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Mini Review

Spectroscopy using Nuclear Magnetic Resonance Cardiovascular Disease Detection and Characterization Using Nuclear Magnetic Resonance Spectroscopy

Shreya David*

lnstitut de Medecine Legale, Strasbourg, France

*Corresponding Author's E-mail: davidshreya0000@yahoo.com

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Abstract

A spectroscopic method for observing the local magnetic fields around atomic nuclei is nuclear magnetic resonance spectroscopy, sometimes referred to as magnetic resonance spectroscopy (MRS) or NMR spectroscopy. The primary subject of this paper is cardiovascular disease, which has atherosclerosis as its underlying cause (Alic AS et al., 2016). It also discusses how nuclear magnetic resonance (NMR) spectroscopy, an analytical method, is being used to better comprehend this subject. The sample is put in a magnetic field, and the nuclear magnetic resonance (NMR) signal is generated by radio waves excitation of the sample's nuclei, which is detected by sensitive radio receivers. A molecule's atom's intra-molecular magnetic field can alter the resonance frequency, providing information about a molecule's electronic structure and its many functional groups. In contemporary organic chemistry, NMR spectroscopy is the only reliable way to identify monomolecular organic molecules since the fields are distinctive or highly specific to particular compounds. The most potent analytical method accessible to biology is nuclear magnetic resonance (NMR) spectroscopy. This review is intended for readers who have little to no experience collecting or analysing NMR spectra and serves as an introduction to the possibilities of this approach (Kelley DR et al., 2010). Instead of imaging applications, we concentrate on spectroscopic ones of the magnetic resonance effect and show how many facets of the NMR phenomenon make it a flexible instrument with which to tackle a variety of biological issues. We go over how 1H NMR spectroscopy is used in mixture analysis and metabolomics, how 13C NMR spectroscopy is used to track isotopomers and calculate the flux through metabolic pathways (referred to as "fluxomics"), and how 31P NMR spectroscopy is used to monitor ATP synthesis and intracellular pH homeostasis in vivo. Additional examples show how NMR spectroscopy can be used to determine macromolecular structures by measuring the bonds and distances that separate individual atoms as well as how it can be used to measure the diffusion and tumbling rates of individual metabolites in order to probe the physical environment of a cell. We conclude by highlighting some of the major obstacles still facing NMR spectroscopy while also pointing out how recent developments, such as stronger magnet fields, cryogenic cooling, microprobes, and hyperpolarization, are providing new opportunities for the field's biological NMR spectroscopists of today (Salmela L et al., 2011).

Keywords: Stable isotope tracers, Stable isotope resolved metabolomics, In vivo NMR, Hyperpolarization, Metabolic network and flux

INTRODUCTION

A common method in chemistry known as nuclear magnetic resonance spectroscopy gives precise details on the composition and distribution of molecules in complicated mixtures like biological fluids or tissue or cell extracts. There are elaborate processes for preparing and analysing common fluids and tissue for such experiments. Magnetic resonance

imaging (MRI) investigations can be supplemented by NMR spectroscopy on solid state materials. These components are classified as either high (often lipid or lipoprotein containing) or low molecular weight entities; this division is employed for the purposes of this research (Chen D et al., 2014). NMR spectroscopy may be used to monitor particular components of complicated matrices. End of 1945 saw the first experimental discovery of nuclear magnetic resonance (NMR), almost simultaneously with work groups led by Edward Purcell of Harvard University and Felix Bloch of Stanford University. The initial report on the first NMR spectra appeared in the same issue of Physical Review in January 1946. The 1952 Nobel Prize in Physics was shared by Bloch and Purcell for their work on nuclear magnetic resonance spectroscopy (Chen Q et al., 2017).

An NMR spectrometer is essentially a microscope and magnetic tomographic device. Initially, NMR spectroscopy was developed to identify chemical properties of small compounds, but fast-growing overall technological developments have made it an incredible tool for analyzing a wide variety of materials, especially proteins (Castelli WP 1988). For organic chemists, nuclear magnetic resonance (NMR) spectroscopy is a vital analytical technique. The NMR has substantially enhanced the research being done in the organic lab. It can provide information about the molecule's structure as well as the sample's composition and purity. One of the NMR techniques that organic chemists utilise the most frequently is proton (1H) NMR. It is possible to determine the structure of a molecule by observing how the protons in it respond to the surrounding chemical environment (Solimene MC 2010).

NMR Spectroscopy Principle

1. The polarisation of magnetic nuclear spins in a magnetic field B0 that is being applied.
2. The alteration of this nuclear spin alignment caused by a radio-frequency (RF) pulse, a weakly oscillating magnetic field.
3. Detection and analysis of the electromagnetic waves that this disruption causes the sample's nucleus to generate.

For tiny compounds, NMR spectra are distinctive, sharp, analytically manageable, and frequently quite predictable. Different functional groups can be easily distinguished from one another, and signals can still be distinguished between identical functional groups with different adjacent substituents (Kanwar G et al., 2014). NMR has essentially taken the role of conventional wet chemistry tests for identification like colour reagents or usual chromatography. The requirement of a relatively significant dose of a purified drug, ranging from 2 to 50 mg, notwithstanding the possibility of recovery through a workup, is a drawback (Bonithon-Kopp C et al., 1990). The sample should ideally be dissolved in a solvent since solids cannot be analysed by NMR without a special magic angle spinning equipment, which may result in less accurately resolved spectra. NMR produces only an averaged spectrum since its timeframe is quite long, making it unsuitable for viewing rapid processes (Hjortland MC et al., 1976).

Applications of NMR spectroscopy

NMR has developed significantly over the past few decades, making it a particularly potent tool for metabolic research. NMR has a number of unrivalled advantages for metabolic studies despite its limitations in sensitivity compared to mass spectrometric methods, most notably the rigour and versatility in structure elucidation, isotope-filtered selection of molecules, and analysis of positional isotopomer distributions in complex mixtures afforded by multinuclear and multidimensional experiments. NMR is also capable of spatially selective in vivo imaging and dynamical metabolic studies in living organisms' tissues. NMR is a tool of choice for examining the dynamics and compartmentation of metabolic pathways and networks, for which our current understanding is woefully inadequate, in combination with the use of stable isotope tracers. With the use of stable isotope-resolved metabolomics (SIRM) analysis, we analyse metabolites and their isotopomer distributions using a variety of direct and isotope-edited 1D and 2D NMR approaches. In order to enable reliable and repeatable NMR-based metabolomics analysis, we additionally emphasise the significance of sample preparation techniques as quick cryoquenching, effective extraction, and chemo selective derivatization. We also show how NMR has been used to achieve systematic and innovative metabolic insights in diverse biological systems, including human subjects, through the use of in vitro, ex vivo, and in vivo metabolic research based on stable isotope tracer technology. As shown in a case study, the route and network information produced by NMR and MS-based tracing of isotopically enriched substrates will be crucial for guiding functional analysis of other omics data to comprehend the control of biochemical systems. NMR should be given more power in systems biochemical research in the future thanks to advancements in NMR reagents and technology that improve detection sensitivity and resolution (Chaudhuri A et al., 2015).

An analytical chemistry method known as nuclear magnetic resonance (NMR) spectroscopy is used in quality control and research to ascertain a sample's composition and purity as well as its molecular structure. For instance, mixtures containing known substances may be quantitatively analysed using NMR. NMR may be used to directly deduce the fundamental structure of unknown substances or to compare against spectrum libraries. Once the fundamental structure has been established, NMR may be used to ascertain the molecule conformation in solution and to investigate molecular-level physical phenomena such conformational exchange, phase shifts, solubility, and diffusion. There are several NMR methods that may be

used to get the required results. Here, the fundamentals of NMR are explained (Chmielecki J et al., 2014). Two distinct sizes of rHDL were employed, and two different tertiary structures for ApoAI were revealed by two-dimensional (2D) NMR spectra of isotope (15N) enriched protein (which offer superior spectral or chemical shift resolution). The NMR data was consistent with the presence of only one kind of ApoAI molecule, showing symmetry in the complex. Therefore, whether ApoAI forms an intramolecular or intermolecular bundle, the double belts of the -helix structure should be the same (Clarke J et al., 2009).

Since Bloch and Purcell first identified the nuclear magnetic resonance phenomenon in solids and liquids in 1945, NMR spectroscopy has established itself as a potent and versatile tool for the determination of macromolecule structure and dynamics for structural biologists, followed more recently by metabolite profiling for the metabolomics field. Due to its element-selective detection, the sensitivity of nuclear spin characteristics to the intra- and intermolecular environment, as well as the reliable and quantitative nature of NMR measurement, NMR has a significant value for molecular structural and quantitative investigation. NMR has been a popular choice for metabolite profiling initiatives [3-6] because of these benefits, and it makes a great teammate for mass spectrometry (MS)-based metabolite profiling. For instance, difficult-to-obtain structural data that NMR analysis offers include functional groups, covalent connections, and non-covalent interactions such as stereochemistry. But when NMR-invisible components (^{32}S, ^{16}O) are present, high-resolution MS offers molecular formula information, which is a crucial parameter for structural NMR research (Onaga LA 2014).

Since the discovery of metabolomics, MS has been increasingly popular in steady-state metabolite profiling because to its higher sensitivity, resolution (including chromatography-based MS and ultra-high resolution MS), and relative simplicity of data interpretation. Only 30% of the research including metabolomics papers in PubMed use NMR analysis. NMR methodologies, on the other hand, offer some special advantages for the next-generation metabolomics applications involving stable isotope tracers for reliable reconstruction of metabolic pathways and networks, including detailed positional isotopomer analysis for enriched metabolites, de novo structure determination of unknown metabolites (both un enriched and enriched), without the need for standards, and in situ analysis of pathway dynamics from cells to whole organisms (Anger F et al., 1977).

CONCLUSION

NMR spectroscopy's intrinsic precision and reliability make it possible to identify minute variations in lipoprotein and metabolic profiles. Analysis of these data can reveal underlying population-level trends, such as those linked to sex, age, and the onset and progression of cardiovascular disease. There is a chance that a path to lessening the burden of this global issue may become obvious as more knowledge is gathered and uses of NMR spectroscopy in cardiovascular disease grow.

REFERENCES

1. Alic AS, Blanquer I, Dopazo J and Ruzafa D (2016). Objective review of de novo stand-alone error correction methods for NGS data. WIREs Comput Mol Sci. 6: 111-146.
2. Kelley DR, Schatz MC, Salzberg SL (2010). Quake: Quality-aware detection and correction of sequencing errors. Genome Biol. 11: R116.
3. Salmela L, Schroder J (2011). Correcting errors in short reads by multiple alignments. Bioinformatics. 27: 1455-1461.
4. Chen D, Hwu WM, Heo Y, Ma J, Wu XL (2014). BLESS: Bloom filter-based error correction solution for high-throughput sequencing reads. Bioinformatics. 30: 1354-1362.
5. Chen Q, Jiang P, Li W, Li J, Wong L, et al (2017). MapReduce for accurate error correction of next generation sequencing data. Bioinformatics. 33: 3844-3851.
6. Castelli WP (1988). Cardiovascular disease in women. Am J Obstet Gynecol. 158:1553-1560.
7. Solimene MC (2010). Coronary heart disease in women: a challenge for the 21st century. Clinics 65:99-106.
8. Kanwar G, Kirad S, Lokesh Chawala L, Jain N (2014). A comparative study of serum lipid profile between premenopausal and postmenopausal women in Kota, Rajasthan, India. IJRANSS 2:61-66.
9. Bonithon-Kopp C, Scarabin P-Y, Darne B, Malmejac A, Guize L (1990). Menopause-related changes in lipoproteins and some other cardiovascular risk factors. Int J Epidemiol.19: 42-48.
10. Hjortland MC, McNamara PM, Kannel WB (1976). Some atherogenic concomitants of menopause: the Framingham study. Am J Epidemiol. 103: 304-311.
11. Chaudhuri A, Manjushree R, Kumar S, Somenath H, Ghosh S (2015). To Study Correlation of Body Fat and Blood Lipids with Autonomic Nervous System Activity in Postmenopausal Indian Women. J Basic Clin Reprod Sc. 4: 59-65
12. Chmielecki J, Meyerson M (2014). DNA sequencing of cancer: what have we learned? Annu Rev Med. 65: 63-79.
13. Clarke J, Wu HC, Jayasinghe L, Patel A, Reid S, et al (2009). Continuous base identification for single-molecule nanopore DNA sequencing. Nat Nanotechnol. 4: 265-270.
14. Onaga LA (2014). Ray Wu as Fifth Business: Demonstrating Collective Memory in the History of DNA Sequencing. Stud His Philos Biol Biomed Sci. 46: 1-14.
15. Anger F, Nicklen S, Coulson AR (1977). DNA sequencing with chain-terminating inhibitors. Proc Natl Acad Sci USA. 74: 5463-5477.