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Title:

Molecular docking analysis of ten plant products for the inhibition of spike glycoprotein and prospective use as anti-COVID compounds

Introduction:

The threat of the COVID-19 pandemic has persisted unabated over the past two years. The current response to maintaining public health has been guided by the vaccination of the population. The success of this policy has been mixed COVID coming back in each region in waves driven by new variants. Given that boosted immune response to COVID-19 owing to the vaccine also having an expiration time, it is important to look at alternative options to protect against COVID-19. In this regard, bioactive substances commonly found in food or food additives present a viable option to shield against consequential COVID-19 infection. We investigate 10 bioactive plant products for possible antiviral use against the SARS-CoV-2 virus, which causes COVID-19 infection.

Methods:

We test these compounds by *in silico* docking to the Spike glycoprotein, one of the major determinants of COVID-19 infection. The AutoDock Vina software was used to scan and score the docking sites on a Spike protein ectodomain model. The top twenty hits were saved for each of the ten compounds and then the common and unique docking sites were delineated noting the putative binding affinity in each case.

Results:

The results show that all ten plant products are high-affinity binders to the Spike protein, the S2 domain being the primary binding site. Very few binding interactions are found on the receptor binding domain, which means that topically used of these molecules such as in nasal spray would not be effective. In the ingestible form, the compounds can bind to the Spike molecule and disable it from driving virus-host fusion, its main function. It can thereby limit the cell-to-cell spread of the virus thus enforcing localization and clearance by the host immune system.

Conclusions:

From this study alone, one can propose Jujuboside B, Glucolepidiin, and Glycyrrhizin as the top three candidates suitable for further trials for COVID-19 mitigation. Linoleic acid need not be considered for any further study.

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