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Structural dynamics at multiple time scales

Paolo Calligari[a], Vania Calandrini[b], Mirko Mori[c], Fatiha Kateb[d], Gerald Kneller[b], Geoffrey Bodenhausen[a,e], Mario Piccioli[c] and Daniel Abergel[a]

[a]Département de Chimie, Ecole Normale Supérieure, 24 rue Lhomond, 75005 Paris, France, [b]Centre de Biophysique Moléculaire, CNRS, Rue Charles Sadron, 45071 Orléans, France, [c]CERM and Department of Chemistry, University of Florence, Via L. Sacconi 3, 50019 Sesto Fiorentino, Italy , [d]Lehrstuhl für Biomolekulare NMR-Spektroskopie, Departement Chemie, Lichtenbergstr. 4, D-85747 Garching, Germany, [e]Institut des Sciences et Ingénierie Chimiques, EPFL, 1015 Lausanne, Switzerland (daniel.abergel@ens.fr)

Spin relaxation measurements in liquids provide most valuable information on internal dynamics of proteins, which is a key factor of their functions. It is therefore important to provide physical models that can serve as a basis for the interpretation of the protein motions. Assuming that these can be related to the structure of the molecule, we recently introduced a model based on a *Network of Coupled Rotators* to describe internal dynamics of proteins from the knowledge of their three-dimensional structures. ^{15}N NMR relaxation rates can thus be predicted and conformational entropies of bond vector calculated. This approach also illustrates the absence of one-to-one relationships between order parameters and *conformational entropies*, and therefore explains the difficulty to relate both quantities from experimental data.[1] Further theoretical developments in the study of protein dynamics demonstrated the presence of multi-scale *fast* internal motions, and this complex behaviour was shown to be accounted for by a simple model based on *fractional Brownian dynamics.*[2] Structural dynamics also involves *microsecond time scale dynamics*, as shown by chemical shift modulation measurements of backbone C'N coherences.[3] These experiments suggest the unusual view of a protein where *slow motions* are present *across the entire backbone, and with characteristics* that can be related to the secondary structure elements. This is clearly in contrast with the conventional picture usually provided by ^{15}N NMR relaxation.

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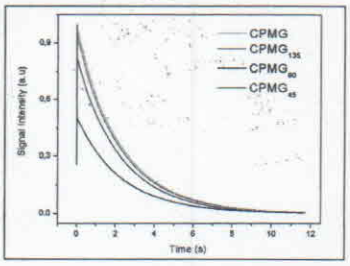
Analysis of CPMG Sequences with Low Refocusing Flip Angles

Fabiana D. Andrade[a], Antonio M. Netto[b] and Luiz A. Colnago[c]

[a]Institute of Chemistry of São Carlos, University of São Paulo, 400 Trab.São-carlense St, 13560-970, São Carlos-SP, Brazil (fabianadiuk@iqsc.usp.br)
[b]Institute of Physics of São Carlos, University of São Paulo, São Carlos-SP, Brazil
[c]EMBRAPA Agricultural Instrumentation, 1452 XV de Novembro St, 13560-970, São Carlos-SP, Brazil

The Carr-Purcell-Meiboom-Gill (CPMG) pulse sequence has been used in many applications. Recently, CPMG has been used in *on-line* measurements[1] where it was applied by long periods. In this case, 180° refocusing pulse can cause undesirable sample heating and equipment overload, which can reduce their durability and erroneous results. Thus, the purpose of this work is the experimental and theoretical analysis of CPMG sequence with low refocusing pulse flip angles (LRFA) using Bloch equation and the effect on the T_2 value under the parameters as magnetic field inhomogeneity, common problems occurred in low magnetic field, in order to use it in NMR *on-line* measurements. This Figure shows the experimental CPMG signals of water obtained on-resonance with refocusing flip angles of 180° (CPMG), 135° ($CPMG_{135}$), 90° ($CPMG_{90}$) and 45° ($CPMG_{45}$) in a less homogeneous field (FWHM=100Hz). However, CPMG signals with LRFA obtained in more homogeneous condition (FWHM=15Hz) were similar for all flip angle studied for experimental and simulated results showing the robustness of CPMG sequence. With this information it is possible to determine a limit to use different flip angles depending on conditions of B_0 inhomogeneous field used, which it can reduce power by more than 75% in *on-line* measurements.



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