Chapter 5
Rational Drug Design and Docking of the RNA Dependent RNA Polymerase Domain of NCoV

It is an urgent requirement of 2020 to develop a drug which can successfully treat the patients of COVID19 and gift them a healthy life back. The development of drugs against COVID is the need of the hour for the scientific community. However Drug development is a long term process requiring drug discovery, testing and validation and cannot be a suitable choice for the current situation. Thus instead of laying a complete focus on discovery of medication it is necessary to repurpose the available and validated drugs which were used previously against other similar virus infections. This chapter focuses on Drug repurposing and selection of suitable drug candidates which have been used previously for other similar infections and validated.

The drugs that were used in the treatment of MERS, SARS, and INFLUENZA etc. can be tried with the COVID19 victims based on their function and similarity to the NCoV. The major proteins of the virus which can be targeted in the disease are the structural proteins including Spike or S protein, Membrane or M protein, Nucleocapsid or N protein, Envelope or E protein etc. as well as the nonstructural proteins including all the NSPs from 1 to 16 and ORFs etc.

Extensive data mining works has revealed the use of ORF1ab and the Structural proteins in the treatment of MERS. Thus the same can be used in the COVID 19 therapy for the current relaxation from the virus. Some of the Drugs that can be repurposed and used for COVID19 treatment include ribavirin, glycyrrhizin and IFN-α.

A. Kumar et al., *Novel Coronavirus 2019*,
SpringerBriefs in Forensic and Medical Bioinformatics,
https://doi.org/10.1007/978-981-15-7918-9_5