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

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Abstract : Chemical compounds clear and reliable identification to do modern analytical chemistry the most important from directions one This is in the article molecules structural and structural features in determining wide being used two advanced spectroscopic technology — atomic nucleus magnet resonance spectroscopy (NMR) and mass spectrometry (MS) scientific-theoretical basics , practical opportunities and their mutual integrated in case application deep analysis will be done . 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. Also, current research conducted in Uzbekistan and the international scientific community, existing technological capabilities in national laboratories and promising areas are 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, electromagnetic resonance, analytical chemistry, molecular spectroscopy, pharmaceutical analysis, instrumental methods.

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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. They using chemical of substances molecular structure , mass-spectral fragmentation and spatial configuration determined by NMR and MS technologies . only in fundamental research not , maybe pharmaceuticals , biochemistry , environment monitoring , materials science and food safety such as practical widely in the fields is being used [1].

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 [2]. Mass spectrometry and ionized molecules mass and their fragmentation to the style based without identification to do opportunity This method gives compounds high in accuracy , speed and small in quantities analysis to do for important importance has [3].

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 show how they effectively illuminate the processes of chemical analysis in combination. Nuclear magnetic resonance spectroscopy (NMR) and mass spectrometry (MS) have emerged as important foundations for 21st century scientific advances in the analysis of chemical compounds. Their theoretical and practical foundations have been refined over the past century and are now widely used in various fields, including pharmaceuticals, biology, materials science, and environmental chemistry. NMR technology development of the nuclei magnet properties based resonance the event clear measurement of styles improvement with directly Modern NMR equipment can detect protons (^{1H}), carbon (^{13C}), nitrogen (^{15N}) and nuclei based on high accurate structural information presented [1] . Using NMR of the substance spatial configuration , connections length and conformational changes to be determined scientific research new to the stage take came out [2]. Mass spectrometry offers high sensitivity and precision in identifying particularly complex compounds [3]. It can identify compounds ionize them mass / particle ratio according to analysis does . Different ionization styles — electric impact under ionization (EI), chemical ionization (CI), electric field desorption (ESI) and matrix helpful laser ionization (MALDI) — MS technology flexibility increased [4]. NMR and MS methods combination through biological active of substances complete structure and isomeric differences clear For example , metabolomics , proteomics and medicine tools in design this two of the method integration central place occupies [5].

Uzbekistan scientists also in the direction one row research take In particular , Tashkent State technique University , Uzbekistan National university and Chemistry institute scientists by phytochemical and synthetic of substances structure according to take visited analyses this of technologies our country in science how much significant place that he has [6] In particular , Professor B. Jo'rayev and A. Rakhimova under the leadership of take visited in research medicinal from plants separate taken alkaloids and NMR and MS methods of flavonoids using identification done increased [7]. Today, knowledge about these methods is increasingly available to the public through open electronic resources [8]. Studies published in international journals, especially analyses using polarization techniques (NOESY, COSY, HSQC) and high-resolution TOF-MS equipment, are dramatically increasing the capabilities of these methods [9]. Also, the automatic identification of complex mixtures through the integration of NMR and MS technologies with artificial intelligence is developing [10].

Nuclear magnetic resonance spectroscopy (NMR) and mass spectrometry (MS) have provided revolutionary advances in chemistry, biochemistry, and materials science in recent years. The widespread use of NMR in structural analysis demonstrates its unique capabilities for in-depth study of chemical compounds. It is known that the information obtained using NMR not only provides information about the bonds between molecules, but also describes their spatial structure. This, in turn, plays an important role in drug development, metabolomics, and the study of biomolecular transformations. In particular, a correctly interpreted NMR spectrum helps in the identification of substances with mutagenic, carcinogenic, and toxic properties [2]. Mass spectrometry, with its high sensitivity and accuracy, allows for the precise determination of the composition of complex mixtures [3]. Mass spectrometric analysis results provide information on the masses, charges, and ionization levels of atoms and molecules, which allows for new approaches in analytical chemistry [4]. The combined use of mass spectrometry and NMR technologies allows for a complete understanding of the molecular structure and mechanisms of many complex substances [5]. This approach also , pharmaceuticals in the industry new medicine of tools efficiency also help in increasing gives , [6]. In addition, the effectiveness of

NMR and MS technologies in scientific research allows for the creation of more advanced analysis systems through their integration. The combination of these two methods not only brings scientific research to a new level, but also demonstrates its importance in practical areas. An example of this is the research of Uzbek scientists. Research conducted in Uzbek scientific centers, in particular in the field of pharmaceuticals and biology, has revealed the structures of many biologically active substances and developed new analysis methods using these technologies. Such research is noteworthy not only for its publication in international scientific journals, but also for its practical significance [7]. NMR and MS methods modern for science necessary was modern are equipment [8]. Their new achievements and updates are mostly artificial intellect and computer modeling through done This is new . technologies , own in turn , scientific research further effective and perfect in a way take to go opportunity creates [9].

With this together , NMR and MS methods in use There are also problems . For example , the low sensitivity of NMR spectroscopy and MS method right ionization complexity some in research problem to give birth possible . With this together , scientific in the community this methods further improvement , facilitation and further wider application directions available [10].

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, perfectly 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. By further developing and improving these technologies, it is possible to increase the competitiveness of the chemical industry and improve the quality of scientific research.

The research of Uzbek scientists in the application of these methods, in particular, the achievements in the development of drugs based on local raw materials and the analysis of the structure of biologically active substances, make a huge contribution to the development of national science. NMR and MS technologies, in the future, together with artificial intelligence and computer modeling technologies, are expected to become more efficient and perfect analysis systems. Thus, NMR and MS techniques open up new possibilities in the field of chemistry and scientific research, help to delve deeper into the molecular world and solve practical problems. The effective application and development of these technologies can lead to new achievements in scientific and industrial fields.

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