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Develop vibrational structural makers for probing the protonation state and hydrogen bonding interactions of tyrosine in proteins and their functional intermediates ANUPAMA THUBAGERE, BEINING NIE, EDWARD MANDA, AIHUA XIE, Oklahoma State University — Proteins are dynamic in nature. In order to understand how a protein performs its function based on laws of physics, it is critical to probe and investigate functionally important structural transitions of the protein. Time-resolved infrared spectroscopy offers excellent time resolution (picoseconds to seconds), and contains extensive structural information. The real challenge is how to extract structural information from time-resolved infrared data. We will report computational methods for developing vibrational structural markers of tyrosine. Using density function theory (DFT) based first principle computational studies combined with experimental data, we found that it is possible to unambiguously determine if the phenolic ring in Tyrosine is neutral or negatively charged based on the frequency of one ring vibrational mode. In addition, we show that it possible to determine the number and nature of hydrogen bonding interactions of a phenolic group in proteins using a combination of C-O stretching and O-H stretching frequencies (2D vibrational spectroscopy).

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