عنوان مقاله:

Molecular Docking and Fragment-Based QSAR Modeling for In Silico Screening of Approved Drugs and Candidate Compounds Against COVID-۱۹

محل انتشار:

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خلاصه مقاله:

Background: Coronavirus disease ۲۰۱۹ (COVID-۱۹) as a serious global health crisis leads to high mortality and morbidity. However, currently, there are no effective vaccines and treatments for COVID-۱۹. Main protease (Mpro) and angiotensin-converting enzyme ۲ (ACE۲) are the best therapeutic targets of COVID-۱۹. Objectives: The main purpose of this study is to investigate the most appropriate drug and candidate compound for proper interaction with Mpro and ACE۲ to inhibit the activity of COVID-۱۹. Methods: In this study, repurposing of approved drugs and screening of candidate compounds using molecular docking and fragment-based QSAR method were performed to discover the potential inhibitors of Mpro and ACE۲. QSAR and docking calculations were performed based on the prediction of the inhibitory activities of ۵-hydroxy indanone derivatives. Based on the results, an optimal structure was proposed to inhibit the activity of COVID-۱۹. Results: Among ۲۶۲۹ DrugBank approved drugs, ۱۱۸ were selected considering the LibDock score and absolute energy for possible drug-Mpro interactions. Furthermore, the top ۴۰ drugs were selected based on screening the results for possible drug- Mpro interactions with AutoDock Vina. Conclusion: Finally, evaluation of the top ۴۰ selected drugs for possible drug-ACE۲ interactions with AutoDock Vina indicated that deslanoside (DB۰۱۰۷۸) can interact effectively with both Mpro and ACE۲. However, prior to conducting clinical trials, further experimental validation is needed.

کلمات کلیدی: