Homology modeling and docking studies of a Delta 9-fatty acid desaturase from a Cold-tolerant Pseudomonas sp AMS8

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Abstract

Membrane-bound fatty acid desaturases perform oxygenated desaturation reactions to insert double bonds within fatty acyl chains in regioselective and stereoselective manners. The Delta 9-fatty acid desaturase strictly creates the first double bond between C9 and 10 positions of most saturated substrates. As the three-dimensional structures of the bacterial membrane fatty acid desaturases are not available, relevant information about the enzymes are derived from their amino acid sequences, site-directed mutagenesis and domain swapping in similar membrane-bound desaturases. The cold-tolerant Pseudomonas sp. AMS8 was found to produce high amount of monounsaturated fatty acids at low temperature. Subsequently, an active Delta 9-fatty acid desaturase was isolated and functionally expressed in Escherichia coli. In this paper we report homology modeling and docking studies of a Delta 9-fatty acid desaturase from a Cold-tolerant Pseudomonas sp. AMS8 for the first time to the best of our knowledge. Three dimensional structure of the enzyme was build using MODELLER version 9.18 using a suitable template. The protein model contained the three conserved-histidine residues typical for all membrane-bound desaturase catalytic activity. The structure was subjected to energy minimization and checked for correctness using Ramachandran plots and ERRAT, which showed a good quality model of 91.6 and 65.0%, respectively. The protein model was used to preform MD simulation and docking of palmitic acid using CHARMM36 force field in GROMACS Version 5 and Autodock tool Version 4.2, respectively. The docking simulation with the lowest binding energy, -6.8 kcal/mol had a number of residues in close contact with the docked palmitic acid namely, Ile26, Tyr95, Val179, Gly180, Pro64, Glu203, His34, His206, His71, Arg182, Thr85, Lys98 and His177. Interestingly, among the binding residues are His34, His71 and His206 from the first, second, and third conserved histidine motif, respectively, which constitute the active site of the enzyme. The results obtained are in compliance with the in vivo activity of the Delta 9-fatty acid desaturase on the membrane phosphohpids.

Keywords

Author Keywords: Cold-tolerant Pseudomonas sp AMS8; Molecular docking; Homology modeling; delta 9-fatty acid desaturase; Palmitic acid

KeyWords Plus: CARRIER PROTEIN-DESATURASE; STEAROYL-COA DESATURASE; FUNCTIONAL EXPRESSION; DIIRON PROTEINS; HETEROLOGOUS EXPRESSION; CRYSTAL-STRUCTURE; SOFTWARE NEWS; IDENTIFICATION; EVOLUTION; HYDROXYLASE

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