Abstract

Human immunodeficiency virus is a retrovirus that causes acquired immunodeficiency syndrome, a condition in humans in which the immune system begins to fail, leading to life threatening opportunistic infections. Reverse transcriptase inhibitors are class of antiretroviral drugs used to treat HIV infection. RTIs inhibit activity of reverse transcriptase, a viral DNA polymerase enzyme that HIV needs to replace. Protein P04585|POL_HV1H2 Gag-Pol polyprotein - Human immunodeficiency virus type 1 (isolate HXB2 group M subtype B) (HIV-1) was docked with RTIs and the free energies of the docking complexes were analyzed. It was concluded that M184V mutations has least impact than that of other mutations and Y115F
mutation has great impact on the drug interaction with Abcavir. This has to be correlated with the real effect on the patients. This serves a best model for evaluating the impact of mutations in changing the folding of protein and further its effect on the inhibition. This is shown by superimposing the wild type structures and mutant structures.

References

- www.expasy.org/prosite

Index Terms

Computer Science  Applied Sciences

Keywords

Reverse transcriptase  Inhibitors