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Computer aided structural based drug design for human herpes viral species

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Introduction: Structural drug design is one of the fields of bioinformatics to finding new medications based on the knowledge of a biological target. This paper is the focus on the development of structure-based drug design for HHV infection that involves choosing the target proteins, visualizing the target structure, identifying the binding site, docking the ligands, and evaluating those using computational techniques. Homology modeling performs for pdb structure of glycoprotein and DNA polymerase of HHV-I and II. On the basis of their properties, twenty one natural molecules were selected for antiviral compounds. Finally, 15 molecules passed the Lipinski rule of five for ligand selection and best of that based on ligand efficiency, binding affinity and inhibitory constant propose for drug target.

Analysis: Structure-based drug design has tremendous potential and an alternative to conventional screening techniques. This drug design method involves bioinformatics, proteomics, biochemistry, and computer modeling of 3-dimensional protein structures. Whole proteomic sequences (DNA polymerase and Envelope glycoprotein B) were downloaded for human herpes virus 1 and 2 from NCBI. The GI numbers of four possible proteins are 386089622, 384597774, 386089624 and 360039889, for comparative modeling using MODELLER9.9. The best model chooses on the basis of DOPE Score and RC Plot analysis. Pymol help to eliminate unwanted part of primary chain and q server request for pocket identification. Proposed antiviral compounds properties were seen using Molinspiration and Lipinski rule of five. Optimized ligands were used to get appropriate interactions with the target protein. The docking of the ligands with the target protein was performed using the Autodock 4.4.

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