

Kaempferol: a potent phytomolecule against SARS-Cov-2

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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 2019-nCoV 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 molecules 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 phytochemical, Kaempferol belonging to the flavanoid group of phytochemical 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.

Introduction

Corona viruses are the group of viruses, which are able to cause diseases in both animal and humans. One of the best examples of previously known coronavirus is severe acute respiratory syndrome (SARS) and the virus strain is known as SARS-CoV. Further new strains of Corona virus are identified, known as severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2). This virus is responsible for causing coronavirus disease 19 (COVID-19). The new coronavirus has spread very rapidly in different parts of the world. 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). SARS-CoV-2 belongs to the beta corona-virus genus (Panda et al., 2016, Lu et al., 2020, Wu et al., 2020). On 11th March, 2020 the World Health Organization (WHO) declared that COVID-19 as a pandemic. A pandemic occurs when, the disease that people are not immune to spread across the large region. Countries including United States of America, Italy had largest outbreak outside China with increased number of infected people leading to death of individuals (Chen et al., 2020, Chan et al., 2020, Li et al., 2020). The pandemic ratio changes very rapidly with fresh data collected on the basis of chemical and serological characteristics of affected case being reported every day (Panigrahi et al., 2016, Panda and Sahoo 2016, Panigrahi et al., 2016). Crystal structure of the SARS-CoV-2 main protease (M^{Pro}) proves to be an outstanding ground for screening specific ligands (Liu et al., 2020). Reportedly, M^{Pro} and other known viral proteins infect the respiratory tract (Wrapp et al., 2020, Lung et al., 2020, Ton et al., 2020). Moreover, M^{Pro} can also be an