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Original Research Article

Molecular Docking of Pyrazole Inhibitors Against Integrase Receptor: A Computational Quantum Approach

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ABSTRACT

HIV/AIDS is an infection caused by a virus. Some drugs are known to be very potent in slowing the virus replication with good binding affinity with the receptor. However, there are some other drugs which have a significant and better docking approach with stronger binding affinity. Pyrazole derivatives are remarkably good and have been reported as better anti-HIV agents because they exhibit stronger binding affinity. In this study, a computational quantum approach was used to understand the binding interaction between the pyrazole derivatives and the receptor (Integrase). Docking is used to predict the bound conformation and binding free energy of small molecules to the target. The docking was carried out on ten pyrazole derivatives and their large negative binding affinity values in **kcal/mol** confirmed that they truly bind the pocket atoms of the receptor. The ligands have good negative binding affinity which showed that they are potent inhibitors for the receptor. The result obtained from the docking of the ligands with the receptor could be useful to design new potent anti-HIV-1 derivatives.

Keywords: Pyrazole Derivatives, Integrase, Binding affinity, Receptor, Ligand.

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