Activity of Neerium indicum against COVID 19 through deactivation of 2019nCoV HR2 Domain (6LVN)

Monalisa Sahu¹, Srimay Pradhan²

¹190705180012@cutm.ac.in

²srimay.pradhan@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Neerium indicum 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 Caffeine helped to prevent COVID 19.

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. Theobromine
- b. Daidzein
- c. Caffeine
- d. Limonene

One of the major enzymes required for the survival of the organism causing COVID 19 is 2019-nCoV 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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