Protein Conformational Entropy is Independent of Solvent.

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Proteins exhibit most of their conformational entropy in individual bond vector motions on the ps-ns timescale. These motions can be examined through determination of the Lipari-Szabo generalized squared order parameter (O^2) using NMR spin relaxation measurements. It is often argued that most protein motions are intimately dependent on the nature of the solvating environment. Here the solvent dependence of the fast protein dynamics is directly assessed. Using the model protein ubiquitin, the order parameters of the backbone and methyl groups are shown to be generally unaffected by up to a six-fold increase in bulk viscosity or by encapsulation in the nanoscale interior of a reverse micelle. In addition, the reverse micelle condition permits direct comparison of protein dynamics to the mobility of the hydration layer; no correlation is observed. The dynamics of aromatic side chains are also assessed and provide an estimate of the length- and timescale of protein motions where solvent dependence is seen. These data demonstrate the solvent independence of conformational entropy, clarifying a long-held misconception in the fundamental behavior of biological macromolecules. Supported by the National Science Foundation.

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Date submitted: 06 Nov 2015
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