Potential Treatment Targets for Covid-19: A Virtual Screening

Karthikeyan, Keerthin (School: Oxford High School)

Purpose: Covid-19, a viral global pandemic caused by the SARS-CoV-2 virus caused 2.72 million deaths (as of 03-22-21) worldwide and more than 543,000 deaths in the United States. The purpose of this project was to identify potential treatment drug targets towards the cure of Covid-19 through virtual screening and confirming their binding affinity through ELISA. Method: For SARS-CoV-2 to infect cells, the viral Spike protein should bind to an ACE2 receptor protein found on the surface of the human host cells. Currently, Remedesivir is the only drug approved by the FDA for the treatment of Covid-19. Drugs/phytochemicals targeting this binding of the Spike protein and ACE2 may offer protection against the viral infection. In this project, several drugs/phytochemicals were docked against spike and N protein of SARS-CoV-2 virus and ACE2, TMPRSS2, and 3CLpro proteins of human cell, to evaluate their inhibitory properties based on their binding affinities. The 3D structure of the proteins was retrieved from the RCSB protein data bank and the ligands (drug molecules) were downloaded from the PUB-CHEM database. Virtual screening was performed using PyRx molecular docking software. The phytochemicals that showed the best docking scores were further characterized through Spike protein-ACE2 binding ELISA method. Results: The docking scores of drugs and phytochemicals for these 5 proteins were tabulated and analyzed with the best binding affinities. Among them, Tenufolin and Isocolumbin exhibited higher binding affinity than Remedesivir. This virtual screening technique of finding new inhibitors to the proteins involved in Sars- CoV 2 infection, helped to identify potential target drugs for Covid-19.