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In silico structure and substrate binding analyses of family 35 Carbohydrate binding Module (Cbm35) from cellulosome of clostridium thermocellum

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CBM35-CtGH26 protein with an accession number (ABN51273.1) is a carbohydrate active modular protein and component of a vast cellulosome of Clostridium thermocellum. Its structural analyses and substrate specificity is unexplored. The molecular architecture of full length protein contains multiple domains viz. signal peptide (1-31), CBM35 (32-134), GH26 (135-507), linker (508-519) and Dockerin type I (520-590). This study mainly focuses on carbohydrate binding module (CBM35) of the protein. CBMs are non catalytic components whose function is to enhance the catalytic efficiency by keeping the substrate in close proximity of the catalytic domain. A good quality 3D structure of CBM35 was generated by using Modeller 9v7. Structure refinement and energy minimization was carried out using loop optimization class of Modeller and by Gromacs (package 2.3), respectively. Ramachandran plot shows that 93% residues lies in most favourable region, 7% residues is in additional allowed region. Structure similarity search of modeled structure into Dali server shows similarity with PDB ID: 2W1W-B and 2VZP-B with RMSD of 1.7 and 1.8, respectively. Multiple Sequence Alignment of representative protein from CBM35s families showed many signature motif residues as conserved. Moreover, the key residues which involve in substrate binding are conserved within subfamily Man-CBM35. Secondary structure of modelled CBM35 showed that it contains 12 β strands and 2 small α helix. Topology diagram showed β-jelly roll fold. Docking study with β-1-4 linked mannotriose and mannopentose identify potential binding sites in CBM35 which shows that key conserved aromatic residues are involved in the substrate specificity.

Biography

Anil Kumar Verma had completed M.Sc. in Industrial Microbiology from the School of Life Sciences, Devi Ahilya Vishwavidyalaya, Indore (MP) in 2009. At present, he is doing PhD at Department of Biotechnology, Indian Institute of Technology Guwahati, Guwahati, Assam-India.