

## Activity of *Barleria lupulina* 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 *Barleria lupulina* 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 Coumarin helped to prevent Herpes.

**Introduction:** *Barleria lupulina* is known for its medicinal activities. The flowers are used internally for the treatment of migraine, internal abscesses, oedema, haemoptysis, herpes, urethral discharges, seminal disorders and reduce obesity.

The plant is classified as follows:

Kingdom	Plantae
Division	Magnoliophyta
Class	Magnoliopsida
Order	Scrophulariales
Family	Acanthaceae
Genus	<i>Barleria</i>
Species	<i>lupulina</i>

Major phytochemicals present in the plant are:

- a. Hesperidin
- b. Epicatechin
- c. Coumarin
- d. Ferulic acid

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.