

Activity of *Caesalpinia sappan* against COVID 19 through deactivation of ADP ribose phosphatase of NSP3 from SARS CoV-2 (6VXS)

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Abstract: An in-silico study was performed to determine the activity of *Caesalpinia sappan* against COVID 19. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate ADP ribose phosphatase of NSP3 from SARS CoV-2 (6VXS) enzyme. It was found that Phenyl isothiocyanate helped to prevent COVID 19.

Introduction: *Caesalpinia sappan* is known for its medicinal activities. This plant has antibacterial and anticoagulant properties. Slivers of heartwood are used for making herbal drinking water in various regions, such as Kerala, Karnataka and Central Java, where it is usually mixed with ginger, cinnamon, and cloves. The heartwood also contains juglone (5-hydroxy-1,4-naphthoquinone), which has antimicrobial activity.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophytes
Class	Angiosperms
Order	Fabales
Family	Fabaceae
Genus	<i>Caesalpinia</i>
Species	<i>sappan</i>

Major phytochemicals present in the plant are:

- Sulforaphane
- Phenyl isothiocyanate
- Digoxin
- Ferulic acid

One of the major enzymes required for the survival of the organism causing COVID 19 is ADP ribose phosphatase of NSP3 from SARS CoV-2 (6VXS) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.