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**Representing the Marginal Stability of Peptides in Coarse Grained Models**[1] MEHMET SAYAR, Koc Univ, CAHIT DALGICDIR, FARHAD RAMEZANGHORBANI, Koc University — Tertiary structure of proteins is only marginally stable; such that the folded structure is separated from local minima by as little as 10 kcal/mol. In particular for intrinsically disordered peptides, this marginal stability is key to understanding their complex behavior. Bottom-up coarse grained (CG) models for proteins/peptides which rely on structural and/or thermodynamic reference data from experiments or all atom simulations inherently focus on the equilibrium structure and fail to capture the conformational dynamics of the molecule. In this study, we present a CG model for a synthetic peptide, LK, which successfully captures the conformational flexibility of the molecule in different environments. LK peptide is composed of leucine and lysine residues and displays a stark conformational transition from a degenerate conformation in dilute solution to a fully stable alpha-helix at macroscopic and molecular interfaces. In this study we demonstrate that by carefully combining atomistic references from both the unfolded and folded states, one can create a CG model that can represent not only the folded state, but also the conformational transitions that the peptide exhibits in response to changes in the environment.

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