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Stretching to Understand Proteins

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Mechanical stretching of single proteins has been studied experimentally for about 50 proteins yielding a variety of force patterns and values of the peak forces. We have performed a theoretical survey of 7749 proteins of known native structure and map out the landscape of possible dynamical behaviors unders stretching at constant speed. The model used is constructed based on the native geometry. It is solved by methods of molecular dynamics and validated by comparing the theoretical predictions to experimental results. We characterize the distribution of peak forces and on correlations with the system size and with the structure classification as characterized by the CATH scheme. We identify proteins with the biggest forces and show that they belong to few topology classes. We determine which protein segments act as mechanical clamps and show that, in most cases, they correspond to long stretches of parallel beta-strands, but other mechanisms are also possible. We then consider stretching by fluid flows. We show that unfolding induced by a uniform flow shows a richer behavior than that in the force clamp. The dynamics of unfolding is found to depend strongly on the selection of the amino acid, usually one of the termini, which is anchored. These features offer potentially wider diagnostic tools to investigate structure of proteins compared to experiments based on the atomic force microscopy.