Field-dependent high-resolution spectral density mapping using a fast, mechanical based shuttle system

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Protein motions are crucial for biological functions, from protein-protein interaction to ligand recognition and enzymatic kinetics. The relaxation properties of a certain biomolecule encode for these motional characteristics. NMR is uniquely suited to study certain relaxation properties at residue-specific or higher resolution. We focus here on the study of spectral density functions as they contain the kinetic information. The use of these techniques requires strong magnetic fields in the case of protein NMR to provide the necessary resolution and sensitivity for a site-specific analysis. Therefore it is challenging to measure relaxation parameters for proteins at low magnetic field strengths. To get a more detailed insight into the spectral density functions. Therefore, to determine the protein dynamics a field-dependent analysis of the relaxation parameters is needed. Shuttle techniques[1, 2] are the method of choice here, since they enable relaxation experiments at low magnetic fields while still having the resolution and sensitivity of a high-field magnet. This is achieved by shuttling the sample between the center position of the magnet where the spectrum is acquired and a second position in the stray field of the magnet where the magnetization relaxes at a lower magnetic field.

In this work we present high-resolution relaxation data acquired with a mechanical-based shuttle system installed at 700 MHz Oxford magnet with a prodigy probe. The sample can be shuttled from the static field of 16.47 T up to a field strength of 0.01 T in about 100 ms. With this set-up we measured ^{15}N longitudinal relaxation rates of the backbone of ubiquitin and protein GB3 at different positions in the stray field of the magnet. The obtained relaxation rates are analysed in respect to their field dependency by fitting the data to known models of the spectral density function[2,3] and the possibility of Non-Lorentzian behaviour[5] at low magnetic field strengths.

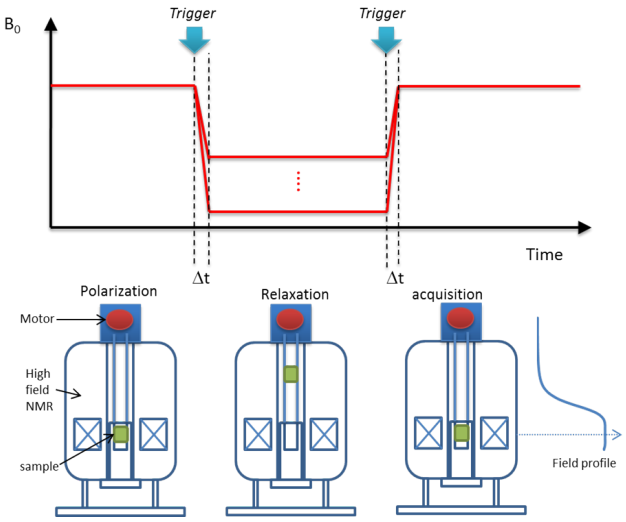

Figure 1: Scheme of shuttle NMR

References

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