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Abstract for an Invited Paper
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integrating Solid State NMR and Computations in Membrane Protein Science

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Helical membrane protein structures are influenced by their native environment. Therefore the characterization of their structure in an environment that models as closely as possible their native environment is critical for achieving not only structural but functional understanding of these proteins. Solid state NMR spectroscopy in liquid crystalline lipid bilayers provides an excellent tool for such characterizations. Two classes of restraints can be obtained - absolute restraints that constrain the structure to a laboratory frame of reference when using uniformly oriented samples (approximately 1° of mosaic spread) and relative restraints that restrain one part of the structure with respect to another part such as torsional and distance restraints. Here, I will discuss unique restraints derived from uniformly oriented samples and the characterization of initial structures utilizing both restraint types, followed by restrained molecular dynamics refinement in the same lipid bilayer environment as that used for the experimental restraint collection. Protein examples will be taken from Influenza virus and Mycobacterium tuberculosis. When available comparisons of structures to those obtained using different membrane mimetic environments will be shown and the causes for structural distortions explained based on an understanding of membrane biophysics and its sophisticated influence on membrane proteins.