In silico molecular docking analysis of plant compounds against VISTA protein: a novel target in cancer

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ABSTRACT

V-domain immunoglobulin suppressor of T-cell activation (VISTA) is a member of B7 protein family and an important immune checkpoint that negatively regulates the T cell mediated inhibition of tumors. VISTA protein is upregulated in melanoma, pancreatic cancer, prostate cancer, colorectal cancer, ovarian cancer, Glioma and fibro sarcoma and various other cancers. Hence identifying novel drugs to target VISTA protein is utmost important in the treatment of cancer. This study involves the docking of plant phytochemicals against VISTA protein (PDB ID 6OIL) to analyze the interactions and orientation of protein ligand complex. Ligand structures obtained from Pubchem were screened for their drug likeness through Lipinski rule of five and those that cleared the Lipinski rule were chosen for further docking studies. All the docked compounds showed good docking results with PatchDock score ranging from 2368 to 4496. Among them capsaicin showed a highest score of 4496 followed by curcumin with 4300. This shows that these plant phytochemicals could be used as potential drug molecules to treat cancer by targeting VISTA protein.

Keywords: VISTA protein, immunoglobulin, fibro sarcoma

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