

Abstract Submitted
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What is the role of native state in thermophilic adaptation ?¹ LUCAS SAWLE, University of Denver, KINGSHUK GHOSH, None — Thermophilic proteins denature at higher temperatures than mesophilic proteins. Among the many hypothesis related to thermophilic adaptation, reduced native state flexibility is one widely believed to be a signature of thermophilic proteins in comparison to their mesophilic homologues. While the majority of existing studies consist of investigating individual proteins, we instead focus on large-scale and detailed modeling of numerous proteins to infer the presence of general principles to thermophilic adaptation. We have curated and constructed the largest dataset of experimentally determined, monomeric, and non-complexed thermophilic-mesophilic homologue pairs. Using this data set of protein pairs, we performed comparative analysis of the native state fluctuations from molecular dynamics simulations at 300K in explicit solvent. From these dynamical fluctuations at short time scales (a cumulative of 150 ns or higher for each protein), we calculated several quantities of interest: i) intraresidue fluctuations, ii) dipole moment fluctuation to calculate dielectric constant, and iii) entropy of contact and cluster distribution. Here, we will present the performance of these different metrics to distinguish thermophiles from mesophiles.

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