Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

What is the Origin of Internal Friction in Unfolded Proteins?

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— The unfolded state is being increasingly recognized as critical to many biological processes. There are many proteins that are found only transiently in the unfolded state, eventually folding into globular structures. Other proteins, called intrinsically disordered proteins (IDPs), may be unfolded even when carrying out important biological functions. Despite its ubiquitousness, the unfolded ensemble is not fully understood. In this work, we have investigated the origin of friction for the unfolded proteins undergoing conformational diffusion. We used extensive all-atom molecular dynamics simulations to study the dynamics of the unfolded cold-shock protein (CSP) from Thermotoga maritima at different solvent viscosities and at different denaturant concentrations. We systematically analyzed the reconfiguration dynamics of relevant structural features such as dihedral angle rotations, hydrogen bonds and hydrophobic contacts forming and breaking. The results of our calculations are broadly consistent with the corresponding experimental measurements. Our findings have important implications for the folding kinetics of proteins, especially under physiological conditions.

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Date submitted: 06 Nov 2013

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