NMR spectroscopy in the characterization of complex glycans

Barbara Mulloy
Glycosciences Laboratory, Imperial College London , UK

NMR spectroscopy is one of the most versatile and powerful physicochemical techniques for structural determinations of complex carbohydrates, providing information on covalent structure, three-dimensional shape, and on interactions with proteins for this class of molecules. Our recent NMR-based studies include the design and verification of neoglycolipid structures for immobilisation of glycans to a surface for microarray analysis, and comparison of the mode of binding of carbohydrate-binding modules (CBMs) of microbial glycoside hydrolases to their glucan substrates. In other studies, the incorporation of lipid-conjugated glycans into micelles allows NMR spectroscopic analysis of the hydrophilic headgroup without any pre-processing or lipid-removal by chemical degradative techniques. A different selection of techniques can be used for the analysis and comparison of highly complex and heterogeneous polysaccharides such as the mammalian glycosaminoglycans, particularly the medically important molecule heparin. Recent events have emphasised the utility of NMR in assuring the identity and purity of heparin samples, from the simplest one-dimensional spectra to complex multi-dimensional diffusion-ordered techniques. Philip A. J. Gorin was one of the pioneers of NMR spectroscopy in structural studies of carbohydrates, beginning in the 1960s and making the most of every advance in the technique (carbon NMR, the introduction of FT-NMR, multidimensional methods etc.) over six decades. The rest of us follow where he led.

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