Abstract

HIV–1 (human immunodeficiency virus type–1) is the pathogenic retrovirus and causative agent of AIDS. When viral RNA is translated into a polypeptide sequence, it is assembled in a long polypeptide chain, which includes several individual proteins namely, reverse transcriptase, protease, integrase, etc. Before these enzymes become functional they have to be cut from polypeptide chain, The dipyrido diazepinone Nevirapine is a potent and highly specific inhibitor of the reverse transcriptase (RT) from human immunodeficiency virus type 1 (HIV-1). In this paper, we implemented better than existing system by virtual screening analysis of HIV-RT from PDB database versus chemical compounds from ZINC database using eHiTS software. Using molecular constraint search, 884 ligands were extracted and docking analysis resulted in 59 best hits.
Virtual Screening of Novel HIV-RT Inhibitors using Zinc Database

References


Index Terms

Keywords

HIV reverse transcriptase protease virtualscreening RMSD Zincdatabase ehits
docking
RCPlot
Clustering