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Infrared Structural Biology: A Tool for Probing Structure and Dynamics of Functional Histidines in Proteins[1] AIHUA XIE, CHARLE LIU, MATTHEW CAVENER, Oklahoma State University — We report a method for structure-function studies of histidine in proteins based on signature infrared signals. The imidazole group of histidine residues are found functionally important in a vast number of catalytic proteins. Knowledge on the protonation states of key histidine side chains in enzymes at rest and during catalytic actions is indispensable to elucidation of the structure-function relationship underlying enzymatic catalysis. We report a rigorous method on how to detect the three protonation states of functionally important histidine imidazole rings in the static and dynamic states of enzymes using infrared structural biology. First principle computational methods based on density functional theory were employed to develop two vibrational structural markers (VSM) of the imidazole group: VSMq for the charged states of the imidazole group, while VSMt for distinguishing the D and E tautomers of charge neutral histidine. The accuracy of the VSMs is assessed by comparison of calculated VSMs with experimental FT-IR data of the 4-ethyl-imidazole model compound. We will discuss how these VSMs may be employed in structure-function studies on functionally important histidine residues in enzymes.

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