عنوان مقاله:

A Molecular Docking Study: Benzoxazolone Derivatives against SARS-CoV-۲ Omicron Subvariant EG.۵.۱

محل انتشار:

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خلاصه مقاله:

In the ongoing COVID-۱۹ pandemic, it is important to develop treatment strategies and new drug candidates that target the interactions between the receptor-binding domains (RBDs) of the currently circulating SARS-CoV-۲ Omicron subvariants-XBB.۱.۵ and EG.۵.۱ and the human ACE۲ receptor. The SARS-CoV-۲ Omicron subvariant EG.۵.۱, currently in circulation, possesses a faster transmission capability compared to other subvariants. It weakens the neutralizing effect of existing monoclonal antibodies and evades vaccine-generated antibodies. Thus, there is a need for new molecules that can target EG.۵.۱ RBD. In this study, the effectiveness of (۸ Compounds) derivatives containing benzoxazolone and piperazine rings, which have previously been reported to have antiviral properties, against XBB.۱.۵ and EG.۵.۱ RBDs, was measured using molecular docking, molecular dynamics simulation, and MM-PBSA methods. For the in silico study, AutoDock Vina, Discovery Studio Visualizer, and GROMACS molecular dynamics software were utilized. According to the results, the compounds were found to be effective against the EG.۵.۱ Omicron subvariant. Among the tested compounds, ۵-chloro-۳-[۴-(۲-bromophenyl)piperazin-۱-ylmethyl]benzoxazol-۲-one (Compound ۸) had the highest affinity and binding energy values for both XBB.۱.۵ and EG.۵.۱ RBDs. In conclusion, the development of Mannich bases containing benzoxazolone and piperazine ring systems will be beneficial against both EG.۵.۱ and future variants of concern.

کلمات کلیدی:

COVID-۱۹س, XBB.۱.۵, EG.۵.۱, ۳ ,ubstituted benzoxazolonesئ olecular docking