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**Calculation of folding rates of two-state proteins supports enhanced structural cooperativity** XIANGHONG QI, JOHN PORTMAN, Department of Physics, Kent State University, Kent, OH, 44242 — The coarse-grained variational model is used to characterize the polymer dynamics of barrier crossing for a set of 28 non-homologous two-state small proteins. When terms that induce minor cooperativity are included in the interaction potential, we find that the behavior of calculated rates are in good agreement with experimental rates in terms of the absolute rate as well as realtionship to native topology. Generally,the structure of the transition state ensemble for the folding and unfolding routes include roughly the same residues, though the distinction between folding and unfolding residues is more pronounced. That is, the main effect of cooperativity is to sharpen the interface of the folding nucleus without significently changing the folding mechanism. Furthermore, the calculated prefactors $1/k_0$ are found to be relatively uniform, with variation in $1/k_0$ less than a factor of five.This calculation justifies the common assumption that $k_0$ is a roughly same for small two-state folding proteins. Using the barrier heights obtained from the model, we find that $1/k_0 \sim 1 - 5\mu$s(with average $\sim 4\mu$s). The relationship between free energy barrier and native state topology and chain length are also considered. The model can be easily to study more subtle aspects of folding such as the variation of the folding rate with stability or solvent viscosity.

Xianghong Qi

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