The Effect of Coronavirus Species on the Binding Strength to a Neutralizing Antibody

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SARS-CoV, SARS-CoV-2, and MERS-CoV are three human coronaviruses (HCoVs). They each cause pathogenic and infectious diseases that have damaged society. The spike (S) protein resides on the HCoV particle's outermost layer with its receptor-binding domain (RBD) being crucial for viral infection. As a result, there is a high demand for antibodies that can inhibit the RBDs and stop viral infection. In this experiment, the HCoV's binding strength to a neutralizing antibody, COVA2-04, is measured by the potential binding energy present between the RBD and COVA2-04. The purpose is to determine whether different HCoV species affect the binding strength to COVA2-04. The experimental hypothesis stated if the SARS-CoV-2 RBD is used, then the binding strength of the virus RBD to COVA2-04 will be the strongest. The crystal structure of SARS-CoV-2 RBD attached to COVA2-04 was downloaded and the other two viral RBD structures were modeled before adding the missing residues to the structure. These structures were then run through Molecular Dynamic (MD) simulations to measure the potential binding energy. There is no control since there is no standard virus species. SARS-CoV-2 had the lowest average amount of potential binding energy to COVA2-04 and the strongest binding to COVA2-04, thus supporting the research hypothesis. In contrast, MERS-CoV had the highest amount of potential binding energy and the weakest binding to COVA2-04. Three t-tests for the results revealed that the data was statistically significant and supported. The results were likely due to COVA2-04 originally being produced to bind to SARS-CoV-2, making their surface structure compatibility the highest. MERS-CoV had the weakest binding to COVA2-04 since it shares the lowest S protein similarity with SARS-CoV-2.

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