

MIRAGE NMR Guidelines

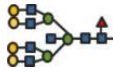
Guidelines for Reporting Nuclear Magnetic Resonance Data on Glycan Structure

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Based on MIRAGE Guidelines ([doi:10.3762/mirage.3](https://doi.org/10.3762/mirage.3))

These guidelines are proposed to comprehensively describe NMR experiments and data obtained for the characterization of glycan composition, glycan conformation and glycan dynamics both for natural and unnatural glycans.

	Description*
1. Sample: Glycan Sample	
Glycan description for defined glycans	Origin: Natural/synthetic/glycoprotein Structural descriptors Glycan sequence, bond regio chemistry (1-2/1-4/1-6) and stereochemistry (α/β) For unnatural glycans describe: reducing-terminal modifications; artificial functional groups; isotopic labelling. Molecular Size (exact mass/average MW) 
Glycan treatment	Natural/synthetic structure Depolymerization: chemical and/or enzymatic
Description of Sample	Concentration Buffer composition Solvent Chemical Shift Reference (e.g. acetone at 2.218 ppm for ^1H and 33.0 ppm for ^{13}C) Stability (temperature and pH requirements)
Quality control	Impurities (natural/chemicals); detection method
2. Spectrometer and Data Processing	
Spectrometer	Magnetic field/cryoprobe y/n
Manufacturer	
Experiments	Indicate: 1D/2D/3D; Name: (^1H , ^1H - ^1H COSY, ^1H - ^1H TOCSY, ^1H - ^1H NOESY, ^1H - ^1H ROESY, ^1H - ^{13}C HSQC, ^1H - ^{13}C HMBC); Specify pulse sequence: (if a pulse sequence is modified report the sequence) Describe specific parameters of the experiments (e.g. number of scans, spectral width, number of increments, mixing time)

Measuring conditions	Temperature
Data processing	Window functions (LB, GB), zero filling, baseline corrections
3. NMR parameters	
Glycan chemical shifts	δ (^1H), δ (^{13}C) list reported y/n
Glycan Js	y/n, J (^1H - ^1H , ^1H - ^{13}C) list reported y/n, J order
Glycan NOEs	y/n, NOE list reported y/n
Glycan relaxation times	y/n, T1, T2 values reported y/n
Glycan RDCs, PCSs, PREs	y/n, RDC (^1H - ^1H , ^1H - ^{13}C) values reported y/n
4. Glycan NMR Data Presentation	
Data presentation	Figures and tables
5. Interpretation and Conclusion from NMR data	
Data interpretation	
Conclusions	

*Only items relevant to NMR experiments need be included in this document which may be cited in manuscripts as a Supplementary Table. Descriptions and references cited here should complement rather than duplicate the content of the Materials and Methods.