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Studies of Protein Folding in Non-Funeled Free Energy Landscapes[1] COREY O'HERN, GREGG LOIS, JERZY BLAWZDZIEWICZ, Department of Mechanical Engineering and Department of Physics, Yale University —
A theoretical framework is developed to understand the dynamics of protein folding. The key insight is that the search for the optimal conformation of the protein is influenced by the rate at which external parameters are adjusted to induce folding. A theory based on this insight predicts that (1) proteins with non-funneled free energy landscapes can fold reliably, (2) reliable folding can occur in equilibrium or out-of-equilibrium, and (3) reliable folding only occurs when the quench rate is below a limiting value, which can be calculated from measurements of the free energy. We test these predictions against numerical simulations of heteropolymers with hydrophobic and hydrophilic interactions and a single energy scale.

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