RESEARCH ARTICLE

IN-SILICO CHARACTERIZATION AND HOMOLOGY MODELING OF PEPCK ENZYME OF *MEDICAGO TRUNCATULA*

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Abstract: Phospho*enol*pyruvate carboxykinase (PEPCK) is an enzyme in the lyase family. PEPCK is an ATP-dependent that is involved in the metabolic pathway of gluconeogenesis. It converts oxaloacetate into phospho*enol*pyruvate and carbon dioxide. In this study, the results of structural and physiochemical study of *Medicago truncatula* PEPCK has explored. The conceptual three-dimensional structure investigated while there was no structural information available in any other database. Computational analysis performed on *Medicago truncatula* PEPCK and developed a three-dimensional structure of PEPCK enzyme using comparative modeling approach. The modeled enzyme includes N-terminal and C-Terminal domains with a mixed α/β topology. The energy of constructing models was minimized and the quality of the models was evaluated by VERRIFY_3D and PROCHECK. Ramachandran plot analysis showed the confirmation of 100 % amino acid residues was within the most favored regions. Multiple sequence alignment of the PEPCK protein sequence of different plant sources revealed the conserved region and constructed a phylogenetic tree. The stability of model checked through Gromacs 4.5. The final three-dimensional structure submitted in the protein model database (PMDB). This study may play keystone role in in-vivo and in-vitro studies.

Keyword Phospho*enol*pyruvate carboxykinase, phylogenetic tree, Gromacs, MD simulation, Homology Modeling

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