

In-silico based inhibition of hiv-1 subtypes by a pholiota squarrosa lectin

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HIV-1 envelope spike consists of GP120 and GP41. GP120 is the site of interaction with the host cell. GP120 protein of HIV-1 is masked with N-glycans, also known as “glycan shield”. N-glycosylation of glycoprotein (GP120) is an important event in HIV-1 infection. The N-glycans affect cell-virus attachment and identification of GP120 by immune system. The blockage of N-glycosylation of HIV-1 glycoprotein can aid in developing therapeutic strategies against HIV-1. The study of N-glycosylation has become an area of extensive research in current areas of research in virus biology. Lectins are carbohydrate binding agents. The lectins that can target N-glycans on the surface of HIV-1 GP120 are potential antiviral agents. The lectin of our interest is a novel Pholiota squarrosa lectin (PhoSL), isolated from mushroom Pholiota squarrosa, that identify N-glycans having α 1,6-linked fucose residues. In HIV-1 glycoprotein, fucose was found associated only with the innermost GLcNAc of N-linked glycans. In this study, the main objective is to observe the possible interactions among Pholiota squarrosa Lectin and GP120 glycans of HIV-1, by using

in-silico based methods. Molecular docking of GP120 of HIV-1 subtypes and the Pholiota squarrosa lectin (PhoSL) was performed by using Patch Dock and Swiss-Model. Interactions between PhoSL and HIV-1 GP120 were analyzed by PLIP (Protein-Ligand Interaction Profiler) server. The molecular docking results showed that the Pholiota squarrosa lectin (PhoSL) can form metal complexes along with non-covalent interactions with GP120 of HIV-1. It can be concluded that the Pholiota squarrosa lectin may serve as a potential agent to block N-glycosylation of HIV-1 glycoprotein. However, empirical data is required to confirm its antiviral potential.

Biography:

I am a Microbiologist and currently working as a Junior Research Fellow at Dr.Panjwani Center for Molecular Medicine and Drug Research (PCMD), International Center For Chemical And Biological Sciences (ICCBS), University Of Karachi - 75270, Karachi, Pakistan.