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Drug Repurposing using Computational Methods to Identify Therapeutic Options for COVID-19

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ABSTRACT

Recently the world has been dealing with the new type of coronavirus called as COVID-19 that in terms of symptoms is similar to the SARS-COVID. The severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2) pandemic has generated a critical need for treatments to reduce morbidity and mortality associated with this disease. However, traditional drug development takes many years, which is not practical solution given the current pandemic. Therefore, a viable option is to repurpose existing drugs. Drug repurposing is a more inexpensive and shorter approach than the traditional drug discovery and development process. The concept of identifying a potent molecule from a library of pre-existing molecules or an already approved drug has become a go-to tactic to accelerate the identification of drugs that can prevent COVID-19. The structural data of several proteins vital for the virus became available shortly after the start of the pandemic. According to the results simeprevir, hesperidin, glecaprivir, glycyrrhizin acid showed highly favorable free binding energies with all tested target proteins. In this review, we discuss the importance of these targets and their available potential inhibitors predicted by the computational approaches. Among the hits identified by computational approaches, 35 candidates were suggested for further evaluation, among which ten drugs are in clinical trials (Phase III and IV) for treating Coronavirus 2019 (COVID-19).

Keywords: COVID-19, SARS-CoV-2, Drug repurposing, Computational approaches, Molecular docking

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