



APPLICATION OF MASS SPECTROMETRY IN ANALYTICAL CHEMISTRY: AN ADVANCED ACADEMIC REVIEW FOR INTERNATIONAL CONFERENCES

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Introduction

Mass spectrometry (MS) in the 21st century has evolved from a highly specialized physicochemical method into a central platform of analytical science. Due to its combination of extremely high sensitivity (down to 10^{-15} – 10^{-18} mol), selectivity, and capability for structural elucidation, MS plays a key role in the development of systems biology, metabolomics, proteomics, pharmacokinetics, and environmental monitoring. Modern mass spectrometric approaches are characterized by integration with chromatography, capillary electrophoresis, and computational methods for big data processing, which allows MS to be considered the core of multi-omics analytical platforms.

Physicochemical Fundamentals of Mass Spectrometry

The foundation of mass spectrometry is based on ionization processes, gas-phase ion dynamics, and their interaction with electromagnetic fields. Ion motion is described by the Lorentz equations, while separation according to the mass-to-charge ratio (m/z) is determined by the parameters of electric and magnetic fields.

A key characteristic is the resolving power (R):

$$R = m \backslash \Delta m$$

where Δm is the minimum mass difference distinguishable by the instrument. Modern high-resolution instruments (Orbitrap, FT-ICR) achieve $R > 10^5$ – 10^6 , enabling precise mass measurements with an error of less than 1 ppm. Another critical parameter is mass accuracy, which determines the ability



to establish the elemental composition of molecules. Advanced Ionization Techniques. Modern research активно employs “soft” ionization methods that minimize fragmentation:

- ESI (Electrospray Ionization)

Enables the transfer of ions from solution into the gas phase without structural destruction. It is used for the analysis of proteins with molecular masses >100 kDa.

- MALDI (Matrix-Assisted Laser Desorption/Ionization)

Effective for the analysis of biopolymers and tissue imaging (MALDI imaging).

- APCI (Atmospheric Pressure Chemical Ionization)

Applied to less polar compounds.

- DESI (Desorption Electrospray Ionization)

Allows direct analysis from the sample surface without prior preparation (ambient MS).

The development of ambient ionization is particularly important, enabling real-time *in situ* analysis.

Tandem Mass Spectrometry (MS/MS)

Tandem MS is a key tool for structural analysis and includes the following stages:

1. Selection of the precursor ion
2. Fragmentation (CID, HCD, ETD)
3. Analysis of product ions

Fragmentation methods:

- CID (Collision-Induced Dissociation)
- HCD (Higher-energy Collisional Dissociation)
- ETD (Electron Transfer Dissociation) — especially important for

the analysis of post-translational modifications of proteins



MS/MS provides structural identification of compounds, including isomers and isobars.

High-Resolution Mass Spectrometry (HRMS)

Modern high-precision systems include:

- Orbitrap
- FT-ICR (Fourier Transform Ion Cyclotron Resonance)

They enable:

- determination of exact mass with an error <1 ppm
- differentiation of compounds with minimal mass differences
- non-target analysis

HRMS is a key tool in exposomics and environmental chemistry.

Hyphenated Techniques: Chromatography–Mass Spectrometry

The combination of MS with separation techniques is a standard approach:

- GC-MS — for volatile compounds
- LC-MS — for thermolabile and polar substances
- UHPLC-MS/MS — high speed and sensitivity

These methods allow the analysis of highly complex matrices such as blood, urine, food products, and soil.

Omics Technologies and Mass Spectrometry

MS is the core of the following fields:

- Proteomics — identification and quantitative analysis of proteins
- Metabolomics — analysis of low-molecular-weight metabolites
- Lipidomics — study of lipid profiles
- Glycomics — analysis of carbohydrates

Approaches used include:

- Targeted analysis (SRM/MRM)
- Untargeted analysis (full scan, data-dependent acquisition)
- Data-independent acquisition (DIA)



Data Processing and Artificial Intelligence

Modern MS generates large datasets (big data) requiring advanced processing:

- spectral deconvolution algorithms
- databases (MassBank, METLIN, HMDB)
- machine learning for pattern recognition
- neural network models for compound identification

AI is actively used for automated spectral annotation and structure prediction.

Advanced Application Areas

- Personalized medicine
 - disease biomarkers
 - pharmacometabolomics
- Exposomics
 - analysis of environmental impacts on the organism
- Pharmaceutical research
 - ADME (absorption, distribution, metabolism, excretion)
- Next-generation forensics
 - rapid detection of drugs and toxins
- Space chemistry and astrobiology
 - analysis of organic compounds in meteorites

Conclusion

Mass spectrometry today is not merely an analytical method but a universal scientific platform integrating physics, chemistry, biology, and informatics. Its development defines the future of analytical science, enabling a transition to high-precision, personalized, and predictive analytics.



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