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Analyzing the structural aspects of Isoprenoid biosynthesis pathway proteins in Ocimum species

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Abstract

Generally thought that the extremely diverse array of secondary metabolites observed within Ocimum species defends against a comparable diverse array of biotic pests, pathogens and herbivores encountered around its natural range. Along with defense the diverse array of secondary metabolite also leads to the therapeutic and remedial property which justifies Ocimum as natural medicinal and aromatic casket. Many of the defense compounds, aroma compounds and medicinal derivatives are secondary metabolites isolated from trichome glands, mainly consist of terpenoids as well as phenylpropanoids. Various pathways fabricating these compounds are known viz. mevalonate pathway (MVA), phenylpropanoid pathway and MEP pathways. The enzyme cascade responsible for various secondary metabolites, need to be explored in various aspects. Here we had studied the MVA pathway enzymes in *O. basilicum* and *O. gratissimum* to figure out variations in enzyme structures due to speciation. Hence, in depth analysis of the transcriptome of *O. basilicum* and *O. gratissimum*, varrying in qualitative and quantitative aspects of essential oil were carried out. The transcriptome data from NCBI server was assembled using bioinformatic approaches. nr database at NCBI repository used for annotation, which assigned 60% contigs to known functions. Contigs corresponding to Mevalonate pathway enzymes are isolated using perl pipelines developed in our lab, which were further assembled using CLC workbench to remove redundancy and make larger stretch of sequence. Blastx of these larger sequences assigned them function and they are mapped to validated sequences to make full length. Data from both species led us to overall seven enzymes (total 14) of MVA pathway. These enzymes are studied in detail for various physio-chemical properties, steriochemical properties and motif/domain for protein-protein interaction (PPI) study. Homolog models of all enzymes were predicted, against templates from RCSB database. Threading approach is used for enzymes whose homologs are not available in public domain. Structure analysis (energy minimization, Ramachandran plot, stereospecificity and PDB cleaning, Root Mean Square deviation) helped to infer that amongst seven enzymes key gene from MVA pathway showed variation at three sites with in active domain. This study opens up new avenue for secondary metabolite pathway prediction and operation analysis, this will help to develop biotechnological logical tools for Ocimum crop improvement.

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