COMPUTATIONAL IDENTIFICATION OF SELECTED BIOACTIVE COMPOUNDS FROM *CEDRUS DEODARA* AS INHIBITORS AGAINST SARS-COV-2 MAIN PROTEASE: A PHARMACOINFORMATICS STUDY

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ABSTRACT

Amid the ongoing Covid-19 pandemic, the quest for potent antiviral treatments intensifies. This study focuses on the potential of bioactive compounds from the Himalayan cedar *Cedrus deodara* against the SARS-CoV-2 virus. Specifically targeting the main protease (M^{Pro}) and spike protein, the study employs docking trials and molecular dynamics simulations. Compounds such as quercetin, dihydrodehydrodiconiferyl alcohol, and cedeodarin exhibit notable binding affinity, surpassing the reference drug favipiravir. Molecular dynamics simulations affirm the stability of these complexes throughout the simulation period. While these findings underscore promising interactions, it is crucial to emphasize the need for further research and experimental validation to fully explore the therapeutic capabilities of *C. deodara* in combatting Covid-19.