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Gas chromatography mass spectrometry (GC-MS): A Tool for the Health Care, Environmental, and Pharmaceutical Industries

Imad Hadi Hameed† [1], Fatima Muhammad Shakhir Najm [2], Atheer Hussein Ali Weiss [3], Maryam Salah Kamel [4]

1College of Biotechnology, Department of medical biotechnology, Al-Qasim Green University, Iraq

2College of Science for Women, Department of Biology, University of Babylon, Iraq

3Al-Farabi University College, Department of Biology, Iraq

4Al-Hilla University College, Department of Applied Medical Physics, Iraq

Abstract: - Analytical techniques like gas chromatography can separate chemicals in complicated combinations according to their polarity. Only substances that are volatile or can be rendered volatile through derivatization with derivatizing agents can be separated. Due to its efficacy, sensitivity, and simplicity, it is one of the most extensively used techniques for compound separation. The difference in partitioning behaviour between the mobile and stationary phases is the basis for compound separation. In this process, a sample is moved through a tube packed with a finely divided solid or a film of liquid by means of a moving gas stream. For the purpose of compound classification, a variety of columns with varying stationary phase compositions have been employed for the purpose of injecting a solvent-containing mixture or sample into the column at a high enough temperature to volatilize the compound

Keywords: GC-MS, Medical, Pharmaceutical, Applications

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Corresponding Author: Imad Hadi Hameed †, College of Biotechnology, Department of medical biotechnology, Al-Qasim Green University, Iraq

Introduction

The acronym GC-MS stands for gas chromatography and mass spectrometry, two methods that work hand in hand. It is more cost-effective to acquire and maintain GC-MS instruments than LC-MS ones. When it comes to clinical specimens, GC-MS is employed more frequently in forensic toxicology than as a standalone instrument in hospital and commercial labs. As sensitive as many modern LC-MS/MS technologies are, GC-MS was used to successfully assess fentanyl in canine plasma as early as 1981 at picogram/mL concentrations. Valdez recently reviewed the literature on GC-MS methods that are optimised for fentanyl and analogues of fentanyl, and his review is highly recommended [1].

The requirement to basify the fentanyl salt in order to enable chromatography and detection is a big downside of GC-MS compared to LC-MS. The most common form of ionisation, known as 70-eV electron impact ionisation (EI), requires molecules to be thermally stable and is considered damaging, often known as a "hard" ionisation process.

Extraction of the free base using an organic solvent follows the basification process. Sample cleanup sometimes involves multiple rounds of basification and extraction, as shown in many approaches [2]. It is possible to skip over some of the extraction processes by using solid phase extraction (SPE). The recovery of fentanyl in spiking investigations was determined to be equivalent when solid-phase extraction, liquid-liquid microextraction (DLLME), and liquid-liquid extraction (LLE) were compared recently [3].

In Selective Ion Monitoring (SIM), the mass filter is not stepped over a broad range of masses but rather data is collected at masses of interest. When run in SIM mode, GC-MS/MS delivers exceptional specificity. Since SIM requires knowledge of the ionisation mechanism of the target molecule, it cannot be used for untargeted analysis. Fentanyl analogues have been detected by GC-MS, which LC-MS/MS has validated and quantified [4]. Actually, GC-MS was the first to find acryl fentanyl on the recreational drug market, and LC-MS, IR, and NMR later corroborated the finding.

Hydride bonding between molecules controls the volatility of many analytes that are seen often. The presence of these linkages makes the transformation from a liquid to a vapour more energy (heat) intensive. Thus, hydrogen bonding effects can be removed, leading to a significant rise in volatility. Alcohols, phenols, carboxylic acids, and amines with high boiling points can now be determined by gas chromatography (GC) using this method. Chromatographic performance can be enhanced by reducing hydrogen bonding, which weakens the link between the molecule and the polar groups in the stationary phase. Consequently, issues with peak tailing and other bad chromatographic behaviours are reduced. It is usual practice to create an appropriate derivative of these hydrogen bonding groups before introducing the analyte to the gas chromatography (GC) system in order to "remove" them. Hydrogen bonding occurs in many alcohols, phenols, and amines, but GC can identify them as acetyl derivatives. Such compounds can be easily prepared by reacting reagents like ethanoic anhydride with a catalyst like hydrochloric acid prior to being introduced to the gas chromatography (GC). Derivatizing chemicals like trifluoro-ethanoic anhydride or N-trifluoroacetyl imidazole can be utilised to produce trifluoro acetyl derivatives of trimethylsilyl compounds, which is likely one of the most widely utilised derivatization procedures. Trimethylchlorosilane (TMS) in pyridine or hexamethyldisilazane (HMDS) and N,O-Bis(trimethylsilyl)trifluoroacetamide (BSTFA) are two of the many different ways that are currently available for their synthesis [5]. Converting carboxylic acids to their methyl esters is another typical procedure for GC analysis of these chemicals. Diazomethane and boron trifluoride in methanolic solutions are two of the most typical ways to get this. Because select ion mode (SIM) is so useful for monitoring the indication, this is a promising strategy for their GC-MS study. However, the McLafferty rearrangement of the methyl ester produces a m/z 74 ion, which is very unusual.

Applications of GC in Metabolomics A

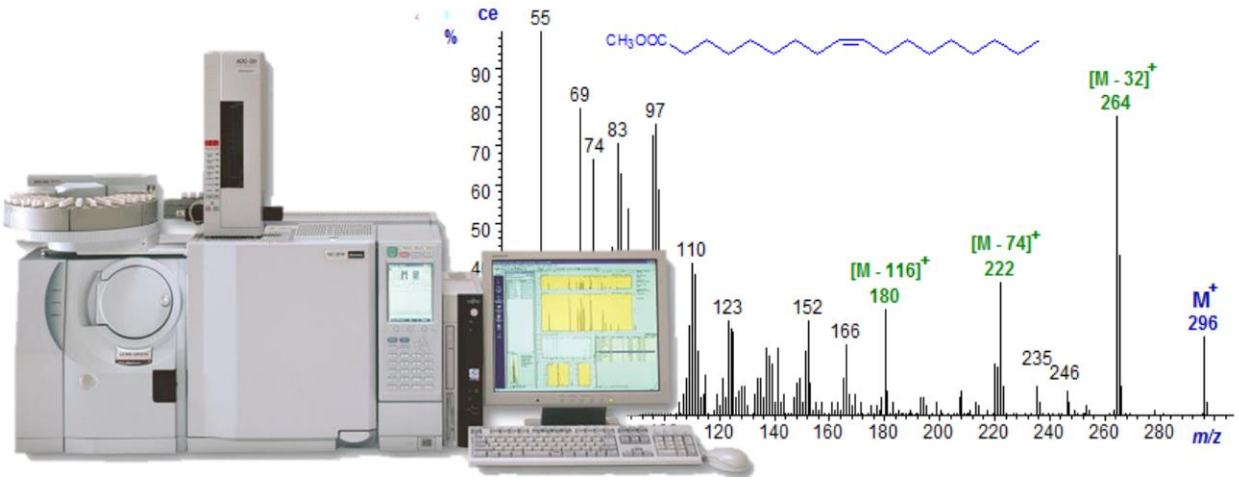
Although gas chromatography coupled with mass spectrometry has not traditionally been linked to studies involving volatile organic molecules, it has found widespread application in metabolomics research. Drug evaluation, clinical toxicology, nutrigenomics, and functional genomics can all benefit from metabolomics research.

High repeatability and strong resolving capabilities are two of GC's most notable characteristics as a separation process. GC is connected to mass spectrometers such the time-of-flight (TOF) device, which can find the exact mass to within four decimal places, and the triple quadruple (QqQ), which can be utilised for quantitative and qualitative analysis [6]. Electron ionisation and chemical ionisation are two methods by which compounds eluting from a GC column become ionised. A wide variety of industries and fields can benefit from this technology, from the food and agricultural sectors to the pharmaceutical and biomarker discovery industries. references [7]. Typically, electron ionisation occurs at a potential of -70 eV. This ionises the samples so that the mass spectrometer can detect them. In order to identify the chemicals, the mass spectra are compared to those already in the database. In order to create 2D databases for compounds that are accurate enough to be shared across analytical platforms, it is possible to capture mass spectra in addition to retention time. One example of a database that serves this purpose is the FeihnLib library. The creation of such databases was facilitated by the early use of GC-MS in metabolomics. Two kinds of metabolomics studies have been targeted, whereas none have been targeted. The goal of non-targeted metabolomics research is to identify the "fingerprint" of an organism's metabolome by detecting and, in many cases, quantifying the

highest number of molecules in a sample. This allows researchers to compare samples and draw valuable biological conclusions [8]. Targeted metabolomics involves comparing the spectra of interest to a library of reference spectra of pure substances in order to identify and quantify the molecules in a specific bio fluid or tissue extract.

Evaluation of Substance Abuse

When combined, GCMS and Headspace provide a powerful analytical tool for narcotics. Examples of this type of analysis include the determination of amphetamine and its metabolites in urine as well as the nicotine content in prescription medications. An improvement in sensitivity of almost 20 times in SIM mode can be achieved by combining GCMS with chemical ionisation and traditional headspace. Because GC MS generates a consistent ionisation, it is much simpler to compare the discovered chemicals to the data in the library [9].



Food science evaluation

Gas chromatography is a trusted tool in the food industry for a variety of tasks, including quantitative and qualitative food analysis, flavour and aroma component analysis, additive analysis, and the detection and analysis of contaminants like pesticides, fumigants, and naturally occurring toxins. Gas chromatography plays an essential role in the food industry's safety regulations by removing any possibility of tainted goods reaching the consumer market. Maintaining a constant aroma, texture, and flavour in food is another important feature that this method guarantees [10]. Although alternative methods are used by the food business, gas chromatography is still the preferred approach because it is easy to use and doesn't cost too much.

Assurance of high-quality

The production of automobiles, chemicals, and pharmaceuticals is among the many industries that heavily utilise gas chromatography as a quality control tool. Gas chromatography is a tool that the pharmaceutical business utilises to make vast amounts of pure goods. Eliminating discrepancies in pharmaceutical products and ensuring the purity of the produced material are the main goals of this procedure [11]. Gas chromatography is also used by the industry to examine chemicals for trace pollutants. The pharmaceutical industry is also seeing increased usage of the approach for chiral chemical separation. According to research, new car interiors emit a high concentration of volatile organic compounds (VOCs). In order to determine how much of a certain chemical is emitted into the air from various interior components such as carpets, door linings, pedals and seat covers, gas chromatography has been utilised by the automotive industry. Toxin levels in modern car interiors are something that scientists are working to lower.

Environmental surveillance

GC-MS is now widely acknowledged as an effective method for detecting and tracing organic contaminants in the natural world. In spite of a dramatic improvement in reliability, the price of GCMS equipment has dropped [12, 13].

Chlorophenols, polycyclic aromatic hydrocarbons (PAHs), sulphur in the air, organo-chlorine pesticides, herbicides, phenols, halogenated pesticides and unleaded petrol are all easily detectable using this method (Figure 2). In bio-mass studies, it can screen lignin breakdown products; in spinach, it can screen insecticides. Derivatization is not necessary for the study of carbamazepine and its metabolites in treated sewage water and steroids, as well as decacyclene, ovalene, and even C60 degradation [14].

Verification of biological and pesticide content

Anaesthetics, alcohols, narcotics, anticonvulsants, antihistamines, anti-epileptic medications, sedative hypnotics, narcotics, and dietary items can all be detected in bio-analysis samples of blood and urine using GC-MS (Figure 5). This method has a wide range of potential applications, including the detection of adulterations, fatty acid profile in microorganisms, free steroids, blood pollutants, serum metabolites, organo-chlorinated pesticides in river water, drinking water, fruit juices, sunflower oil, and other similar substances [15].

Medical Treatment and Pharmaceutical Uses

Gas chromatography-mass spectrometry screening techniques can now identify newborns with dozens of congenital metabolic illnesses, sometimes known as inborn errors of metabolism. Even at low concentrations, GC-MS may identify substances in urine [16]. People with metabolic problems often have these substances, which are ordinarily absent. Similar to how a urine test administered at birth can identify metabolic problems with a high degree of certainty, this method is simple, quick, and accurate. Metabolic activity can be determined using GCMS in conjunction with isotope labelling of metabolites. Isotope ratio mass spectrometers (IRMSs)—MSs equipped with detectors tailored to measure a small number of target ions and provide results as ratios—form the basis of most applications using 13C labelling and the measurement of 13C-12C ratios. The ability to identify oils in topical medications is a great asset. Analytical research and development [17-19], quality control, production, pilot plant departments for API, bulk pharmaceuticals, and formulations are some of the many areas of the pharmaceutical industry that make extensive use of GC-MS. Method and process development, as well as the detection of API contaminants, make use of it. Research in medicinal chemistry (compound synthesis and characterisation), pharmaceutical analysis (impurity profiling, stability testing), pharmacognosy, pharmaceutical process control, pharmaceutical biotechnology, and related fields relies heavily on it. See references.

Conclusion:

Chromatography and its hyphenated techniques are significant platform techniques in modern technology and chemical statistical methodologies, which play an important role in quality research and assessment of TCM. High chromatographic resolution, sensitivity, and repeatability are three reasons why GC-MS is becoming more prominent in TCM research. The data generated by GC-MS analysis of TCM is rich with information, but it takes a lot of skill and knowledge to interpret the results and link them to biological function. We anticipate that the coverage of TCM will be substantially improved with the adoption of enhanced fibre properties and extraction conditions, in conjunction with advancements in chemometric data analysis.

Forensic analytical gas chromatography has long been regarded as the "gold standard" because to its maturity and reliability. New technologies that are just as reliable and have comparable capabilities have not arisen to the point where these methods are no longer useful in forensic science. However, as this paper shows, researchers are increasingly focusing on novel and unconventional areas to study, rather than new technology. The development of more sensitive GC and GC-MS instruments appears to be a contributing factor, since it enables the use of smaller sample quantities and, by extension, the possibility of new types of samples. Sweat analysis has the potential to replace the currently used methods of analysing urine, blood, and hair for the identification of narcotics and other chemicals. The comparably non-invasive cerumen sample also has its benefits; it has a longer detection window than urine but a shorter one than reported for hair, and it may be less contaminated than urine. Evidence of exposure throughout pregnancy and in the baby's first year can be gleaned from meconium as well as breast milk.

Beyond its typical use in determining polymeric materials, Py-GC-MS has demonstrated the ability to investigate the chemistry and byproducts produced during the smoking of some commonly used medicines. As a result of feeding on both enriched and naturally occurring quantities of meat discovered in autopsy samples, it has been demonstrated that it is feasible to determine narcotics in insects. Potentially applicable to drug detection in various contexts, this is an intriguing new study. Giving the bug the freedom to use its innate senses to find its way about and report back with details. Similarly, it may be possible to conduct future research into the possibilities of detecting explosive and drug residues in various animals and plants.

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