

Abstract

In Silico Evaluation of Interactions of Triterpenes in *Momordica charantia* on Proteins Involved in Angiogenesis [†]

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Abstract: Angiogenesis is important process that play active role in tumorigenesis. VEGFR-1, a member of the tyrosine kinase receptor family, is known as the receptor for VEGF ligands in tumor cells. SPARC protein has recently been shown to play a role in metastasis in various types of cancer. *Momordica charantia*; is a valuable plant used quite often in traditional medicine. Triterpenes from that plant appear to be promising in in vitro cancer studies. In this study; triterpenes in fruit and seed of *M. charantia* were selected according to literature. The 3D structure files of triterpenes were obtained from PubChem. The structure files of ligands were prepared with various programs and converted to the appropriate file format. X-ray diffraction structure files of proteins were obtained from RCSB PDB. These structure files were made suitable for molecular docking studies. Docking was performed with the AutoDock Tool (downloaded from autodock.scripps.edu/resources/adt), and the results were scored using the Vina program. According to the in silico analysis; It has been found that various triterpenes which can be obtained from *M. charantia* can co-inhibit VEGFR-1 and SPARC proteins. These results show that these triterpenes are promising in terms of new therapeutic routes for aggressive cancer therapy.

Keywords: angiogenesis; molecular docking; VEGFR-1; SPARC; bioinformatics



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