In-silico docking and QSAR analysis of HIV protease inhibitors as anti-dengue drugs

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Till date little success has been achieved in antiviral therapy against Dengue virus. The NS3 viral protease, required for virus replication is a potential target for antiviral drugs. This work is a computational prediction of some of the potential HIV protease inhibitors against NS3 protease of Dengue virus followed by activity study of the molecules by taking different types of molecular descriptors. Total 19 inhibitors were obtained from Pubchem database. After energy minimization of molecules the docking study was carried out with NS3 protease of dengue virus as a receptor .The docking evaluates the binding affinity and ligand having Pubchem database id CID 482206 and CID 484561 shows the highest binding affinity i.e., -400.88. All the docked ligands were observed to share a similar position and confirmation with the receptor. Although HIV and Dengue belongs to different families of virus but the docking results suggest that some HIV protease inhibitor could be used as antiviral drug against the Dengue virus. In order to study the activity of these selected potential drug molecules, QSAR analysis has been performed by taking some of the physiochemical and structural descriptors. The effect was calculated for each type of descriptors by taking Andrews affinity as a dependent variable. Multiple regression equation models were built using Minitab Tools.

Biography

Mr. Prangya Ranjan Rout has completed his Bachelor Degree in engineering from Biju Pattnaik University of Technology,(B.P.U.T) Odisha in the year 2009. At present he is a research scholar at National Institute of Technology, Rourkela pursuing his Master of Technology Degree. He is working on the Project "In-silico docking and QSAR analysis of HIV protease inhibitors against Dengue virus NS3 protease" under supervision of Prof G.R. Satpathy and Raghunath Satpathy.