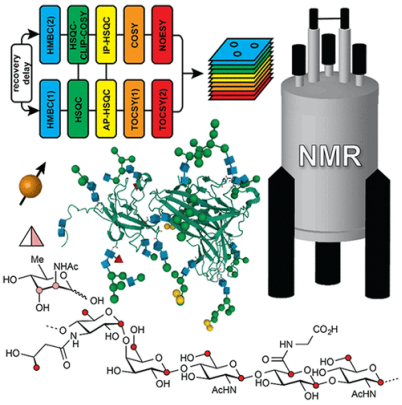


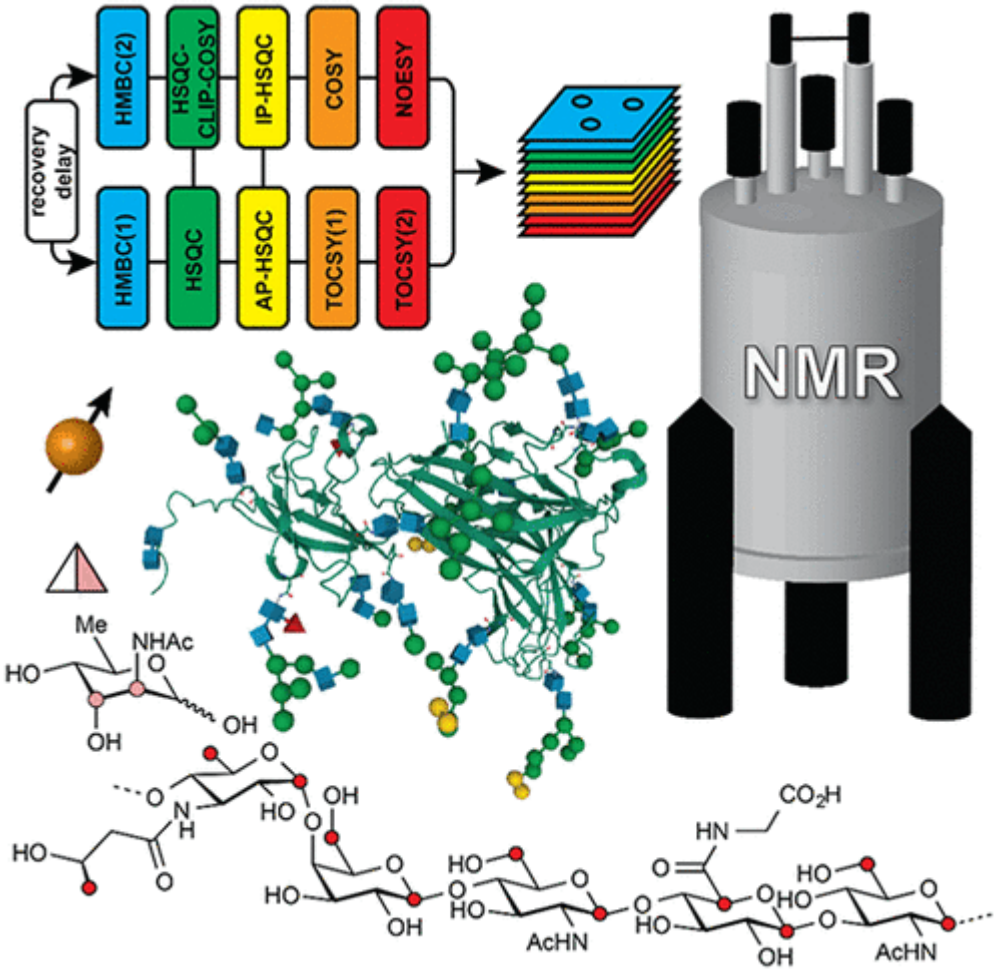
Primary Structure of Glycans by NMR Spectroscopy

Description

Glycans, carbohydrate molecules in the realm of biology, are present as biomedically important glycoconjugates, and a distinctive aspect is that their structures, in many instances, are branched. In determining the primary structure of a glycan, the sugar components, including the absolute configuration and ring form, anomeric configuration, linkage(s), sequence, and substituents, should be elucidated. Solution-state NMR spectroscopy offers a unique opportunity to resolve all these aspects at atomic resolution. During the last two decades, NMR experiments and spectrometer hardware advancements have enabled the unravelling of carbohydrate structures more efficiently. These developments applicable to glycans include :

- NMR experiments that reduce spectral overlap,
- use selective excitations,
- record tilted projections of multidimensional spectra,
- acquire spectra by multiple receivers,
- utilize polarization by fast-pulsing techniques,
- concatenate pulse-sequence modules to acquire several spectra in a single measurement,
- acquire pure shift correlated spectra devoid of scalar couplings,
- employ stable isotope labeling to efficiently obtain homo- and/or heteronuclear correlations,

• rely on dipolar cross-correlated interactions for sequential information.



Refined computer programs for NMR spin simulation and chemical shift prediction aid the structural elucidation of glycans, which are notorious for their limited spectral dispersion. Hardware developments include cryogenically cold probes and dynamic nuclear polarization techniques, resulting in enhanced sensitivity and ultrahigh field NMR spectrometers with a 1H NMR resonance frequency higher than 1 GHz, thus improving the resolution of resonances. Such developments have made and will make it possible to elucidate carbohydrate structure in great detail, thereby forming the basis for understanding how glycans interact with other molecules.

Category

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