Effects of Renal Osmolytes on Water Structure and Dynamics: Time-Resolved Vibrational Spectroscopy and MD simulation

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Osmolytes are an integral part of living organism e.g., the kidney uses sorbitol, trimethylglycine, taurine and myo-inositol to counter the deleterious effects of urea and salt. Therefore, understanding the effects of renal osmolytes on water structure and dynamics is of great importance. Our measurement results show that protecting osmolytes, e.g., trimethylglycine and sorbitol, significantly modulate the water hydrogen-bonding network structure and its dynamics, though the magnitude and spatial extent of osmolyte-induced perturbation greatly vary. In contrast, urea behaves neutrally towards local water hydrogen-bonding network structure and dynamics. These experimental findings are further confirmed by concentration-dependent molecular dynamics simulations of all the aqueous renal osmolyte solutions and by applying spectral graph theoretical method to analyze hydrogen-bond network and osmolyte aggregation structures. It was found that protecting osmolytes studied here show strong concentration-dependent behaviours (vibrational frequencies and lifetimes of two different infrared probes), while denaturant does not. Our findings highlight the significance of the alteration of hydrogen bonding network of water under biologically relevant environment, often encountered in real biological systems.