Mapping ligand binding and solvent-dependent structural features in a protein via biomolecular NMR

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Biomolecular NMR spectroscopy is able to elucidate residue-specific properties within proteins in solution, ranging from highly detailed tertiary-structural information to secondary-structural integrity, in-depth assessment of motional properties, and mapping of intermolecular interactions.

In this module, you will have the chance to experience a first contact to bio-NMR. You will learn (1) how to acquire and interpret an HSQC spectrum of an isotope-labeled protein, (2) how interatomic distances can reveal structural information, (3) how the interaction surfaces of binders to the protein can be mapped, and (4) how solvent-specific properties can influence the local structure, i. e., in particular, which structural properties remain after unfolding using a denaturant.

The practical course requires basic knowledge of protein structure and magnetic-resonance spectroscopy. We will explain basic principles of bioNMR, in particular encoding of resonance frequencies in multi-dimensional experiments, magnetization transfer, and Fourier transformation, and you will be exposed to spectrometer handling and using bioNMR-specific software for data processing and analyses. This will give you an overview about the power and beauty of NMR for proteins in structural biology and beyond.