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Modulators of heterogeneous protein surface water dynamics

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The hydration water that solvates proteins is a major factor in driving or enabling biological events, including protein-protein and protein-ligand interactions. We investigate the role of the protein surface in modulating the hydration water fluctuations on both the picosecond and nanosecond timescale with an emerging experimental NMR technique known as Overhauser Dynamic Nuclear Polarization (ODNP). We carry out site-specific ODNP measurements of the hydration water fluctuations along the surface of Chemotaxis Y (CheY), and correlate the measured fluctuations to hydropathic and topological properties of the CheY surface as derived from molecular dynamics (MD) simulation. Furthermore, we compare hydration water fluctuations measured on the CheY surface to that of other globular proteins, as well as intrinsically disordered proteins, peptides, and liposome surfaces to systematically test characteristic effects of the biomolecular surface on the hydration water dynamics. Our results suggest that the labile (ps) hydration water fluctuations are modulated by the chemical nature of the surface, while the bound (ns) water fluctuations are present on surfaces that feature a rough topology and chemical heterogeneity such as the surface of a folded and structured protein.

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