BITS :: Call for Abstracts 2021 - Oral communication

Type	Oral communication
Session	Bioinformatics challenges in the SARS-Cov-2/COVID-19 pandemic
Title	Molecular dissection of the inter-chain interface of the human Angiotensin-Converting Enzyme 2 (ACE2) receptor with the SARS-CoV-2 Spike-protein
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Motivation

The COVID-19 pandemic has prompted many researchers to deepen knowledge of the interaction mechanisms that allow the coronavirus attack to the human target cells. It is well recognized that human ACE2 acts as a cellular receptor of the Spike-protein (Sp) characterizing the virus surface, as for the past coronavirus epidemics. The molecular interactions with Sp are of crucial importance for the successful coronavirus attack, and their complete understanding can be useful for the definition of the mechanism of action as well as for ascertaining possible interaction differences in the case of ACE2 or Sp variants.

Methods

We in silico analyzed the structural features of the chain interface in ACE2/SARS-CoV-2 Sp complexes, described at atomic level by different crystallographic structures available in the RCSB PDB. We observed the surface interactions by PyMol v1.3, PDBePISA and COCOMAPS, and investigated at visual level the molecular interactions by DiscoveryStudio v20.1.0.

Results

The results of the structural analysis on the crystallographic complexes of ACE2/SARS-CoV-2 Sp defined what amino acid residues interact with the chain-chain interface. Their physiological roles and structural features were investigated in detail and will be presented together with a comparative analysis that evidenced differences between the interaction of ACE2 with Sp of SARS-CoV-2 and SARS-CoV (previously characterized), with potential implications on the different health impact of the most recent coronavirus.

Info

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Figure

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Availability	-

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