Activity of Scoparia dulcis 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 Scoparia dulcis 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 Pelletierine and Digoxin helped to prevent Herpes.

Introduction: Scoparia dulcis is known for its medicinal activities. It is considered a weed in many areas but used as medicinal herb for a wide range of uses including treatment for digestive problems, pulmonary conditions, fever, skin disorders, hypertension, hemorrhoids, diarrhea, dysentery, insect bites, anemia, albuminuria, diabetes, herpes, etc.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Lamiales
Family	Plantaginaceae
Genus	Scoparia
Species	dulcis

Major phytochemicals present in the plant are:

- a. Pelletierine
- b. Digoxin
- c. Rosmarinic acid
- d. Campesterol

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.

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