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Insilico antiviral activity of quassinoids and HIV protease, a protein ligand interaction

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Quassinoids are the naturally available plant extracts which exhibit a wide range of biological activities that include anti malarial, anti amoebic, antitumor and antiviral properties etc. These bioactive phytochemical agents belong to the triterpene chemical family. The main active groups of Quassinoids are Ailanthionone, Glaucorubinone and Holacanthone besides Benzoquinone, Canthin, Dehydroglaucarubinone, Glaucarubine, Simarolide, Sitosole and Melianone. The picrasane skeleton, a pentacyclic derivative of the Quassinoids have shown a remarkable antiviral activities. The present experiment aims to study the binding affinity of the Quassinoid analogues (Ligand) and HIV protease, (Protein) a potential drug target for HIV. HIV Protease (HIV PR) cleaves newly synthesized polyproteins to create the mature protein components of an infectious HIV virion. In the absence of the effect of HIV PR, the virions are uninfectious and hence acts as a drug target. The quassinoid acting as a ligand for the present study, were drawn using chemsketch. The protein for the present study is imported from PDB [Protein Data Bank]. 68 quassinoid analogues were designed and were docked with HIV Protease .The docking results showed compound 15 to be the best ligand for HIV protease.

Biography

R.D. Shailima Vardhini is currently pursuing P.hD. from CMJ University, India. She has published research articles in various reputed international journals. Her research interests include Cancer Biology and Bioinformatics.

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