Activity of Lippia alba 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 Lippia alba 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 Pelargonidin and Caffeine helped to prevent Herpes.

Introduction: Lippia alba is known for its medicinal activities. A tea made from the leaves is used to treat intestinal and respiratory disturbances, including influenza and herpes. A well-sugared infusion is drunk to bring relief of heart problems and to soothe tachycardia.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Equisetopsida
Order	Lamiales
Family	Verbenaceae
Genus	Lippia
Species	alba

Major phytochemicals present in the plant are:

- a. Pelargonidin
- b. Caffeine
- c. Curcumin
- d. Ascorbic acid

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.