ANALYTICAL SEMINAR

Advances in 2D IR spectroscopy of proteins: utilizing transition dipole strength calculations to enhance structural analysis

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219 BRL

Using 2D IR spectroscopy to calculate absolute transition dipole strength (TDS) spectra, we can detect changes to protein structure that arise from post-translational modifications, mutations, or interactions with surfaces without the need for site-specific labels. The application of TDS analysis to both highly ordered protein aggregates and minimally ordered soluble peptides will be presented. Through these examples, we demonstrate TDS spectra as a label-free method to detect structural polymorphs in samples that appear identical by traditional spectroscopic methods. This talk will also address current challenges in the application of TDS to noisy or weak signals and our efforts to use machine learning approaches to improve both precision and accuracy.

Lauren Buchanan is an expert in ultrafast vibrational spectroscopy and biophysical chemistry. She joined Vanderbilt University in 2016 as an Assistant Professor in the Department of Chemistry at Vanderbilt University. She earned her Ph.D. with Martin T. Zanni at the University of Wisconsin – Madison in 2013, followed by a postdoctoral fellowship with Richard P. Van Duyne at Northwestern University. Dr. Buchanan's research program focuses on developing new approaches for using two-dimensional infrared (2D IR) spectroscopy to study protein structure and dynamics that are difficult to observe using traditional biophysical methods. Some of the topics that the Buchanan group is pursuing include 1) understanding the role of amino acid sequence on protein folding and self-assembly in order to guide rational design of peptide nanomaterials, 2) determining the detailed molecular-level changes to protein secondary, tertiary, and quaternary structure that occur when proteins adsorb onto nanoparticles, and 3) elucidating the self-assembly mechanisms of both functional and pathogenic amyloid proteins in biological environments by developing unnatural amino acids as site-specific structural probes.

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