

**W0215**

**Determining the Structures of Peptides in Membranes Using Diffraction and MD Simulations.** S. H. White, Dept. of Physiology and Biophysics, Univ. of California at Irvine, Irvine, CA 92697.

Quantitative structural images of peptides in oriented arrays of fluid lipid bilayers are necessary for interpreting thermodynamic measurements of peptide-bilayer energetics in molecular terms. Lamellar x-ray and neutron diffraction provide a starting point for obtaining structural images. But the high thermal motion of fluid bilayers limits “structures” to so-called bilayer profiles, representing a time-averaged projection of the unit-cell contents onto an axis normal to the bilayer plane. Specific deuteration of lipid structural groups combined with neutron diffraction difference methods allow these profiles to be decomposed into a collection of groups (phosphates, carbonyls, etc.) representing transbilayer probability distribution functions. We are extending the power of this method to include x-ray data, a joint-refinement protocol, and molecular dynamics simulations. Our goal is to convert 1-D experimental data into 3-D images. Importantly, these images will be dynamic, which will permit the ensembles of peptide-lipid structures to be explored in detail. Research supported by the NIH: GM46283, GM68002, & RR14812.