Activity of Swertia chirata 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 Swertia chirata 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 Theobromine and Limoene helped to prevent Herpes.

Introduction: Swertia chirata is known for its medicinal activities. People use the parts that grow above the ground to make medicine. Chirata is used for fever, constipation, herpes, upset stomach, loss of appetite, intestinal worms, skin diseases, and cancer.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Gentianales
Family	Gentianaceae
Genus	Swertia
Species	chirayita

Major phytochemicals present in the plant are:

- a. Theobromine
- b. Limonene
- c. Naringin
- d. Limonene

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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