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Commentary

Computational Analysis of COVID-19 Theraprutic Targets and Human Proteins

Jyotshna Patnaik*

Department of Life Science, Sambalpur University, Jyoti Vihar, Burla, Odisha, India

ABOUT THE STUDY

Novel zoonotic viruses pose a serious concern to people because they have the potential to spread quickly and cause substantial pathology. Numerous viral illness outbreaks, including those caused by Ebola, Zika, Nipah, Avian Influenza (H7N9), H1N1, Severe Acute Respiratory Syndrome Coronavirus 1 (SARSCoV1), and Middle East Respiratory Syndrome Coronavirus, have occurred throughout the past few decades (MERS-CoV). In the Chinese city of Wuhan, strange pneumonia cases start to appear at the end of 2019. The sickness was dubbed "coronavirus disease-19" after a novel coronavirus, later known as the cause of severe acute respiratory syndrome coronavirus 2 (SARS-CoV2), was identified (COVID19). The worst pandemic on record, COVID-19 has killed an average of 3% of its victims and has so far afflicted 35 million people worldwide.

The SARS-CoV2, SARS-CoV1, and MERS-CoV are all members of the genus and family Coronaviridae. Although bats are thought to be the source of SARS-CoV1 and SARS-CoV2, it is still unclear what intermediary host SARS-CoV2 was transmitted to before it reached humans. According to a sequence analysis, SARS-CoV2 is comparable to the coronavirus seen in Malayan pangolins (*Manis javanica*). The positive-sense, single-stranded RNA SARSCoV2 genome measures 29.8–29.9 kb and has a 5′ cap and 3′ polyA tail. The genome of this organism is divided into two sections that each encode structural and Non-Structural Proteins (Nsp). The first segment is directly translated into polyprotein 1a (486 kDa) or 1ab (790 kDa) (ORF1a, ORF1ab) by ribosomal frame shifting, resulting in the production of non-structural proteins and the establishment of the Replication-Transcription Complex (RTC).

Spike (S), Membrane (M), Envelope (E), and Nucleocapsid (N) proteins are the four primary structural proteins that are encoded by the second segment at the 3′ end of the genome. SARS-CoV2 enters the host cell through receptor-mediated endocytosis, which is triggered by the Spike protein's interaction to the ACE2 receptor. The viral particle's covering is then removed, releasing the genome, which is then translated to produce complex proteins needed for protein replication and transcription. The full length negative sense RNA is then produced by the viral RTC complex and is then translated into the whole genome. Near the ER and Golgi interface, the structural proteins and viral genome are put together to form virions, which are then exocytosed out of the cell by vesicles.

Clinical symptoms and underlying molecular pathways driving illness development are still poorly understood in full. Currently, the therapeutic protocol for the illness consists of symptomatic care and medications approved for emergency use, including remdesivir, favipiravir, and ivermectin, among others. Worldwide attempts are still being made to create SARS-CoV2 vaccines and medications. Repurposing of existing medications is one of the best and fastest methods to find prospective therapeutic candidates based on similarities and information from different coronaviruses. In this situation, new compounds that target viral proteins can be swiftly identified using computational approaches, providing possibilities for repurposing. As a result, numerous researches using a variety of these techniques have been reported during the COVID epidemic.

The medications that have a high affinity for viral proteins (structural and non-structural) and that can successfully block viral entry as well as post-entry processes including viral genome replication and transcription. The viral proteases and methyl transferase, which are essential for viral entry, replication, and transcription, as well as spike protein, can bind to capreomycin with high affinity. This makes capreomycin a promising candidate with potential to inhibit SARS-CoV2 at multiple stages of the viral lifecycle.

Correspondence to: Jyotshna Patnaik, Department of Life Science, Sambalpur University, Jyoti Vihar, Burla, Odisha, India, E-mail: jyoshnaik@gmail.com

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