

Systematic review on role of structure based drug design (SBDD) in the identification of anti-viral

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Perspective

Introduction

The outbreak of existing public health distress is threatening the entire world with emergence and rapid spread of severe acute respiratory syndrome coronavirus the novel coronavirus disease 2019 is mild in most people. However, in some elderly people with co-morbid conditions, it may progress to pneumonia, acute respiratory distress syndrome and multi organ dysfunction leading to death. COVID-19 has caused global panic in the healthcare sector and has become one of the biggest threats to the global economy [1]. Drug discovery researchers are expected to contribute rapidly than ever before. The complete genome sequence of coronavirus had been reported barely a month after the identification of first patient.

This systematic review provides an overview of the novel coronavirus, its pathology of replication, and role of structure based drug design, available drug targets and recent advances in in-silico drug discovery for the prevention of COVID-19. SARS-CoV-2 main protease, RNA dependent RNA polymerase and spike protein are the potential targets, which are currently explored for the drug development.

In early December 2019, an outbreak of novel coronavirus disease 2019 occurred in Wuhan City, China caused by a novel severe acute respiratory syndrome coronavirus [2-5]. Ever since its emergence in China, the infectious disease has progressed into a serious threat, wreaking havoc around the world. On March 11, 2020, the World Health Organization declared COVID-19 outbreak a global pandemic. It has now reached almost every country in the world, closing borders, shutting down institutions, work places, ceasing economic activity and forcing entire continents to act on emergency response protocols.

Description

Structure based drug design (SBDD)

SBDD is one of the inherent tools of the principal industrial drug discovery programs. The tool helps in overcoming the limitations of conventional drug discovery process by accelerating it. Comparatively, lower amount of time, cost, and labour is spent in the computational drug design and can have a huge impact in the discovery of the new drug molecules.

Tools used for SBDD

SBDD approach includes important stages of drug discovery such as 'hit identification' and 'hit-to-lead' optimization. The initial phase comprises the identification of a number of chemical molecules, known as 'hits', that ideally exhibit some range of potential effect along with specificity against the particular biological target

Computational drug repurposing

Drug repurposing is a strategy for identifying new uses and indications for existing or failed drugs. Potential targets/proteins of COVID-19 for development of therapeutic agents.

The drugs or therapies acting on coronavirus can be categorized on the basis of bispecific pathways including inhibition of functional proteins involved in RNA synthesis Blockage of the structural protein Responsible for binding to human cell receptors Alteration of factors that restore host innate immunity and acts on host's receptor or enzyme to prevent entry of virus into the cell.

Conclusions

SBDD is a faster, highly cost effective and efficient tool for the lead drug discovery in comparison to the traditional approaches. It has rapidly gained the acceptance of researchers to design and optimize ligands and can greatly influence the discovery of new drug molecules for the treatment of COVID-19. Over past two decades, technological advancements in experimental approaches including computational, X-ray crystallography and NMR etc.

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