Structural insight into interaction and conformation mechanisms of Serratia marcescens lysine decarboxylase (SmcadA)

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Abstract

Inducible lysine decarboxylases (LDCs) are essential in various cellular processes of microorganisms and plants, especially under acid stress, which induces expression of genes encoding LDCs. In this study, a novel Serratia marcesenes LDC (SmcadA) was successfully expressed in E. coli and structural modeling showed the protein as a decamer with a molecular weight of approximately 75 kDa. Further structural analysis of the protein network interactions showed that specific N-terminal and C-terminal residues with significant node size-degree correlation and high color intensity possessed high values of betweenness, suggesting they played a key role in protein function and activity. Molecular dynamics simulations further revealed that hydrogen bonds were vital interactions for stabilization of cofactor PLP and formation of intermediates, hence improved biocatalysis. Furthermore, mutations coffered structural changes of the protein residues and PLP hence altered the type of interacting residues with the ligand, causing changes in conformation of PLP. Moreover, temperature also induced changes in orientation of cofactor PLP and amino acid residues. This work therefore demonstrates the role of protein-ligand interactions in altering cofactor and binding site residue conformations thus contributing to improved biocatalysis.

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