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MD Simulation and Topological Data Analysis of High Temperature Activity of an Enzyme

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Applying a novel computational technique to the structure of Candida Antarctica Lipase B, which is an efficient catalyst with a wide range of applications, this study investigates the potential for its industrial applications owing to its activity under extreme conditions. We examined the molecular effects of distinct solvents on the stability of CalB at high temperatures, aiming to contribute to its unusual performance. Applying the persistent homology tool from algebraic topology we proposed to recognize the relationship between the topology-function of these macromolecules and uncover how local modifications in the amino acid interaction network structure correlate to activity at the scale of the entire protein network. Originally, MD simulations were carried out to address the molecular impacts of different solvents on the structural stability of CalB at a range of temperatures. We tracked conformational changes of an alpha helix (alpha-5), which its function previously is considered as the lipase lid and is thought to be responsible for the activity of the protein both in polar (water), and nonpolar (glycerol) solvents at high temperature. Notably, the native lipase fold was maintained in a non-polar solvent (glycerol) even at high temperatures, representing the enhancement of lipase's thermostability in glycerol. Topologically we distinguish the topological feature this conformational change emerge in the amino acid network in its active state and compared its topology to inactive network. Hence, we noted the presence of a relationship between local topological features of the network and the global activity of the protein

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