Probing the vibrational dynamics of proteins in liquid water by terahertz absorption spectroscopy

NGUYEN QUANG VINH, Department of Physics, UCSB, KEVIN W. PLAXCO, Department of Chemistry and Biochemistry, UCSB, S. JAMES ALLEN, Department of Physics, UCSB — Biomolecules solvated in their biologically milieu are expected to exhibit strong absorption in the terahertz range that contain information on their global and subglobal collective vibrational modes and global dynamical correlations among solvent water molecules and the protein. Measurements in this region, however, are challenging due to due to the strong absorption of water and often sever interference artifacts. In response, we have developed, with Virginia Diode Inc., a highly sensitive Vector Network Analyzer system for probing collective dynamics in aqueous solution. Using this we explore the complex dielectric response from 0.07 to 0.70 THz that directly probes such questions as the hydration level around proteins and the large scale vibrational modes of biological polymers. We make a direct comparison to the existing molecular dynamic simulations and normal mode calculations and investigate the dependence of the low frequency dynamics on protein concentration and solvent pH. Our measurements shed light on the macromolecular motions in a biologically relevant water environment.

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