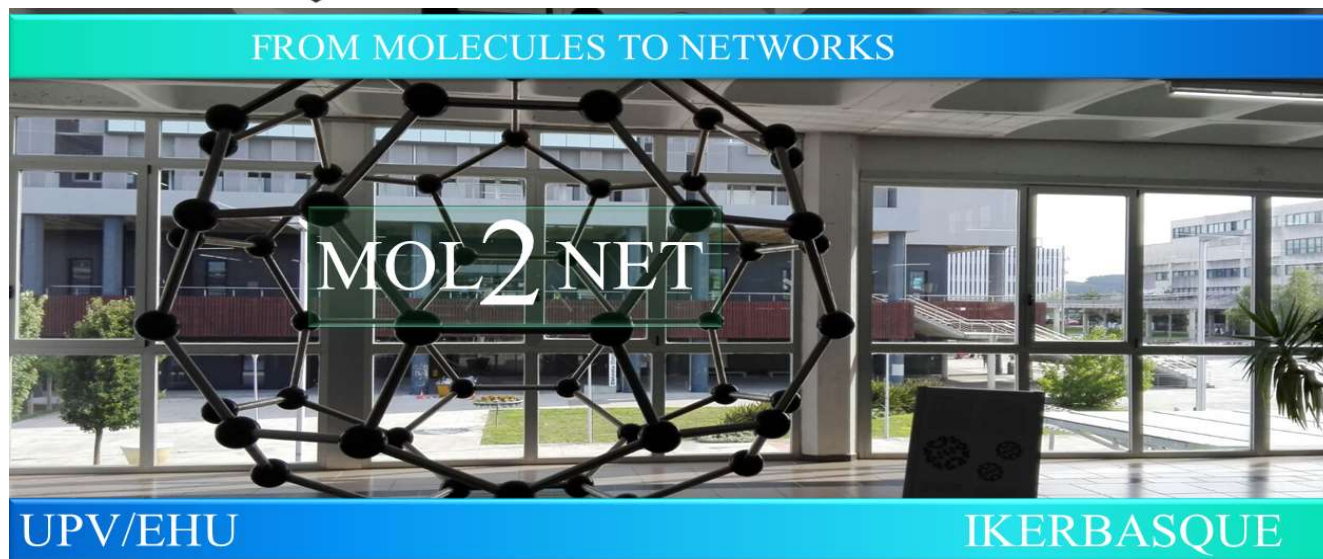




MOL2NET'21, Conference on Molecular, Biomedical & Computational Sciences and Engineering, 7th ed.



Repurposing Drugs to Find HIV-1 Protease Inhibitors: A Virtual Study

Raphael Onuku (raphael.onuku@unn.edu.ng) *, Ngozi Nwodo (ngozi.nwodo@unn.edu.ng)

Akachukwu Ibezim (akachukwu.ibezi@unn.edu.ng)

Department of Pharmaceutical and Medicinal Chemistry, Faculty of Pharmaceutical Sciences, University of Nigeria

Abstract

Edit

Abstract

HIV-1 protease, a homodimer, has attracted the interest of many researchers due to its essential role in HIV replication and subsequent functional activities. It hydrolyses different viral proteins into their functional form to help in maturing the virus for further extending the disease propagation. The present workflow in this research was designed to identify potential HIV-1 protease inhibitors from library of approved drugs (1,428 compounds) using computational techniques in Computer-Aided-Drug-Design (CADD). The inhibitory potency of the dataset was evaluated using the lowest theoretical binding energies of the target-ligand complex. Software and tools such as Molecular Operating Environment (MOE), AutoDock Vina, Discovery Studio used in CADD were employed during the process of this work. This study suggest the possibility of repurposing some current drugs (from the library) to having potential HIV Protease inhibitory effect.