Chapter 49
Molecular Docking Study of Expansin Proteins in Fibers of Medicinal Plants Calotropis Procera

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ABSTRACT

Calotropis procera is used in several traditional medicines to treat a variety of diseases. Calotropis is also used as a homeopathic medicine. The bast fiber can substitute cotton wool for surgical or stuffing purposes. This fiber can be used as an excellent model system to study the genes involved in fiber elongation. Expansins are typically 250-275 amino acids long, pH-dependent cell wall-loosening proteins required for cell wall expansion in many developmental processes. Four Expansin A proteins are present in fast growing Calotropis procera fibers. Expansins proteins disrupt the cellulose-hemicellulose network transiently, allowing slippage of cell wall polymers. But the molecular mechanism by which expansin loosens the cellulosic network is not yet established. To understand of the role of protein expansins in the xyloglucan-cellulose, different computational biology techniques are used. Molecular docking analysis of protein expansins with ligand xylose present in xyloglucan shows that arginine and serine are responsible for protein-ligand interactions.

INTRODUCTION

The *Calotropis procera*, a well-known medicinal plant, contents seed fibers which can provide an excellent model system to study the genes involved in fiber elongation, fineness and strength. The floss from the seed capsules is used as a stuffing material in mattresses etc. The floss from the seeds, which is about 2 - 3.5 cm long, white silky and strong, is used as an inferior stuffing for mattresses and pillows, may be substituted as cotton wool for surgical purposes (Tropical,2018). Earlier scientists have identified

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four homologs of Expansin gene i.e. CpEXPA1, CpEXPA2, CpEXPA3 and CpEXPA4 from the cDNA library obtained from fast growing *Calotropis procera* fibers (Cheema et al, 2010). These homologous genes represent typical Expansin A family. Each of these four expansin genes have two conserved domains known as GH45 like domain and the putative polysaccharide binding domain. The amino acid sequencing of these homologous genes shows the presence of three conserved motifs e.g. eight cysteine residues at N-terminus, four tryptophan residues at C-terminus and a Histidine-Phenylalanine-Aspartate motif in the center of the sequence. The presence of N-terminal signal peptide sequence containing hydrophobic amino acids and a transmembrane region in all four expansin proteins suggests that they are secretory proteins.

Primary cell walls in plants consist of layers of cellulose microfibrils embedded in a hydrophilic matrix made up of pectins and xyloglucans in most land plants. Microfibrils are linked together with pectins and xyloglucans by noncovalent interactions. Plant cell wall loosening during its growth does not occur at selective sites where cellulose microfibrils make close contact with xyloglucan molecules. These specific sites appear to be the targets of plant expansins during cell wall expansion (Cosgrove, 2015). The widening of plant cells requires shear (slippage) of the structural polymers within the plant cell wall, which must simultaneously maintain sufficient strength to withstand high turgor pressure. Plant protein expansin, has a unique ability of inducing cell-wall expansion without hydrolytic breakdown of the major structural components e.g. cellulose microfibrils, xyloglucan etc. of the cell wall (McQueen-Mason, et al, 1992, 1995). Gene expression analysis indicates that expansin transcript abundance is utmost during cell growth and during fruit softening (Shcherban, et al, 1995).

Computational approaches are frequently used for the sequence analysis and functional characterization of proteins (Webb & Sali, 2014), (Sehar, et al, 2013). Various structural and physicochemical properties of proteins can be illustrated by using computational tools when the crystal structure of interested protein is not available (Karumuri, & Bandopadhyay, 2014). Although precise and accurate structure of proteins can be guaranteed by experimental methods but the disadvantage is that the experimental laboratory-based methods are time consuming and large amount of purified protein is required for this purpose.

In this context, structural aspects of expansin proteins from *Calotropis procera* are studied, considering the interaction with plant cell wall carbohydrate molecule e.g. xylose molecule have been carried out in this work. The results obtained might be helpful to identify the role of expansin in cell elongation. The proteins are subjected to several online and desktop-based bioinformatics tools to study physico-chemical properties. The 3D structures of these proteins are modeled using homology modeling approach. The predicted structures are used for docking analysis with monosaccharide xylose.

MATERIALS AND METHODS

Generation of Structural Models of Expansin Proteins in *Calotropis Procera*

Four expansin protein sequences of *Calotropis procera* are extracted from UNIPROT database. Using FASTA sequences of these proteins e.g. CpEXPA1, CpEXPA2, CpEXPA3 and CpEXPA4, homology modeled structures are derived from SWISS-MODEL (Arnold, et al, 2006) evaluating by GMQE score. A phylogenetic tree has been built up with these sequences.