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Dipolar Relaxation of Water Protons in the Vicinity of a Collagen-like Peptide

Type II collagen is the most abundant macromolecule in articular cartilage. In the tissue collagen forms anisotropic, fibrillous structures. Longitudinal relaxation is generally thought to be isotropic in articular cartilage [1]. We investigate the conditions needed to observe the anisotropy of the collagen network in the longitudinal relaxation time T_1.

We have computed longitudinal relaxation rates R_1^{intra} of water protons due to intramolecular ^{1}H-^{1}H dipole-dipole coupling from molecular dynamics simulations of a dissolved collagen-like peptide 1QSU [2]. The effects of peptide orientation with respect to the main magnetic field and residual dipolar interaction were included in the analysis. Movements of different spin pairs were assumed to be uncorrelated. Comparisons were made to results from simulations of bulk water.

Overall, the intramolecular dipole-dipole couplings were estimated to be the largest contributor to the proton relaxation. We found that for the water molecules in the first hydration layer of the peptide, R_1^{intra} has a clear minimum when the long axis of the peptide is oriented perpendicular to the main magnetic field. This anisotropy was mostly lost in the second hydration layer. The intermolecular couplings were estimated to have a smaller, and nearly isotropic contributions to the relaxation, comparable to relaxation rates in bulk water.

Since the anisotropy in relaxation rates was only seen for the intramolecular couplings in the first hydration layer of the peptide, we expect that quite severe confinement of water molecules and uniform alignment of their macromolecular environment would be needed to observe the anisotropy in experimentally determined T_1.

[1] N. Hänninen, J. Rautiainen, L. Rieppo, S. Saarakkala and M. J. Nissi, Sci. Rep. 7, 9606 (2017).
[2] R. Z. Kramer, M. G. Venugopal, J. Bella, P. Mayville, B. Brodsky and H. M. Berman, J. Mol. Biol. 301, 1191 (2000).

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