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Intermediate couplings: NMR at the solids-liquids interface

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Anisotropic interactions like dipolar couplings and chemical shift anisotropy have long offered solid-state NMR spectroscopists valuable structural information. Recently, solution-state NMR structural studies have begun to exploit residual dipolar couplings of biological molecules in weakly anisotropic solutions. These residual couplings are about 0.1% of the coupling magnitudes observed in the solid state, allowing simple, high-resolution NMR spectra to be retained. In this work, we examine the membrane-associated opioid, leucine enkephalin (lenk), in which the ordering is ten times larger than that for residual dipolar coupling experiments, requiring a combination of solution-state and solid-state NMR techniques. We adapted conventional solid-state NMR techniques like adiabatic cross- polarization and REDOR for use with such a system, and measured small amide bond dipolar couplings in order to determine the orientation of the amide bonds (and therefore the peptide) with respect to the membrane surface. However, the couplings measured indicate large structural rearrangements on the surface and contradict the published structures obtained by NOESY constraints, a reminder that such methods are of limited use in the presence of large-scale dynamics.