

Homology modeling of antiviral protein (CA-SRI) from *Clerodendrum aculeatum* L.

*Heena Gaur, Shuchi Negi, Divya Shrivastava, H. N. Verma, Abhijeet Singh and Devendra Jain**

Institute of Biotechnology and Allied Sciences, Seedling Academy of Design, Technology and Management, Jagatpura, Jaipur (302025), INDIA

The leaves of *Clerodendrum aculeatum* contain an endogenous virus inhibitor protein (CA-SRI), a 34 kDa Basic protein, which confer systemic resistance in several plants against plant viruses. The virus inhibiting protein have been studied in many plants and all belongs to a class of proteins called ribosome inactivating proteins (RIPs). Unlike other virus inhibiting proteins, CA-SRI induces a strong systemic resistance in susceptible plants. Structure-based protein engineering may pave the way for directed evolution of variants with enhanced potency and stability of the proteins.

In the present study homology modeling of CA-SRI was done using Deep View software. The template for CA-SRI (Accession number CAA65328) protein sequence was selected using ExPdb template search. The raw sequence of the CA-SRI was superimposed over the Pokeweed antiviral protein PDB template (1qciB). The superimposed model was submitted to the SWISS Model server. After receiving the CA-SRI model, energy minimization was done using Gromos96. The threading energy and force field energy were calculated. Further energy minimization was done by building loops in unallowable residues calculated by Ramachandran plot. The homology model of CA-SRI made by us along with the 1qciB model from the SWISS-MODEL repository was used for comparative analysis. The homology model of CA-SRI was validated with PROCHECK and WHATIF programs. Further Prosite scan revealed that CA-SRI is having SHIGA_RICIN motif (Shiga/Ricin ribosomal inactivating toxins active site signature). A homology model of CA-SRI developed by us is available in Protein Model Database (WWW.mi.caspur.it/PMBD/) with accession no. PM0074969.