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HOMOLOGY MODELING AND VALIDATION OF REPLICATION ASSOCIATED PROTEIN (REP) OF SRI LANKAN CASSAVA MOSAIC VIRUS (SLCMV)

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ABSTRACT

Cassava mosaic disease caused by Sri Lankan cassava mosaic virus (SLCMV) is a major biotic threat to cassava production in Sri Lanka. SLCMV is a bipartite begomo virus and its occurrence was first reported in Sri Lanka in year 2002. Rep protein encoded by AC 1 gene of SLCMV plays a vital role in viral replication. Through the current work, Rep protein of Sri Lankan Cassava Mosaic Virus (SLCMV) was modelled and validated using *in silico* methods. At first the amino acid sequence of the Rep was retrieved from the GenBank (AJ890226) and constructed its Protein Data Bank (PDB) file using 3D-JIGASAW (Protein Comparative Model Server). PDB file of a template (PDBID: 1L2M) with percentage identity of 73% and e value of $8e^{-83}$ to query sequence was also retrieved from the same database. Using Swiss Model server 3D model of the protein was generated and stereo chemical consistency of the model was determined using RAMPAGE and ProSA-web servers. The Ramachandran plot generated by the RAMPAGE server had 87.33% of amino acid residues in the most favored region, implying the model is a near good quality model (90%). Moreover, allowed and outlier regions contained 12.3% and 1.4% residues respectively. Using ProSA-web and Verify-3D servers the predicted model was validated. Accordingly, ProSA-web resulted in a Z score values of -4.90 and -5.03 for Rep and 1L2M indicating that the Rep bears the native characteristics similar to the available structures in the database. The Verify-3D server output showed a better averaged 3D/ID score > = 0.2 of 85.14% (Template= 87.29%) which is higher than the minimum requirement (80%) while the profile score plot showed a value more than 0 (model=0.56, template =0.66) indicating the acceptability of the structure. The predicted model needs to be experimentally validated using X-ray crystallography and the findings of this study will potentially be used in designing antiviral agents in order to control SLCMV.

Keywords: Sri Lankan cassava mosaic virus (SLCMV), Replication associated protein (Rep), In silico, Homology modelling, model validation