

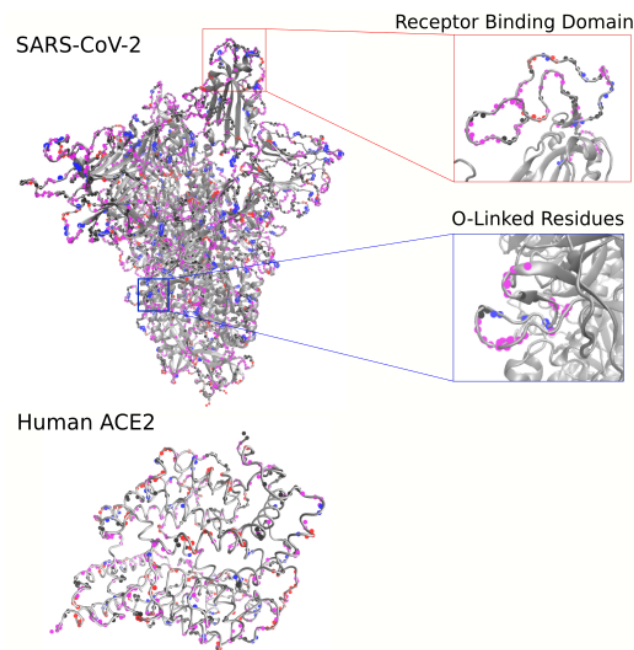
Protein Surface Printer for Exploring Protein Domains

Yang Li, Baofu Qiao and Monica Olvera de la Cruz, *J Chem Inf Model*, 2020, DOI: 10.1021/acs.jcim.0c00582

A program, Protein Surface Printer (PSP), was developed for extracting and quantitatively analyzing the surface domain information. PSP features its broad compatibility for multiple file formats from different software, atomistic resolution analysis and on-the-fly analysis.

Protein surface domains are surface area where amino acids with similar polarities or charges distribute together to form domain-like structures. Surface domains are found to significantly impact the protein-protein interactions and protein-ligand binding, such as the formation of a core (protein)–shell (polymer) reverse micellar structure. Inspired by the properties of surface domains, PSP was developed to quantitatively analyze the surface domains, which can help us further understand protein interactions.

In the paper, a case study was conducted using PSP on the spike proteins of SARS-CoV-2 and its relative SARS-CoV, as well as the human binding receptor ACE2.



Protein surface domains of SARS-CoV-2 spike protein, its RBD, O-linked residues and human receptor ACE2