

Activity of Peganum harmala against Herpes through deactivation of Herpes Simplex virus Type II Protease (1AT3)

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Abstract: An in-silico study was performed to determine the activity of Peganum harmala against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes Simplex virus Type II Protease (1AT3) enzyme. It was found that Myricetin and Theobromine helped to prevent Herpes.

Introduction: Peganum harmala is known for its medicinal activities. It has been used as an analgesic, emmenagogue, and abortifacient agent. Leaf was used to cure herpes. In a certain region of India the root was applied to kill body lice.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Sapindales
Family	Nitrariaceae
Genus	Peganum
Species	harmala

Major phytochemicals present in the plant are:

- a. Genistein
- b. Myricetin
- c. Theobromine
- d. Quercetin

One of the major enzymes required for the survival of the organism causing Herpes is Herpes Simplex virus Type II Protease (1AT3) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.