Abstract Submitted
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Protein dynamics from structural ensembles: Diffusive and activated contributions in a linear mode description[1] JEREMY COPPERMAN, MARINA GUENZA, University of Oregon — We have developed a coarse-grained linear Langevin equation for protein dynamics, which describes proteins as semiflexible objects collapsed into the free energy well representing the folded state of the protein. Fundamental to this approach is the inclusion of internal dissipation, absent in any rigid-body hydrodynamical modeling scheme. The normal mode analytical solution naturally separates into global modes describing the anisotropic tumbling of the object, and internal modes which contain both diffusive and activated glass-like contributions. We show how cooperativity in the dynamical modes is related to the energy barriers to mode diffusion. While molecular dynamic simulations generate the most accurate structural ensembles, we show how sets of NMR conformers can be used to generate the structural ensemble needed as input to the theory, making the approach truly predictive in nature. Results are in good agreement when compared with both nuclear magnetic resonance relaxation, and time correlation functions calculated from molecular dynamic simulations.

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