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Stability versus flexibility in the dimerization kinetics and thermodynamics of the GCN4 Leucine zipper DIPAK RIMAL, YANXIN LIU, PREM CHAPAGAIN, BERNARD GERSTMAN, Florida International University, THEORETICAL AND COMPUTATIONAL BIOPHYSICS TEAM — We present results of computer simulations that show that too much stability of the native state can have the unwanted side-effect of slower and less reliable folding. The time spent in non-native configurations depends on both the depth of the valleys in the energy landscape and the probability for visiting various regions of the landscape. We present computational results for dimerization of the GCN4 Leucine zipper in which both the helical propensities and the ionic interactions are varied in strength. The results show that when interactions are too strong, they not only beneficially stabilize the native state, but also stabilize non-native configurations that act as kinetic traps. In some cases, intermediate structures become so rigid that the peptide does not have the flexibility necessary to fold to the native state. In other situations, such as high temperature, the chain has superfluous flexibility and can form non-native bonds. If these non-native bonds are too strong, the peptide spends significant time in contorted non-native configurations and folding is slowed and less efficient. Therefore, efficient folding must be a compromise between stability and flexibility.

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