COVID-19: A Computational Study

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The outbreak of a new coronavirus SARS-CoV-2 (severe acute respiratory syndrome–coronavirus 2) has caused a global COVID-19 (coronavirus disease 2019) pandemic, resulting in millions of infections and deaths around the world. Through unprecedented scientific endeavors, several vaccines, drugs and antibodies have been developed and are widely used, but the fight against COVID-19 continues as more and more variants of concern such as Delta and Omicron emerge. To understand the side effects caused by vaccines and therapeutic agents, and to develop more effective treatments, a deeper understanding of the molecular interactions of SARS-CoV-2 with them and human cells is required. In this talk, advances in combating COVID-19 using computational methods will be discussed. We will focus on the following problems:

1.   Binding of the spike protein to human Angiotensin-converting enzyme 2 (ACE2) before entering the cell for replication: Binding free energy and free energy landscape

2.   Interactions of antibodies with the spike protein of SARS-CoV-2.

3.   SARS-CoV-2 non-structural protein 1 can stall mRNA translation in host ribosomes.