

RESIDUAL DIPOLAR COUPLING CONSTANTS IN THE CONFORMATIONAL ANALYSIS OF CARBOHYDRATES

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NMR spectroscopy of small molecules oriented in liquid crystals is a well-established method for obtaining accurate information about molecular geometry [1]. However, it is only after the introduction of *dilute liquid crystalline media* [2] that residual dipolar couplings (RDCs) could be applied in the structural analysis of biomolecules, including carbohydrates. The very low order imposed on the solute molecules in such media leads to small RDCs of up to several Hz. Providing these can be measured accurately with a similar relative precession to that of dipolar couplings obtained in strong liquid crystal (up to thousands of Hz), small RDCs should yield accurate solution structure of small molecules.

We have developed methods for precise measurement of proton-proton [3a], one-bond [3b] and long-range proton-carbon [3c] RDCs in dilute liquid crystalline media. These methods, which measure coupling constants with a precision of a *few hundreds of a Hz*, were used in determination of the first solution structure of a monosaccharide, methyl β -D-xylopyranoside (**I**) [3c]. We discuss this example and compare our solution structure with a published neutron diffraction structure of **I**.

We have recently extended our methodology for the measurement of small ¹H-¹H RDCs to systems with crowded ¹H spectra. We illustrated these methods using a heparin-derived fully sulphated tetrasaccharide and report on our progress towards the conformational analysis of this flexible molecule using various dipolar and scalar coupling constants.

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