

Effective inhibitory effect of alliin against the SARS-Cov-2 main protease

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Abstract

The deadly infectious 2019 Novel corona-virus (2019-nCoV) also referred to as severe acute respiratory syndrome Corona-virus 2 (SARS-CoV-2) that took stem in Wuhan, China has spread all over the globe within no time. It is the cause of the increasing death rate of people. This challenging situation requires development of pharmacophore for efficient treatment against severe acute SARS-CoV-2. The available crystal structure of SARS-CoV-2 main protease (M^{pro}) can be used effectively for fast *in silico* docking. This may result into identification of active biomolecules including phytochemicals. *In silico* Molecular Docking revealed that the phytochemical, Alliin effectively binds to the active pocket of the SARS-CoV-2 main protease.

Keywords: 2019-nCoV, SARS-CoV-2, SARS-CoV-2 main protease, docking, phytochemicals, Alliin.

Introduction

The pandemic situation caused due to the 2019-nCoV represents a severe public health calamity across the globe. The city of Wuhan was the epicentre where the outbreak of this human pathogen emerged, and resulted to human ailment, termed as COVID-19 (Chen et al., 2020, Huang et al., 2020). Coronavirus belongs to the family of Coronaviridae including 4 genera i.e. Alpha coronavirus, Beta coronavirus, Delta coronavirus, Gamma coronavirus. Among these, Beta coronavirus are severe acute respiratory syndrome coronavirus (SARS-CoV) and Middle East respiratory syndrome corona virus (MERS-Cove), which have engulfed more than 10,000 people around the globe in past two decades. SARS-CoV-2 belongs to Beta corona virus comprising of a positive single stranded RNA genome having 29,903 base pairs (Panda et al., 2016, Lu et al., 2020, Wu et al., 2020). These also show the characteristics of having genes encoding 3C-like proteins, RNA dependant RNA polymerase, 2'-O-ribose methyltransferase, spike protein, envelope protein, nucleocapsid phosphor protein and several unknown proteins. 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 (Chen et al., 2020, Chan et al., 2020, Li et al., 2020). The virus shows the symptoms such as fever, dry cough and difficulty in breathing. However, the treatment cannot be achieved by developing drugs against at this current time as it will take many years (Panigrahi et al., 2016, Panda and Sahoo 2016, Panigrahi et al., 2016). Thus a strategy of rapid application of drug is necessary at this very moment. Crystal structure of the SARS-CoV-2 main protease (M^{pro}) proves to be an exceptional ground for screening specific ligands (Liu et al., 2020). SARS-CoV-2 main protease can be beleaguered for developing antibodies, diagnostics and vaccines. Reportedly, M^{pro} and other known viral proteins are defining features paving the path of virus from entry to infection in the host cell (Wrapp et al., 2020, Lung et al., 2020, Ton et al., 2020). Moreover, M^{pro} can also be an effectual target to diminish the viral replications within the host cells since it facilitates the synthesis of functional viral proteins. The effectiveness of traditional medications on the restriction of COVID-19 growth does not have any scientific back up as of now, since the underlying molecular mechanisms are unclear. 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). The phytochemicals are fundamentally bioactive compounds and has the potential to amend cellular physiology (Sahoo et al., 2020a,b). Here, we report that Alliin, a phytochemical mostly enriched in some selected plants binds into the active site of the SARS-CoV-2 main protease as revealed by the *in*