

Abstract Submitted
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Develop Infrared Structural Biology for Probing Structural Dynamics of Protein Functions¹ AIHUA XIE, ZHOUYANG KANG, OLIVER CAUSEY, CHARLE LIU, Oklahoma State University — Protein functions are carried out through a series of structural transitions. Lack of knowledge on functionally important structural motions of proteins impedes our understanding of protein functions. Infrared structural biology is an emerging technology with powerful applications for protein structural dynamics. One key element of infrared structural biology is the development of vibrational structural marker (VSM) database library that translates infrared spectroscopic signals into specific structural information. We report the development of VSM for probing the type, geometry and strength of hydrogen bonding interactions of buried COO- side chains of Asp and Glu in proteins. Quantum theory based first principle computational studies combined with bioinformatic hydrogen bond analysis are employed in this study. We will discuss the applications of VSM in mechanistic studies of protein functions. Infrared structural biology is expected to emerge as a powerful technique for elucidating the functional mechanism of a broad range of proteins, including water soluble and membrane proteins.

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