Exploration of phytochemicals as active medicines against COVID-19 via molecular docking.

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Abstract

Molecular docking approaches were used to identify the best bioactive phytochemicals from several medicinal plants, indicating a possible pre-clinical drug discovery against SARS-CoV-2 viral infection. To compute binding affinity at SARS-active CoV-2's sites, researchers performed in silico screening of bioactive phytochemicals with the two druggable targets of the virus using basic precision/extra precision molecular docking methods. Scientists were forced to look for new antiviral treatments after the SARS-CoV-19 pandemics and the insufficiency of targeted medications. The current state of knowledge about plant extracts containing polyphenols that inhibit Covid-19 is presented. Natural phytochemicals originating from plants have the potential to establish coronavirus therapy and preventive research employing extracts and/or specific compounds. The polyphenolic medicines have the ability to block the coronavirus protein, which is required for virus infection and reproduction. After a thorough examination of isolated phytochemicals, the molecular descriptors, docking score, active sites, and FMOs energies were compared to those of commonly used COVID-19 medicines.

Keywords: Drug, Molecular docking, Phytochemicals.

Introduction

The World Health Organization has designated the severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2) infection, also known as new coronavirus disease 2019 (COVID-19), to be a pandemic. This globally spreading viral virus serves as a stark reminder of humanity's susceptibility to an unseen foe. SARS, Ebola, and the Middle East respiratory syndrome were all highly infectious zoonotic viral infections that caused millions of deaths in the past. These viruses, on the other hand, have been successfully confined without triggering a worldwide epidemic. In contrast, the current COVID-19 is highly contagious, and over million people have been infected worldwide, with a lower mortality rate than previously [1].

COVID-19 patients have been linked to a variety of neurological symptoms and pulmonary manifestations. Headache, fever, nausea, pneumonia, loss of smell, unconsciousness, ataxia, epilepsy, neuralgia, and cerebrovascular and musculoskeletal disorders are the most common neurological manifestations. This virus causes acute encephalopathy and acute hemorrhagic necrotizing encephalopathy in some patients, which can lead to a breakdown of the blood–brain barrier [2].

In the pharmaceutical industry, bioactive phytochemical substances are well-known for generating treatments for inflammatory, cancer, and infectious disorders. Antiviral treatments for chikungunya, HIV, influenza, dengue fever, and SARS are all being developed using phytochemicals derived from various natural sources. Alkaloids, flavones, flavonols, fatty acids, tannins, and terpenes, among other phytochemicals from flora and wildlife, were examined for their antiviral action. Apart from the lipophilic and hydrophilic groups seen in other anti-viral medications, highlighted critical pharmacophoric chemical properties for anti-SARS-CoV-1 infection such as hydrophobic groups, electron donors (hydroxyl), and carbohydrate moieties [3].

Furthermore, anti-viral activities of bioactive phytochemicals from medicinally essential plant sources such as green tea, turmeric, gooseberry, and basil have recently been proven in various computational and in vitro investigations against SARS-CoV-2. Despite extensive experimental measures involving extraction, chemical complexity, and diversity of natural compounds, it is worth noting that the development of bioactive natural products is more desirable than particular vaccine design for this novel virus at this time. The primary goal of this study is to find the best phytochemical by conducting a literature research and generating new medications from various wild edible fruit plants, as well as determining the protein structures of various plant metabolites. The molecular docking grid box was first created by specifying the reported active sites of both the spike protein and the Mpro crystal

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structure using the Glide grid generating feature of the Schrödinger software [4].

Glide molecular docking was done in two steps: Standard Precision (SP) docking, which entails screening ligands that can bind to proteins, and Extreme Precision (XP) docking, which involves using a stringent scoring system to exclude false-positive hits. In prior research, we had success with the docking approach utilising the GLIDE module. The docking score of bioactive phytochemicals from various medicinal plants against SARS-CoV-2 protein targets was used to rate them [5].

The interaction between the viral spike protein and the ACE2 host cell receptor, which allows SARS-CoV-2 to enter the human host epithelial cell, has been widely researched. The spike protein of SARS-CoV-2 has been found to be ten times more powerful than SARS-CoV. In the current context, spike protein is a prime druggable target for blocking SARS-CoV-2 viral entrance into the host cell. Many investigations are being conducted in order to find appropriate inhibitors that target the SARS-CoV-2 spike protein.

Conclusion

Traditional medicinal herbs have been revealed to contain phytochemicals that could be used to produce newer, safer treatments. To find chemicals that could be employed in the creation of new drugs and as inhibitors of therapeutically significant enzymes. Using structure-based phytochemical modelling approaches, the current research will be used to find the optimal phytochemical molecule for blocking two critical SARS-CoV-2 functional druggable targets. The binding affinity of important constituent's phyllaemblicin C, phyllaemblicin B, procyanidin B1 and cinnamtannin B1 compounds from diverse medicinal plants was shown by molecular docking and MD simulations of one minute intervals of these complexes.

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