

Comparing Unfolding and Folding Pathways for Eglin C, SH3, and C1-2  
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We tested folding dynamics of three representative proteins: Eglin C (1CSE), SH3 (1NLO), and Chymotrypsin Inhibitor 2 (1YPC) investigating their thermodynamic pathways for unfolding and folding. We posit that a significant correlation in the frequencies of contact maps will depict similarities in folding and unfolding pathways. Using discrete molecular dynamics (DMD), we performed molecular dynamics simulations of the unfolding and folding pathways at complementary temperature ranges. We have collated data for 10 simulations for folding and unfolding trajectories of the three proteins and have generated the corresponding contact maps. Using this data, we design a cross-correlation metric for analyzing the frequencies of contact maps and compare the unfolding and folding pathways.