Reg. No: RJ17D0105798 ISSN NO: 2582-0648

HEB

Journal of Research in Indian Medicine
An Official Publication of Bureau for Health & Education Status Upliftment
(Constitutionally Entitled As Health-Education, Bureau)

JRIM

Drug Design and Discovery for SARS-CoV-2: In-Silico Molecular Docking of suitable phytochemicals via targeting of Spike Protein and RNA Dependant RNA Polymerase

By Shreyas Mukherjee, Samrat Mukherjee

Under the guidance of Dr. Jyoti Bala, Rapture Biotech

Email Id: serviceheb@gmail.com

ABSTRACT

The coronavirus disease 19 (COVID-19) is a highly transmittable and pathogenic viral infection caused by severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2), which caused global pandemic. Genomic analysis revealed that SARS-CoV-2 is phylogenetically related to severe acute respiratory syndrome-like (SARS-like) bat viruses. The intermediate source of origin and transfer to humans is not known, however, the rapid human to human transfer has been widely confirmed. Few broad-spectrum antiviral drugs have been evaluated against COVID-19 in clinical trials, resulted in clinical recovery. In the current research paper, we summarize and comparatively analyse the emergence and pathogenicity of COVID-19 infection and previous human coronaviruses including severe acute respiratory syndrome coronavirus (SARS-CoV). We also discuss the approaches for developing effective solutions and therapeutic combinations to cope with this viral outbreak. Since the process of a novel drug discovery and development has always been a very challenging and time-consuming task, computer aided drug design (CADD) also known as in-silico screening has become a powerful technique to increase the efficiency of the drug discovery process. In this research, suitable ligands have been identified and receptors such as RNA dependant RNA Polymerase were targeted by virtual screening of phytochemicals, namely Curcumin, Quercetin, Kaempferol, Rosoxacin and Ridogrel, using CADD methods. All chosen phytochemicals Lipinski's rule and especially Curcumin shows promise as it scored 3268 and 3596 in blind docking with Spike Protein and RDRP domains respectively. This research holds significant prospects for the designing of therapeutic agents against Covid-19 which can be further tested in-vitro and in-vivo to prove their efficiency.

Access this Article Online	Quick Response Code:
Website:http://heb-nic.in/jrim	
Received on 20/12/2021	
Accepted on 31/12/2021 © HEB All rights reserved	