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Hydrophobic Hydration of Stimulus-Responsive Polyproteins Measured by Single Molecule Force Spectroscopy

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We present a new procedure to reduce and analyze force-extension data obtained by single molecule force spectroscopy (SMFS). This approach allows, for the first time, to infer effects of solvent quality and minor changes in molecular architecture on molecular-elasticity of individual (bio)macromolecules. Specifically, we show how changes in the effective Kuhn segment length can be used to interpret the hydrophobic hydration behavior of elastin-like polypeptides (ELPs). Our results are intriguing as they suggest that SMFS in combination with our analysis procedure can be used to study the subtleties of polypeptide-water interactions on the single molecule level. We also report on the force-induced cis-trans isomerization of prolines, which are repeated every fifth residue in the main chain of ELPs. We present evidence for this mechanism by Monte Carlo simulations of the force-extension curves using an elastically coupled two-state system. Our results suggest that SMFS could be used to assay proline cis-trans isomerization in proteins and may thus have significant potential diagnostic utility.