

# Structural analysis of the woodland strawberry COI1-JAZ1 co-receptor for the plant hormone jasmonoyl-isoleucine

Valenzuela-Riffo F.

Garrido-Bigotes A.

Figueroa P.M.

Morales-Quintana L.

Figueroa C.R.

The phytohormone jasmonoyl-isoleucine (JA-Ile) regulates fundamental plant processes. *Fragaria vesca*, the woodland strawberry, is a model plant for the Rosaceae family, in which the JA-Ile perception is poorly understood at the molecular level. JA-Ile promotes binding of JAZ repressor to COI1 protein in *Arabidopsis* to activate jasmonate (JA)-dependent responses. The aim of this work was to understand the molecular basis of the interaction between the *F. vesca* COI1 (FvCOI1) and JAZ1 (FvJAZ1) promoted by JA-Ile using a computational approach. Multiple sequence alignments and phylogenetic analyses of amino acid sequences were performed for FvCOI1, FvJAZ1 and their ortholog sequences. 3D structures for FvCOI1 and FvJAZ1 proteins were built by methods of homology modeling, using AtCOI1-JA-Ile-AtJAZ1 as template and then they were further refined and validated by molecular dynamics (MD) simulation. A molecular docking approach along with MDS analysis were used to gain insights into the interaction between a putative degron-like sequence present in FvJAZ1 with the FvCOI1-JA-Ile complex. FvCOI1 and FvJAZ1 showed high and moderate sequence identity, respectively, with the corresponding ortholog proteins from other plant species including apple, grape, tomato and *Arabidopsis*. Moreover, the FvJAZ1 has a variant C-terminal IPMQRK sequence instead of the canonical LPIARR degron sequence located in the Jas domain of AtJAZ1. The MD simulation results showed that the FvCOI1-JA-Ile-FvJAZ1 complex was stable, and the IPMQRK peptide of FvJAZ1 directly interacted with FvCOI1 and JA-Ile. The present research provides novel insight into the molecular interactions among key JA-signaling components in the model plant *F. vesca*, being few examples of characterized JA-Ile receptors at a structural

level in plants. © 2018 Elsevier Inc.

CORONATINE INSENSITIVE1 protein

Fragaria vesca

Jasmonate signaling

JASMONATE ZIM-DOMAIN repressor

Jasmonoyl-isoleucine

Molecular dynamics simulations

Molecular modeling

Amino acids

Fruits

Molecular modeling

Plants (botany)

Proteins

Coronatine

Fragaria

Jasmonate signaling

Jasmonates

Jasmonoyl-isoleucine

Molecular dynamics simulations

Molecular dynamics

coronatine

coronatine insensitive1 protein

jasmonoyl isoleucine

phytohormone

unclassified drug

cyclopentane derivative

isoleucine

jasmonoyl-isoleucine

ligand

multiprotein complex

phytohormone

plant protein

protein binding

amino acid sequence

apple

Arabidopsis

Arabidopsis thaliana

Article

controlled study

fruit ripening

grape

molecular docking

molecular dynamics

molecular interaction

nonhuman

phylogeny

priority journal

protein analysis

protein conformation

protein interaction

protein structure

sequence alignment

strawberry

tomato

X ray diffraction

chemistry

conformation

DNA sequence

Fragaria

genetics

metabolism

molecular model

protein domain

structure activity relation

Amino Acid Sequence

Cyclopentanes

Fragaria

Isoleucine

Ligands

Models, Molecular

Molecular Conformation

Multiprotein Complexes

Plant Growth Regulators

Plant Proteins

Protein Binding

Protein Interaction Domains and Motifs

Sequence Analysis, DNA

Structure-Activity Relationship