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A Brief Study of Mass Spectrometry of Natural Products

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Abstract

Objective: The physical and chemical data of the pure substance can be analysed to determine the structure. In the current era of structural elucidation, NMR spectroscopy and mass spectroscopy, especially the various types of 2D NMR, are used extensively, while infrared (IR) and ultraviolet spectroscopy (UV) are main tool to recognize the functional groups in the structure. The correlation of key chemicals in chromatograph peaks with individual mass spectra is commonly accomplished using HPLC mass spectrometry (LCMS). For most chemicals studied, LCMS ionisation procedures are chemically mild, and strong molecular ion peaks are detected. MS (mass spectrometry) is a technique for determining a substance's molecular mass, formula, and fragmentation pattern. The most widely deployed techniques in mass spectrometry are electrospray ionisation mass spectrometry, chemical ionization mass spectrometry, chemical ionisation mass spectrometry, and fast atom bombardment mass spectrometry. Our paper discusses in brief how mass spectrometry can be used to study and analyze natural products in a scientific manner. Mass spectrometry, which has been used to study complex biological systems for more than a century, is currently at a critical crossroads. We'll be looking at how the mass spectrometry business is expected to change over the next decade, emphasising the natural products industry's increasing techniques and technology. This research aims to provide a fast summary of how mass spectrometry is used in many disciplines.

Material and Methods: This review study relies on three search engines, Pub Med, Science Direct, Google Scholar, and printed material from the library, to do the best literature research possible.

Conclusion: We highlight growing mass spectrometric methodologies and technologies employed by the natural product field in this viewpoint piece and provide a glimpse into the future directions in which the mass spectrometry field will migrate over the next decade.

Introduction

In chemistry, mass spectrometry is used to analyze materials, identify new molecules, and determine a molecule's structural and chemical properties. The fragmentation pattern, molecular mass, and molecular formula are all reported. Among the most popular equipment for applying mass spectrometric analyses are electrospray ionization mass spectrometry (ESIMS), electron impact mass spectrometry (EIMS), chemical ionization mass spectrometry (CIMS) and fast atom bombardment mass spectrometry (FABMS).

Mass spectrometry has a limited detection capability, but it has a wide variety of uses in industries like chemical, pharmaceutical, biotechnology, and food, to name a few. It's widely utilized in environmental and medicinal research and molecular biology. The fast growth of mass spectrometry over the past century and a diverse set of procedures and

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equipment have enabled qualitative and quantitative analysis of practically all compounds present in natural products [1, 2]. Because extracts from biological matrices containing natural products are typically mixed with various chemicals, GC or LC coupled systems are frequently used [3, 4]. New techniques like Electrospray Ionization have expanded the variety of studied biomolecules, including those with large molecular weights [5]. Similarly, sophisticated mass analysers allow for the analysis of molecular ions or fractionated ions with high resolution [6]. The purpose of this study is to offer a concise overview of how mass spectrometry is employed throughout a wide range of fields.

Essential oils

The molecular composition of essential oils can be studied relatively quickly because they are volatile metabolites. Thus, studies of the chemical composition of these natural products usually achieve a percentage greater than 90% [7, 8]. Having both mass spectra and retention indices evaluated is an effective way of acquiring information that can be verified using specific databases in the case of compounds with this type of structure [9]. There may also be the possibility of determining biochemical properties through GC/MS analysis of molecules, such as antibiotics or antioxidants, isolated with a TLC method [10].

Fatty acids

Gas chromatography coupled to mass spectra (GC-MS) is typically employed to obtain structural information about fatty acids. Proper derivatives can be used to locate structural properties like branches, rings, the position and kind of heteroatoms, and double bonds. Although the large molecular weight molecules are non-volatile, this is solved using chemical derivatization methods, generating methyl or ethyl esters [11-13]. Various plant species include saturated and unsaturated fatty acids; GC/MS typically carries out studies. This methodology is used to examine a variety of nutritional and pharmaceutically essential species, including Plukenetia volubilis [14], Borrago officinalis [15], and fish oil [16].

Aromas and flavours

Due to their volatile nature, GC/MS equipment is well suited for studying the chemistry of fruits and vegetables, given their aromas and flavours are essential for distinguishing their taste. Because most of these compounds are highly volatile and cannot be removed from the vapour stream, they must first be extracted using non-polar solvents or injected directly into the headspace in chromatographic systems [17, 18].

Phenols and polyphenols

A small number of phenolic compounds can be directly analyzed by the GC/MS instrument, generally those compounds with low molecular weight [29]. It is noted that most phenolic and polyphenolic compounds are non-volatile and can be monitored using two different analytical protocols for their structure determination. The first entails a chemical derivatization process, using a mechanism known as sylitation, which renders these compounds volatile [20–21]. In the second, mass spectrometry is combined with HPLC, allowing many tests to be performed after separating them into one column. The advantage of the electrospray ionization technique is the possibility of ionizing molecules that lack volatility [22, 23]. Compared to the conventional ionization technique, the electrospray ionization technique is superior because it can ionize molecules that are not volatile. A material's m/z value may be calculated more accurately using mass spectrometers with a better resolution than the quadrupole or orbitrap, leading to a greater degree of precision in compound identification [24–26].

Alkaloids

The alkaloids belong to a group of natural products in a wide range of structurally diverse chemical forms. A secondary characteristic of alkaloids is nitrogen's presence in their structure, which provides a mechanism for their active properties. In addition to their biological properties, these compounds have a diverse range of physiological effects. They are widely used as pharmaceuticals due to their wide range of bodily functions. Alkaloids, which are active substances found in plants, have been recognized as one of the most critical sources of alkaloids for centuries. Some of the most well-known alkaloids, such as morphine, quinine, strychnine, nicotine, and cocaine, are derived from various plants. As mentioned above, some alkaloids such as nicotine

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and others present in tobacco may be analyzed directly using the GC/MS equipment [27], caffeine and xanthine alkaloids [28, 29], and other compounds such as tropane alkaloids can also be separated using gas chromatography [30]. The most frequently used method in the test of these metabolites is the LC/ MS in its diverse variants, such as the LC/MS [31], LC/MS-MS [32], some with a more excellent mass resolution, such as the HPLC-TOF-MS [33].

The most often used method for assessing these metabolites has been discovered to be liquid chromatography/mass spectrometry (LC/MS), which has been improved using various approaches, for instance, the LC/MS-MS [31, 32], and even HPLC-TOF-MS [43]. It may be possible to discover new structures of this type of molecule using mass spectrometry such as Orbitrap [34].

Cannabinols

It is known that cannabinoids are a family of natural products containing more than 70 compounds, out of which THC and CBD [35] are some of the most vital. Since discovering the endocannabinoids 1 and 2, these phytochemicals have attracted considerable attention in the medical field [36]. GC/MS systems can determine the properties of these compounds in a highly accurate manner because of their high solubility in nonpolar solvents and volatility at the injection temperature [37, 38]. These substances may also be analyzed with LC/MS [39–40].

Conclusions

Mass spectrometry can examine almost all natural compounds, and its great sensitivity and comprehensive structural information make it an indispensable tool in research and product development labs. Equipment with high-resolution analyzers can give us with incredibly precise values of molecular ions, allowing us to distinguish the nature of the molecules. There is now a wide range of equipment that may be used in conjunction with LC or GC separation systems, which is perfect for natural extracts, which are typically a mixture of compounds from various sources. Similarly, the combination of ionisation and analyzer approaches has been able to give instrumental variability, which has now made it a popular tool for discovering novel natural structures.

Since its inception more than a century ago, mass spectrometry has been used to investigate biological molecules. However, the field is presently at a crossroads. Over the next decade, we'll be looking at how the mass spectrometry market is projected to develop, with a focus on the natural products industry's expanding use of methods and technology. In this perspective essay, we discuss the mass spectrometric approaches and technologies used by the natural product industry, as well as the future directions in which the mass spectrometry field is expected to migrate over the next decade.

Authors' Contribution

Conceived and designed the analysis: IUR, LM. Collected the data: IUR, LM, SZ. Contributed data or analysis tools: IUR, LM, MA. Performed the analysis: IUR, LM, SZ. Paper written by: IUR, LM

Conflict of interest

The authors have no conflicts of interest to declare.

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