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Review Article

NMR Libraries of Natural and Synthetic Monosaccharides

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A B S T R A C T

Nuclear Magnetic Resonance (NMR) spectroscopy is a cornerstone analytical technique for the structural elucidation of monosaccharides, which are the fundamental building blocks of complex carbohydrates. Due to their structural diversity, including variations in stereochemistry, ring forms (furanose and pyranose), and functional group modifications, accurate identification of monosaccharides remains a significant challenge in glycoscience. To address this, NMR libraries of natural and synthetic monosaccharides have been developed, providing reference spectra for a wide range of sugar molecules under standardized conditions. These libraries typically include both 1D (^{1}H, ^{13}C) and 2D (COSY, HSQC, HMBC, TOCSY) NMR data, enabling comprehensive structural comparisons. Such databases are essential tools for rapid identification, quality control in carbohydrate synthesis, and the interpretation of complex biological mixtures, such as plant extracts or glycoproteins. Synthetic monosaccharides, often labeled or derivatized, are especially useful in expanding NMR libraries to include rare or unstable structures not readily found in nature. Moreover, computational tools and software are now integrated with these spectral databases, improving automated peak assignments and structure prediction. These resources facilitate the study of carbohydrate-related biological processes, such as pathogen recognition, cell signaling, and energy metabolism. The development and continuous updating of NMR libraries not only streamline structural analysis but also contribute to standardization efforts in carbohydrate research. As the demand for glycan-based therapeutics and diagnostics grows, the role of comprehensive NMR libraries becomes increasingly vital in supporting both fundamental research and applied sciences.

Keywords- Glycoscience, carbohydrates, monosaccharides, NMR spectroscopy, spectral library.

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INTRODUCTION

The structural elucidation of natural compounds present in minute quantities became feasible only after the advent of Nuclear Magnetic Resonance (NMR) spectroscopy, a non-invasive and highly informative tool for structure determination of both natural products and synthetic compounds[1]. The introduction of Fourier Transform (FT) techniques marked a significant advancement in NMR, drastically reducing the amount of sample required for analysis and improving sensitivity and resolution. NMR has since become indispensable in studying bioactive molecules from both synthetic and natural sources[2]. In the structural characterization of such compounds, a variety of NMR experiments are routinely employed. Initially limited to one-dimensional ^{1}H NMR, the field has expanded to include ^{13}C NMR and sophisticated two-dimensional techniques such as ^{1}H-^{1}H COSY, NOESY, HSQC, and HMBC, along with multidimensional experiments. These advanced methods enable unambiguous interpretation of complex, overlapping signals, particularly in oligosaccharides and other structurally rich molecules. NMR spectral data provide detailed insights into molecular structures, functional groups, conformational dynamics, and stereochemistry. The development of pulse field gradient (PFG) techniques has further enhanced the scope and precision of NMR, making it a powerful approach for structural, conformational, and stereochemical analysis across a wide range of chemical entities[3].

During the course of investigation, it was observed that the field of carbohydrate chemistry, now broadly encompassed under the domain of glycobiology[4], is among the most challenging areas in natural product research. Carbohydrates and carbohydrate-containing moieties such as glycosides, glycoproteins, oligosaccharides and glycoconjugates have

emerged as a vital class of biomolecules due to their diverse biological functions[5]. Understanding the stereochemical architecture of these compounds is essential, as their biological activity is often highly structure-dependent. To achieve this, detailed conformational and configurational analyses must be conducted, primarily through specially designed Nuclear Magnetic Resonance (NMR) experiments. These NMR-based techniques are crucial for elucidating the three-dimensional structures and stereochemistry of complex carbohydrate molecules with high precision.

Carbohydrates play a crucial role in numerous biological recognition processes[6], disease development, and various applications in the food and pharmaceutical industries. Despite their importance, the biological functions and mechanisms of carbohydrates remain poorly understood. Among all classes of biomolecules, carbohydrates are arguably the least explored, primarily due to their synthetic complexity, structural heterogeneity, and limited natural availability[7]. Their synthesis and manipulation present significant challenges, and subtle differences in stereochemistry and inter-residue linkages contribute to their structural diversity[8]. Notably, the information-carrying capacity of carbohydrates surpasses that of proteins, largely due to their branched architectures. It has been proposed that carbohydrates carry a "hidden code" essential for biological recognition. The addition of carbohydrate moieties to organic compounds often enhances their water solubility, bioavailability, and reduces toxicity, making them attractive candidates for therapeutic development[9]. Consequently, the study of carbohydrate-mediated bioactive compounds is increasingly recognized as critical for biomedical research. To develop carbohydrate-based therapeutics, it is essential to understand the behavior and mechanisms of carbohydrate functions at the molecular level. Recent advancements in glycochemistry have begun to overcome previous limitations, particularly in the large-scale synthesis of complex carbohydrates. However, elucidating the structures of complex oligosaccharides remains a formidable task. Nuclear Magnetic Resonance (NMR) spectroscopy stands out as the most powerful and widely used technique for the identification and characterization of known and novel oligosaccharides and glycoconjugates[10]. Given the complexity and significance of these molecules, it is both timely and necessary to review the latest NMR techniques and their applications in carbohydrate research.

NMR library

To date, researchers lack a universally accepted and systematic method that enables stepwise structural assignment of carbohydrates with high precision. Among the available analytical techniques, Nuclear Magnetic Resonance (NMR) spectroscopy remains the only non-invasive, successful, and powerful method for the direct structural elucidation of these biologically significant molecules. However, one major limitation of NMR in carbohydrate analysis is the narrow chemical shift range exhibited by the protons and carbons in various monosaccharides, which often leads to overlapping signals and ambiguity in interpretation. Although significant progress has been made with the development of advanced two-dimensional and three-dimensional NMR experiments to address the structural complexity of oligosaccharides, a comprehensive and detailed spectral library of chemical shifts and related data specific to monosaccharide units within oligosaccharide moieties is still lacking. The absence of such a resource continues to hinder accurate and efficient structural assignments, emphasizing the need for a curated NMR database to support research in glycochemistry and glycobiology.

The ^{1}H and ^{13}C NMR data which is available in the literature and procured from synthetic compounds and natural products has been compiled in the following tables.

Table 1: ^{1}H chemical shifts and coupling constants of D-aldohexoses[11]

D-Hexopyranoses	H-1	H-2	H-3	H-4	H-5	H-6	H-6'
α-glucose	5.09 (J=3.6)	3.41(J=9.5)	3.61(J=9.5)	3.29(J=9.5)	3.72	3.72(J=2.8)	3.63(J=5.7, 12.8)
β-glucose	4.51(J=7.8)	3.13(J=9.5)	3.37(J=9.5)	3.30(J=9.5)	3.35	3.75(J=2.8)	3.60(J=5.7, 12.8)
α-galactose	5.16(J=3.8)	3.72(J=10.0)	3.77(J=3.8)	3.90(J=1.0)	4.00	3.70(J=6.4)	3.62(J=6.4)
β-galactose	4.48(J=8.0)	3.41(J=10.0)	3.56(J=3.8)	3.84(J=1.0)	3.61	3.70(J=3.8)	3.62(J=7.8)
α-mannose	5.05(J=1.8)	3.79(J=3.8)	3.72(J=10.0)	3.52(J=9.8)	3.70	3.74(J=2.8)	3.63(J=6.8, 12.2)
β-mannose	4.77(J=1.5)	3.85(J=3.8)	3.53(J=10.0)	3.44(J=9.8)	3.25	3.74(J=2.8)	3.60(J=6.8, 12.2)
β-allose	4.76(J=8.5)	3.30(J=3.3)	4.05(J=3.2)	3.51(J=9.5)	3.66	3.76(J=2.4)	3.57(J=6.0, 12.8)
β-gulose	4.76(J=8.3)	3.52(J=3.6)	3.95(J=3.6)	3.70(J=0.8)	3.92	3.62(J=6.0)	3.58(J=6.0)

Table 2: ^{1}H chemical shifts and coupling constants of D-aldopentoses[12-14]

D- Pentopyranoses	H-1	H-2	H-3	H-4	H-5a	H-5e
β-xylose	4.47(J=7.8)	3.14(J=9.2)	3.33(J=9.0)	3.51	3.82(J=5.6)	3.22(J=10.5, 11.4)
α-xylose	5.09(J=3.6)	3.42(J=9.0)	3.48(J=9.0)	3.52	3.58(J=7.5)	3.57(J=7.5)
β-arabinose	5.12(J=3.6)	3.70(J=9.3)	3.77(J=9.8)	3.89	3.54(J=2.5)	3.91(J=1.7, 13.5)
α-arabinose	4.40(J=7.8)	3.40(J=9.8)	3.55(J=3.6)	3.83	3.78(J=1.8)	3.57(J=1.3, 13.0)
β-ribose	4.75(J=2.1)	3.71(J=3.0)	3.83(J=3.0)	3.77	3.82(J=5.3)	3.50(J=2.6, 12.4)
α-ribose	4.81(J=6.5)	3.41(J=3.3)	3.98(J=3.2)	3.77	3.72(J=4.4)	3.57(J=8.8, 11.4)
β-lyxose	4.89(J=4.9)	3.69(J=3.6)	3.78(J=7.8)	3.73	3.71(J=3.8)	3.58(J=7.2, 12.1)

α-lyxose	4.74(J=1.1)	3.81(J=2.7)	3.53(J=8.5)		3.84(J=5.1)	3.15(J=9.1, 11.7)

Table 3: [1]H chemical shifts and coupling constants of methyl-D-pentosides[15-17]

D-pentopyranosides	H-1	H-2	H-3	H-4	H-5e	H-5a	OMe
α-arabinose	4.16(J=8.0)	3.43(J=10.0)	3.57(J=3.9)	3.85	3.82(J=2.8, 13.8)	3.57(J=1.0)	3.44
β-arabinose	4.72(J=2.8)	3.74(J=10.0)	3.72(J=3.0)	3.89	3.55(J=2.3, 13.0)	3.77(J=1.0)	3.30
α-lyxose	4.58(J=3.2)	3.77(J=3.8)	3.68(J=4.0)	3.76	3.69(J=4.8, 12.0)	3.42(J=9.0)	3.32
β-lyxose	4.51(J=2.2)	3.14(J=3.8)	3.60(J=7.5)	3.75	3.89(J=4.0, 12.5)	3.23(J=7.5)	3.37
α-ribose	4.51(J=3.0)	3.70(J=3.2)	3.86(J=3.2)	3.72	3.47	3.68	3.35
β-ribose	4.52(J=5.1)	3.51(J=3.4)	3.91(J=3.4)	3.79	3.74(J=3.5, 12.5)	3.61(J=7.0)	3.37
α-xylose	4.67(J=3.4)	3.44(J=10.0)	3.53	3.47	3.59(J=5.0, 11.0)	3.39(J=11.0)	3.30
β-xylose	4.21(J=7.9)	3.14(J=9.5)	3.33(J=9.5)	3.51	3.88(J=5.5, 12.3)	3.21(J=11.0)	3.44

Table 4: [13]C chemical shifts of D-Hexopyranoses[18]

D-Hexopyranoses	C-1	C-2	C-3	C-4	C-5	C-6
α-Allose	93.7	67.9	72.0	66.9	67.7	61.6
β-Allose	94.3	72.2	72.0	67.7	74.4	62.1
α-Altrose	94.7	71.2	71.1	66.0	72.0	61.6
β-Altrose	92.6	71.6	71.3	65.2	75.0	62.5
α-Galactose	93.2	69.4	70.2	70.3	71.4	62.2
β-Glactose	97.3	72.9	73.8	69.7	76.0	62.0
α-Glucose	92.9	72.5	73.8	70.6	72.3	61.6
β-Glucose	96.7	75.1	76.7	70.6	76.8	61.7
α-Gulose	93.6	65.5	71.6	70.2	67.2	61.7
β-Gulose	94.6	69.9	72.0	70.2	74.6	61.8
α-Idose	93.2	73.6	72.7	72.6	73.6	59.4
β-Idose	93.9	71.1	68.8	70.6	75.6	62.1
α-Mannose	95.0	71.7	71.3	68.0	73.4	62.1
β-Mannose	94.6	72.3	74.1	67.8	77.2	62.1
α-Talose	95.5	71.7	70.6	66.0	72.0	62.4
β-Talose	95.0	72.5	69.6	69.4	76.5	62.2

Table 5: [13]C chemical shifts of D-Pentopyranoses[18]

D-Pentopyranoses	C-1	C-2	C-3	C-4	C-5
α-Arabinose	97.6	72.9	73.5	69.6	67.2
β-Arabinose	93.4	69.5	69.5	69.5	63.4
α-Lyxose	94.9	71.0	71.4	68.4	63.9
β-Lyxose	95.0	70.9	73.5	67.4	65.0
α-Ribose	94.3	70.8	70.1	68.1	63.8
β-Ribose	94.7	71.8	69.7	68.2	63.8
α-Xylose	93.1	72.5	73.9	70.4	61.9
β-Xylose	97.5	75.1	76.8	70.2	66.1

Table 6: [13]C chemical shifts of methyl aldosides[18]

D-Hexopyranosides	C-1	C-2	C-3	C-4	C-5	C-6	OMe
α-Allose	100.0	68.3	72.1	68.0	67.3	61.7	56.3
β-Allose	101.9	72.2	71.4	68.0	74.8	62.2	58.0
α-Altrose	101.1	70.0	70.0	64.8	70.0	61.3	55.4
β-Altrose	100.4	70.7	70.2	65.6	75.6	61.7	57.7
α-Galactose	100.1	69.2	70.5	70.2	71.6	62.2	56.0
β-Galactose	104.5	71.7	73.8	69.7	76.0	62.0	58.1
α-Glucose	100.0	72.7	74.1	70.6	72.5	61.6	55.9
β-Glucose	104.0	74.1	76.8	70.6	76.8	61.8	58.1
α-Gulose	100.4	65.5	71.4	70.4	67.3	62.0	56.3
β-Gulose	102.6	69.1	72.3	70.5	74.9	62.1	58.1
α-Idose	101.5	70.9	71.8	70.3	70.8	60.2	55.8
α-Mannose	101.9	71.2	71.8	68.0	73.7	62.1	55.9
β-Mannose	101.3	70.6	73.3	67.1	76.6	61.4	56.9
α-Talose	102.2	70.7	66.2	70.3	72.1	62.3	55.6

Table 7: [13]C chemical shifts of methyl aldosides[19]

D-Pentopyranosides	C-1	C-2	C-3	C-4	C-5	OMe
α-Arabinose	107.0	73.9	75.6	71.5	69.3	60.0
β-Arabinose	103.0	72.1	70.1	71.4	65.7	58.1
α-Lyxose	102.0	70.4	71.6	67.4	63.3	55.9
α –Ribose	100.4	69.2	70.4	67.4	60.8	56.7
β –Ribose	103.1	71.0	68.6	68.6	63.9	57.0

α –Xylose	100.6	72.3	74.3	70.4	62.0	56.0
β –Xylose	105.1	74.0	76.9	70.4	66.3	58.3

CONCLUSION

Nuclear Magnetic Resonance (NMR) spectroscopy remains an indispensable tool for the structural elucidation of natural and synthetic monosaccharides. Despite the structural complexity and limited chemical shift dispersion in carbohydrate spectra, NMR offers unparalleled insights into the stereochemistry, conformation, and connectivity of sugar units. While advanced multi-dimensional NMR techniques have significantly enhanced our ability to analyze these molecules, the absence of a comprehensive and standardized NMR spectral library for monosaccharides continues to pose a challenge. Developing well-curated libraries containing detailed chemical shift data and associated spectral patterns of various monosaccharide derivatives, both natural and synthetic, will greatly facilitate accurate structure assignments, promote consistency in carbohydrate research, and accelerate progress in glycobiology, drug development, and related disciplines. As the demand for carbohydrate-based therapeutics and diagnostics continues to grow, the creation and use of such NMR libraries will be vital for advancing both fundamental and applied glycoscience.

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Conflicts of interest

The author declares no conflict of interest.

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