

Computational study of FaEXPA1, a strawberry alpha expansin protein, through molecular modeling and molecular dynamics simulation studies

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Changes in the cellulose-hemicellulose fraction take place during ripening of strawberry fruit and are associated with the activity of a set of proteins and hydrolytic enzymes. Expansins are proteins located in the cell wall with no catalytic activity. In this context, FaEXPA1 was previously reported to have a high accumulation rate during fruit ripening in three different strawberry cultivars. In order to understand at the molecular level the expansin mechanism mode, a 3D model of FaEXPA1 protein was built by comparative modeling. FaEXPA1 protein model displayed two domains, a cellulose-binding domain with a β -sandwich structure, and a second domain that included a HFD motif with a similar structure to the catalytic core of endoglucanase V from *Humicola insolens*. Additionally, in the center of the structure, an open groove was formed. Finally, using a cellulose polymer as a ligand, the protein-ligand interaction was evaluated by molecular dynamic (MD) simulation. Two MD simulations showed that FaEXPA1 can interact with cellulose via the flat aromatic surface of its binding domain D2, composed mainly of residues Trp99 and Trp225. In addition, FaEXPA1 formed a high number of hydrogen bonds with the glycan chain and the Asn81, Phe114 and Asn211 residues. © 2018 Elsevier Ltd

Cellulose

Expansin protein

Molecular dynamic simulation

Plant cell wall

Strawberry

Catalyst activity

Cellulose

Computational chemistry

Fruits

Hydrogen bonds

Ligands

Plants (botany)

Proteins

Walls (structural partitions)

Comparative modeling

Computational studies

Hemicellulose fraction

Molecular dynamics simulations

Plant cell wall

Protein-ligand interactions

Strawberry

Strawberry cultivars

Molecular dynamics

Binding

Cellulose

Fruits

Hydrogen Bonds

Ligands

Proteins

Residues

Ripening

cellulose

ligand

plant protein

protein binding

amino acid sequence

binding site

chemistry

Fragaria

genetics

hydrogen bond

metabolism

molecular dynamics

mutation

Amino Acid Sequence

Binding Sites

Cellulose

Fragaria

Hydrogen Bonding

Ligands

Molecular Dynamics Simulation

Mutation

Plant Proteins

Protein Binding