

Abstract Submitted  
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**Time-resolved infrared structural biology: from active-site structural dynamics to proton transfer mechanism of photoactive yellow protein** SHUO DAI, LORAND KELEMEN, ZHOUYANG KANG, WOUTER HOFF, AIHUA XIE, Oklahoma State University, Stillwater, OK 74078 — Proton transfer is a fundamental process in biology. We employ photoactive yellow protein (PYP), a bacterial blue light receptor protein, as an ideal model system to study the physical mechanism of intra-molecular proton transfer in proteins. We employ time-resolved step-scan FTIR spectroscopy to detect functionally important structural changes in the active site of PYP before and after proton transfer from Glu46 to the negatively charged phenolic group of the *p*-coumaric acid chromophore in PYP, which occurs on a 250 microsecond time scale. In addition, we employ a combination of isotope editing and site-specific mutations to identify the vibrational modes and structural origins of infrared signals, and we develop and utilize vibrational structural markers to translate infrared signals to structural information. We will demonstrate the power of time-resolved infrared structural biology in structure-function studies of proteins and in proton transfer mechanism in photoactive yellow protein.

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