NMR spectroscopy as a tool – How we can use it to probe protein structures and function

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For many scientists, solution-state nuclear magnetic resonance (NMR) spectroscopy is associated with structure elucidation of small molecules in organic chemistry, or at best, extends to characterization of the 3D structure of proteins. But structural elucidation represents just one facet of NMR spectroscopy and when we are working with a solution, we can freely change the conditions and then follow the resulting changes in biological molecules. This approach can be used to study an enzymes affinity for metal ions, pK_a of individual amino acids, and interaction with a substrate. It is possible to characterize protein-substrate interactions from both the protein and substrate point of view. Furthermore, substrate modification and degradation can be followed directly in the NMR tube in real time and the starting and end products can also be characterized by NMR spectroscopy. Altogether, this provides detailed information, which is a vital part for understanding the enzymatic process in question. We can also take advantage of the resonance frequency of our NMR instrument, which is at the same time scale as molecular motions and allows us to study protein mobility. In short - NMR spectroscopy serves as a tool providing key information for structure and functional understanding of proteins, substrates, and their interplay.