

RESEARCH ARTICLE

***In silico* Molecular Docking Analysis of some Terpenoids against 3CLpro of SARS-CoV-2**

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ABSTRACT:

The recent pandemic of coronavirus disease 2019 (COVID-19) caused by severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2) has raised global health concerns. The main viral protease called 3-chymotrypsin-like cysteine protease (3CLpro) plays an important role in viral replication by polyproteins processing that are translated from viral RNA. Therefore, the present *in silico* docking study aimed to assess the inhibitory actions of various terpenoids against 3CLpro of SARS-CoV-2. Molecular docking was performed using ArgusLab 4.0.1. a computational docking program and the protein-ligand interaction was visualized by using Pymol 1.7 software. The inhibitory activity of terpenoids like abietic acid, ferruginol, rosmarinic acid, zingiberine, sugiol, kaempferol and betulinic acid was tested against 3CLpro (PDB ID: 6M2N) using molecular docking paradigm while antiviral drugs- remdesivir, darunavir and hydroxychloroquine- were used as standards for comparison. All phyto-constituents showed an effective binding interaction with 6M2N, and the binding affinity was ranged from – 8.854 to –13.398 as compared to remdesivir, darunavir and hydroxychloroquine. Amongst tested compounds, abietic acid, ferruginol and betulinic acid exhibited promising enzyme interaction. Results indicate that based upon the binding energy of abietic acid, ferruginol and betulinic acid could be efficient SARS-CoV-2 3CLpro inhibitors. This is supported by the fact that the effects of some terpenoidal phytochemicals especially abietic acid, ferruginol and betulinic acid showed promising enzyme interaction as compared to remdesivir and darunavir. Therefore, further studies are warranted to confirm the effectiveness of abietic acid, ferruginol and betulinic acid for the therapy of COVID-19.

KEYWORDS: COVID-19, 3CL^{pro}, terpenoids, molecular docking.

INTRODUCTION:

The severe acute respiratory syndrome corona virus 2 (SARS-CoV-2) triggered coronavirus disease 2019 (COVID-19) is currently the rapidly spreading disease across the globe. The virus has been mainly emerged as human-to-human contact-transmitted pathogen. Moreover, it can also be spread through the air if respiratory droplets of infected person reach the mouth,

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