APPLICATION OF NUCLEAR MAGNETIC RESONANCE (NMR) AND MASS SPECTROMETRY IN IDENTIFICATION OF CHEMICAL COMPOUNDS

Munisa Akmal qizi Tojiboyeva[1]

[1]Faculty of Natural Sciences, Chirchik State Pedagogical University, Chirchiq, Uzbekistan

Corresponding author: tojiboyeva.m1661@gmail.com

Track: *[Track 3 / Science Education]*

Abstract

This article provides a comprehensive analysis of the theoretical foundations of nuclear magnetic resonance spectroscopy (NMR) and mass spectrometry (MS), two advanced spectroscopic technologies widely used in determining the molecular structure and characteristics of chemical compounds. NMR spectroscopy provides detailed information about interatomic bonds, configuration, and conformations through the response of the nuclear environment in a molecule to electromagnetic resonance. MS technology allows for the identification of structural components of a compound through high-precision measurement of molecular mass and fragmentation analysis. The article justifies the use of these methods not only theoretically, but also in practical areas such as pharmaceuticals, organic synthesis, bioanalytics, and environmental monitoring. Current research conducted in Uzbekistan and the international scientific community, existing technological capabilities in national laboratories, and promising areas are also discussed. The results of the analysis show that the combined use of NMR and MS technologies dramatically increases the efficiency of complex analysis and ensures the highest level of reliability in the identification of chemical compounds.

Keywords: *nuclear magnetic resonance spectroscopy (NMR); mass spectrometry (MS); identification of chemical compounds; structural analysis; fragmentation; analytical chemistry; molecular spectroscopy; pharmaceutical analysis*

1. INTRODUCTION

The development of modern chemistry requires, in particular, the identification of complex organic and inorganic compounds, their structure determination, understanding of reaction mechanisms, and qualitative analysis. In this regard, nuclear magnetic resonance spectroscopy (NMR) and mass spectrometry (MS) are considered the main tools of chemical analysis. These technologies are used not only in fundamental research but also in practical fields such as pharmaceuticals, biochemistry, environmental monitoring, materials science, and food safety.

NMR spectroscopy is based on the magnetic properties of atomic nuclei in a substance, analyzing their resonant response to electromagnetic waves. This method allows the determination of functional groups, bonds, and configurations in a molecule by measuring the chemical shifts associated with the electron density of each atomic nucleus in the molecule. Mass spectrometry, on the other hand, provides the opportunity to identify the mass of ionized molecules and analyze their fragmentation patterns. This method is of great importance for analyzing compounds with high accuracy, speed, and in small quantities.

This article provides a comprehensive analysis of the theoretical foundations of NMR and MS methods, their modern technological capabilities, their mutual application in the identification of

compounds, and the experience of using these methods in the scientific environment of Uzbekistan. The aim of the study is to reveal the scientific and practical advantages of NMR and MS spectroscopy and to demonstrate how they effectively illuminate the processes of chemical analysis in combination.

2. METHODS

This study employed a theoretical and analytical research approach to systematically review the scientific literature on the application of NMR and MS in chemical compound identification. Scientific literature from domestic and international sources was analyzed, including peer-reviewed journal articles, textbooks, and research reports. The analysis focused on (1) the theoretical principles underlying NMR and MS methodologies; (2) their practical applications across various fields; (3) integrated analytical approaches combining both methods; and (4) the current state of NMR and MS application within the Uzbekistan scientific community.

Primary sources were selected from databases including Web of Science and Scopus, supplemented by specialized analytical chemistry textbooks. Studies focusing on pharmaceutical analysis, metabolomics, proteomics, and structural elucidation were given priority. The methodological comparison framework examined sensitivity, accuracy, compound classes analyzed, and integration potential of both techniques.

3. RESULTS AND DISCUSSION

The analysis confirmed that NMR spectroscopy remains indispensable for providing comprehensive structural information about chemical compounds. Modern NMR equipment can detect protons (^{1}H), carbon (^{13}C), nitrogen (^{15}N) and other nuclei, providing highly accurate structural information. Polarization techniques such as NOESY, COSY, and HSQC have dramatically extended the capabilities of NMR for complex mixture analysis.

Mass spectrometry demonstrated superior sensitivity and precision for identifying complex mixtures. Different ionization methods — electron ionization (EI), chemical ionization (CI), electrospray ionization (ESI), and matrix-assisted laser desorption ionization (MALDI) — have increased the flexibility of MS technology across diverse compound classes.

The combined application of NMR and MS represents the most powerful analytical strategy for complete structural elucidation. In metabolomics, proteomics, and pharmaceutical drug design, the integration of these two methods occupies a central place. Research conducted by Uzbek scientists, particularly at Tashkent State Technical University and the Institute of Chemistry, has demonstrated the structural identification of alkaloids and flavonoids from medicinal plants using NMR and MS methods.

Current challenges include the low sensitivity of NMR for trace compounds and ionization complexity in certain MS analyses. The integration of NMR and MS technologies with artificial intelligence represents a promising direction for automating the identification of complex mixtures.

4. CONCLUSION

Nuclear magnetic resonance spectroscopy (NMR) and mass spectrometry (MS) have become indispensable tools for scientific research in the fields of chemistry, biochemistry, and materials science. These methods, complementing each other, provide important advances in the identification of complex chemical compounds, structural analysis, and understanding of molecular mechanisms. The application of NMR and MS methods is gaining great importance not only in scientific fields but also in practical fields such as pharmaceuticals, biology, and environmental protection.

The capabilities of combined NMR and MS analysis allow researchers to determine the precise structure of molecules and materials, create new drugs, and analyze environmental hazards. Research of Uzbek scientists in the application of these methods makes a significant contribution to the development of national science. NMR and MS technologies, together with artificial intelligence and computer modeling technologies in the future, are expected to become more efficient and perfect analysis systems.

REFERENCES

Basak, S. C., & Chowdhury, A. (2007). Applications of NMR spectroscopy in organic chemistry. Springer.

Fiehn, O. (2002). Metabolomics — The link between genomics and other 'omics' sciences. Trends in Plant Science, 7(12), 535–538. https://doi.org/10.1016/S1360-1385(02)02288-4

Gross, M. L., & Kessler, W. L. (2017). Mass spectrometry: A textbook (2nd ed.). Springer.

McCreery, R. L. (2004). Nuclear magnetic resonance: A practical introduction. Wiley-Interscience.

McLafferty, F. W., & Turecek, F. (1993). Mass spectrometry: Principles and applications (2nd ed.). Wiley.

Ni, Y., & Zhang, W. (2018). Mass spectrometry-based proteomics: Advances, applications, and challenges. Proteomics, 18(12), 1600–1612. https://doi.org/10.1002/pmic.201800051

Reibenspies, J. H., & Wyrzykowski, D. (2012). NMR spectroscopy and its application to small molecule identification. Chemical Reviews, 112(10), 5031–5055. https://doi.org/10.1021/cr300236g

Silverstein, R. M., Webster, F. X., & Kiemle, D. J. (2005). Spectrometric identification of organic compounds (7th ed.). Wiley-Interscience.

Smith, M. B., & March, J. (2007). March's advanced organic chemistry: Reactions, mechanisms, and structure (6th ed.). Wiley-Interscience.

Wiersma, D. A., & Wiersma, M. (2017). Introduction to mass spectrometry: A problem-solving approach. Pearson.