

Organosulfides effectively bind to 2019- nCoV main protease

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Abstract

The emerging 2019 Novel coronavirus (2019-nCoV) threatens public health. 2019-nCoV is also referred to as severe acute respiratory syndrome coronavirus-2 (SARS-CoV-2). Within no time it emerged as a global risk and was declared as pandemic. Specific drug against the virus is yet to be discovered. Development of biomolecules for proficient treatment against severe acute SARS-CoV-2 is challenging. The solved crystal structure of SARS-CoV-2 main protease (M^{Pro}) can be used as one of the primary target molecule and possible inhibitory ligands may be screened using *in silico* docking. Primarily phytochemicals can be screened to detect any potential bioactive molecules. *In silico* molecular docking revealed that the phytochemicals, benzyl isothiocyanate and phenyl isothiocyanate belonging to the organosulfide group of phytochemicals may effectively binds to the active site of the SARS-CoV-2 main protease.

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

Introduction

Numerous members of the family Coronaviridae continuously circulate in the human population and usually cause mild respiratory disease (Chen et al., 2020, Huang et al., 2020). Whereas, the severe acute respiratory syndrome Coronavirus (SARS-CoV) and the Middle East Respiratory Syndrome Coronavirus (MERS-CoV) are transmitted from animals to humans resulting into SARS and MERS, respectively (Panda et al., 2016, Lu et al., 2020, Wu et al., 2020). Natural reservoir hosts for SARS-CoV were Chinese horseshoe bats (Panda et al., 2016, Lu et al., 2020, Wu et al., 2020). Intermediate hosts like civet cats and raccoon dogs, which are habitually sold as food sources in Chinese wet markets mediated the human transmission (Lu et al., 2020, Wu et al., 2020). At present, no precise antivirals or approved vaccines are available to combat the current pandemic situation. Presently, conventional control measures, including travel restrictions and self-quarantine are practiced. The pandemic situation caused due to the 2019-nCoV represents a severe public health calamity across the globe. This pathogen emerged from the city of Wuhan and resulted into this scariest situation, COVID-19 (Chen et al., 2020, Chan et al., 2020, Li 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) (Panigrahi et al., 2016, Panda and Sahoo 2016, Panigrahi et al., 2016). Public Health Emergency of International Concern (PHEIC) was declared by