Infectious Disorders - Drug Targets

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Research Article

Molecular Docking of Phytochemical Compounds of Momordica charantia as Potential Inhibitors against SARS-CoV-2

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Abstract

Background: Coronavirus disease 2019 (COVID-19) has been recently declared as a global public health emergency, where the infection is caused by SARS-CoV-2. Nowadays, there is no specific treatment to cure this infection. The main protease (Mpro) of SARS-CoV-2 and SARS spike glycoprotein- human ACE2 complex have been recognized as suitable targets for treatment, including COVID-19 vaccines.

Objective: In our current study, we identified the potential of Momordica charantia as a prospective alternative and a choice in dietary food during a pandemic.

Materials and Methods: A total of 16 bioactive compounds of Momordica charantia were screened for activity against 6LU7 and 6CS2 with AutoDockVina.

Results: We found that momordicoside B showed the lowest binding energy compared to other compounds. In addition, kuguaglycoside A and cucurbitadienol showed better profiles for drug-like properties based on Lipinski's rule of five.

Conclusion: Our result indicates that these molecules can be further explored as promising candidates against SARS-CoV-2 or Momordica charantia can be used as one of the best food alternatives to be consumed during the pandemic.

Keywords: Antiviral, COVID-19, molecular docking, Momordica charantia, SARS-CoV-2, phytochemical compounds.

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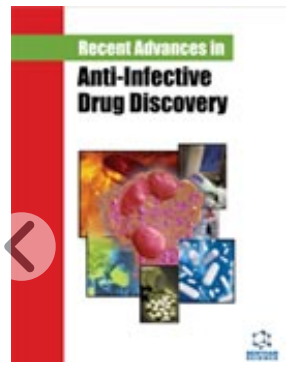

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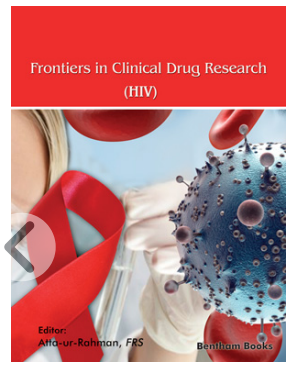

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