Potent Inhibitors for SARS-COV-2 Main Protease: An in-Silico Study for Drug Development

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Abstract

The emergent of the new coronavirus (SARS-CoV-2) and consequently the viral infection that spread widely affecting hundreds of thousands across the entire world has developed a global health concern. Coronaviruses infect humans causing highly prevalent diseases. The current work is an effort to examine commercially available drugs in order to repurpose them against SARS-CoV-2 by the means of structure-based in-silico screening. The present study focusses on testing the repurposing efficacy of the currently used drugs against SARS-CoV-2 main protease. The main proteases from the coronavirus are essential for the viral replication and are involved in the polyprotein cleavage and immune regulation, making them attractive and effective targets for the development of antiviral drugs. Number of approved anti-viral drugs were tested as potential SARS-CoV-2 virus inhibitors using molecular docking analysis by examining the free natural affinity of the binding ligand to the active-site pocket and catalytic residues without forcing the docking of ligand to active site. SARS-CoV-2 protease solved structure (6LU7) is targeted by repurposed drugs. The molecular docking analysis results have shown that the binding of Remdesivir and Mycophenolic acid acyl glucuronide with the protein drug target has optimal binding features suggesting further experimental consideration for their treatment effectiveness.

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