

Secondary and Super Secondary Structure of Prefusion Conformation of Spike Protein of SARS-CoV-2: A Computational Structure Profiling

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The spread of the COVID-19 infectious disease that is caused by the SARS-CoV-2 virus (severe acute respiratory syndrome coronavirus 2) has been a huge threat to the people of Sri Lanka and worldwide. It has stirred a global health crisis since 2019 which has led to the declaration of a public health emergency of international concern by the World Health Organisation. Owing to its novelty, there is a lack of effective therapeutic options to combat the viral infection. To better appreciate key secondary level interactions leading to the structural complexity, a computational structural analysis of secondary and super secondary structures (motifs) of the SARS-CoV-2 S protein (RCSB PDB ID: 5X5B) was carried out. The three-dimensional prefusion structure of the S protein was first structurally characterized using the ProFunc server tool, followed by analysis of molecular graphics of secondary and super secondary structures as well as torsion angles of helical sequences using RasMol program and STRIDE visual assignment tool, respectively. Three distinguished protein chains namely A, B and C were identified from the prefusion three-dimensional structure of the SARS-CoV-2 spike glycoprotein. The protein chain A is represented with the identical chains of B and C with 1033 protein residues. Among the 14 β sheets of the chain A, 9 are observed to be formed from more than two strands. The present work identifies a special region of irregular β sheet in the S protein of the prefusion conformation which is experimentally verified in previous optical spectra studies of SARS-CoV-2 proteins. Helical turns show a large deviation from an ideal helix by 9.8 Å. Interhelical interactions are observed to experience the highest negative interaction angle of magnitude 162.80°. The most occurring non-flexible β turns may or may not be stabilized by hydrogen bonds. This study emphasizes the need for further investigation of fused conformation of SARS-CoV-2 virus in the light of current urgency of establishing optimal treatment strategies for COVID-19.

Keywords: SARS-CoV-2; Computational analysis; Prefusion conformation; Spike protein