Molecular docking and molecular dynamics studies of sars-cov-2 inhibitors: Crocin, digitoxigenin, beta-eudesmol and favipiravir: Comparative study

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Abstract
In this study, Crocin, Digitoxigenin, Beta-Eudesmol, and Favipiravir were docked in the active site of SARS-CoV-2 main protease (PDB code: 6LU7). The docking study was followed by Molecular Dynamics simulation. The result indicates that Crocin and Digitoxigenin are the structures with the best affinity in the studied enzyme's binding site. Still, Molecular Dynamics simulation showed that Digitoxigenin is the molecule that fits better in the active site of the main protease. Therefore, this molecule could have a more potent antiviral treatment of COVID-19 than the other three studied compounds. © 2021 by the authors.

Author keywords
Beta-Eudesmol; Crocin; Digitoxigenin; Favipiravir; SARS-CoV-2