Predicting Virus-Human Interactions To Facilitate the Design of Anti-Coronavirus Vaccines and Therapeutics

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Infectious diseases are a leading cause of mortality worldwide. Among the major pathogens, SARS-CoV-2 is a coronavirus causing the current COVID-19 pandemic. MERS-CoV and SARS-CoV also belong to the family of coronavirus, which are known to cause the Middle East respiratory syndrome (MERS) and severe acute respiratory syndrome (SARS), respectively. The goal of this research was to discover the common human targets of coronaviruses to facilitate the development of anti-coronavirus medicines. My hypothesis was that different coronaviruses share some common target proteins in the human body and identification of these targets and their interactions with viral proteins would provide valuable information for the design of novel vaccines and therapeutics against coronaviruses. In this project, I identified the interactions of human proteins with eight viral strains including MERS-CoV, SARS-CoV, SARS-CoV-2 and its variants (alpha, beta, gamma, delta and omicron). The viral and human protein sequences were downloaded from NCBI GenBank and Uniprot, respectively, and their interactions were analyzed using the PredHPI platform. The results showed that MERS-CoV and SARS-CoV interact with 242 and 129 human proteins, respectively. SARS-CoV-2 and its variants target 90 human proteins. All tested coronaviruses interact with 44 common human proteins such as peptidyl-prolyl cis-trans isomerases through their N, S and M proteins as well as RNA replicase. With these common human targets, I performed a virtual drug screening and identified 38 anti-coronavirus drug candidates from DrugBank. This project thus provides a novel approach for discovery of common human proteins targeted by different coronaviruses and yielded some promising molecules for development of new antiviral therapeutics.