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Characterization of protein hydration by solution NMR spectroscopy

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A comprehensive understanding of the interactions between protein molecules and hydration water remains elusive. Solution nuclear magnetic resonance (NMR) spectroscopy has been proposed as a means to characterize these interactions but is plagued with artifacts when employed in bulk aqueous solution. Encapsulation of proteins in reverse micelles prepared in short chain alkane solvents can overcome these technical limitations. Application of this approach has revealed that the interaction of water with the surface of protein molecules is quite heterogeneous with some regions of the protein having long-lived interactions while other regions show relatively transient hydration. Results from several proteins will be presented including ubiquitin, staphylococcal nuclease, interleukin 1beta, hen egg white lysozyme (HEWL) and T4 lysozyme. Ubiquitin and interleukin 1beta are signaling proteins and interact with other proteins through formation of dry protein-protein interfaces. Interestingly, the protein surfaces of the free proteins show relatively slowed (restricted) motion at the surface, which is indicative of low residual entropy. Other regions of the protein surface have relatively high mobility water. These results are consistent with the idea that proteins have evolved to maximize the hydrophobic effect in optimization of binding with protein partners. As predicted by simulation and theory, we find that hydration of internal hydrophobic cavities of interleukin 1beta and T4 lysozyme is highly disfavored. In contrast, the hydrophilic polar cavity of HEWL is occupied by water. Initial structural correlations suggest that hydration of alpha helical structure is characterized by relatively mobile water while those of beta strands and loops are more ordered and slowed. These and other results from this set of proteins reveals that the dynamical and structural character of hydration of proteins is heterogeneous and complex. Supported by the National Science Foundation.