

Deciphering the flexibility and dynamics of *Geobacillus zalihae* strain T1 lipase at high temperatures by molecular dynamics simulation.

ABSTRACT

The stability of biocatalysts is an important criterion for a sustainable industrial operation economically. T1 lipase is a thermoalkalophilic enzyme derived from *Geobacillus zalihae* strain T1 (T1 lipase) that was isolated from palm oil mill effluent (POME) in Malaysia. We report here the results of high temperatures molecular dynamics (MD) simulations of T1 lipase in explicit solvent. We found that the N-terminal moiety of this enzyme was accompanied by a large flexibility and dynamics during temperature-induced unfolding simulations which preceded and followed by clear structural changes in two specific regions; the small domain (consisting of helices alpha3 and alpha5, strands beta1 and beta2, and connecting loops) and the main catalytic domain or core domain (consisting of helices alpha6- alpha9 and connecting loops which located above the active site) of the enzyme. The results suggest that the small domain of model enzyme is a critical region to the thermostability of this organism.

Keyword: Thermostability; Thermoalkalophilic enzyme; Lipase; Protein Dynamics; Flexibility.