World Academy of Science, Engineering and Technology
International Journal of Biomedical and Biological Engineering
Vol:19, No:01, 2025

The Omicron Variant BA.2.86.1 of SARS- 2 CoV-2 Demonstrates an Altered Interaction Network and Dynamic Features to Enhance the Interaction with the hACE2

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Abstract : The SARS-CoV-2 variant BA.2.86 (Omicron) has emerged with unique mutations that may increase its transmission and infectivity. This study investigates how these mutations alter the Omicron receptor-binding domain's interaction network and dynamic properties (RBD) compared to the wild-type virus, focusing on its binding affinity to the human ACE2 (hACE2) receptor. Protein-protein docking and all-atom molecular dynamics simulations were used to analyze structural and dynamic differences. Despite the structural similarity to the wild-type virus, the Omicron variant exhibits a distinct interaction network involving new residues that enhance its binding capacity. The dynamic analysis reveals increased flexibility in the RBD, particularly in loop regions crucial for hACE2 interaction. Mutations significantly alter the secondary structure, leading to greater flexibility and conformational adaptability compared to the wild type. Binding free energy calculations confirm that the Omicron RBD has a higher binding affinity (-70.47 kcal/mol) to hACE2 than the wild-type RBD (-61.38 kcal/mol). These results suggest that the altered interaction network and enhanced dynamics of the Omicron variant contribute to its increased infectivity, providing insights for the development of targeted therapeutics and vaccines.

Keywords : SARS-CoV-2, molecular dynamic simulation, receptor binding domain, vaccine
Conference Title : ICBAHS 2025 : International Conference on Biomedical and Health Sciences
Conference Location : San Diego, United States
Conference Dates : January 16-17, 2025