Investigating a peptide chameleon sequence using Replica Exchange Molecular Dynamics.

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Chameleon sequences, defined by their ability to adopt multiple secondary structures, have been implicated in several disease causing agents such as prions and aggregate forming proteins [1]. The existence of such sequences demonstrates the significance of non-local interactions in the native structures of proteins. The 23-residue sequence in this study is stable in two different protein folds, as an alpha helix and beta sheet [2]. We use Replica Exchange Molecular Dynamics to sample conformational space of this sequence.

1. Meiler and Baker. (2003) *PNAS* **100**(21), 12105-12110.
2. He et al. (2008) *PNAS* **105**(38), 14412-14417.