Study of the structure and binding site features of FaEXPA2, an ?-expansin protein involved in strawberry fruit softening

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Tissue softening accompanies the ripening of many fruits and initiates the processes of irreversible deterioration. Expansins are plant cell wall proteins that have been proposed to disrupt hydrogen bonds within the cell wall polymer matrix. Several authors have shown that FaEXPA2 is a key gene that shows an increased expression level during ripening and softening of the strawberry fruit. For this reason, FaEXPA2 is frequently used as a molecular marker of softening in strawberry fruit, and changes in its relative expression have been related to changes in fruit firmness. In this context, we previously reported that FaEXPA2 has a high accumulation rate during fruit ripening in four different strawberry cultivars; however, the molecular mechanism of FaEXPA2 or expansins in general is not yet clear. Herein, a 3D model of the FaEXPA2 protein was built by comparative modeling to understand how FaEXPA2 interacts with different cell wall components at the molecular level. First, the structure was shown to display two domains characteristic of the other expansins that were previously described. The protein-ligand interaction was evaluated by molecular dynamic (MD) simulation using four different long ligands (a cellulose fiber, two of the more important xyloglucan (XG) fibers found in strawberry (XXXG and XXFG type), and a pectin (homogalacturonic acid type)). The results showed that FaEXPA2 formed a more stable complex with cellulose than other ligands via the different residues present in the open groove surface of its two domains, while FaEXPA2 did not interact with the pectin ligand.

Expansin protein

Fruit softening

Molecular dynamic simulation

Protein-ligand interaction

Strawberry

3D modeling

Cellulose

Deterioration

Hydrogen bonds

Ligands

Molecular dynamics

Plants (botany)

Proteins

Walls (structural partitions)

Accumulation rates

Cell wall polymers

Cell-wall components

Comparative modeling

Molecular mechanism

Protein-ligand interactions

Ripening and softening

Strawberry cultivars

Fruits

Cellulose

Degradation

Fruits

Hydrogen Bonds

Ligands

Proteins