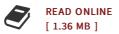# CYSTEINE PROTEINASE (CP- 30) PROTEIN OF TRICHOMONAS VAGINALIS

By Misra, Rahul / Talari, Jayachandra P.

Condition: New. Publisher/Verlag: LAP Lambert Academic Publishing | In-silico Homology Modeling and Docking study | CP30 protein plays an important role in the establishment of host parasite relationship in Trichomoniasis. In the present work, single letter amino acid sequence of CP30 protein of T. vaginalis (ACC.No.NP_057852) was retrieved from protein database of NCBI, taken as a target protein sequence. Modeling of 3D structure of CP30 protein performed related to the target sequence using PSI-BLAST.As a consequence of number of hits, potential template structure (PDB-ID: 1K30), followed by calculation for energy and root mean square deviation (RMSD) of the specific model. Subsequently, various inhibitors were docked employing AutoDock to CP30 protein structure determined by comparative homology modeling. Auto Dock 3.05' was used for docking and calculation of the energy maps. From inhibitor optimization and docking studies, suitable inhibitor sphingosine is hunted. CP30 binds by the designed inhibitor; it may be very successful drug for CP30 protein inhibition. This work on inhibitor optimization will be a platform for the further studies on molecular mechanism of HIV infection & for most cost effective drug designing & for finding the inhibitor against this sexual transmitting disease. | Format: Paperback | Language/Sprache: english | 72...

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