Basic Concepts

Mass Spectrometry (MS) is an analytical technique used to determine the molecular mass and structure of a compound.

It involves ionizing a sample, separating the ions based on their mass-to-charge ratio (m/z), and detecting them to generate a mass spectrum.

Mass Detectors

Electron Multiplier: Converts ions into electrons, amplifying the signal for detection.

Faraday Cup: Collects and measures the current generated by ions striking a metal surface.

Photomultiplier Tube (PMT): Converts ions into photons, which are then amplified and detected.

Applications

Identification of Unknown Compounds: MS can be used to determine the elemental composition and structure of an unknown compound.

Quantitative Analysis: MS can measure the abundance of specific compounds in a sample using techniques like Selected Ion Monitoring (SIM) or Multiple Reaction Monitoring (MRM).

Proteomics: MS is extensively used to analyze proteins, peptides, and post-translational modifications.

Ionization Techniques

Electron Ionization (EI): Involves bombarding the sample with high-energy electrons, resulting in the formation of radical cations (M+•).

Electrospray Ionization (ESI): Suitable for polar and large molecules. It involves the formation of charged droplets from a nebulized sample, which subsequently undergo desolvation to form ions.

Matrix-Assisted Laser Desorption/Ionization (MALDI): Suitable for large biomolecules. Involves co-crystallizing the sample with a matrix compound and using a laser to ionize the analyte.

Tandem Mass Spectrometry (MS/MS)

MS/MS involves performing multiple stages of mass spectrometry, usually involving precursor ion selection, fragmentation, and product ion analysis.

Common techniques include Collision-Induced Dissociation (CID) and Electron Transfer Dissociation (ETD).

Mass Analyzers

Time-of-Flight (TOF): Measures the time taken for ions to reach the detector based on their m/z ratio.

Quadrupole: Uses a combination of direct current (DC) and radio frequency (RF) voltages to selectively transmit ions of a specific m/z ratio.

Ion Trap: Uses an electric field to trap and store ions, allowing their m/z ratios to be selectively scanned.

Data Interpretation

Molecular Ion (M+•): Represents the intact molecule after ionization.

Base Peak: The most intense peak in a mass spectrum, assigned a relative abundance of 100%.

Fragmentation: The process of breaking down the molecular ion into smaller fragments, providing structural information.

Isotopes: Different forms of an element with varying numbers of neutrons, resulting in peaks at different m/z values.

Also Read

Mass Spectrometry (MS) – Principle, Parts, Working, Steps, Uses

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