Molecular scaffolds from mother nature as possible lead compounds in drug design and discovery against coronaviruses: A landscape analysis of published literature and molecular docking studies

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A B S T R A C T

The recent outbreak of viral infections led to an unanimous for highlighting the importance of its virulence to the mitigation of public health globally. The classification of novel drugs and efficient therapies against these in-fectious viruses is need of hour. The emergence of SARS-CoV-2 caused by a novel acute respiratory syndrome virus (SARS-CoV) which has taken the whole world by storm as it has transformed into a global pandemic. The lethal virulence in a global health threat to present public which has already affected millions of people. Despite the development of vaccines potential vaccines are repurposed drugs for treatment. As health emergency need more attention due to the inefficacy of these vaccines and indeed the emergence of novel and virulent strains of SARS-CoV-2. Due to enormous structural diversity and biological significance, natural products are considered as a renowned source of bioactive compounds and a natural product-based drug discovery is considered a substantial proportion of the pharmaceutical market potential to the therapeutic uses of infectious diseases and oncology. The naturally occurring bioactive natural phytochemicals including flavonoids, terpenoids and peptides have gained much attraction in virtual docking studies to develop new drugs against potential targets for the treatment of SARS-CoV. In this review we describe various potential natural products such as flavonoids, terpenoids and peptides which can target the lethal virus. Due to which method to use such quench environmental virus when compared to the other conventional methods which can find and test methods. Based on this in silico approach, various natural products have been recently identified which might have a potential to inhibit SARS-CoV-2 outbreak. These natural products have been shown by computational studies to interact with spike protein of the novel coronavirus. The spike protein has been shown to bind to a neuroendocrine protein called angiotensin converting enzyme-2 (ACE2), this protein acts as a receptor for the viral spike protein. The comprehensive review also covers providing a summary of the activity and your own experimental and data. This review also highlights the potential of natural medicine that can be developed into possible lead compounds against the new threat of the novel coronavirus. Most natural products and to highlight natural source of potential ther-apeutics mainly covering the potential of these natural products as possible lead compounds in drug discovery. The review article intends to provide a starting point for the research analysis that are needed for the design and development of therapeutic drugs from natural products, their synthesis or semi-synthetic derivatives and unidentified phytochemicals. The current study will be highly helpful for scientists who are working in natural to work on novel anti-drugs from natural sources.

1. Introduction

Coronaviruses (CoVs) are RNA enveloped family of viruses mostly found in mammals and birds [1]. The virus infection causes fatal re-piratory or mainly disorders and has can cause both neurological and liver disorders [2]. Species-specific effects of CoV's are observed in

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