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A role for quercetin in coronavirus disease 2019 (COVID-19)

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Abstract

Several months ago, an outbreak of pneumonia of unknown aetiology was detected in Wuhan City (China) and the aetiological agent of the atypical pneumonia was isolated by the Chinese authorities as novel coronavirus (2019-nCoV or SARS-CoV-2). The WHO announced this new disease was to be known as "COVID-19." When looking for new antiviral compounds, knowledge of the main viral proteins is fundamental. The major druggable targets of SARS-CoV-2 include 3-chymotrypsin-like protease (3CLpro), papain-like protease (PLpro), RNA-dependent RNA polymerase, and spike (S) protein. Quercetin inhibits 3CLpro and PLpro with a docking binding energy corresponding to -6.25 and -4.62 kcal/mol, respectively. Quercetin has a theoretical, but significant, capability to interfere with SARS-CoV-2 replication, with the results showing this to be the fifth best compound out of 18 candidates. On the basis of the clinical COVID-19 manifestations, the multifaceted aspect of quercetin as both antiinflammatory and thrombin-inhibitory actions, should be taken into consideration.

Keywords: COVID-19; SARS-CoV-2; infectious diseases; nutraceutical; quercetin.

Figures

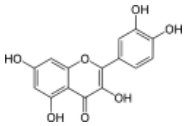

FIGURE 1 Chemical structure of quercetin

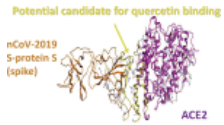

FIGURE 2 A reasonable target for structure-based...

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