Joint Event

21st International Conference on
Structural Biology

13th International Conference on
Emerging Infectious Diseases

October 17, 2022

WEBINAR

In silico evaluation of SNPs at the interface of ACE2 forming the ligand-receptor complex with the spike protein

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Severe Acute Respiratory Syndrome Coronavirus 2 (SARS-CoV-2) has recently emerged in China and caused the disease COVID-19, the virus spread rapidly around the world, causing a global outbreak. Protein-protein binding assays have confirmed that Angiotensin-Converting Enzyme 2 (ACE2) is the cellular receptor through which the virus invades the host cell. The severity of the symptoms and the rapid progression of the disease have led to in-depth investigation of this virus, suggesting a response by which some populations are more susceptible to the entry of the SARS-CoV-2 virus and this may be due to polymorphisms of a Single Nucleotide (SNP) present in various populations in this case in the ACE2 receptor. In this study, nsSNPs present in the ACE2 interface were selected, the amino acid changes corresponding to each nsSNP were made from the base model that form the ACE2-SARS- CoV-2 complex, the binding energy and the binding constant were calculated. protein-protein interaction dissociation. The results of the analysis indicate that the presence of the Asp355Asn and Ser19Pro variants in ACE2 decrease the binding affinity in the protein-protein complex, therefore, we suggest a lower susceptibility to COVID-19 disease. However, the Glu329Gly and Glu37Lys variants indicate an increase in binding affinity according to the physicochemical parameters evaluated, so their presence in ACE2 would possibly increase susceptibility to COVID-19 disease.

Biography

Alejandro A. Gutiérrez-Hernández is a student in Autonomous University of Zacatecas, Mexico. He is interested in working with Pathology and Molecular Diagnosis Laboratory, Academic Unit of Chemical Sciences.

Received: October 05, 2022; **Accepted**: October 07, 2022; **Published**: October 17, 2022