Comparative in silico study of the differences in the structure and ligand interaction properties of three alpha-expansin proteins from Fragaria chiloensis fruit

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Expansins are cell wall proteins associated with several processes, including changes in the cell wall during ripening of fruit, which matches softening of the fruit. We have previously reported an increase in expression of specific expansins transcripts during softening of Fragaria chiloensis fruit. Here, we characterized three ?-expansins. Their full-length sequences were obtained, and through qRT-PCR (real-time PCR) analyses, their transcript accumulation during softening of F. chiloensis fruit was confirmed. Interestingly, differential but overlapping expression patterns were observed. With the aim of elucidating their roles, 3D protein models were built using comparative modeling methodology. The models obtained were similar and displayed cellulose binding module(CBM) with a ?-sandwich structure, and a catalytic domain comparable to the catalytic core of protein of the family 45 glycosyl hydrolase. An open groove located at the central part of each expansin was described; however, the shape and size are different. Their protein?ligand interactions were evaluated, showing favorable binding affinity energies with xyloglucan, homogalacturonan, and cellulose, cellulose being the best ligand. However, small differences were observed between the protein?ligand conformations. Molecular mechanics-generalized Born-surface area (MM-GBSA) analyses indicate the major contribution of van der Waals forces and non-polar interactions. The data provide a dynamic view of interaction between expansins and cellulose as putative cell wall

ligands at the molecular scale. Communicated by Ramaswamy H. Sarma.

fruit ripening

molecular dynamics simulations

molecular modeling

plant cell wall

RT-qPCR

alpha expansin

cellulose

glucan

glycosidase

homogalacturonan

plant protein

polymer

polysaccharide

unclassified drug

xyloglucan

ligand

pectin

plant protein

polygalacturonic acid

xylan

Article

binding affinity

catalysis

cell wall

comparative study

computer model

controlled study

energy

Fragaria

Fragaria chiloensis

genetic analysis

nonhuman

priority journal

protein analysis

protein expression

protein interaction

protein protein interaction

protein structure

quantitative analysis

reverse transcription polymerase chain reaction

surface area

chemistry

fruit

gene expression regulation

molecular dynamics

physiology

protein conformation

Cell Wall

Cellulose

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Fruit

Gene Expression Regulation, Plant

Glucans

Ligands

Molecular Dynamics Simulation

Pectins

Plant Proteins

Protein Conformation

Xylans