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Research Articles

# Artecanin of *Laurus nobilis* is a novel inhibitor of SARS-CoV-2 main protease with highly desirable druglikeness

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## Abstract

Main protease ($M^{pro}$) is a critical enzyme in the life cycle of severe acute respiratory syndrome Coronavirus −2 (SARS-CoV-2). Due to its essential role in the maturation of the polyproteins, the necessity to inhibit $M^{pro}$ is one of the essential means to prevent the outbreak of COVID-19. In this context, this study was conducted on the natural

compounds of medicinal plants that are commonly available in the Middle East to find out the most potent one to inhibit $M^{pro}$ with the best bioavailability and druglikeness

from PubChem database and docked against $M^{pro}$. Thirty compounds with the highest docking scores with $M^{pro}$ were chosen for further virtual screening. Variable druglikeness and toxicity potentials of these compounds were evaluated using SwissADME and Protox servers respectively. Out of these virtually screened compounds, artecanin was predicted to exhibit the most favourable druglikeness potentials, accompanied by no predicted hepatoxicity, carcinogenicity, mutagenicity, and cytotoxicity. Molecular dynamics (MD) simulations showed that $M^{pro}$-artecanin complex exhibited comparable stability with that observed in the ligand-free $M^{pro}$. This study revealed for the first time that artecanin from *Laurus nobilis* provided a novel static and dynamic inhibition for $M^{pro}$ with excellent safety, oral bioavailability, and pharmacokinetic profile. This study suggested the ability of artecanin to be used as a potential natural inhibitor that can be used to block or at least counteract the SARS-CoV-2 invasion.

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