

Potential Drug Leads for SARS-CoV2 from Phytochemicals of Aerva lanata: An in silico approach

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Abstract

COVID-19 outbreak is the recently reported worldwide pandemic threat. As part of our interventions with molecular simulation approaches, we report the inhibitory effect of thirty compounds reported from the sacred plant Aerva lanata and compare their activity with the one of the present medication, hydroxy chloroquine, on the main protease (PDB:6YB7) of SARS-CoV-2. Our studies pointed out the effectiveness of the plant with twenty seven compounds having potential activity against the main protease compared to the reference HCQ. The robustness of some of the phytochemicals such as ervoside, which is only present in Aerva lanata computed to have very high anticoronavirus activity. The results are indicative of potential natural antiviral source, which subsidizes in thwarting the invasion of coronavirus into the human body. Many phytochemicals which are computed to be effective towards SARS-CoV-2 in this study are used as drugs for various other diseases. Perhaps these compounds could be attractive for the management of COVID-19, but clinical trials must be performed in order to validate this observation.

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