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Title:	Thermostability of In Vitro Evolved Bacillus subtilis Lipase A: A Network and Dynamics Perspective
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Abstract:	Proteins in thermophilic organisms remain stable and function optimally at high temperatures. Owing to their important applicability in many industrial processes, such thermostable proteins have been studied extensively, and several structural factors attributed to their enhanced stability. How these factors render the emergent property of thermostability to proteins, even in situations where no significant changes occur in their three-dimensional structures in comparison to their mesophilic counter-parts, has remained an intriguing question. In this study we treat Lipase A from Bacillus subtilis and its six thermostable mutants in a unified manner and address the problem with a combined complex network-based analysis and molecular dynamic studies to find commonality in their properties. The Protein Contact Networks (PCN) of the wild-type and six mutant Lipase A structures developed at a mesoscopic scale were analyzed at global network and local node (residue) level using network parameters and community structure analysis. The comparative PCN analysis of all proteins pointed towards important role of specific residues in the enhanced thermostability. Network analysis results were corroborated with finer-scale molecular dynamics simulations at both room and high temperatures. Our results show that this combined approach at two scales can uncover small but important changes in the local conformations that add up to stabilize the protein structure in thermostable mutants, even when overall conformation differences among them are negligible. Our analysis not only supports the experimentally determined stabilizing factors, but also unveils the important role of contacts, distributed throughout the protein, that lead to thermostability. We propose that this combined mesoscopic-network and fine-grained molecular dynamics approach is a convenient and useful scheme not only to study allosteric changes leading to protein stability in the face of negligible over-all conformational changes due to mutations, but also in other molecular networks where change in function does not accompany significant change in the network structure.
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