Chapter 11
Harnessing the Capability of CADD Methods in the Prediction of Anti-COVID Drug Likeliness

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ABSTRACT

The COVID-19 pandemic has claimed many lives and added to the social, economic, and psychological distress. The contagious disease has quickly spread to almost 200 countries following the regional outbreak in China. As the number of infected populations increases exponentially, there is a pressing demand for anti-COVID drugs and vaccines. Virtual screening provides possible leads while extensively cutting down the time and resources required for ab-initio drug design. The chapter aims to highlight the various computer-aided drug design methods to predict an anti-COVID drug molecule.

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1. INTRODUCTION

Nearly the entire year 2020 was marred by the deleterious effect of the pandemic, COVID 19 infection. The infection claimed many lives and added to the social, economic, and psychological distress. The contagious disease that had an initial regional outbreak in Wuhan, China, quickly spread to almost all countries. The World Health Organization declared the disease as a pandemic in March 2020. As the number of infected populations increased exponentially, the medical research fraternity faced pressing demand for anti-COVID therapeutic solutions like drugs and vaccines. Despite some recent success claims in vaccine development, the search for an ideal drug candidate continues. Predominantly, three drugs that have ambiguous success include hydroxyquinoline- an antimalarial drug with quinoline as the pharmacophore, remedesivir- a nucleoside analog with an interfering role in RNA replication, and dexamethasone- a steroid that modulates the inflammatory response. However, as none of the above candidates are "the drug" against COVID-19, the scientists continue searching for drugs. With limited workforce resources due to the infected personnel or preventive lockdown and time-pressures for early therapeutic solutions, computer-aided drug design emerged as a preferred tool with many scientific reports that focussed on drug repurposing using screening methods.

Researchers applied computational screening methods to the FDA approved drugs to cut down on cost and time as the already tested and approved drugs were assumed to be safe for immediate clinical application. Media reports included mega-projects of Scripps Research, US announcing compound library screening of over 14000 drugs, the screening of drugs for augmenting remedisivir by Calibr scientist, and many more.

The quantum of the reported work in a short span is unparallel. However, in the absence of uniform protocols, though the protocol may be complete and standardized in itself, there have been contradictory and ambiguous findings. The reliability of the screening data hence needs to be ascertained. Further, as the predicted drugs, especially the established antivirals, did not elicit desired results in clinical settings, the scientists were forced to include varied categories of the molecules while screening. While mining extensive databases with varied scaffolds, newer screening protocols based extensively on machine learning methods were also developed. The chapter aims to highlight the various computer-aided drug design methods to predict an anti-COVID drug molecule. (Figure 1)

Metal Artifact Reduction: A Problem of Tremendous Importance in Medical Imaging

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