2D IR spectroscopy of the CD3ζ transmembrane peptide

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Membrane peptides serve a variety of functions in cell biology including acting as antimicrobial drugs and as models for the transmembrane segments of proteins. In this talk, experiments will be presented using heterodyned 2D IR spectroscopy and $^{13}C=^{18}O$ isotope labeling to study the conformational and environmental heterogeneity of a 27-residue peptide in lipid vesicles that encompasses the transmembrane domain of the T-cell receptor CD3ζ. In membranes, this peptide forms a tetramer transmembrane helical bundle with the helices pointing 12° to the membrane normal. Using $^{13}C=^{18}O$ isotope labeling, the amide I modes of 10 different residues have been labeled along the length of the peptide spanning the width of the membrane. The $^{13}C=^{18}O$ label shifts the amide I band about 60 cm^{-1}, spectrally isolating it from the remaining residues. For each of the 10 residues, heterodyned 2D IR spectra have been collected using an echo pulse sequence and each spectrum has been fit to extract the inhomogeneous and homogeneous linewidths. We find that the homogeneous linewidths of all the labeled residues are the same to within our resolution, but that the inhomogeneous linewidth of residues near the center of the peptide are narrower than for residues at the ends. The data are interpreted based on a structural model of the bundle, the heterogeneous environment of the membrane itself, and with a force-force correlation function calculated from molecular dynamics simulations.