Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Connecting thermal and mechanical protein (un)folding landscapes LI SUN, JEFFREY NOEL, Rice University, JOANNA SULKOWSKA, University of Warsaw, HERBERT LEVINE, JOSÉ ONUCHIC, Rice University —
Molecular dynamics simulations supplement single-molecule pulling experiments by providing the possibility of examining the full free energy landscape using many coordinates. Here, we use an all-atom structure-based model to study the force and temperature dependence of the unfolding of the protein filamin by applying force at both termini. The unfolding time-force relation τ(F) indicates that the unfolding behavior can be characterized into three regimes: barrier-limited low- and intermediate-force regimes, and a barrierless high-force regime. Slope changes of τ(F) separate the three regimes. We show that the behavior of τ(F) can be understood from a two-dimensional free energy landscape projected onto the extension X and the fraction of native contacts Q. In the low-force regime, the unfolding rate is roughly force-independent due to the small (even negative) separation in X between the native ensemble and transition state ensemble (TSE). In the intermediate-force regime, force sufficiently separates the TSE from the native ensemble such that τ(F) roughly follows an exponential relation. The TSE becomes increasingly structured with force. The high-force regime is characterized by barrierless unfolding, approaching a time limit of around 10 μs.

Li Sun
Rice University

Date submitted: 11 Nov 2014 Electronic form version 1.4