Site-selective Infrared Spectroscopy to Investigate Protein Conformations and Dynamics

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Protein dynamics, the population of and interconversion among multiple states, can be fundamental to function. However, to fully uncover their role, experimental approaches for characterizing protein dynamics must contend with both the complex spatial heterogeneity of proteins and the rapid interconversion of potentially important conformational states. To address these challenges, our group combines the inherent temporal resolution of linear and twodimensional infrared spectroscopy with the spatial resolution afforded by site-selective incorporation of vibrational reporter groups with frequency-resolved absorptions. This enables capture of even rapid dynamics at local environments in proteins. I will share how we have applied this approach to investigate the functional role of dynamics in protein molecular recognition and catalysis.