عنوان مقاله:

In silico Study to Identification of Potential SARS-CoV-۲ Main Protease Inhibitors: Virtual Drug Screening and Molecular Docking with AutoDock Vina and Molegro Virtual Docker

محل انتشار:

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خلاصه مقاله:

Coronavirus disease ۲۰۱۹ (COVID-۱۹) has emerged in Wuhan, China, and because of fast transmission, it has led to its extensive prevalence in almost all countries, which has made it a global crisis. Drug repurposing is considered a fast way to discover new applications of the current drugs. This study aims to recognize a possible small molecule as a primary protease inhibitor versus the main protease protein of SARS-CoV-۲ by computational programs. Virtual screening procedures like using Molegro Virtual Docker, AutoDock Tool, and AutoDock Vina, were done for more than ۱۶۰۰ FDA-approved medicines downloaded from the ZINC database, were employed to characterize new implied molecule inhibitors for the recently published crystal structure of the main protease protein of SARS-CoV-۲. Virtual screening results indicated, many drugs including ARBs, cephalosporins, some kinase inhibitors, HMG CoA reductase, and leukotriene receptor antagonist, may inhibit the main protease of SARS-COV-۲. Velpatasvir, Molnupiravir, and Ivermectin were selected by virtual screening methods for further studies to find an efficient ligand for the treatment of COVID-۱۹. Due to some other beneficial features, including anti-infectious, anti-inflammatory properties, and ADME profile, they could be a promising drug nominee for repurposing to the treatment of COVID-۱۹. Velpatasvir was selected by some virtual screening methods for further studies to find a suitable ligand for the treatment of COVID-۱۹. Furthermore, more studies need to approve this data and finally clinical trial needs to be done to examine the efficacy of Velpatasvir for the treatment of covid-۱۹ as an anti-viral agent.

کلمات کلیدی:

Velpatasvir, Virtual screening, Covid-۱۹, molecular docking, Repurpose, main protease inhibitor