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Protein structure predictions for coronavirus non-structural protein 1 (nsp1)

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The recently discovered SARS-CoV2 virus provoked a severe coronavirus pandemic (COVID-19). Understanding the structure and function of viral proteins is essential for comprehending viral infection and pathogenesis and developing treatment and prevention techniques. The coronavirus non-structural protein 1 (nsp1) is a crucial feature with a wide range of involvement in virus-host interactions and various sequence, structure, and functional mode characteristics. This research aims to reveal the structural conformational changes of nsp1 to aid in prediction by developing a homology model utilising SWISS-Model and I-Tasser and evaluating the best model. PROCHECK, PROSA, Errat, and Verify3D investigated and validated all predicted models corresponding to the nsp1 homologs of SARS-CoV1, SARS-CoV2, and MERS-CoV. SWISS-Model homology modeling for SARS-CoV2 resulted in 94.6% of builds being in the most favorable region, 5.7% in the authorised region, 0% in the liberally permitted zone, and 0% in the denied region. The i-Tasser model had a significantly lower percentage of builds in the most favourable region (61.1%), higher percentages in the authorised region (28.9%), a relatively higher percentage in the liberally permitted zone (6.0%), and a relatively higher percentage in the denied region (4.0%). It was observed that SARS-CoV1 nsp1 and MERS-CoV nsp1 in SWISS-Model showed higher PROCHECK values than I-Tasser. The PROCHECK, ProSA Z-score, Errat, and Verify3D results demonstrated that the SWISS-Model is reliable and solid enough to be utilised in future research.

Keywords: Protein modeling, Bioinformatics, Structure and function analysis, Immunoinformatic, COVID-19.

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