Chapter 7
Evolutionary and Structural Studies of NCoV and SARS CoV-Spike proteins and their association with ACE2 Receptor

Abstract Severe acute respiratory syndrome coronavirus-2 (SARS-CoV-2)/Novel Corona Virus Disease-19 (nCOVID-19)/COVID-19 has only been discovered recently, and so our understanding of the disease epidemiology is continuously evolving. WHO has declared it a worldwide pandemic with high morbidity and significant mortality, hence it has been announced as the global health and wealth emergency. At present there is no any specific therapy available to fight against this virus, hence the drug repositioning is the most challenging to entire scientific community. The aim of this study is to determine the mutation(s) in the sequence of the spike protein, which plays a significant role in transmission from human to human. By using bioinformatics approach first we analyzed spike protein sequence of four nearest coronavirus family that include COVID-19, bat coronavirus RaTG13, pangolian coronavirus and SARS CoV, to determine phylogenetic distance between them. The homology modeling of COVID-19 spike protein has been done by iTASSER. and the protein-protein docking with human receptor ACE2 by Frodock web based docking tool showing the less binding energy of COVID-19 (−12.7 kcal/mol) in comparison with SARS CoV (10.3 kcal/mol). Further, the superimposed structure of COVID-19 and SARS CoV viruses has been performed to find the mutational site in association with human ACE2 protein. The extensive and detailed computational analyses approaches help to identify conserved region of COVID-19 and SARS CoV. Hence, our present data might help to identify potential target site and to develop antiviral drugs/vaccine to combat this pandemic.

Keywords COVID-19 · SARS CoV · ACE2 receptor · Protein docking

7.1 Introduction

Currently, the emergency has been declared by WHO due to novel human coronavirus sporadic outbreaks in different countries. The first case of novel coronavirus (nCoV-19) has been detected in China in December, 2019, where, patients presenting with viral pneumonia like symptom caused by severe acute respiratory syndrome

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