Activity of Cyperus rotundus against Herpes through deactivation of Thymidine Kinase of Herpes Simplex virus (1KIM)

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Abstract: An in-silico study was performed to determine the activity of Cyperus rotundus against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme. It was found that Pelargonidin helped to prevent Herpes.

Introduction: Cyperus rotundus is known for its medicinal activities. It is a medicinal herb traditionally used to treat various clinical conditions at home such as diarrhea, diabetes, pyresis, herpes, inflammation, malaria, and stomach and bowel disorders.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Poales
Family	Cyperaceae
Genus	Cyperus
Species	rotundus

Major phytochemicals present in the plant are:

- a. Ellagic acid
- b. Gallic acid
- c. Pelargonidin
- d. Limonene

One of the major enzymes required for the survival of the organism causing Herpes is Thymidine Kinase of Herpes Simplex virus (1KIM) 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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