عنوان مقاله:

Coronavirus (SARS-CoV-۲) Deactivation via Spike Glycoprotein Shielding by Old Drugs: Molecular Docking Approach

محل انتشار:

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خلاصه مقاله:

Today the disease of COVID-۱۹ comprises the most serious problem against human health worldwide with a high rate of virulence and mortality. The disease is caused by the SARS-CoV-۲ virus from the beta coronavirus family. The virus makes use of its surface glycoprotein named S protein or spike to enter the human cells. The virus is attached to its receptor of angiotensin-converting enzyme ۲ on the cell surface via its receptor-binding domain and fused after cleavage at S۲' site that is carried out by surface protease. Vaccines or drugs interfering with S protein binding or blocking the cleavage sites of S protein could be considered as a treat to get rid of the infection. In the current work and through molecular docking and molecular dynamics experiments, ۱۴ drugs were selected based on their molecular weights among ۱۰۰ drugs to study their shielding potency toward S protein binding sites. The obtained results indicate that fidaxomicin, niclosamide, and flubendazole bind specifically to the S۲' cleavage site; while ivermectin, rapamycin, heparin, azithromycin, clarithromycin, and erythromycin bind both receptor-binding domain and S۲' and can prevent virus attachment to its receptor and may be useful as a prophylactic candidate for COVID-۱۹ management after clinical approval.

کلمات کلیدی:

COVID-۱۹, Docking, Heparin, Ivermectin, Clarithromycin, Erythromycin