

## News &amp; Comments

## *Tinospora cordifolia*: Potential Herb for antiviral drugs against Coronavirus

Muneeb Abbasi

*Tinospora cordifolia* is an immunomodulator that affects humoral, cellular, and nonspecific immune responses. *Tinospora cordifolia* includes macromolecular polysaccharides that modulate host immunity by acting on the receptor specifically, activating the signal pathway, and secreting macrophages, T cells and B cells, natural killer cells, and cytokines. *Tinospora cordifolia* boosts melatonin levels in the pineal gland, as well as essential immunomodulatory cytokines such as interleukin-2, interleukin-10, and TNF- $\alpha$ . The aqueous extracts also boost the immune system and impact cytokine synthesis<sup>3</sup>. It also contains vitamin C, which helps to strengthen the immune system. The pathophysiology of pneumonia is a complex reaction in which a viral infection triggers an immunogenic response or cytokine storm, which results in severe tissue destruction, defective coagulation, pulmonary inflammation, and the creation of microvascular thrombus. In the therapy of COVID-19 patients, various methods are considered, including reduction of the inflammatory response, antioxidant effects, and immunomodulatory effects. *Tinospora cordifolia* holds a special place in India, where hundreds of tribal people use it to treat a variety of maladies such as cough, fever, ear discomfort, fractured bone, cancer, asthma, leucorrhoea, anti-snake venom, acidity, and skin disease. Alkaloids, diterpenoid lactones, glycosides, sesquiterpenoids, polysaccharides, steroids, phenolic, and aliphatic chemicals found in *Tinospora cordifolia* have immunomodulatory, antioxidant, anti-inflammatory, analgesic, antipyretic, hypoglycaemic, antibacterial, and anticancer properties.

The study was carried out simultaneously at Meerut Institute of Engineering and Technology, Meerut, India and Taif University, Taif, Saudi Arabia from July 2020-2021. The 3-D structure of all the compounds was determined using Cresset's Flare 4.0. These built structures were subjected to extensive optimizations. In this study used two enzymes: Mpro from the virus-cell and ACE-2 receptor from the host cell. To construct the protein structure for docking analysis, the Protein Preparation Wizard was employed. The correct bond ordering was assigned, and hydrogen atoms were provided to the protein. An interaction grid for protein structure was created during docking. For Mpro protein, a grid was built at the active site of chain A. (6LU7). The bound inhibitor AXX5804 was used as the reference structure for identifying the active site in the receptor grid for ACE-2 protein (1R4L).

The 3-D structure of all the compounds was determined using Cresset's Flare 4.0. These built structures were subjected to extensive optimizations. In this investigation, two enzymes were used: Mpro from the virus-cell and ACE-2 receptor from the host cell. To construct the protein structure for docking analysis, the Protein Preparation Wizard was employed. The correct bond ordering was assigned, and hydrogen atoms were provided to the protein. An interaction grid for protein structure was created during



docking. For Mpro protein, a grid was built at the active site of chain A. (6LU7). Docking with the COVID-19 Mpro and ACE-2 was investigated in this study. Chloroquine has also been demonstrated to exhibit anti-SARS-CoV action, which could be linked to the decrease of ACE-2 glycosylation. At low pH38, these drugs have been shown to interfere with post-translational modification of viral proteases and glycosyltransferase in the endoplasmic reticulum or trans-Golgi complex vesicles.

Using Chloroquine as a reference drug, docking of chemical components from *Tinospora cordifolia* and *Withania somnifera* against Mpro and ACE-2 was done. Chemical components from *Tinospora cordifolia* and *Withania somnifera* have been shown to inhibit viral Mpro and human ACE-2 receptors in this investigation.

This research shows that plant-derived chemical components can suppress ACE-2 and Mpro more effectively than certain available medicines, making them useful for COVID-19 prophylaxis and therapy. These phytochemicals can more efficiently bind to ACE-2 and Mpro and act as inhibitors.

As a result, antiviral medicines against Coronavirus could be developed using these bioactive components in the future.

#### **JOURNAL REFERENCE**

Chaudhary, A., R. Tomar, S.M.B. Asdaq, M. Imran and S.I. Alaqel et al., 2022. In silico screening of phytochemicals as potential inhibitors of SARS-CoV-2 Mpro and human ACE-2. *Int. J. Pharmacol.*, 18: 104-115.

#### **KEYWORDS**

*Tinospora cordifolia*: , macromolecular polysaccharides, host immunity, melatonin levels, maladies, AXX5804, ACE-2 protein

