Title

Structural and transcriptional characterization of pyruvate decarboxylase (PDC) gene family during strawberry fruit ripening process

Abstract

Strawberry is one of the most popular fruits in the world, because their high fruit quality, especially with respect to the combination of aroma, flavor, color, and nutritional compounds. Pyruvate decarboxylase (PDC) is the first of two enzymes specifically required for ethanolic fermentation and catalyzes the decarboxylation of pyruvate to yield acetaldehyde and CO2. The ethanol, an important alcohol which acts as a precursor for the ester and other alcohols formation in strawberry, is produced by the PDC. The objective was found all different PDCs genes present in the strawberry genome and investigate PDC gene expression and ligand-protein interactions in strawberry fruit. Volatile organic compounds were evaluated during the development of the fruit. After this, eight FaPDC were identified with four genes that increase the relative expression during fruit ripening process. Molecular dynamics simulations were performed to analyze the behavior of Pyr and TPP ligands within the catalytic and regulatory sites of the PDC proteins. Results indicated that energy-restrained simulations exhibited minor fluctuations in ligand-protein interactions, while unrestrained simulations revealed crucial insights into ligand affinity. TPP consistently displayed strong interactions with the catalytic site, emphasizing its pivotal role in enzymatic activity. However, FaPDC6 and FaPDC9 exhibited decreased pyruvate affinity initially, suggesting unique binding characteristics requiring further investigation. Finally, the present study contributes significantly to understanding PDC gene expression and the intricate molecular dynamics underlying strawberry fruit ripening, shedding light on potential targets for further research in this critical biological pathway.

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