عنوان مقاله:

Investigation of some natural extract compounds against COVID-۱۹ by Molecular Docking study

محل انتشار:

اولین همایش بین المللی و دهمین همایش ملی بیوانفورماتیک ایران (سال: 1400)

تعداد صفحات اصل مقاله: 1

نویسندگان:

Akbar Vaseghi - *Demarteman of Nanobiotechnology, Faculty of Biological Sciences, Tarbiat Modares University, Tehran, Iran*

Sanaz Soltangheis - *Department of Chemical engineering, University of Mohaghegh, Ardabil, Iran*

Reza Ashrafi Parchin - *Excir Faravaran Sabalan company, Ardabil Science and Technology Park, Ardabil, Iran*

Kosar Rezaee Chamanie - *Department of Biology, Faculty of Science, University of Guilan, Rasht, Iran*

Majid Sadeghizadeh - *Demarteman of Nanobiotechnology, Faculty of Biological Sciences, Tarbiat Modares University, Tehran, Iran*

خلاصه مقاله:

We used the molecular docking technique on the ACE۲, Heat Shock Protein A۵ substrate-binding domain b(HSPA۵ SBDb), proteins in the human body, and the main protease (PDB۶LU۷) protein of SARS-CoV-۲.We describe from silico studies on the host-cell receptor recognized by the viral spike protein that leads toan essential foundation about SARS-CoV-۲ resistance of individual compounds. In this study, ۱۱ naturalcompounds, which have antiviral properties according to previous studies, have been selected as smallmolecules candidates in the molecular docking study of spike and PDB۶LU۷ proteins of SARS-CoV۲ andalso ACE۲, TMPRSS۲, and HSPA۵ proteins in human cells. Binding constants of CAPE, Apigenin,Acacetin, Rutin, Chrysin, Galangin, Kaempferol, Quercetin, Artepillin c, Cinnamic acid, Prenyl caffeate, andthree drugs as conventional antivirus include Oseltamivir, Heparan sulfate, and Acyclovir were measuredusing the AutoDock ۴.۲ molecular docking program. The results showed a high binding affinity for the Rutin,Galangin, and Quercetin to the ACE۲, HSPA۵, TMPRSS۲, and ۶LU۷ protein from -۸.۱ to -۱۰.۷ kcal/mol.Also, Chrysin had the best inhibition potentials among the studied molecules with high binding energy -۹.۴kcal/mol from S protein. Our studies showed that rutin had the best inhibition potentials among the studiedmolecules with high binding energy again ACE۲, HSPA۵, TMPRSS۲, ۶LU۷, and S protein. Among thesecompounds, Rutin might compete with Covid-۱۹ for ACE۲, HSPA۵, TMPRSS۲, ۶LU۷, and S proteins andmight prevent or delay the entry of Covid-۱۹ into the cell. It is followed by myricetin, caffeic acid phenethylester, hesperetin, and pinocembrin. In conclusion, the high potential of polyphenolic agents and flavonoidsin propolis to bind to human and viral proteins associated with the SARS-CoV-۲ pandemic indicates that hashigh potential in the treatment of Covid-۱۹.

کلمات کلیدی:

SARS-CoV-۲, natural compounds, Molecular Docking