عنوان مقاله:

Docking of helicase, main protease, papain-like protease, and RNA-dependent RNA polymerase of SARS-CoV-۲ by theaflavin-۳-gallate

محل انتشار:

مجله جنبه های زیستی میکرو نانو, دوره 2, شماره 3 (سال: 1402)

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خلاصه مقاله:

Polyphenol phytochemicals have obtained huge attention owing to their numerous therapeutic applications. Green, oolong, and black teas are the main sources of abundant polyphenols. Theaflavins are a large group of polyphenols isolated from oolong and black tea. Theaflavins have shown various therapeutic advantages, specifically antimicrobial activity. Hear, the antiviral effect of theaflavin-۳-gallate as one the main theaflavins against severe acute respiratory syndrome coronavirus ۲ (SARS-CoV-۲) has been investigated by molecular docking study. This study exhibited the best binding affinity for the interaction of the theaflavin-۳-gallate ligand with SARS-CoV-۲ helicase NSP۱۳ with a Vina score of -۱۰.۳ kcal/mol compared with theaflavin-۳-gallate and spike protein S۱ complex with a lowest binding affinity of -۸.۲ kcal/mol. For a better understanding of the antiviral activity of theaflavin-۳-gallate compound, experimental in vitro .and in vivo studies about other bioactive compounds and drugs are needed

کلمات کلیدی:

theaflavins, polyphenols, Theaflavin-۳-gallate, Oolong tea, Black tea, Helicase NSP۱۳