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Polymer dynamics and the folding rates of fast folding proteins

JOHN PORTMAN, Kent State University — In recent years, minimal models of fast folding proteins has enabled considerable agreement between computation, theory, and experiment. The assumptions associated with most simple models of fast folding proteins (Go-models) give rather robust results in terms of coarse grained description of the transition state ensemble. One aspect of the folding mechanism that has received less attention is describing the conformational dynamics responsible for the folding rate prefactor, k_0 . Here, we consider the distribution of prefactors of fast folding proteins: does local dynamics influence k_0 , or can one reasonably expect that k_0 is essentially the same regardless of contact order or mean structure of the transition state ensemble. We address this question by considering the folding routes of a wide variety of fast folding proteins using a polymer based model in which structural ensembles are parameterized by the degree of localization about the native structure.

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