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A new perspective of protein hydration & solvent slaving from solution NMR

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The interactions of proteins with water are fundamental to their structure, dynamics and function. Historically, characterization of the location and residence times of hydration waters of proteins in solution has been difficult. Confinement within the nanoscale interior of a reverse micelle allows detection of protein-water interactions using solution NMR techniques. Complications that normally arise from short residence times, hydrogen exchange and long-range dipolar coupling are overcome by the nature of the reverse micelle sample. Characterization of ubiquitin demonstrates that encapsulation within a reverse micelle allows detection of dozens of hydration waters. Comparison of NOE and ROE intensities indicate a considerable range of hydration water dynamics on the protein surface. A clustering of different hydration dynamics is evident. These clusters also correlate with the surface that is involved in protein-protein interactions suggesting that evolution has maximized the hydrophobic effect (i.e. entropy gain of water). Similar studies of other proteins will also be presented. In addition, the coupling of the motion of water at the surface and in the bulk has long been thought to “slave” the motions of the protein. Site-resolved measurement of this has been lacking. Here we show that the confinement of ubiquitin within the high-viscosity water core of a reverse micelle affects internal protein motion in only small and subtle ways. This may require a revision of the “solvent slaving” model for protein motion. Supported by the NIH and the NSF.