Elasticity and Coarse-grained Models of Protein Secondary Structures

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Abstract

From explicit molecular dynamics simulations, we compute the elastic properties of α-helices and β-sheets. The elastic constants are extracted from the MD data and are inputs of coarse-grained models of secondary structures. We investigate the sequence, solvent and boundary condition dependencies of the elastic constants. The coarse-grained models are then used to predict the response of the secondary structures to applied forces. For α-helices, we find that a semiflexible rod model is able to predict the conformation and bending properties of the coiled-coil protein motif.