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# Repositioning Therapeutics For SARS-CoV-2: Virtual Screening Of Plant-based Anti-HIV Compounds As Possible Inhibitors Against COVID-19 Viral RdRp.

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## Abstract:

Background: Coronavirus disease 2019 (COVID-19) has caused a global pandemic with a high mortality and morbidity rate worldwide. The COVID-19 vaccines that are currently in development or already approved are expected to provide at least some protection against the emerging variants of the virus, but the mutations may reduce the efficacy of the existing vaccines. Purified phytochemicals from medicinal plants provide a helpful framework for discovering new therapeutic leads as they have long been employed in traditional medicine to treat many disorders.

Objective: The objectives of the study are to exploit the anti-HIV bioactive compounds against SARS-CoV-2 RNA-dependent RNA polymerase (RdRp) through molecular docking studies and to evaluate the Absorption, Distribution, Metabolism, Excretion, and Toxicity (ADMET) properties of potential compounds.

Methods: Molecular docking was performed to study the interaction of ligands with the target sites of RdRp protein (PDB: 6M71) using AutoDock Vina. The ADMET properties of potential compounds were predicted using the pkCSM platform.

Results: A total of 151 phytochemicals derived from the medicinal plants with recognized antiviral activity and 18 anti-HIV drugs were virtually screened against COVID-19 viral RdRp to identify putative inhibitors that facilitate the development of potential anti-COVID-19 drug candidates. The computational studies identified 34 compounds and three drugs inhibiting viral RdRp with binding energies ranging from -10.2 to -8.5 kcal/mol. Among them, five compounds, namely Michellamine B, Quercetin 3-O-(2'',6''-digalloyl)-beta-Dgalactopyranoside, Corilagin, Hypericin, and 1,2,3,4,6-Penta-O-galloyl-beta-D-glucose residues, bound efficiently with the binding site of RdRp. Besides, Lopinavir, Maraviroc, and Remdesivir drugs also inhibited SARS-CoV-2 polymerase. In addition, the ADMET properties of top potential compounds were also predicted in comparison to the drugs.

Conclusion: The present study suggested that these potential drug candidates can be further subjected to in vitro and in vivo studies that may help develop effective anti-COVID-19 drugs.