Providing Complete Mass Spectrometry Solutions

Mass spectrometry is a powerful analytical tool for chemical analysis and life sciences. It can be used to identify unknown compounds, to quantify known compounds, and to obtain information about chemical structure. The ability of mass spectrometry to do all of this for minute amounts of chemicals—often less than a billionth of a gram—make it a highly useful analytical technique in both established and emerging branches of science.

Mass spectrometers are often used in connection with devices that can separate a mixture of chemicals via either a gas phase, in which the sample is vaporized (gas chromatography, or GC), or a liquid phase, in which the sample is dissolved in a solvent (liquid chromatography, or LC; capillary electrophoresis, or CE; and supercritical fluid chromatography, or SFC).

With each of these techniques, the complex mixture that enters the separation device exits into the mass spectrometer as a series of partially or totally separated chemical entities. This separation process makes it far easier to identify each compound in the original sample.

Agilent has long been a leading supplier of gas chromatographs, liquid chromatographs, and mass spectrometers as well as combined GC/MS and LC/MS systems. Agilent is a leading supplier of CE/MS solutions that combine the orthogonal, high separation efficiency of CE with molecular weight and structural information of mass spectrometry for complex sample matrices. Agilent also offers SFC/MS instruments, which are well suited for chiral separations and hydrophobic molecules such as lipids.

Agilent is also the leading supplier of inductively coupled plasma mass spectrometry (ICP-MS) instruments, used for the separation and detection of individual inorganic analytes rather than organic compounds. With its high-temperature plasma ion source and sensitive ion-counting detector, ICP-MS enables scientists to characterize the elemental composition of samples from sub-ng/L (part per trillion) to % levels. ICP-MS can also be used as a sensitive, specific detector for GC, LC, or CE. This allows identification and quantitation of organic compounds that contain a heteroatom that can be measured by ICP-MS.

These products have earned a reputation for excellent performance, reliability, and ease of use. Agilent also provides

HOW IT WORKS

All matter is composed of elements or mixtures of elements combined to form organic molecules or inorganic compounds. Mass spectrometry, or MS, can be used to measure the organic or inorganic composition of a sample by separating and detecting which molecules or compounds are present. In the “source” of the mass spectrometer, molecules or elemental atoms are transformed (ionized) to give charged molecules, fragments of molecules or individual elemental ions, which have a characteristic mass-to-charge ratio (m/z). These ions are transferred into a vacuum system where the mass spectrometer is located. Electrical fields are used to guide and deflect the ions allowing separation of the mixture of ions based upon differences in each ion’s m/z.

A plot of the intensity (response) of each ion versus m/z is called a mass spectrum. An elemental mass spectrum shows the peak intensity (counts) for each element’s characteristic atomic mass (m/z 75 for arsenic, m/z 238 for uranium, and so on), allowing quantitation of the concentration of each element. When an organic molecule fragments into smaller ions, the sum of all of the ions plotted as a mass spectrum gives a spectral fingerprint for the structure of the original compound. Each ion carries specific information about the original molecule with an indication of the structure of that ion. Scientists can compare organic mass spectra to commercial MS databases to identify chemicals the way detectives use fingerprints to identify people.
unmatched expertise in support solutions, application development, and data interpretation tools.

APPLICATIONS

Mass spectrometry has an extremely wide range of molecular and elemental applications.

Pharmaceuticals: Mass spectrometry plays an important role in the entire lifecycle of a drug, from discovery to development to manufacturing. In drug discovery, LC/MS systems are the method of choice for identifying and characterizing drug candidates produced by combinatorial chemistry or extracted from natural products. LC/MS is also a primary tool used to check the quality of drug compounds and the presence of organic contaminants during manufacturing. Similarly, ICP-MS is used in drug development and to measure the levels of inorganic contaminants and catalyst residues (elemental impurities) in drug products, to confirm compliance with regulatory limits.

Biopharmaceuticals: Mass spectrometry is growing in importance as a tool to confirm intact protein mass, major glycoforms, and other post-translational modifications. These are critical measurements for characterizing therapeutic proteins and understanding their efficacy and stability. Protein and peptide quantitation is an emerging application for both ICP-MS and LC-ICP-MS, where the protein can be quantified based on the measured response for phosphorus. Furthermore, laser ablation ICP-MS supports bio imaging of tagged proteins making it possible to map the distribution of the metal containing protein tissue.

Proteomics: Proteomics is the large-scale analysis of proteins for disease research and drug discovery. MS analysis is a fundamental tool for proteomic research. In addition to LC/MS instruments for identifying and quantifying proteins in biological samples, Agilent has developed wide range of complementary technologies to help researchers prepare, separate, analyze, identify, and interpret challenging protein samples.

Metabolomics: In this area of research, scientists study large sets of metabolites found in biological samples at a given time, looking for correlations with good health or various diseases. Agilent is a leading provider of tools to metabolomics scientists, including sample-preparation supplies, GC/MS, LC/MS, CE/MS, and LC-ICP-MS instruments, software for identifying compounds using metabolite databases and libraries, and software for comparing samples and projecting the results onto biological pathways.

Environment: The ability to identify and quantify pollutants is essential to maintaining a healthy environment. Agilent is the worldwide leader in GC/MS, the mainstay of environmental testing for organic pollutants, used to detect volatile and semivolatile organic compounds such as pesticides and poly-aromatic hydrocarbons. The company’s LC/MS systems, a popular complement to GC/MS, are used to analyze nonvolatile chemicals and more fragile chemicals that may thermally degrade during GC/MS analysis. Agilent’s ICP-MS is the premier instrument for analysis of inorganic environmental contaminants and, coupled to a chromatography system, ICP-MS also provides accurate trace analysis for organometallic compounds such as methyl mercury and organo tin.

Food safety: Testing food for harmful chemicals and bacteria is a vital aspect of public safety and international trade. Agilent GC/MS, LC/MS, and ICP-MS systems are widely used to detect and analyze additives, residues, contaminates, essential nutrient elements, and toxic trace elements in agricultural products, foods, and beverages. Several factors are driving the growing need for food testing: global trade, stringent regulations, and increased public awareness of food-safety issues.

Forensics: Agilent is the leading provider of GC/MS systems for drug screening and toxicology worldwide. Forensic scientists also use the company’s LC/MS systems as a complement to GC/MS. Agilent’s ICP-MS systems can be used to identify the presence of toxic elements in poisoning cases, analyze gunshot residue and scene of crime debris, and, coupled to laser-ablation technology, provide direct measurement of solid samples and elemental fingerprinting of materials in forensic investigations.
**Hydrocarbon processing and energy research:** Companies in the hydrocarbon-processing industry produce petroleum, petrochemicals, plastics, fine and specialty chemicals, natural gas, industrial gas, and fuel cells. These enterprises routinely use Agilent mass spectrometers, particularly GC/MS systems, to analyze product quality and process performance. ICP-MS is used to monitor the levels of environmental contaminants in fuels, confirm the levels of fuel additives, and measure metals that may act as catalyst poisons. Agilent MS systems are also widely used to analyze feedstocks, intermediate products, and finished biofuels.

**Semiconductors:** Agilent provides high-performance ICP-MS and GC/MS instrumentation to accurately identify and quantify trace level contaminants in the ultra-high purity materials used in semiconductor fabrication. Major applications include the characterization of ultra-pure water and bulk and process chemicals used in manufacturing semiconductors, the analysis of organic and metal contaminants on the surface of silicon wafers, and the analysis of volatile organic solvents used when manufacturing disk drives, circuit boards, and other electronic components.

**KEY PRODUCT LINES**

**Agilent’s GC/MS** portfolio includes the most sensitive, selective, reliable, and feature-rich systems on the market.

**Agilent’s LC/MS** systems provide unparalleled capabilities for reliable, reproducible analysis of a wide variety of analytes.

**Agilent ICP-MS and ICP-QQQ** instruments deliver exceptional sensitivity, freedom from interferences, and accurate routine analysis of complex, high-matrix samples. Coupled to a chromatographic separation device (LC, GC, CE), ICP-MS provides high sensitivity and very specific quantitation of organometallic compounds.

**Agilent CE/MS** solution provides an orthogonal approach that is an ideal complement to chromatographic LC/MS analysis.

**Agilent’s SFC/MS** solution provides the researcher the ability to easily switch between HPLC and SFC techniques to find the best separation for a given sample.

**Agilent MassHunter Workstation** provides a comprehensive portfolio of software for LC/MS, CE/MS, ICP-MSGC/MS, and SFC/MS. It offers a single, consistent user experience across all Agilent MS platforms.

**The Agilent 1260 Infinity HPLC-Chip/MS** system is a reusable microfluidic chip-based technology for high sensitivity nanospray LC/MS. Comprehensive integration of columns and connectors combined with intuitive operation make this high performance chip the perfect option for many applications, including proteomics and small molecule analysis.

**The mAb-Glyco chip kit** significantly increases productivity in N-glycan related applications by combining trapping of sample, enzymatic cleavage, and separation of glycans with MS detection. A custom chip program delivers user-defined capabilities to scientists for increased efficiency and flexibility beyond the Agilent standard chip program.