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COVID-19 RESEARCH NEWSLETTER

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Dynamics of the ACE2 - SARS-CoV-2/SARS-CoV spike protein interface

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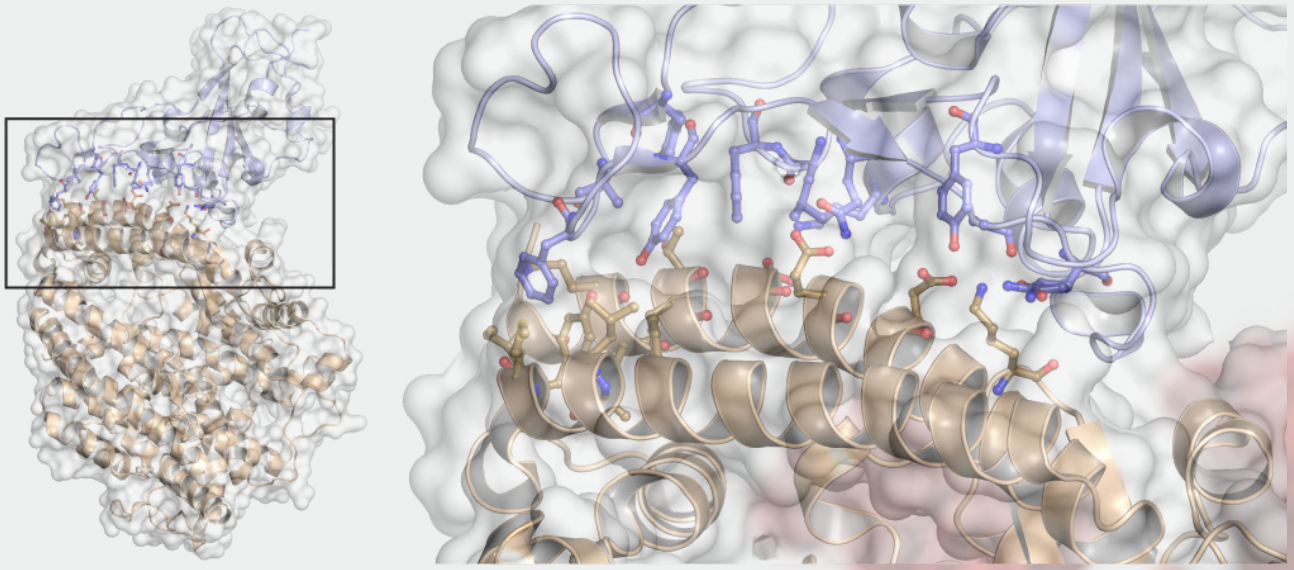

The coronavirus disease 2019 (COVID-19) pandemic, caused by the severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2), is a major global health concern. In some ways, the SARS-CoV-2 is similar to the SARS-CoV, another betacoronavirus that caused the SARS outbreak in 2002. Structural biology techniques have been used to produce static atomic-level structures that depict how the SARS-CoV-2 and SARS-CoV spike protein interact with its primary host target, which is the angiotensin converting enzyme 2 (ACE2). Molecular recognition, binding and function are dynamic processes. To gain a deeper insight into this, the researchers performed several long molecular dynamics simulations to evaluate the structural stability and interfacial interactions between the spike protein of SARS-CoV-2 and SARS-CoV bound to ACE2.

In spite of the remarkable similarity, they found that the SARS-CoV-2 and SARS-CoV utilize unique strategies to achieve stable binding to ACE2. Several intermolecular contacts formed, broke and reformed in the interface during the simulations. Differences were observed between the amino acids that consistently interacted with ACE2. Notably, a stable salt bridge between Lys417 of SARS-CoV-2 spike protein and Asp30 of ACE2 as well as three stable hydrogen bonds between Tyr449, Gln493 and Gln498 of SARS-CoV-2 and Asp38, Glu35 and Lys353, respectively, of ACE2 were observed, which were absent in the SARS-CoV-ACE2 interface. Additionally, the researchers performed free energy calculations to estimate the binding affinity of the SARS-CoV-2 and SARS-CoV spike proteins. This was observed to be more favourable in the case of SARS-CoV-2 supporting a stronger binding in SARS-CoV-2. Such stable interactions are vital for host identification and viral entry. Therefore, these results should assist the attempts of designing potential drugs and vaccines that target this interface.

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If you are interested in sharing your COVID-19 releated research, please send your contribution to research.office@uaeu.ac.ae

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