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Molecular dynamics of Lentil and Fava Bean proteins investigated by ^{1}H NMR relaxometry

Faisal Sheraz Shah[1], Pedro J. Sebastião[2], Özlem Özmutlu Karslioglu[3], Danuta Kruk[1*]

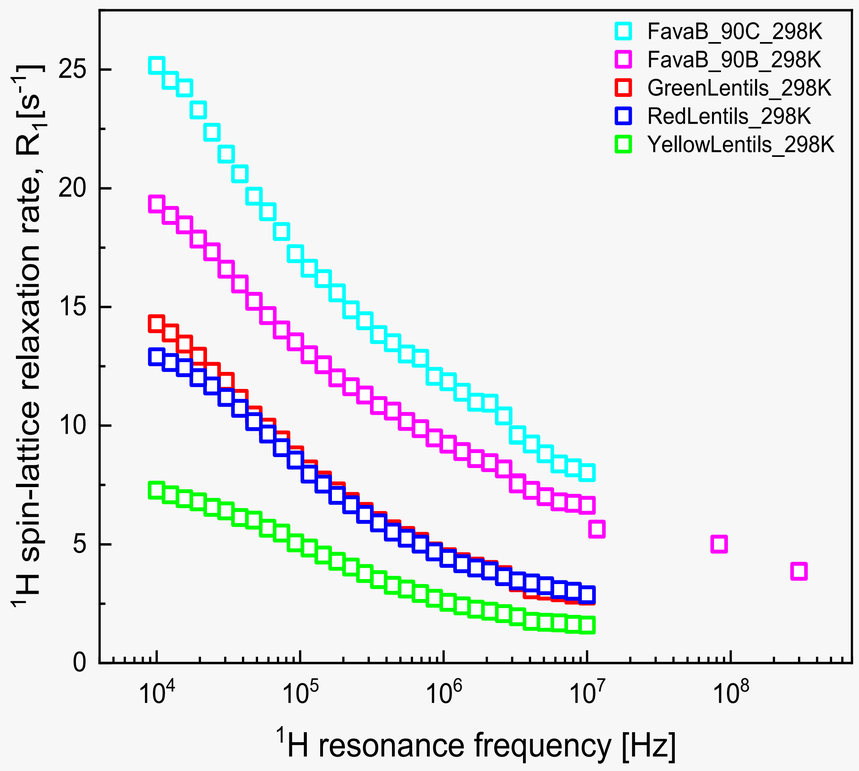
[1]*Department of Physics and Biophysics, University of Warmia and Mazury in Olsztyn, Oczapowskiego 4, 10-719 Olsztyn, Poland*

[2]*CeFEMA and Department of Physics, Instituto Superior Técnico, University of Lisbon, 1049-001 Lisbon, Portugal*

[3]*Institute of Food Technology, University of Applied Sciences Weihenstephan-Triesdorf, Am Staudengarten 11, 85354 Freising, Germany*

Introduction

- The dynamic properties of plant proteins play a crucial role in determining their functionality in food systems and bioprocessing applications. In this study, we employed ^{1}H NMR relaxometry to investigate the molecular mobility of protein systems derived from lentils and fava beans.
- We used Fast Field Cycling (FFC) techniques to measure the spin-lattice relaxation rates (R_1) across a wide frequency range (10 kHz to 10 MHz). For higher frequencies, conventional inversion-recovery pulse sequences were applied. These relaxation profiles provide insight into molecular motions and interactions within the legume protein systems.
- ^{1}H spin-lattice relaxation rate R_1 for 5 legume samples at 298K have been analyzed. All samples show the frequency dispersion where the relaxation rate R_1 decreases with increasing resonance frequency.



Theory and Experimental Results

We used two diffusion contributions with one *BPP* for rotations as a theoretical model to made the fits and get the required parameters and is given as:

$$R_1^{Total}(\omega_L) = R^{BPP}(\omega_L, \tau_R) + R_1^{SD}(\omega_L, \tau_{D1}) + R_1^{SD}(\omega_L, \tau_{D2}) \quad (1)$$

$$R_1^i(\omega, \tau) = A^i[\, J^i(\omega, \tau) + 4\, J^i(2\omega, \tau)] \quad (2)$$

$i \equiv BPP;\ SD$

$$J^{BPP}(\omega, \tau) = \frac{\tau}{1+\omega^2\tau^2} \quad (3)$$

This relaxation rate was first obtained by N. Bloembergen, E. M. Purcell, and R. V. Pound and is often denoted the *BPP* relaxation model (Eq.3).

The spectral density for the self diffusion contribution of the Freed model is expressed in Eq.4.

$$J^{SD}(\omega, \tau) = 72\,\frac{3}{4\pi}\int_0^\infty \frac{\mu^2}{81-9\mu^2-2\mu^4+\mu^6}\,\frac{\mu^2\tau}{\mu^4+(\omega\tau)^2}\,d\mu \quad (4)$$

$$\tau_D = \frac{d^2}{2D}$$

τ is the correlation time, ω is the Larmor angular frequency, A denotes an effective dipole-dipole coupling constant. The parameter d is the distance of closest approach of the interacting nuclei.

Tab.1. Parameters obtained by fitting the relaxation dispersion data in terms of Equation (1).

Label	T(K)	chi²t	NP	n	reff (m)	τ_1 (s)	d (m)	d_1 (m)	D (m²/s)	D_1 (m²/s)
FavaB_90C	298	1.5043	10	6.68×10^{28}	1.75×10^{-10}	2.35×10^{-10}	9.52×10^{-10}	3.18×10^{-9}	6.29×10^{-12}	1.06×10^{-12}
FavaB_90B	298	1.0569	10	6.68×10^{28}	1.70×10^{-10}	1.74×10^{-10}	1.17×10^{-9}	3.58×10^{-9}	6.89×10^{-12}	1.30×10^{-12}
Green_Lentils	298	2.4999	10	6.68×10^{28}	2.13×10^{-10}	2.84×10^{-10}	1.46×10^{-10}	3.31×10^{-9}	7.74×10^{-12}	1.45×10^{-12}
Red_Lentils	298	0.9103	10	6.68×10^{28}	1.77×10^{-10}	1.00×10^{-10}	1.51×10^{-10}	3.03×10^{-9}	9.79×10^{-12}	1.83×10^{-12}
Yellow_Lentils	298	1.7932	10	6.68×10^{28}	2.29×10^{-10}	2.52×10^{-10}	1.80×10^{-10}	3.46×10^{-9}	1.25×10^{-11}	3.26×10^{-12}

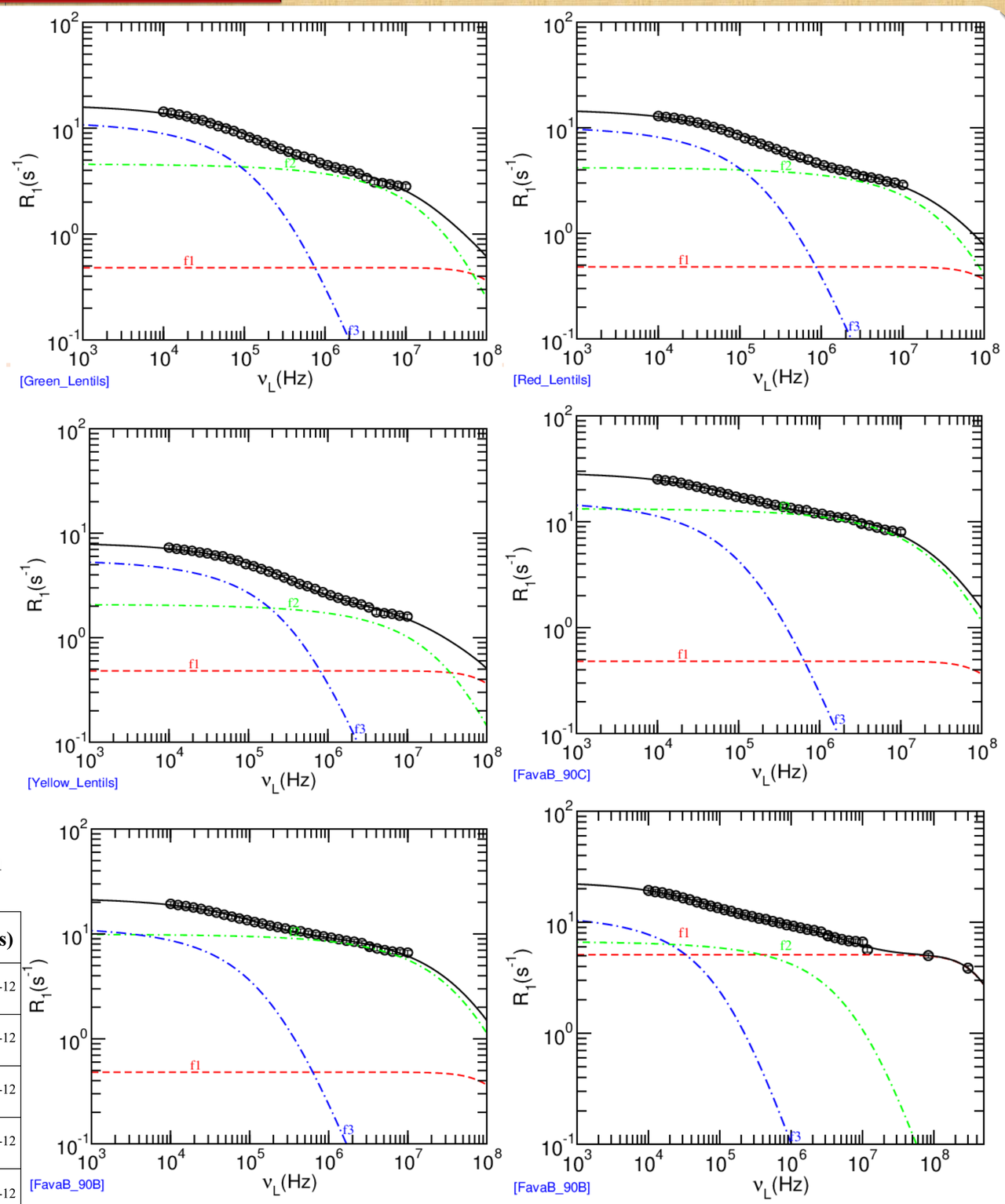


Fig.1. ^{1}H spin-lattice relaxation rate R_1 for 5 legume samples at 298K for all. Fits of the overall relaxation rate in terms of Equation (1). The parameters are given in Table 1.

Conclusions: With this integrated approach, we aim at obtaining a deeper understanding of protein hydration dynamics and its dependence on protein type, structure and water content. This work will continue with the high field measurements on all samples to obtain equivalent model accuracy on all systems.

References:

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2. Hwang, Lian-Pin, and Jack H. Freed. "Dynamic effects of pair correlation functions on spin relaxation by translational diffusion in liquids." The Journal of Chemical Physics 63.9 (1975): 4017-4025.