

Structural adaptation of cold-active RTX lipase from pseudomonas sp. Strain AMS8 revealed via homology and molecular dynamics simulation approaches

ABSTRACT

The psychrophilic enzyme is an interesting subject to study due to its special ability to adapt to extreme temperatures, unlike typical enzymes. Utilizing computer-aided software, the predicted structure and function of the enzyme lipase AMS8 (LipAMS8) (isolated from the psychrophilic *Pseudomonas* sp., obtained from the Antarctic soil) are studied. The enzyme shows significant sequence similarities with lipases from *Pseudomonas* sp. MIS38 and *Serratia marcescens*. These similarities aid in the prediction of the 3D molecular structure of the enzyme. In this study, 12 ns MD simulation is performed at different temperatures for structural flexibility and stability analysis. The results show that the enzyme is most stable at 0°C and 5°C. In terms of stability and flexibility, the catalytic domain (N-terminus) maintained its stability more than the noncatalytic domain (C-terminus), but the non-catalytic domain showed higher flexibility than the catalytic domain. The analysis of the structure and function of LipAMS8 provides new insights into the structural adaptation of this protein at low temperatures. The information obtained could be a useful tool for low temperature industrial applications and molecular engineering purposes, in the near future.

Keyword: Lipase AMS8; LipAMS8; Structural adaptation; Molecular dynamic simulation.