Biomolecules against SARS-CoV-2 Main protease, RdRp and the RBM of its spike glycoprotein: an *In Silico* approach

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Abstract

Severe acute respiratory syndrome coronavirus 2 emerged in Wuhan, China, in December 2019, marking the onset of a profound global health crisis. The unprecedented scale of the ensuing pandemic prompted an urgent need for innovative strategies to combat COVID-19. In response, researchers and scientists worldwide directed their efforts towards identifying effective preventive and therapeutic measures. Among these, natural products have gained prominence due to their potential in offering a holistic approach to tackling the virus. This study undertook a rigorous computational approach to sift through a vast array of natural compounds, aiming to pinpoint those with promising antiviral properties against the SARS-CoV-2 Main Protease, RdRp and the RBM of the spike glycoprotein. Through sophisticated molecular docking simulations, the study investigated the intricate interplay between selected natural compounds and the virus targets. This analysis encompassed diverse factors such as binding affinity, interaction dynamics, and structural compatibility within the active sites of the target protein. The encouraging results provide a solid foundation for further in-depth exploration, including experimental validation and refinement of these compounds as potential therapeutic agents against COVID-19. The identification of novel natural antiviral compounds presents a beacon of hope for global health, offering new avenues for combatting SARS-CoV-2 and future potential viral threats. As these findings pave the way for future drug design strategies, they reinforce the collaborative and interdisciplinary approach needed to triumph over the challenges posed by COVID-19.

Keywords: SARS-CoV-2, COVID-19, Main protease, RdRp, Spike Glycoprotein, Antiviral, Biomolecules, Molecular dynamics.