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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 themolecular effects of distinct solvents on the stability of CalB at high temperatures, aiming to con-tribute to its unusual performance. Applying the persistent homology tool from algebraic topologywe proposed to recognize the relationship between the topology-function of these macromoleculesand uncover how local modifications in the amino acid interaction network structure correlate toactivity at the scale of the entire protein network. Originally, MD simulations were carried out toaddress the molecular impacts of different solvents on the structural stability of CalB at a range oftemperatures. We tracked conformational changes of an alpha helix (alpha-5), which its functionpreviously is considered as the lipase lid and is thought to be responsible for the activity of the pro-tein both in polar(water), and nonpolar(glycerol) solvents at high temperature. Notably, the nativelipase fold was maintained in a non-polar solvent (glycerol) even at high temperatures, representingthe enhancement of lipase's thermostability in glycerol. Topologically we distinguish the topologicalfeature this conformational change emerge in the amino acid network in its active state and com-pared its topology to inactive network. Hence, we noted the presence of a relationship betweenlocal topological features of the network and the global activity of the protein

Authors: TAJIK, samin (brock university); Dr HARROUN, Thad

Presenter: TAJIK, samin (brock university)

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