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Computational Prediction of the Effect of S477N Mutation on the RBD Binding Affinity and Structural Characteristic, A Molecular Dynamics Study

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Abstract : The COVID-19 pandemic, caused by SARS-CoV-2, has led to significant concerns worldwide due to its catastrophic effects on public health. The SARS-CoV-2 infection is initiated with the binding of the receptor-binding domain (RBD) in its spike protein to the ACE2 receptor in the host cell membrane. Due to the error-prone entity of the viral RNA-dependent polymerase complex, the virus genome, including the coding region for the RBD, acquires new mutations, leading to the appearance of multiple variants. These variants can potentially impact transmission, virulence, antigenicity and evasive immune properties. S477N mutation located in the RBD has been observed in the SARS-CoV-2 omicron (B.1.1. 529) variant. In this study, we investigated the consequences of S477N mutation at the molecular level using computational approaches such as molecular dynamics simulation, protein-protein interaction analysis, immunoinformatics and free energy computation. We showed that displacement of Ser with Asn increases the stability of the spike protein and its affinity to ACE2 and thus increases the transmission potential of the virus. This mutation changes the folding and secondary structure of the spike protein. Also, it reduces antibody neutralization, raising concern about re-infection, vaccine breakthrough and therapeutic values.

Keywords : S477N, COVID-19, molecular dynamic, SARS-COV2 mutations
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