Activity of Adansonia digitata 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 Adansonia digitata 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 Resveratrol and Peonidin helped to prevent Herpes.

Introduction: Adansonia digitata is known for its medicinal activities. The various parts of the plant (leaves, bark and seeds) are used to cure tuberculosis, fever, microbial infections, diarrhea and herpes.

The plant is classified as follows:

Kingdom	Plantae
Division	Magnoliophyta
Class	Magnoliopsida
Order	Malvales
Family	Bombacaceae
Genus	Adansonia
Species	digitata

Major phytochemicals present in the plant are:

a. Resveratrol
b. Phenyl isothiocyanate
c. Capsaicin
d. Peonidin

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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