

## 2D IR LINE SHAPES FOR DETERMINING THE STRUCTURE OF A PEPTIDE IN A BILAYER

ANN MARIE WOYS, Y. S. LIN, J. S. SKINNER, M. T. ZANNI, *Department of Chemistry, University of Wisconsin, Madison, WI 53706*; A. S. REDDY, J. J. DE PABLO, *Department of Chemical Engineering, University of Wisconsin, Madison, Wisconsin 53706*.

Structure of the antimicrobial peptide, ovispirin, on a lipid bilayer was determined using 2D IR spectroscopy and spectra calculated from molecular dynamics simulations.<sup>a</sup> Ovispirin is an 18 residue amphipathic peptide that binds parallel to the membrane in a mostly alpha helical conformation. 15 of the 18 residues were <sup>13</sup>C<sup>18</sup>O isotopically labeled on the backbone to isolate the amide I vibration at each position. 2D IR spectra were collected for each labeled peptide in 3:1 POPC/POPG vesicles, and peak width along the diagonal was measured. The diagonal line width is sensitive to the vibrators electrostatic environment, which varies through the bilayer. We observe an oscillatory line width spanning 10 to 24 cm<sup>-1</sup> and with a period of nearly 3.6 residues. To further investigate the position of ovispirin in a bilayer, molecular dynamics simulations determined the peptide depth to be just below the lipid headgroups. The trajectory of ovispirin at this depth was used to calculate 2D IR spectra, from which the diagonal line width is measured. Both experimental and simulated line widths are similar in periodicity and suggest a kink in the peptide backbone and the tilt in the bilayer.

---

<sup>a</sup>A. Woys, Y. S. Lin, A. S. Reddy, W. Xiong, J. J. de Pablo, J. S. Skinner, and M. T. Zanni, *JACS* 132, 2832-2838 (2010).