Activity of Holoptelea integrifolia 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 Holoptelea integrifolia 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 Limonene helped to prevent Herpes.

Introduction: Holoptelea integrifolia is known for its medicinal activities. The plant Holoptelea integrifolia is used traditionally for the treatment of inflammation, gastritis, dyspepsia, colic, intestinal worms, vomiting, wound healing, leprosy, diabetes, hemorrhoids, herpes, dysmenorrhea, and rheumatism.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Rosales
Family	Ulmaceae
Genus	Holoptelea
Species	integrifolia

Major phytochemicals present in the plant are:

- a. Naringin
- b. Limonene
- c. Glutathione
- d. Malvidin

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.

ISSN: 2395-6216