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Infrared Structural Biology of Proteins: Development of Vibrational Structural Markers for Probing the Structural Dynamics of COO- of Asp/Glu in Proteins ZHOUYANG KANG, AIHUA XIE, Department of Physics, Oklahoma State University — Asp and Glu often play critical roles in the active sites of proteins. Probing the structural dynamics of functionally important Asp and/or Glu provides crucial information for protein functionality. Time-resolved infrared structural biology offers strong advantages for its high structural sensitivity and broad dynamic range (ps to ks). In order to connect the vibrational frequencies to specific structures of COO- groups, such as the number, type, and geometry of hydrogen bond interactions, we develop two vibrational structural markers (VSM), built on the symmetric and asymmetric COO- stretching frequencies. Extensive quantum physics (density functional theory) based computational studies, combined with 13C isotopic editing of Asp/Glu and experimental FTIR data on Asp/Glu in proteins, are used to establish a unique correlation between the symmetric and asymmetric COO- vibrations with more than 10 types of hydrogen bonding interactions. Development of the COO- VSM markers enhances the power of time-resolved infrared structural biology for the study of functionally important structural dynamics of COO- in proteins, including rhodopsin for biological signaling, bacteriorhodopsin for proton transfer, photosystem II for energy transformation, and HIV protease for enzymatic catalysis.

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