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In Silico Study of Antiviral Drugs Against Three Important Proteins of Sars-Cov-2 Using Molecular Docking Method

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Abstract : Object: In the last two decades, the recent outbreak of Coronavirus (SARS-CoV-2) imposed a global pandemic in the world. Despite the increasing prevalence of the disease, there are no effective drugs to treat it. A suitable and rapid way to afford an effective drug and treat the global pandemic is a computational drug study. This study used molecular docking methods to examine the potential inhibition of over 50 antiviral drugs against three fundamental proteins of SARS-CoV-2. METHODS: Through a literature review, three important proteins (a key protease, RNA-dependent RNA polymerase (RdRp), and spike) were selected as drug targets. Three-dimensional (3D) structures of protease, spike, and RdRP proteins were obtained from the Protein Data Bank. Protein had minimal energy. Over 50 antiviral drugs were considered candidates for protein inhibition and their 3D structures were obtained from drug banks. The Autodock 4.2 software was used to define the molecular docking settings and run the algorithm. RESULTS: Five drugs, including indinavir, lopinavir, saquinavir, nelfinavir, and remdesivir, exhibited the highest inhibitory potency against all three proteins based on the binding energies and drug binding positions deduced from docking and hydrogen-bonding analysis. Conclusions: According to the results, among the drugs mentioned, saquinavir and lopinavir showed the highest inhibitory potency against all three proteins compared to other drugs. It may enter laboratory phase studies as a dual-drug treatment to inhibit SARS-CoV-2.

Keywords : covid-19, drug repositioning, molecular docking, lopinavir, saquinavir
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