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Protein Folding and Unfolding Dynamics from Direct Energy Landscape Sampling Simulations NATHAN WALTER, YANG ZHANG, University of Illinois at Urbana-Champaign — Attempts to capture the protein folding-unfolding process at the atomic scale are limited due to the temporal constraints of molecular dynamics simulations. Herein, we circumvent this temporal limitation by using a history-dependent metadynamics algorithm to directly sample the potential-energy landscape of several proteins. Previous applications of the original metadynamics method to proteins penalized select collective variables or dihedral angles of the protein assumed to be the principles to the folding process. Rather, our method penalizes the full coordinate space of the protein resulting in a 3N-dimensional sampled energy-landscape. The sampled timescale of the landscape is orders of magnitude longer than molecular dynamics simulations, which allows the observation of the folding and unfolding process multiple times during the simulation. From the sampled energy landscape, we can predict the folded state of the protein, and the activation barrier and the timescale associated with the folding and unfolding processes of the protein. Herein, we will present these findings for several well-studied proteins, to validate our results, and several new proteins, as a novel extension.

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