Abstract

Human immunodeficiency virus type 1 protease (HIV-1 PR) is an essential enzyme for the replication cycle of HIV. HIV-1 PR inhibitors have been extensively investigated as anti-AIDS drugs. In the presence of HIV-1 protease inhibitors, the virion is unable to mature. Natural compounds are important sources of drugs. The present investigation concentrates on discovering anti-HIV compounds that are present in Mappia foetida, a medicinal plant belonging to Icacinaceae family. Here, we selected Phytochemicals of Mappia foetida- Root identified by the method of Gas chromatography–mass spectrometry (GC-MS Method) to dock against the enzyme HIV-1 protease (PDB ID: 3HAU). The resulted enzyme-substrate interaction energies shows that those compounds are active against HIV-1 protease and further research on plant Mappia foetida will be useful in drug designing against HIV.

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**Index Terms**

Computer Science  Biomedical

**Keywords**

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