عنوان مقاله:

Molecular Docking Analysis of Anti-Severe Acute Respiratory Syndrome-Coronavirus ۲ Ligands against Spike Glycoprotein and the ۳-Chymotrypsin-Like Protease

محل انتشار:

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خلاصه مقاله:

Background: The severe acute respiratory syndrome-like disease coronavirus disease ۲۰۱۹ (COVID-۱۹) is a disastrous global pandemic with ۱۶,۲۸۸,۴۹۰ infected cases and ۶۴۹,۸۸۴ deaths. Until now, no effective treatments are found. Methods: The virus uses the ۳-chymotrypsin-like protease for inducing the activity of the viral polyproteins and the spike (S) glycoprotein for human cell entry through the human angiotensin-converting enzyme ۲ receptor. Blocking the active binding sites of these molecules might be beneficial for decreasing the activity of the virus and suppressing the viral entry to the human cells. Here, docking methods were used to identify a group of ligands may perform the blocking operations. Results: The results revealed the strongest binding affinities, sorted high to low, for tadalafil (Cialis) (phosphodiesterase type ۵ inhibitor, tirofiban (antiplatelet), paraxanthine (central nervous system stimulant), dexamethasone, gentian violet cation (triphenylmethane), salbutamol, and amlodipine (calcium channel blocker). Conclusion: These substances may provide vital help for further clinical investigation in fighting against the current global pandemic of the COVID-۱۹.

کلمات کلیدی:

Cialis, coronavirus disease ۲۰۱۹, dexamethasone, ligands, salbutamol, severe acute respiratory syndrome-coronavirus ۲