The role of lid in protein-solvent interaction of the simulated solvent stable thermostable lipase from Bacillus strain 42 in water-solvent mixtures.

ABSTRACT

Lip 42 lipase, isolated from Bacillus sp. strain 42 was previously shown to be stable in polar organic solvent such as dimethyl sulfoxide (DMSO). Stabilities in different solvent compositions were studied based on 400C pre-incubation in solvent, and the purified lipase was shown to retain at least 100% residual activity in up to 45% v/v DMSO. In 60% v/v DMSO, 68% of residual activity was retained, however, this dramatically reduced to 6.5% at 65% v/v DMSO. Activity enhancements were recorded at lower solvent compositions (less than 45% v/v solvent), whereby, at 30% v/v DMSO, enhancement was as much as 35%. Based on these solvent stability profile, molecular dynamic simulations were then carried out in the presence of water, 60% v/v DMSO + 40% v/v water and 100% v/v DMSO, by using a structure predicted from a highly homologous (97%) lipase (PDB:1JI3). Results showed that the flexibility changes in the helix-loop-helix motif covering catalytic triad were found to be associated with a hydrophobic cluster region. The presence of 60% v/v DMSO resulted in the disorganization of the cluster, accompanied with nonnative H-bonds formations. The cluster was retained in 100% v/v DMSO which resembled to that of water simulation. Mutant form of Lip 42, V171S contained residue substitution in the cluster and within helix-loop-helix motif. At 500C pre-incubation, the mutant lost as much of the high temperature enhancements observed in low DMSO compositions. This indicated the potential role of hydrophobic residues in helix-loop-helix motif and the cluster in interfacial activation.

Keyword: Solvent stable lipase; Thermostable; Protein-solvent interaction; Helix-loop-helix; Interfacial activation