

# New NMR experimental techniques: Protein structural compactness and transient conformational exchange dynamics

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Atomic resolution and dynamic information of biological macromolecules are mandatory to understand their biological function at molecular level. However macromolecules are dynamic ensembles so alternative high-energy conformations can play important function roles. Therefore, there is a real demand of new experimental techniques that provide access to study dynamic properties of macromolecules by NMR.

Intrinsically disordered proteins (IDPs) are characterized by high local mobility and lack of stable three-dimensional structure allowing them to interact with a large variety of binding partners. We propose taking advantage on the different relaxation dynamics of IDPs and globular proteins to understand the structural compactness and solvent accessibility by new NMR experiments based on a set of selective measurements of  $T_1$  relaxation delays (I).

NMR spectroscopy is a unique technique to study conformational dynamics over a wide-range of time scales, from picoseconds to hours. Real-Time NMR provides information of transient populated states based on the acquisition of NMR experiments with fast-pulsing methods. On the other hand relaxation-dispersion (RD) methods enable detection of conformational exchange dynamics of excited protein states that take place on the micro- to millisecond time scale but. Then we propose to combine both techniques as a powerful tool to study site-resolved conformational dynamics occurring in timely unstable or transient populated protein states (II).

(I) Tomas Hosek, Sergio Gil-Caballero, Roberta Pierattelli, Bernhard Brutscher and Isabella C. Felli, Journal of Magnetic Resonance, (254) 2015, 19-26.

(II) Rémi Franco, Sergio Gil-Caballero, Isabel Ayala, Adrien Favier and Bernhard Brutscher, J. Am. Chem Soc, (139) 2017, 1065-1068.

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