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GC-MS Technique and its Analytical Applications in Science and Technology

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Abstract

GC-MS is highly effective and versatile analytical techniques with numerous scientific applications to cater the field of applied Sciences and Technology. This review elaborates the significant uses of this technique. It is a very useful for quality control, analytical research, impurity profiling and maintenance for human welfare and development.

Keywords: Gas Chromatography; Mass Spectrometry; Applied sciences; Environmental monitoring

Introduction

Gas Chromatography–Mass Spectrometry (GC-MS) is a hyphenated analytical technique that combines the separation properties of gas-liquid chromatography with the detection feature of mass spectrometry to identify different substances within a test sample (Figure 1). GC is used to separate the volatile and thermally stable substitutes in a sample whereas GC-MS fragments the analyte to be identified on the basis of its mass. The further addition of mass spectrometer in it leads to GC-MS/MS. Superior performance is achieved by single and triple quadrupole modes [1-3].

Advantages of GC-MS

GC requires the analyte to have significant vapor pressure between 30 and 300°C. GC presents a insufficient proof of the nature of the detected compounds. The identification is based on retention time matching that may be inaccurate or misleading. GC-MS represents the mass of a given particle (Da) to the number (z) of electrostatic charges (e) that the particle carries. The term m/z is measured in DA/e. GC-MS commonly uses electron impact (EI) and chemical ionization (CI) techniques. The main features of enhanced molecular ion, improved confidence in sample identification, significantly increased range of thermally labile and low volatility samples amenable for analysis, much faster analysis, improved sensitivity particularly for compounds that are hard to analyze and the many other features and options provide compelling reasons to use the GC-MS in broad range of areas [4,5].

Applications of GC-MS

Environmental monitoring

GC-MS has become a highly recommended tool for monitoring and tracking organic pollutants in the environment. The cost of GC-MS equipment has decreased whereas the reliability has markedly increased. The determination of chloro-phenols in water and soil, polycyclic aromatic hydrocarbons (PAH), unleaded gasoline, dioxins, dibenzofurans (Figure 2), organo-chlorine pesticides, herbicides, phenols, halogenated pesticides, sulphur in air is very convenient to be screened by this technique. It can be used to screen the degradation products of lignin in bio-mass research, pesticides in spinach. Analysis of decacyclene, ovalene and even C_{60} degradation analysis of carbamazepine and its metabolites in treated sewage water and steroid can be done without derivatization [6,7].

Food, beverage, flavor and fragrance analysis

Foods and beverages have several aromatic compounds existing naturally in native state or formed while processing. GC-MS is exclusively used for the analysis of esters, fatty acids, alcohols, aldehydes, terpenes etc. GC-MS is also used to detect and measure contaminants, spoilage and adulteration of food, oil, butter, ghee that could be harmful and should to be controlled and checked as regulated by governmental agencies. It is used in the analysis of piperine (Figure 3), spearmint oil, lavender oil, essential oil, fragrance reference standards, perfumes, chiral compounds in essential oils, fragrances, menthol, allergens, olive oil, lemon oil, peppermint oil, yiang oil, straw berry syrup, butter triglycerides, residual pesticides in food and wine [8,9].

Forensic and criminal cases

GC-MS can analyze the particles from suspect to correlate his involvement in case. The analysis of fire debris using GC-MS can be established by American Society for Testing Materials (ASTM) standard for fire debris analysis. It is the key tool used in sports anti-doping laboratories to test athlete's urine samples for prohibited performance-enhancing drugs like anabolic steroids. It is also commonly used in forensic toxicology to find poisons, steroids (Figure 4) in biological specimens of suspects, victims, or the deceased [10,11].

Biological and pesticides detections

GC-MS is exclusively used in bio-analysis of blood, urine for the presence of barbiturates, narcotics, alcohols, residual solvents, drugs like anesthetics, anticonvulsant, antihistamine, anti-epileptic drug, sedative hypnotics, narcotics and food items (Figure 5). This technique could be used for detecting adulterations, fatty acid profiling in microbes, presence of free steroids, blood pollutants, metabolites in serum, organo-chlorinated pesticides in river water, drinking water, soft drinks by head space, pesticides in sunflower oil etc. [12].

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Figure 1: A typical GC-MS with head space of Shimadzu Company

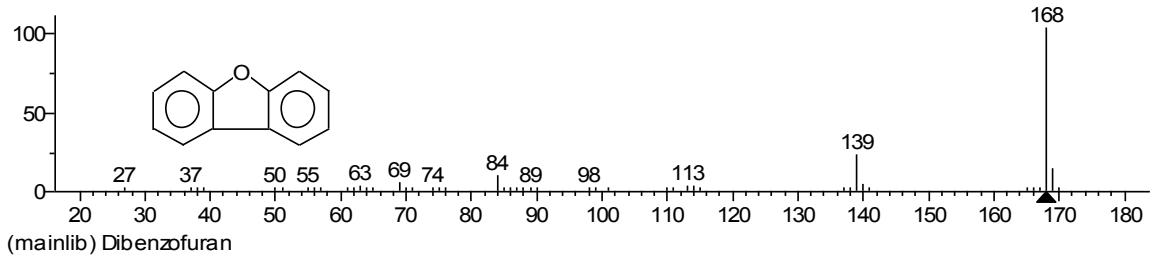

Figure 2: The GC-MS spectrum of Dibenzofuran (Formula: $C_{12}H_8O$, MW: 168) with x-axis *m/z* ratio and y-axis as intensity.

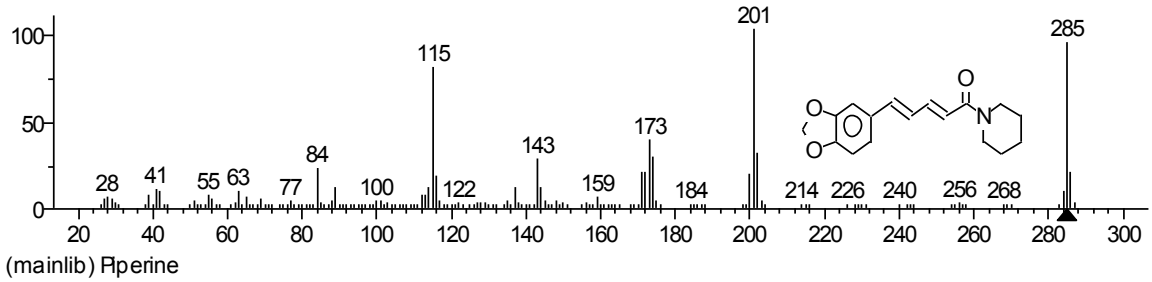

Figure 3: The GC-MS spectrum of Piperine (Formula: $C_{17}H_{19}NO_3$, MW: 285) with x-axis *m/z* ratio and y-axis as intensity.

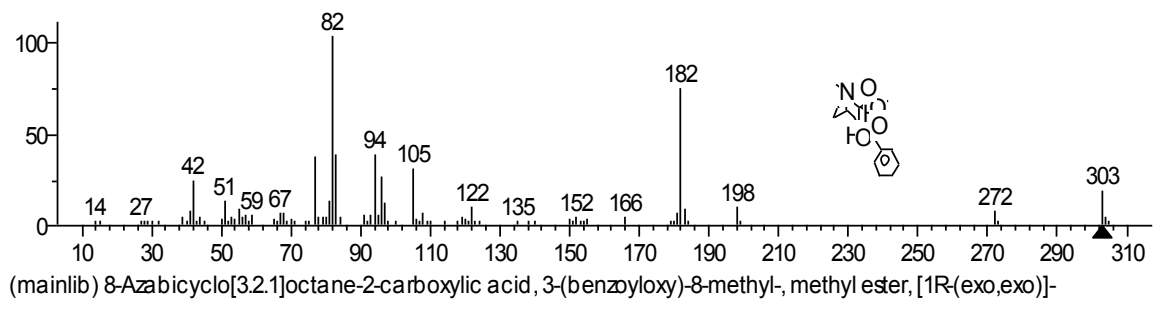

Figure 4: The GC-MS spectrum of Cocaine (Formula: $C_{17}H_{21}NO_4$, MW: 303) with x-axis *m/z* ratio and y-axis as intensity.

Security and chemical warfare agent detection

Explosive detection systems have become a part of all United State airports, GC-MS. Is an essential part of chemical analysis unit. For enhancing capability in homeland security and public health preparedness, traditional GC-MS units with the transmission quadrupole mass spectrometers, as well as those with cylindrical ion trap (CIT-MS) and toroidal ion trap (T-ITMS) mass spectrometers have been modified for field portability and near real-time detection of chemical warfare agents (CWA) such as sarin, soman, and VX [13,14] (Figure 6).

Astro chemistry and Geo chemical Research

Several GC-MS have left earth for the astro chemistry studies. Two were taken to Mars planet by the Viking program. Scientist

analyzed the atmosphere of Venus with GC-MS. The Huygens probe of the Cassini-Huygens mission landed one GC-MS on Saturn's largest moon, Titan. The material in the comet 67P/Churyumov-Gerasimenko will be analyzed by the Rosetta mission with a chiral GC-MS in 2014.

Significantly enhanced molecular ions, major isomer and structurally significant mass spectral peaks, extended range of low volatility hydrocarbons that are amenable for analysis and unique isotope ratio information make GC-MS valuable for organic geochemical applications [15,16].

Medicine and Pharmaceutical Applications

Dozens of congenital metabolic diseases called as inborn error of metabolism are now detectable in newborn by screening tests using gas chromatography–mass spectrometry. GC-MS can determine compounds in urine even in minor concentration. These compounds are normally not present but appear in individuals suffering from metabolic disorders. This is easy, effective and efficient way to diagnose the problem like in case of genetic metabolic disorders by a urine test at birth. In combination with isotopic labeling of metabolite, the GC-MS is used for determining metabolic activity. Most applications are based on the use of ^{13}C labeling and the measurement of ^{13}C-^{12}C ratios with an isotope ratio mass spectrometer (IRMS); an MS with a detector designed to measure a few select ions and return values as ratios. It is useful to detect oils in creams, ointments, lotion etc.

GC-MS is widely used in pharmaceutical industries for analytical research and development, quality control, quality assurance, production, pilot plants departments for active pharmaceutical ingredients (API), bulk drugs and formulations. It is used for process and method development, identification of impurities in API. It is an integral part of research associated with medicinal chemistry (synthesis and characterization of compounds), pharmaceutical analysis (stability testing, impurity profiling), pharmacognosy, pharmaceutical process control (Figure 7), pharmaceutical biotechnology etc. [17,18].

Petrochemical and hydrocarbons analysis

Significantly enhanced molecular ions that are always observed, isomer and structurally significant mass spectral peaks and extended range of low volatilite hydrocarbons that are amenable for analysis including waxes up to $C_{74}H_{150}$ makes the GC-MS a most valuable technique. Broad range of petrochemicals, fuels and hydrocarbon mixtures, including gasoline, kerosene, naphthenic acids, diesel fuel (Figures 8A and 8B), various oil types, transformer oil, biodiesel, wax and broad range of geochemical samples can be analyzed by GC-MS [19].

Clinical toxicology

Enhanced molecular ions, extended range of compounds amenable for analysis, superior sensitivity for compounds and faster analysis are the main attractive features of the clinical toxicology. The toxin and venoms are identified by GC-MS. It is extensively used in clinical toxicology [20].

Academic research

As a unique and powerful technology the GC-MS provides a rare opportunity to perform the analysis of new compounds for characterization and identification of synthesized or derivatized compound. It is widely used in pure and applied sciences like Chemistry, Polymers, Nanotechnology and Biotechnology etc. It yields useful information that can be used in research publication internationally [21,22].

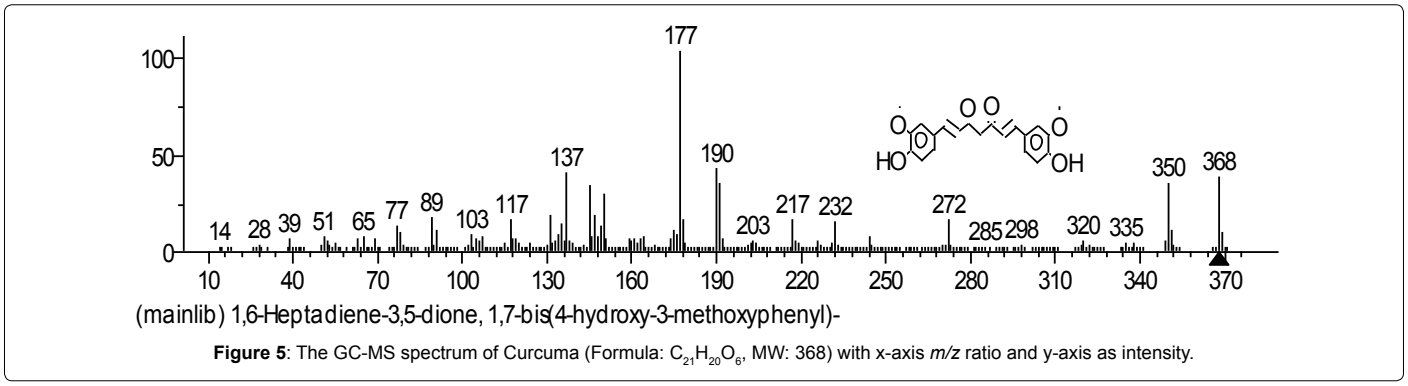

Figure 5: The GC-MS spectrum of Curcuma (Formula: $C_{21}H_{20}O_6$, MW: 368) with x-axis *m/z* ratio and y-axis as intensity.

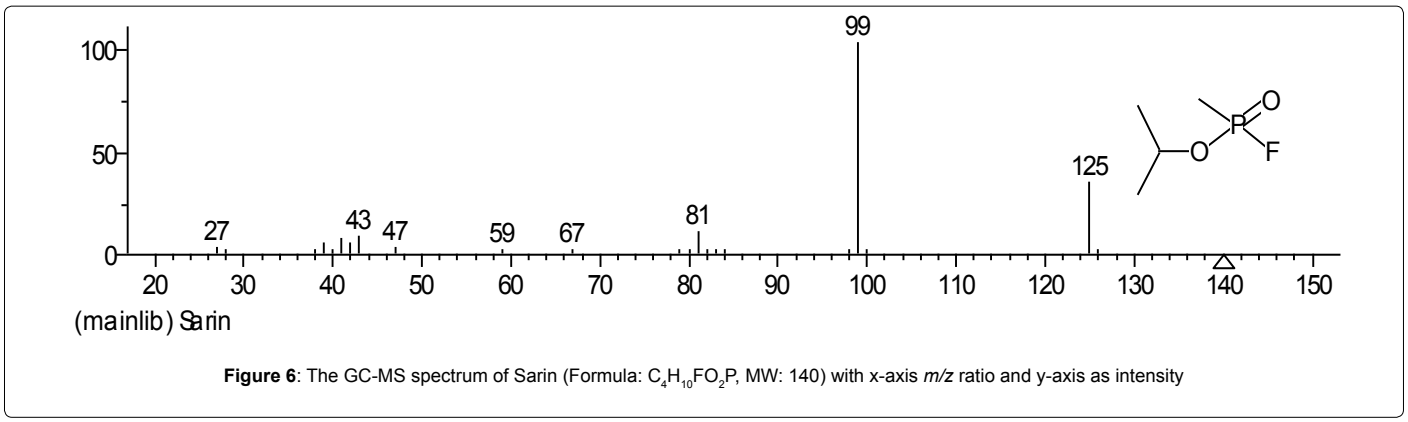

Figure 6: The GC-MS spectrum of Sarin (Formula: $C_4H_{10}FO_2P$, MW: 140) with x-axis *m/z* ratio and y-axis as intensity

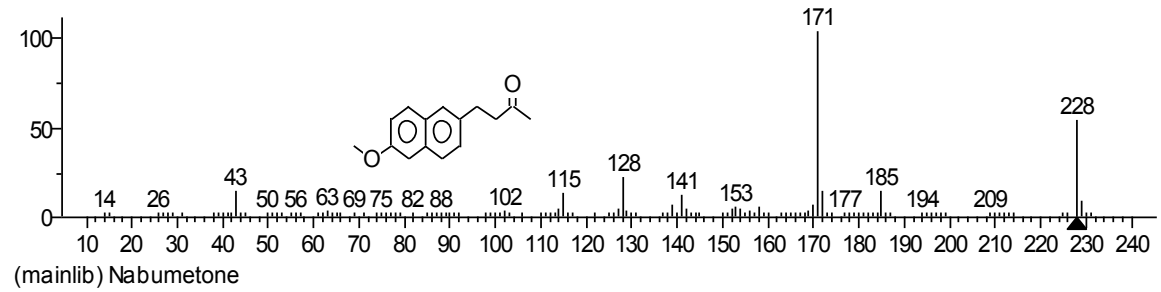

Figure 7: The GC-MS spectrum of Nabumetone (Formula: $C_{15}H_{16}O_2$, MW: 228) with x-axis *m/z* ratio and y-axis as intensity

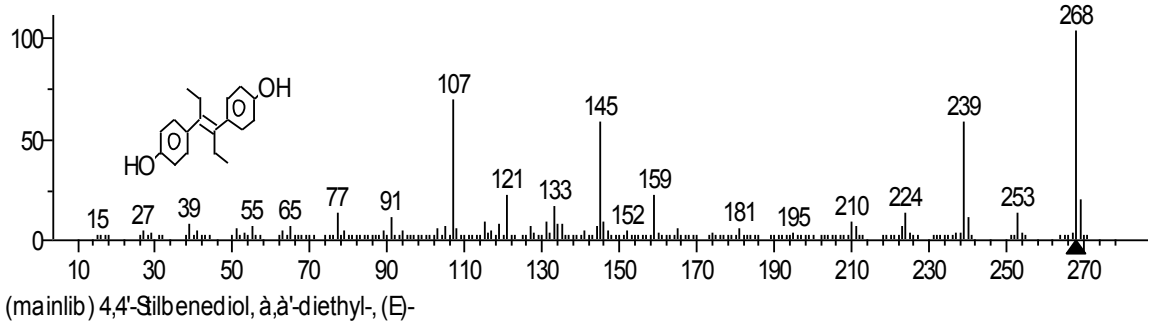

Figure 8A: The GC-MS spectrum of Diesel (Formula: $C_{18}H_{20}O_2$, MW: 268) with x-axis *m/z* ratio and y-axis as intensity.

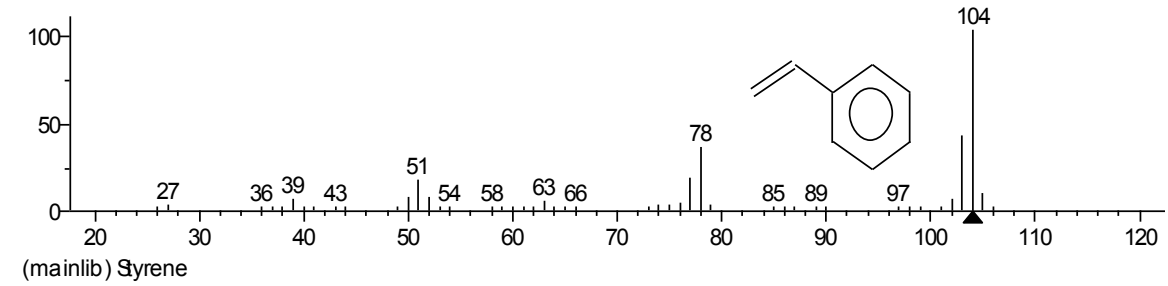

Figure 8B: The GC-MS spectrum of Diesel (Formula: C_8H_8, MW: 104) with x-axis *m/z* ratio and y-axis as intensity.

Industrial applications

GC-MS is used in industries for the analysis of aromatic solvents, inorganic gases, amino alcohol in water, impurities in styrene, glycol, diols, xylene, allergens in cosmetics etc. GC-MS is used for the characterization of formic acid in acetic acid for industrial use. In Industries acetic acid is important intermediate in coal chemical synthesis. It is used in the production of poly ethylene, cellulose acetate and poly vinyl as well as synthesic fiber and fabrics [23].

Energy and fuel applications

GC-MS is used for the analysis of aromatic solvents, sulphur, impurities in polypropylene, sulphur in menthane, natural gases, 1,3 butadiene, ethylene, gas oil, unleaded gasoline, polyethene, diesel.oil, unleaded gasoline, polyethylene, diesel, modified biomass, grafted polymers etc. [24].

GC-MS has triggered a new arena of research and taken to new heights of impactful presentation and characterization of compounds by its wide range of applications [25-27].

Conclusions

GC-MS is an advanced technique that cannot be compared with other modern analytical equipment but can be complemented by mass spectrophotometer to achieve GC-MS/MS. It has broad range of applications that caters to academic research, quality control as-well as industrial applications. Its concise, efficient, automated system gives fast, reproducible and effective results that serve a key role in advancement of Science and Technology. This versatile analytical technique could be explored for better prospects in future.

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