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Title of Manuscript: Molecular docking of phytochemical compounds of Momordica charantia as potential inhibitor against SARS-CoV-2

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Volume 22, Issue 3, 2022

Published on: 15 February, 2022

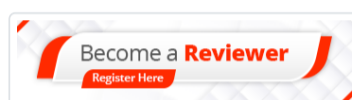
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Abstract

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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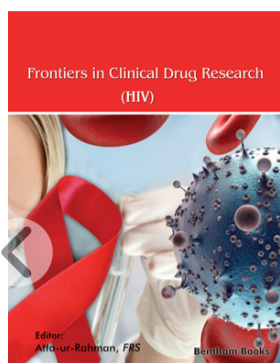
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(Formerly Current Drug Targets - Infectious Disorders)

ISSN (Print): 1871-5265

ISSN (Online): 2212-3989

Volume 22, Issue 8, 2022

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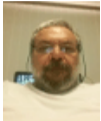


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