Activity of Barleria prionitis against COVID 19 through deactivation of 2019nCoV HR2 Domain (6LVN)

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Abstract: An in-silico study was performed to determine the activity of Barleria prionitis against COVID 19. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate 2019-nCoV HR2 Domain (6LVN) enzyme. It was found that Benzyl isothiocyanate helped to prevent COVID 19.

Introduction: Barleria prionitis is known for its medicinal activities. It is used for various medicinal purposes in ayurvedic medicine. The juice of the leaves is applied to feet to prevent maceration and cracking in the monsoon season. Its leaves are known to contain 6-Hydroxyflavone, one of the chemical compounds that is a noncompetitive inhibitor of the protein cytochrome P450 2C9.

Kingdom	Plantae
Division	Tracheophytes
Class	Angiosperms
Order	Lamiales
Family	Acanthaceae
Genus	Barleria
Species	prionitis

The plant is classified as follows:

Major phytochemicals present in the plant are:

- a. Rosmarinic acid
- b. Daidzein
- c. Benzyl isothiocyanate
- d. Quercetin

One of the major enzymes required for the survival of the organism causing COVID 19 is 2019nCoV HR2 Domain (6LVN) 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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