

In Silico Characterization of Tomato leaf curl Joydebpur virus (ToLCJV) DNA-A Proteins

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ABSTRACT

We retrieved six proteins sequences of *Tomato leaf curl Joydebpur virus* (ToLCJV) DNA-A [FJ345402] from GenBank-NCBI (ACJ03821, ACJ03822, ACJ03823, ACJ03824, ACJ03825 and ACJ03826) and were used for computational modeling structure prediction. Ramachandran plot of ACJ03826-AC4 had maximum 73.3 % and ACJ03822-AV1 had 71 % residues in core region therefore these models cannot be place in a good quality category. ACJ03824-AC2 had only 18.6 % residues in core and 13.6% residues in disallowed region therefore it was least stable protein. Verify-3D graph profile scores for selected ToLCJV proteins were greater than zero therefore all the Verify-3D graph corresponds to acceptable environment of the model. Findings of the present study provide base for docking and *In-Silico* anti-Begomoviral compound designing.

Key words: *In-Silico*, ToLCJV, GenBank

INTRODUCTION

Geminiviruses are plant viruses that belong to the family *Geminiviridae* Fauquet *et al.*, 2005) and this family classified into four genera (*Mastrevirus*, *Curtovirus*, *Topocuvirus* and *Begomovirus*) based on structure of genome, host range and insect vector (Stanley *et al.*, 2005). *Begomovirus* is the largest genus of family *Geminiviridae* (Dhakar *et al.*, 2010) and obligatory transmitted by the whitefly *Bemisia tabaci* Sidhu *et al.*, 2009; Govindappa *et al.*, 2011) that are common in the tropical and subtropical regions of the world. The aim of the study was, characterization of six proteins of ToLCJV DNA-A [FJ345402] and development of the foundation for the protein-protein or protein-ligand docking study for anti-ToLCJV agent designing because the infection of ToLCJV in tomato cause major yield loss.

MATERIALS AND METHOD

The FASTA sequences of all these six portions were uploaded on the I-TASSER (version 3.0) protein comparative modeling server that powered by POPULUS for PDB files building (<http://bmm.cancerresearchuk.org/~populus/>). The predicted models were validated with PROCHECK (<http://www.ebi.ac.uk/thornton-srv/software/PROCHECK/>) for identification of stereochemical quality of a protein structure by analyzing residue-by-residue geometry and overall structure geometry (Laskowski *et al.*, 1996). The predicted models were uploaded on Verify 3D (http://nihserver.mbi.ucla.edu/Verify_3D/) server that analyzes the compatibility of an atomic model (3D) with its own amino acid sequence (1D). PDB files of proteins were used for the ribbon structure prediction using UCSF Chimera software.

RESULTS AND DISCUSSION

Accession No and Protein	Ramachandran Plot regions				Main-chain Parameters			Residue Properties					
	Core %	Allowed %	Gener %	Dball %	Better	Inside	Worse	Max. deviation	Bad contacts	Bond length	Dihedrals	Covalent	Overall
ACJ03822-AV1	71.0	22.6	4.8	1.6	2	0	4	9.3	36	21.4	-0.68	-1.50	-0.96
ACJ03821-AV2	62.4	29.0	7.5	1.1	3	0	3	7.7	22	7.6	-0.57	-0.80	-0.64
ACJ03823-AV3	71.0	22.6	6.5	0.0	3	0	3	17.3	8	22.9	-0.68	-1.37	-0.93
ACJ03825-AC1	63.8	24.4	7.5	4.4	2	0	4	8.6	45	10.8	-0.66	-0.86	-0.73
ACJ03824-AC2	18.6	47.5	20.3	13.6	2	0	4	17.9	18	8.9	-1.23	-1.61	-1.31
ACJ03826-AC4	73.3	21.7	5.0	0.0	3	0	3	10.4	11	6.4	-0.50	-0.49	-0.49

Table 1: Ramachandran plot results of the six proteins of *Tomato leaf curl Joydebpur virus* (ToLCJV) DNA-A [FJ345402].

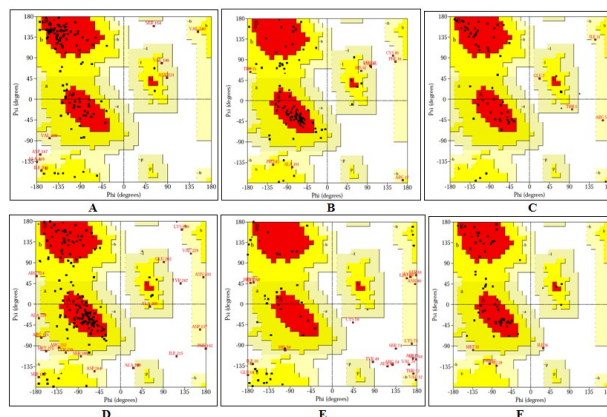


Fig. 1: Ramachandran plots of ACJ03822-AV1 (a), ACJ03821-AV2 (b), ACJ03823-AV3 (c), ACJ03825-AC1 (d), ACJ03824-AC2 (e) and ACJ03826-AC4 (f) proteins of *Tomato leaf curl Joydebpur virus* (ToLCJV) DNA-A [FJ345402].

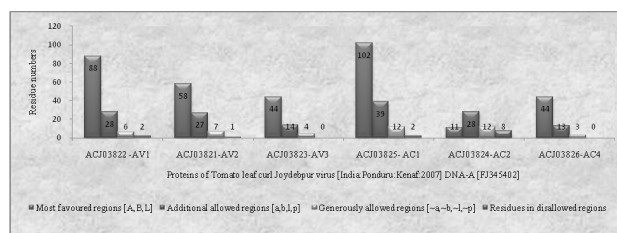


Fig. 2: Histogram of Ramachandran plot residues distribution for proteins of *Tomato leaf curl Joydebpur virus* (ToLCJV) DNA-A [FJ345402].

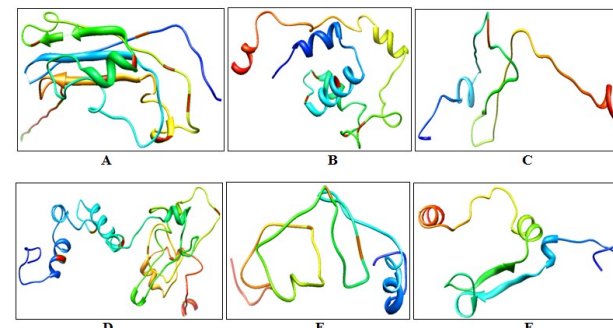


Fig. 3: Ribbon structure of ACJ03822-AV1 (a), ACJ03821-AV2 (b), ACJ03823-AV3 (c), ACJ03825-AC1 (d), ACJ03824-AC2 (e) and ACJ03826-AC4 (f) of *Tomato leaf curl Joydebpur virus* (ToLCJV) DNA-A [FJ345402]. Structure designed by using UCSF Chimera.

CONCLUSION

Computational modeling is the tool for the prediction of structure of protein from its sequence by using *In Silico* approach and by this way we overcome the limitations of X-Ray crystallography and NMR (Nuclear Magnetic Resonance). Characterization of six proteins of ToLCJV DNA-A [FJ345402] build a foundation for docking study for anti-ToLCJV agent designing because the infection of ToLCJV in tomato cause major yield loss.

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