Abstract Submitted
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Probing the dynamics of biomolecules in liquid water by terahertz spectroscopy[1] NGUYEN VINH, JIM ALLEN, Physics Department, UCSB, KEVIN PLAXCO, Department of Chemistry and Biochemistry, UCSB — Decades of molecular dynamics and normal mode calculations suggest that proteins are rife with collective vibrational modes with ps to ns time constants. Given that proteins are "decorated" with charged groups, these motions should lead to oscillating dipoles that, in turn, will lead to strong gigahertz to terahertz absorption. Investigation of these harmonic motions by absorption spectroscopy, however, is extremely challenging due to the strong absorption of water. In response, we have developed a sensitive Vector Network Analyzer based spectrometer that operates from 65 to 700 GHz and can measure both the absorbance and refractive index of protein solutions. In order to extract the complex dielectric response of the protein in solution we employ an effective medium approximation for the mixture of the protein and aqueous buffer. The extracted dielectric response suggests that each protein molecule is surrounded by a tightly held layer of 164 +/- 5 water molecules that behave as if they are an integral part of the protein. The size of this hydration shell and the dielectric response of the solvated protein are all independent of protein concentration. Our measured dielectric response, however, does not agree with published computation models of the protein: the measurements indicate a low frequency cutoff in the density of modes of ∼250 GHz.

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