First Report on In-silico de novo Design and Interaction studies on Novel COVID-19 Proteins

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Abstract

The paper presents the incorporation of *in silico* missenses and studies the effect of missenses to understand its effect on the Ligand-Protein interactions, of COVID-19 protein. *In silico* protein-ligand interaction, studies are being used to understand and investigate the drug-likeness of various molecules. 19 novel COVID-19 proteins are designed by inducing *in silico* missenses by mutating N691 amino acid residue in 7bv2 protein, the only residue forming H-bond with the ligand molecule in the parent protein. The work illustrates the effects of *in silico-induced* mutation on various interactions such as H-Bond, VDW, π-alkyl interactions, and changes in the number and type of surrounding amino acid residues. The results have suggested a common pattern of behavior on mutation with T, V, W, and Y. Further, it is observed that the number and type of amino acid residues increase on mutation, suggesting future possibilities to understand the effect of natural mutation on the binding of a ligand molecule with the protein.

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