Activity of Neerium indicum 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 Neerium indicum 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 Myricetin helped to prevent Herpes.

Introduction: Neerium indicum is known for its medicinal activities. Nerium indicum has many medicinal properties like bitter, acrid, astringent, anthelmintic, aphrodisiac, stomachic, febrifuge, diuretic, emetic, expectorant, cardio tonic, anticancer etc which is used in the treatment of cardiac asthma, renal and vesicle calculi, chronic stomach, skin related problems, snake bites joint pains, leprosy, cancer, ulcers etc. Leaves and flowers are also used to treat malaria. Leaves and bark is treated as insecticide, rat poison and parasitic.

The plant is classified as follows:

Kingdom	Plantae
Division	Magnoliophyta
Class	Magnoliopsida
Order	Gentianales
Family	Apocynaceae
Genus	Nerium
Species	indicum

Major phytochemicals present in the plant are:

- a. Myricetin
- b. Peonidin
- c. Curcumin
- d. Ascorbic 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.

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