Activity of Melia azaderach 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 Melia azaderach 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 Zingiberene helped to prevent Herpes.

Introduction: Melia azaderach is known for its medicinal activities. The leaf juice is anthelmintic, antilithic, diuretic, herpes and emmenagogue.

The plant is classified as follows:

Kingdom	Plantae
Division	Magnoliophyta
Class	Magnoliopsida
Order	Sapindales
Family	Meliaceae
Genus	Melia
Species	azedarach

Major phytochemicals present in the plant are:

- a. Zingiberene
- b. Ursolic acid
- c. Astaxanthin
- d. Digoxin

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.

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