Activity of Aglai odorata 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 Aglai odorata 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 Benzyl isothiocyanate helped to prevent Herpes.

Introduction: Aglai odorata is known for its medicinal activities. Aglaia species are used in traditional medicine: leaves to treat wounds, fever, headache, asthma, jaundice, and as a tonic e.g. after childbirth; flowers against fever, asthma, jaundice and herpes.

The plant is classified as follows:

Kingdom	Plantae
Division	Magnoliophyta
Class	Magnoliopsida
Order	Sapindales
Family	Meliaceae
Genus	Aglai
Species	odorata

Major phytochemicals present in the plant are:

- a. Morphine
- b. Myricetin
- c. Peonidin
- d. Benzyl isothiocyanate

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.

ISSN: 2395-6216