Unlocking the Potential of Antibodies Against SARS-COV-2: A Pipeline for Fast and Accurate Mapping of Interaction Sites with Free Energy Analysis

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In this study, we employed free energy interaction analysis to identify key interaction sites between SARS-COV-2 and antibody structures. Specifically, we generated a pipeline for efficient mapping of these interaction sites that can be used for multiple system pairs, or for a single pair using parallelized computing. Our pipeline significantly reduces the time and effort required for this analysis, making it a feasible approach for large-scale studies. Our results demonstrate that the interaction between SARS-COV-2 and antibody structures can be mapped with high accuracy using free energy interaction analysis [1].

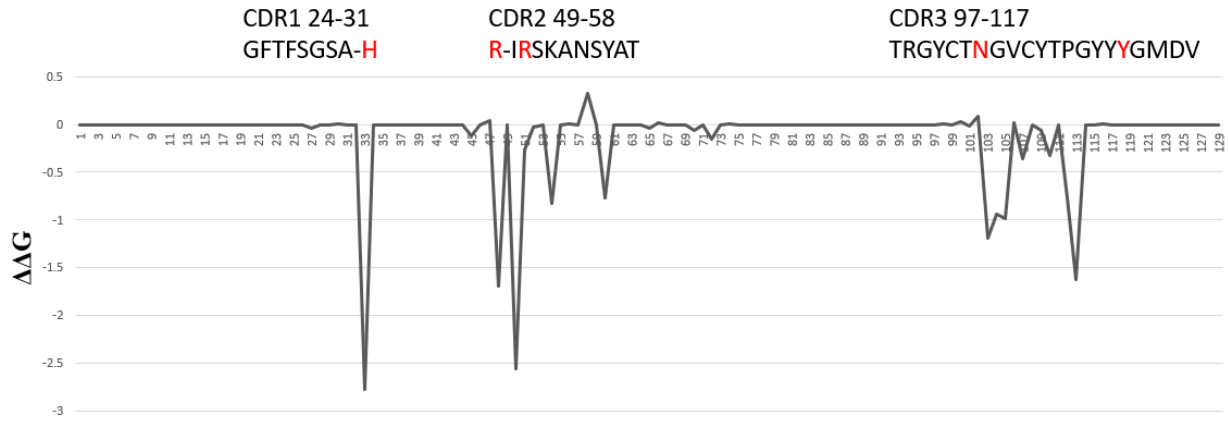

Fig. 1 Free energy mapping of an Anti-SARS-CoV-2 antibody binding interface. The most influential residues for each position are marked red and visualized on the antibody's paratope.

The technology can also be used to study protein-protein interactions in general. By mapping the key interaction sites between proteins, researchers can gain insights into the mechanism of interaction and the structural features of the protein complex. This information can help to identify potential drug targets and facilitate the design of peptide inhibitors that disrupt the protein-protein interaction [2]. For example, it could be used to study interactions between viral proteins and host proteins, as well as interactions between different signaling molecules.

Overall, the technology has the potential to significantly improve the understanding of protein-protein interactions and accelerate the development of effective therapies for a range of diseases.

[1] Schymkowitz J, Borg J, Stricher F, Nys R, Rousseau F, Serrano L. The FoldX web server: an online force field. Nucleic Acids Res. 2005 Jul 1;33(Web Server issue):W382-8. doi: 10.1093/nar/gki387
[2] Weißenborn L, Richel E, Hüseman H, Welzer J, Beck S, Schäfer S, Sticht H, Überla K, Eichler J. Smaller, Stronger, More Stable: Peptide Variants of a SARS-CoV-2 Neutralizing Miniprotein. Int J Mol Sci. 2022 Jun 4;23(11):6309. doi: 10.3390/ijms23116309