

Chapter 1 : GC-MS And Its Applications |authorSTREAM

Gas chromatography-mass spectrometry (GC-MS) is a hybrid analytical technique that couples the separation capabilities of GC with the detection properties of MS to provide a higher efficiency of.

History[edit] The first on-line coupling of gas chromatography to a mass spectrometer was reported in In , Electronic Associates, Inc. EAI , a leading U. Chou, Michael Story, and William Fies. The GC-MS is composed of two major building blocks: The difference in the chemical properties between different molecules in a mixture and their relative affinity for the stationary phase of the column will promote separation of the molecules as the sample travels the length of the column. The molecules are retained by the column and then elute come off from the column at different times called the retention time , and this allows the mass spectrometer downstream to capture, ionize, accelerate, deflect, and detect the ionized molecules separately. The mass spectrometer does this by breaking each molecule into ionized fragments and detecting these fragments using their mass-to-charge ratio. GC-MS schematic These two components, used together, allow a much finer degree of substance identification than either unit used separately. It is not possible to make an accurate identification of a particular molecule by gas chromatography or mass spectrometry alone. The mass spectrometry process normally requires a very pure sample while gas chromatography using a traditional detector e. Flame ionization detector cannot differentiate between multiple molecules that happen to take the same amount of time to travel through the column i. Sometimes two different molecules can also have a similar pattern of ionized fragments in a mass spectrometer mass spectrum. Combining the two processes reduces the possibility of error, as it is extremely unlikely that two different molecules will behave in the same way in both a gas chromatograph and a mass spectrometer. Therefore, when an identifying mass spectrum appears at a characteristic retention time in a GC-MS analysis, it typically increases certainty that the analyte of interest is in the sample. The target analytes are extracted and mixed with water and introduced into an airtight chamber. An inert gas such as Nitrogen N₂ is bubbled through the water; this is known as purging or sparging. The volatile compounds move into the headspace above the water and are drawn along a pressure gradient caused by the introduction of the purge gas out of the chamber. The trap is a column of adsorbent material at ambient temperature that holds the compounds by returning them to the liquid phase. The trap is then heated and the sample compounds are introduced to the GC-MS column via a volatiles interface, which is a split inlet system. In this system the inert gas is bubbled through the water until the concentrations of organic compounds in the vapor phase are at equilibrium with concentrations in the aqueous phase. The gas phase is then analysed directly. Another relatively common detector is the ion trap mass spectrometer. Additionally one may find a magnetic sector mass spectrometer, however these particular instruments are expensive and bulky and not typically found in high-throughput service laboratories. Other detectors may be encountered such as time of flight TOF , tandem quadrupoles MS-MS see below , or in the case of an ion trap MS_n where n indicates the number mass spectrometry stages. The first quadrupole Q1 is connected with a collision cell Q2 and another quadrupole Q3. Types of analysis include product ion scan, precursor ion scan, selected reaction monitoring SRM sometimes referred to as multiple reaction monitoring MRM and neutral loss scan. When Q1 is in static mode looking at one mass only as in SIM , and Q3 is in scanning mode, one obtains a so-called product ion spectrum also called "daughter spectrum". From this spectrum, one can select a prominent product ion which can be the product ion for the chosen precursor ion. The pair is called a "transition" and forms the basis for SRM. SRM is highly specific and virtually eliminates matrix background. Ionization[edit] After the molecules travel the length of the column, pass through the transfer line and enter into the mass spectrometer they are ionized by various methods with typically only one method being used at any given time. Once the sample is fragmented it will then be detected, usually by an electron multiplier , which essentially turns the ionized mass fragment into an electrical signal that is then detected. The ionization technique chosen is independent of using full scan or SIM. Block diagram for gas chromatography using electron ionization for collecting mass spectrum. Electron ionization[edit] By far the most common and perhaps standard form of ionization is electron ionization EI. The molecules enter into the MS the source is a

quadrupole or the ion trap itself in an ion trap MS where they are bombarded with free electrons emitted from a filament, not unlike the filament one would find in a standard light bulb. The electrons bombard the molecules, causing the molecule to fragment in a characteristic and reproducible way. Hard ionization is considered by mass spectrometrists as the employ of molecular electron bombardment, whereas "soft ionization" is charge by molecular collision with an introduced gas. The molecular fragmentation pattern is dependent upon the electron energy applied to the system, typically 70 eV electron Volts. Spectral library searches employ matching algorithms such as Probability Based Matching [10] and dot-product [11] matching that are used with methods of analysis written by many method standardization agencies. Cold electron ionization[edit] The "hard ionization" process of electron ionization can be softened by the cooling of the molecules before their ionization, resulting in mass spectra that are richer in information. Collisions with the make up gas at the expanding supersonic jet reduce the internal vibrational and rotational energy of the analyte molecules, hence reducing the degree of fragmentation caused by the electrons during the ionization process. The enhanced molecular ions increase the identification probabilities of both known and unknown compounds, amplify isomer mass spectral effects and enable the use of isotope abundance analysis for the elucidation of elemental formulae. Chemical ionization In chemical ionization a reagent gas, typically methane or ammonia is introduced into the mass spectrometer. A softer ionization fragments the molecule to a lower degree than the hard ionization of EI. One of the main benefits of using chemical ionization is that a mass fragment closely corresponding to the molecular weight of the analyte of interest is produced. In positive chemical ionization PCI the reagent gas interacts with the target molecule, most often with a proton exchange. This produces the species in relatively high amounts. In negative chemical ionization NCI the reagent gas decreases the impact of the free electrons on the target analyte. This decreased energy typically leaves the fragment in great supply. Analysis[edit] A mass spectrometer is typically utilized in one of two ways: The typical GC-MS instrument is capable of performing both functions either individually or concomitantly, depending on the setup of the particular instrument. The primary goal of instrument analysis is to quantify an amount of substance. This is done by comparing the relative concentrations among the atomic masses in the generated spectrum. Two kinds of analysis are possible, comparative and original. Comparative analysis essentially compares the given spectrum to a spectrum library to see if its characteristics are present for some sample in the library. This is best performed by a computer because there are a myriad of visual distortions that can take place due to variations in scale. Computers can also simultaneously correlate more data such as the retention times identified by GC , to more accurately relate certain data. Deep learning was shown to lead to promising results in the identification of VOCs from raw GC-MS data [18] Another method of analysis measures the peaks in relation to one another. The total mass of the unknown compound is normally indicated by the parent peak. The value of this parent peak can be used to fit with a chemical formula containing the various elements which are believed to be in the compound. The isotope pattern in the spectrum, which is unique for elements that have many natural isotopes, can also be used to identify the various elements present. Once a chemical formula has been matched to the spectrum, the molecular structure and bonding can be identified, and must be consistent with the characteristics recorded by GC-MS. Typically, this identification is done automatically by programs which come with the instrument, given a list of the elements which could be present in the sample. Conversely, selective ion monitoring SIM only monitors selected ions associated with a specific substance. This is done on the assumption that at a given retention time, a set of ions is characteristic of a certain compound. This is a fast and efficient analysis, especially if the analyst has previous information about a sample or is only looking for a few specific substances. When the amount of information collected about the ions in a given gas chromatographic peak decreases, the sensitivity of the analysis increases. So, SIM analysis allows for a smaller quantity of a compound to be detected and measured, but the degree of certainty about the identity of that compound is reduced. The determination of what range to use is largely dictated by what one anticipates being in the sample while being cognizant of the solvent and other possible interferences. Additionally if one is to use a large scan range then sensitivity of the instrument is decreased due to performing fewer scans per second since each scan will have to detect a wide range of mass fragments. Full scan is useful in determining unknown compounds in a sample. It provides more information than SIM

when it comes to confirming or resolving compounds in a sample. During instrument method development it may be common to first analyze test solutions in full scan mode to determine the retention time and the mass fragment fingerprint before moving to a SIM instrument method. Selective ion monitoring[edit] In selective ion monitoring SIM certain ion fragments are entered into the instrument method and only those mass fragments are detected by the mass spectrometer. The advantages of SIM are that the detection limit is lower since the instrument is only looking at a small number of fragments e. More scans can take place each second. Since only a few mass fragments of interest are being monitored, matrix interferences are typically lower. To additionally confirm the likelihood of a potentially positive result, it is relatively important to be sure that the ion ratios of the various mass fragments are comparable to a known reference standard. Applications[edit] Environmental monitoring and cleanup[edit] GC-MS is becoming the tool of choice for tracking organic pollutants in the environment. The cost of GC-MS equipment has decreased significantly, and the reliability has increased at the same time, which has contributed to its increased adoption in environmental studies. Criminal forensics[edit] GC-MS can analyze the particles from a human body in order to help link a criminal to a crime. Law enforcement[edit] GC-MS is increasingly used for detection of illegal narcotics, and may eventually supplant drug-sniffing dogs. It involves identifying an acid metabolite of tetrahydrocannabinol THC , the active ingredient in marijuana, in urine samples by employing derivatization in the sample preparation. In drug screening, GC-MS methods frequently utilize liquid-liquid extraction as a part of sample preparation, in which target compounds are extracted from blood plasma. These systems run on a host of technologies, many of them based on GC-MS. Chemical warfare agent detection[edit] As part of the post-September 11 drive towards increased capability in homeland security and public health preparedness, traditional GC-MS units with 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. Chemical engineering[edit] GC-MS is used for the analysis of unknown organic compound mixtures. One critical use of this technology is the use of GC-MS to determine the composition of bio-oils processed from raw biomass. GC-MS is extensively used for the analysis of these compounds which include esters , fatty acids , alcohols , aldehydes , terpenes etc. It is also used to detect and measure contaminants from spoilage or adulteration which may be harmful and which is often controlled by governmental agencies, for example pesticides. Two were brought to Mars by the Viking program. GC-MS can determine compounds in urine even in minor concentration. These compounds are normally not present but appear in individuals suffering with metabolic disorders. This is increasingly becoming a common way to diagnose IEM for earlier diagnosis and institution of treatment eventually leading to a better outcome. It is now possible to test a newborn for over genetic metabolic disorders by a urine test at birth based on GC-MS. In combination with isotopic labeling of metabolic compounds, the GC-MS is used for determining metabolic activity. Most applications are based on the use of ^{13}C as the labeling and the measurement of ^{13}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.

Chapter 2 : GCMS Application Data Sheet : SHIMADZU (Shimadzu Corporation)

Instrumentation 2 The GC-MS is composed of two major building blocks: the gas chromatograph and the mass spectrometer The gas chromatograph utilizes a capillary column which depends on the column's dimensions (length, diameter, film thickness) as well as the phase properties.

Advanced Search Abstract The development of one comprehensive gas chromatographic-triple quadrupole mass spectrometric GC-MS-MS method for the analysis of nerve agents and their breakdown products can pose a challenge due to significant differences in analyte volatility. Nerve agent breakdown products typically have a low volatility, requiring a derivatization step prior to analysis by gas chromatography GC. However, nerve agent parent compounds are generally more volatile, which eliminates the need for derivatization and allows for direct analysis. Therefore, the analysis of these analytes is typically performed using separate analytical methods. This may require the use of multiple columns composed of different stationary phases to ensure the most efficient separation. Chromatographic separation and multiple-reaction mode electron ionization detection of the nerve agents and silylated breakdown product derivatives were performed using an Agilent A gas chromatography GC equipped with a mid-polarity column, coupled to a triple quadrupole mass spectrometry system. The feasibility of this method for nerve agent and breakdown product detection in real samples was demonstrated using nerve agent-spiked human plasma at various exposure times 3 min, 1 h and 24 h. Five of the six nerve agents and all six breakdown products were successfully detected. This robust method has utility as a rapid screening tool to identify a specific nerve agent in a potential exposure event by simultaneous detection of the parent and or its corresponding breakdown product in plasma. First developed in , they gained popularity during World War II as they were synthesized as weapons of war. Recent nerve agent use has been reported in the news 1 , 2. Several months later, there was a suspected sarin attack on Syrian civilians by the Syrian government. It is the inhibition of AChE that poses a serious threat to human health. AChE enzymes catalyze the breakdown of acetylcholine, which is necessary for nerve impulse transmission. Exposure to these extremely toxic chemicals can typically be characterized by miosis, salivation and convulsions and other neurological manifestations that can ultimately result in death. There is a short latency period, dependent on dose and route, so symptoms can present in minutes 3. The V series agents are the most toxic of the nerve agents, with low volatility, and are highly stable and persistent in the environment. Primary routes of exposure are skin, eye and inhalation 4. However, their high volatility makes them highly lethal when inhalation is the route of exposure. AChE-adducted and BChE-adducted nerve agents can persist for as short as minutes to days typically G agents before they undergo an irreversible aging process, spontaneous enzymatic reactivation or hydrolysis 6. AChE-adducted and BChE-adducted nerve agents can be found in the red blood cells and plasma of humans, respectively. The reactivation and hydrolysis processes form alkyl methylphosphonic acid AMPA breakdown products in the blood, which are rapidly excreted in the urine 7. The AMPAs can each serve as a marker of exposure, since they can be found in biological matrices such as urine, plasma and serum. They are less toxic and less volatile than their precursor; therefore they require derivatization for detection by GC. Structural depiction of nerve agents and their corresponding breakdown products. View large Download slide Structural depiction of nerve agents and their corresponding breakdown products. The existing detection schemes for nerve agents or their breakdown products include chromatographic, electrochemical, colorimetric and spectrometric techniques 8 While a myriad of published methods have successfully detected nerve agents or AMPAs, currently no single method can simultaneously detect both the nerve agent and breakdown product. The nerve agents are mostly volatile, making GC the more suitable approach. On the other hand, liquid chromatography is ideal for the breakdown products. Each of these limitations likely contributes to the absence of a comprehensive method. This present paper describes a method that can simultaneously detect GC-amenable nerve agents and non-volatile polar breakdown products in an individual sample using one column. The GC is suitable for chromatographic separation of both nerve agents and breakdown products with the use of a mid-polarity column and the application of a derivatizing reagent. The nerve agents remain intact and maintain their volatility. This paper

will present a rapid Hydrochloric acid HCl molecular biology grade, The structures of each compound are illustrated in Figure 1. Pooled plasma with sodium heparin was purchased from Bioreclamation Hicksville, NY. A seven-point calibration curve was prepared in IPA at concentrations ranging from 1. The derivatization step was completed each day for the inter-day study. Instrument analysis Analysis was performed using an Agilent A GC system coupled to a triple quadrupole mass spectrometry system. Helium carrier gas was set to a flow rate of 1. Multiple-reaction monitoring MRM mode was selected for the acquisition of data, to minimize interferences from the matrix, resulting in improved sensitivity and selectivity of the CWA. Positive electron impact ionization was employed using the parameters summarized in Table I.

Chapter 3 : Introduction to hyphenated techniques and their applications in pharmacy

spectrometry (GC-MS) is an analytical method that combines the features of gas-liquid chromatography and mass spectrometry to identify different substances within.

This represents the latest in technology. Its development was aided through research sponsored by the National Research Council of Canada. The methods used also comply with ASTM guidelines. Our services have been designed specifically for the needs of the Arson Investigator and have been thoroughly designed through interviews with investigators. This includes the pre-sampling information, detailed chain-of-custody, legal sample tracking, review by a Chartered Chemist, to a concise and carefully laid out final report. Our instrumentation is the most sensitive available. This is important for samples that have been in the field, held in storage for months, and for highly weathered samples. This analysis has improved sensitivity, but most importantly, results in new daughter ion mass spectra. This significantly improves the confidence in the identification of ignitable liquid components. This re-analysis will be at no extra charge to the client. Introduction Activation Laboratories Ltd. We use this as a secondary confirmation analysis on weak, complex, or highly weathered samples. This method is designed to provide a better analysis for weak, highly weathered or older samples. It is particularly well suited for the detection of gasoline and can be used on any sample. This technique is increasingly becoming the analytical tool of choice when analyzing target compounds in very complex matrices. How Does it Work? These selected precursor ions or parent ions are then induced to further dissociate by collision with Helium molecules. The resultant unique product ion spectrum provides confirmation of the target analyte. As gasoline is one of the more common distillates used by arsonists, the identification of gasoline in fire debris samples is important. The question has been posed. The hydrocarbons detected must also be present in ratios that define a fingerprint to each other that is then similar to a known ignitable liquid reference materials that has been obtained and analyzed under the same conditions. How defensible is it in court? It has been used in the Environmental and Pharmaceutical fields as well as in the Drug Testing area of the Forensic field. This method has been presented in court in the analyses of fire debris in How does it compare to the sensitivity of the K9? Our goal is to complement the use of the K9, and ideally obtain a similar level of sensitivity and specificity. In our observations we believe we are approaching the sensitivity of the average K9 on relatively typical fire debris.

Chapter 4 : GC-MS: an ideal tool for forensic analysis

Gas chromatography-mass spectrometry (GC-MS) is an analytical method that combines the features of gas-chromatography and mass spectrometry to identify different substances within a test sample.

Stephen Harrison, Linde Gas Viewed: GC-MS can be harnessed across the entire value chain in the oil and petrochemical arena, from the prospecting stage to the refining process to monitor and improve quality, to final refined and formulated fuels and lubricants, as well as to ensure compliance with environmental standards, and even as a forensic tool in criminal cases in which fuel has been used to perpetrate arson. Conducting quantitative work alone on a sample with unknown content can be fruitless. The qualitative method is especially relevant to research applications and lays the correct foundation for the analysis. Only when it is known which chemicals are present can the quantitative analysis be performed. The GC principle is that molecules in a sample separate in the chromatography column because of differences in their chemical properties. The MS breaks the components as they exist from the column into ionised species and separates these based on their mass-to-charge ratio. This is the great advantage of the combination of GC as the first separation step and the MS as the qualitative detector. It is one of few techniques to determine exactly what is in a sample. Characterised by its quick screening abilities, GC-MS has been widely heralded as the gold standard for forensic substance identification. On the same standing with GC-MS, liquid chromatography-mass spectrometry LC-MS is also a qualitative analytical chemistry technique that combines the physical separation capabilities of high-performance liquid chromatography with the qualitative analysis capabilities of mass spectrometry. Both techniques involve using a mass spectrometry detector, but GC-MS is used to screen a sample using a gaseous-phase component separation process in the gas chromatography column, while LC-MS is able to detect and identify chemicals using a liquid- phase component separation process in the liquid chromatography column. The medium in which the sample exists and is most effectively separated in the chromatography column, gaseous or liquid, determines which technique is more appropriate. However, GC-MS is preferred when quick screening is required because the column separation is generally faster in the gaseous phase. Sample preparation In the petrochemical sector, GC-MS can be dynamically applied across a broad range of applications. However, critical to the success of the analytical process is the correct handling and preparation of the sample. Samples requiring GC-MS analysis could include heavy liquids, such as tars, which behave like solids, or solids such as coal. In cases like this, analysts are able to use Pyrolysis mass spectrometry MS to convert the sample into the gaseous phase required for characterisation by GC-MS. Pyrolysis MS is an important technique in the overall analysis armoury and has been hailed for its ability to analyse small amounts of material with minimum sample preparation to obtain, within minutes, fingerprint data that can be used for identification and typing. Pyrolysis MS samples are heated up so rapidly to very high temperatures that they convert from solid to gaseous phase instantaneously and can then be passed through the GC-MS process. Another sample preparation technique is called thermal desorption mass spectrometry TDMS. This technique involves collecting desorbed molecules from a surface when the surface temperature is increased and then introducing these individual components into the GC-MS process. This method is commonly used to analyse volatile organic compounds, commonly the source of odours in the ambient air, either inside a building or outside in the open air. Samples are collected using thermal desorption tubes. As drilling proceeds, exploration personnel need to determine the value of the resources they come across. GC-MS will be able to tell you exactly what you have uncovered. It is the perfect tool for determining the quality of the stream of crude oil or natural gas emanating from the well. A significant part of the financial valuation of petrochemical companies is based on the reserves that companies believe they hold – much more than the value of their processing assets, ships or oil rigs. It is all about the potential value of the oil field that the company has rights to. Therefore, an accurate assessment of the quality of these reserves is absolutely critical for a fundamental evaluation of the reserves being declared. A technique such as GC-MS can play a fundamental role in quantifying the value of such oil field reserves. The most typical use of GC-MS in the petrochemical industry it is for process troubleshooting. The composition of crude oil is never consistent,

creating the opportunity for operational problems to arise as raw material feedstock changes between incoming crude oil batches. Production pressures require the source of the problem to be identified as quickly as possible and very often the best way to achieve this is to use GC-MS as a forensic tool to identify the presence and type of chemical responsible and at what point it entered the process.

Chapter 5 : Gas chromatography – mass spectrometry - Wikipedia

Major Applications of GC-MS with Cold EI. GC-MS with Cold EI (also known as Supersonic GC-MS) can be applied with few major advantages to practically all GC-MS analysis types as demonstrated in it over publications and applications listed below.

Presentation Transcript PowerPoint Presentation: Introduction 1 Gas chromatography-Mass spectroscopy GC-MS is one of the so-called hyphenated analytical technique As the name implies, it is actually two techniques that are combined to form a single method of analyzing mixtures of chemicals Gas chromatography is a technique capable of separating, detecting and partially characterizing the organic compounds particularly when present in small quantity. Mass spectroscopy provides some definite structural information from in small quantity. Principle of GC-MS 2 The sample solution is injected into the GC inlet where it is vaporized and swept onto a chromatographic column by the carrier gas usually helium. The sample flows through the column and the compounds comprising the mixture of interest are separated by virtue of their relative interaction with the coating of the column stationary phase and the carrier gas mobile phase. The latter part of the column passes through a heated transfer line and ends at the entrance to ion source where compounds eluting from the column are converted to ions. This allows the mass spectrometer downstream to capture, ionize, accelerate, deflect, and detect the ionized molecules separately. The solvent must be volatile and organic for example, hexane or dichloromethane. Amount Depending on the ionization method, analytical sensitivities of 1 to pg per component are routine. Preparation Sample preparation can range from simply dissolving some of the sample in a suitable solvent to extensive. Clean up procedures using various forms of liquid chromatography. Limitation - small micromolar composition of the solute. Procedure still useful for qualitative analysis of multi-component. Interfacing GC with Spectroscopic Methods: The flow rate is usually small enough to feed directly into the ionization chamber of the Mass Spectrometer. Packed columns use a jet separator, which removes the carrier gas for the analyte. Lighter helium molecules are deflected by vacuum and pumped away. Use to identify components present in natural and biological systems. The GC effluent enters the vacuum region, those molecules which continue in the same direction enter the second capillary tube and continue to the ion source. Jet Separator The carrier gas molecules are more easily diverted from the linear path by collisions. The analyte molecules are much larger and carry more momentum. The surface of the separator must be inactive and a reasonably even temperature. Analysis A mass spectrometer is typically utilized in one of two ways: Environmental Monitoring and Cleanup GC-MS is becoming the tool of choice for tracking organic pollutants in the environment. The cost of GC-MS equipment has decreased significantly, and the reliability has increased at the same time, which has contributed to its increased adoption in environmental studies. There are some compounds for which GC-MS is not sufficiently sensitive, including certain pesticides and herbicides, but for most organic analysis of environmental samples, including many major classes of pesticides, it is very sensitive and effective. Portable GC units can be used to detect pollutants in the air, and they are currently used for vapor intrusion investigations. Criminal Forensics GC-MS can analyze the particles from a human body in order to help link a criminal to a crime. Law Enforcement GC-MS is increasingly used for detection of illegal narcotics, and may eventually supplant drug-sniffing dogs. Security A post-September 11 development, explosive detection systems have become a part of all US airports. These systems run on a host of technologies, many of them based on GC-MS. Two were brought to Mars by the Viking program. Medicine Dozens of congenital metabolic diseases also known as Inborn error of metabolism are now detectable by newborn screening tests, especially the testing using gas chromatography-mass spectrometry. These compounds are normally not present but appear in individuals suffering with metabolic disorders. This is an increasingly becoming a common way to diagnose IEM for earlier diagnosis and institution of treatment eventually leading to a better outcome. In combination with isotopic labeling of metabolic compounds, the GC-MS is used for determining metabolic activity. Food, Beverage and Perfume Analysis Foods and beverages contain numerous aromatic compounds, some naturally present in the raw materials and some forming during processing. GC-MS is extensively used for the analysis of these compounds which include

esters, fatty acids, alcohols, aldehydes, terpenes etc. It is also used to detect and measure contaminants from spoilage or adulteration which may be harmful and which is often controlled by governmental agencies, for example pesticides. LimitationS Only compounds with vapor pressures exceeding about 10^{-10} torr can be analyzed by gas chromatography-mass spectrometry GC-MS. Determining positional substitution on aromatic rings is often difficult. Certain isomeric compounds cannot be distinguished by mass spectrometry for example, naphthalene versus azulene, but they can often be separated chromatographically. References gas chromatography-mass spectroscopy from Wikipedia, The free encyclopedia. Principles and Instrumentation of gas chromatography-mass spectroscopy by W. Gas chromatography by U.

Chapter 6 : Applications - E2M | Bruker

The Application of a Single-Column GC-MS-MS Method for the Rapid Analysis of Chemical Warfare Agents and Breakdown Products Sheena A Young US Army Medical Research Institute of Chemical Defense, Ricketts Point Road, MD, USA.

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 with Cold EI in broad range of areas including: Petrochemical and hydrocarbons analysis Service and institution GC-MS analysis Entomology research Forensic analysis arson, explosives, drugs, unknowns High end research GC-MS Pesticide analysis, food safety and quality Pharmaceutical and drug analysis Clinical toxicology Food oils and fragrance We have experience with an extensive range of GC-MS with Cold EI applications, and perhaps one or few among those overlap with your field of interest. Thus, please communicate with us about your challenging applications and we shall be happy to develop a SMB GC-MS with Cold EI method for your application and needs, based on our discussions and your samples. We shall analyze your samples and provide you with a file of the results and our further suggestions and recommendations for your consideration. Note that the Aviv Analytical SMB GC-MS can serve as an alternative to many LC-MS analyses with several advantages including the ability to use library for easy sample identification plus isotope abundance analysis, having fragment information with extended structural and isomer information in a low cost single quad system, having uniform semi quantitative response unlike ESI that can provide semi-quantitative data for unknowns without calibration, elimination of ion suppression effects and the fact that GC-MS has a one easy-to-employ method that encompasses most of its applications in contrast to LC-MS that requires lengthy method development for each new sample.

Petrochemical and hydrocarbons analysis: Significantly enhanced molecular ions that are always observed, isomer and structurally significant mass spectral peaks and extended range of low volatility hydrocarbons that are amenable for analysis including waxes up to C₇₄H makes the SMB GC-MS with Cold EI a most valuable GC-MS, particularly in comparison with standard GC-MS that often fails to enable hydrocarbon identification due to lack of molecular ions. We analyzed broad range of petrochemicals, fuels and hydrocarbon mixtures, including gasoline, kerosene, naphthenic acids, diesel fuel, various oil types, transformer oil, Biodiesel, wax and broad range of geochemical samples. A special isomer abundance analysis method was developed for fuel characterization. We shall be happy to show you our results and demonstrate the capabilities of the SMB on your sample. For detailed information please read A. The combination of extended range and enhanced molecular ion is demonstrated in the enclosed Wax by SMB Figure. Enhanced and trustworthy molecular ions, extended range of thermally labile compounds amenable for analysis including all the major labile explosives, isotope abundance analysis software for improved sample identification, ChromatoProbe solid sample introduction device connected simultaneously with another column, Open Probe and ultra fast GC-MS analysis make GC-MS with Cold EI the ideal Forensic GC-MS system. Touch the sample, push it inside the GC-MS and get in a few seconds an accurate answer on the type of mixture or compound analyzed. Enhanced molecular ions, extended range of compounds amenable for analysis, superior sensitivity particularly for compounds that are the bottleneck of the whole analysis and faster analysis are the main attractive features of the GC-MS with Cold EI. Examples include much lower LOD for phthalates such as dinonylphthalate and didecylphthalate in the method analysis or much larger PAHs amenable for analysis such as decacyclene, ovalene and even C₆₀, degradation free analysis of carbamazepine and its metabolites in treated sewage water and steroid analysis without derivatization. Pesticide analysis and food safety: Enhanced molecular ions, extended range of pesticides amenable for analysis, superior sensitivity for those pesticides that are the bottleneck of the whole analysis and faster analysis are the main attractive features of the SMB GC-MS with Cold EI. The enhanced molecular ion and lack of ion source peak tailing and degradation can further serve for improved sensitivity and selectivity. Isotope abundance analysis provides greater confidence level in the

pesticide identification. For further information please read M. Pharmaceutical and drug analysis: In addition, unlike LC-MS the SMB GC-MS with Cold EI provides quantitative information on drug synthesis yield and on the abundance of drug contamination, it has no ion suppression effects and the analysis are fast, under 8 min analysis cycle time. Our SMB is the only mass spectrometry system with uniform, approximately compound independent response, which as a result enables the quantitative determination of drug impurities without their identification and response calibration. Enhanced molecular ions, extended range of compounds amenable for analysis, superior sensitivity for compounds that are the bottleneck of the whole analysis and faster analysis are the main attractive features of GC-MS with Cold EI for clinical toxicology. Enhanced molecular ions, isotope abundance analysis software for improved unknown sample identification, unique isomer mass spectral effects and compatibility with pulsed flow modulation GCxGC-MS make GC-MS with Cold EI the ideal GC-MS for the food and fragrance industry as an information generation machine. High end research GC-MS: GC-MS with Cold EI can be used in all types of research and enable you to lead the way and obtain cutting edge new results. Please communicate with us and we shall be happy to analyze your challenging sample and demonstrate how GC-MS with Cold EI can help you. Service and institution GC-MS: Enhanced and trustworthy molecular ions, significant structural and isomer mass spectral effects, TAMI isotope abundance analysis software for improved sample identification and for the provision of elemental formulas as required for journal publications and significantly extended range of low volatility and thermally labile compounds amenable for analysis are all attractive features of GC-MS with Cold EI for service and institution GC-MS. Combined with the provision of fast, real time analysis what else can be requested from institutional service GC-MS. It is truly the ideal GC-MS for institutes. Thus, this technology was extensively evaluated and proved its effectiveness and usefulness in broad range of applications. Please brows through the list of applications below to find your specific application or area of interest and please ask us about it as we also worked on many other unlisted applications. We shall be happy to discuss your challenging application and analyze your sample thus please contact us about having any of the application below and about information on your specific application with the SMB. Aviv Amirav, Alexander B. Fialkov, Urs Steiner, Steven J. Spectrom , Marina Poliak, Alexander B. Iliia Brondz, Alexander B. Importance of 5-Hydroxytryptophane pathway in biogenesis of alkaloids in mushrooms" Trends in Chromatography Chan "Resolving detailed molecular structures in complex organic mixtures and modelling their secondary organic aerosol formation", Atmospheric Environment , Uri Keshet, Alexander B. Amirav "The pre-separation of oxygen containing compounds in oxidised heavy paraffinic fractions for identification by Supersonic Molecular Beams Mass Spectrometry".

Chapter 7 : GCMS | Gas Chromatography Mass Spectrometry Instruments | PerkinElmer

Gas chromatography-mass spectrometry (GC-MS) is used to gain qualitative results of detected metabolites for biological samples as it provides superior distinguish ability, detection sensitivity.

Chapter 8 : Aviv Analytical - Major Applications of GC-MS with Cold EI

Today, gas chromatography/mass spectrometry (GC/MS) is a well-established technique used routinely in many industrial applications for the analysis of volatile and semivolatile materials.

Chapter 9 : Application Finder | Agilent

What is GC/MS/MS? Gas Chromatography coupled to Tandem Mass Spectrometry (GC/MS/MS) is used to separate the organic compounds in the mixture (fire debris). This technique is increasingly becoming the analytical tool of choice when analyzing target compounds in very complex matrices.