# The Blocking Ability of Daidzen against the Active Pocket of the SARS-Cov-2 Enzyme

Gagan Kumar Panigrahi[1,a], Annapurna Sahoo[1,a] and Kunja Bihari Satapathy[1]*
[1]School of Applied Sciences, Centurion University of Technology and Management, Odisha, India

[a]Author's contributed equally

*Corresponding Author's email: kunjabihari.satapathy@cutm.ac.in

**Abstract**

2019 Novel corona-virus (2019-nCoV) came up as a worldwide risk factor and put the entire human species into unrest. Till date, specific drug against the virus is not available. The current state of affair demands the development of anti-viral molecules against 2019-nCoV. The three dimensional structure of SARS-CoV-2 main protease ($M^{pro}$) can be used for high throughput screening of potential chemicals by *in silico* docking. This may result into identification of active biomolecules like phytochemicals. *In silico* Molecular Docking revealed that the phytochemical, Daidzein which belongs to isoflavone category effectively binds to the active pocket of the severe acute respiratory syndrome Corona-virus 2 (SARS- CoV-2) or the 2019-nCoV main protease.

**Keywords:** 2019-nCoV, SARS-CoV-2 main protease, SARS-CoV-2, *in silico*, molecular docking, phytochemicals.

## Introduction

Owing to the spread of 2019-nCoV which resulted into the pandemic situation represents a severe public health crisis. Outbreak of this human pathogen emerged in the city of Wuhan, and resulted to human illness, termed as COVID-19 (Chen et al., 2020, Huang et al., 2020). SARS-CoV-2 belongs to the Beta corona-virus genus, closely related to the previously identified severe acute respiratory syndrome corona-virus (SARS-CoV) [3,4]. Public Health Emergency of International Concern (PHEIC) was declared by the World Health Organization (WHO) owing to its fast rate of transmission within the humans (Panda et al., 2016, Lu et al., 2020, Wu et al., 2020). Novel coronavirus induces respiratory disease and around 10-15% patients have acute respiratory distress syndrome, which is triggered primarily by cytokines. It has been reported that the neutrophilic extracellular traps (NET) contributes to organ damage and mortality in COVID-19. NET is also linked to pulmonary diseases, thrombosis, mucous secretions and cytokine production. NETs may be well targeted to reduce the clinical severity of COVID-19. The severity of COVID-19 depends upon the pandemic spread and unprecedented pressure on health care system (Chen et al., 2020, Chan et al., 2020, Li et al., 2020). Crystal structure of the SARS-CoV-2 main protease ($M^{pro}$) can be effectively used for screening specific ligands (Liu et al., 2020). $M^{pro}$ and other known viral proteins are defining features which allow the virus to enter and infect the host cell (Wrapp et al., 2020, Lung et al., 2020, Ton et al., 2020). $M^{pro}$ can be an effective target to diminish the viral replications within the host cells since it facilitates the synthesis of functional viral proteins (Panigrahi et al., 2016, Panda and Sahoo 2016, Panigrahi et al., 2016). Effective curative measures against SARS-CoV-2 are lacking. Plants are enriched with tremendous defense response capabilities (Panigrahi and Satapathy 2020, Panigrahi et al., 2021). Elaborated defense mechanism(s) in plants need to be explored (Panigrahi and Satapathy 2020a, 2020b, 2020c). Phytochemicals which are fundamentally bioactive compounds and has the potential to amend cellular physiology may be screened against the viral proteins (Sahoo et al., 2020a,b). Here, we report that Daidzein, a phytochemical binds to the active site of the SARS-CoV-2 main protease as revealed by the *in silico* molecular docking and thus further studies may reveal the effectiveness of Daidzein to be used as COVID-19 therapeutics.

## Methods


ISSN: 2395-6216