# Design and in silico identification of potential inhibitors against SARS-CoV-2 main protease. A preliminary study.

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SARS-ongoing CoV-2's worldwide outbreak has been identified as a global public health issue due to its daily high rates of morbidity and mortality. There is a need to discover a powerful medication against SARS-CoV-2 due to the virus' quick spread and resurgence. Due to their serious side effects, drugs like Remdisivir and Hydroxychloroquine have received more focus and still are under investigation. Therefore, the aim of the present work is to identify novel, potent inhibitors against the main protease SARS-CoV-2. In this study, with the aid of molecular docking studies, ADME properties and molecular dynamic simulations, we designed and selected molecules with a high probability to be potent inhibitors of main protease SARS-CoV-2. The molecular docking study results revealed that compound **12** had higher binding affinity among the 85 designed compounds compared to co-crystal native ligand inhibitor N3 with an optimal pharmacokinetic profile. Moreover, the molecular dynamics simulations have shown that compound **1** stably possesses good binding susceptibility and strong interactions with essential residues of SARS-CoV-2 main protease. Finally, the findings of the present work imply that selected compounds were predicted to be potent inhibitors against SARS-CoV-2. However, additional biological research is required to prove the prediction results.