted from PDB to evaluate the binding efficiency of various molecules towards the active site. And these values were compared with commercially available FDA approved HIV drugs Ritonavir, Saquinavir, Amprenavir, Indinavir, Lopinavir, Nelfinavir. The final docking and toxicity prediction studies proves that these novel drug molecules were satisfied all drug likeness rules, which are violated by FDA approved drugs, and have the binding energies and predicted inhibitory constant Ki nearly similar to commercially available drugs.

KEYWORDS: HIV, HIV-1 Protease, Anti Retroviral Drugs, Drug Designing, Docking, Predicted Toxicity Studies