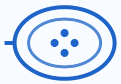
Mass Analyzers: Comprehensive Guide

Quadrupole Filters

- Four parallel rods with RF/DC voltages
- Sequential ion transmission
- Good for targeted analysis

Time-of-Flight (TOF)

- Velocity-based separation
- High mass accuracy
- Unlimited mass range



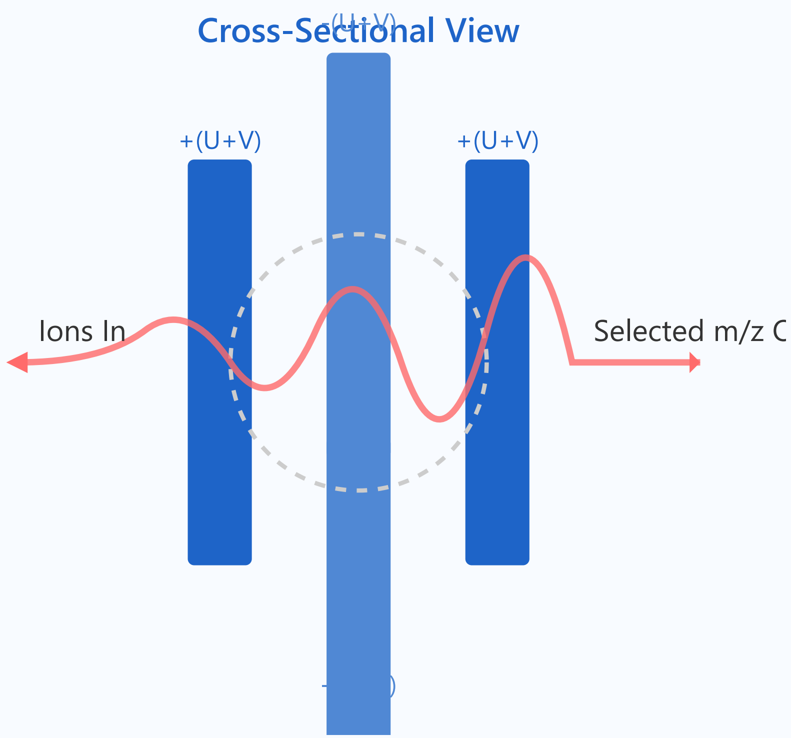
Orbitrap Technology

- Ion orbital trapping
- Ultra-high resolution (>100,000)
- Excellent mass accuracy (<1 ppm)

Ion Trap & Hybrid

- 3D ion confinement
- Multiple MS/MS stages
- Q-TOF, Q-Orbitrap combinations

1 Quadrupole Mass Filters



Operating Principle

Quadrupole mass filters consist of four parallel cylindrical or hyperbolic rods arranged symmetrically. Opposite rods are electrically connected and have the same polarity. A combination of DC (U) and RF (V cos ωt) voltages is applied to create an oscillating electric field.

Ions entering the quadrupole experience forces in both x and y directions. Only ions with a specific mass-to-charge ratio (m/z) maintain a stable trajectory and pass through to the detector. All other ions have unstable trajectories and collide with the rods.

⚡ **Mass Selection**
Scanning U and V while maintaining their ratio allows sequential transmission of different m/z values

🎯 **Resolution**
Unit resolution (1 Da) is typical, adequate for most quantitative applications

Scan Speed
Fast scanning capability (up to 10,000 Da/s) enables rapid analysis

Common Applications

- Quantitative analysis in LC-MS/MS (triple quadrupole)
- Environmental monitoring and pesticide analysis
- Pharmaceutical drug quantification
- Clinical diagnostics and therapeutic drug monitoring

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2 Time-of-Flight (TOF) Mass Analyzers

Operating Principle

TOF analyzers separate ions based on their velocities in a field-free flight tube. Ions are accelerated by an electric field to a kinetic energy determined by their charge. Since $KE = \frac{1}{2}mv^2$, ions with different m/z ratios achieve different velocities.

Lighter ions travel faster and reach the detector first, while heavier ions arrive later. The time of flight is directly proportional to the square root of the m/z ratio: t ∝ √(m/z). This simple relationship enables very wide mass range analysis.

📊 **Mass Range**

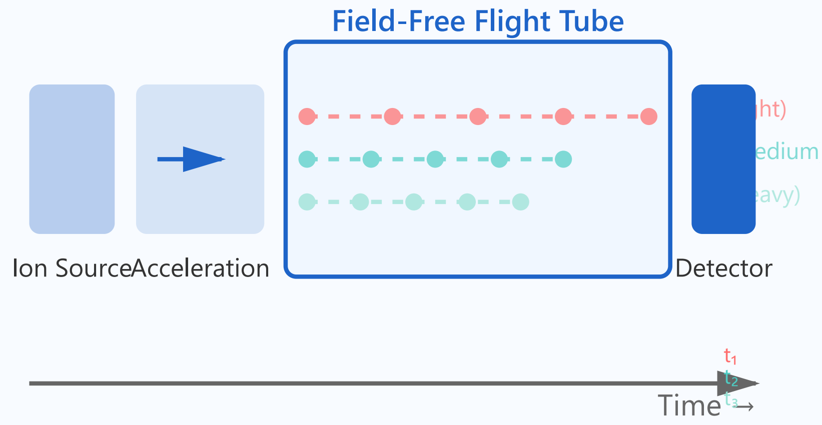
Theoretically unlimited mass range, routinely measures up to 500,000 Da for proteins

🎯 **Accuracy**

High mass accuracy (2-5 ppm) enables confident molecular formula determination

⚡ **Speed**

Complete spectrum acquisition in microseconds, ideal for fast chromatography

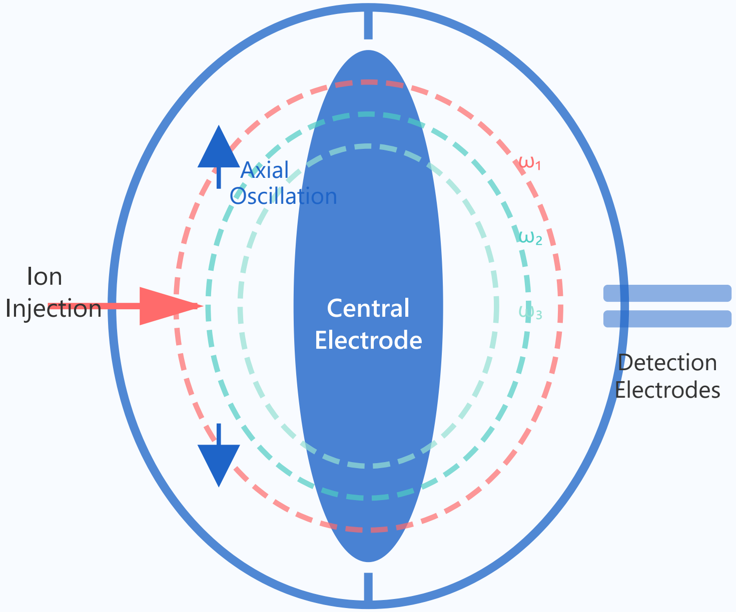


Common Applications

- Proteomics and intact protein analysis
- Metabolomics and lipidomics screening
- High-resolution accurate mass (HRAM) analysis
- MALDI imaging mass spectrometry
- Polymer and synthetic molecule characterization

3 Orbitrap Mass Analyzers

Orbitrap Cross-Section



Operating Principle

The Orbitrap consists of a central spindle-shaped electrode surrounded by two outer barrel-shaped electrodes. Ions are injected tangentially and trapped in stable orbits around the central electrode, simultaneously rotating and oscillating along the axis.

The frequency of axial oscillation is independent of the ion's energy and spatial distribution, depending only on the m/z ratio. Image current detection measures these oscillation frequencies using Fourier transformation, similar to FT-ICR, providing ultra-high resolution mass spectra.

🔬 **Resolution**
Ultra-high resolving power (>500,000 at m/z 200), enabling separation of isobaric compounds

🎯 **Mass Accuracy**
Sub-ppm mass accuracy (<1 ppm) with external calibration, <3 ppm without calibration

📈 **Dynamic Range**
Wide dynamic range (>5000:1) allows detection of both abundant and trace compounds

Common Applications

- High-resolution proteomics and top-down protein analysis
- Small molecule identification and structure elucidation
- Metabolomics with accurate mass measurements
- Complex mixture analysis and petroleomics
- Pharmacokinetics and drug metabolism studies

4 Ion Trap and Hybrid Mass Analyzers

Operating Principle

Ion traps confine ions in three dimensions using a combination of RF and DC electric fields. The 3D quadrupole ion trap consists of a ring electrode and two end-cap electrodes. Ions are trapped in stable trajectories at the center and can be stored for extended periods.

Hybrid instruments combine different analyzer types to leverage their complementary strengths. Q-TOF combines quadrupole selection with TOF analysis, while Q-Orbitrap pairs quadrupole filtering with Orbitrap detection. These combinations enable sophisticated MS/MS experiments with high sensitivity and resolution.

MS^n Capability

Multiple stages of fragmentation (MS^2 to MS^{10}) in ion traps for detailed structural analysis

Sensitivity

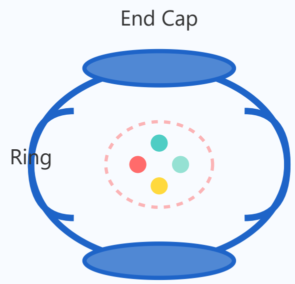
Ion accumulation and focusing improves detection limits, especially for low-abundance species

Versatility

Hybrid systems combine selectivity, sensitivity, accuracy, and resolution in one instrument

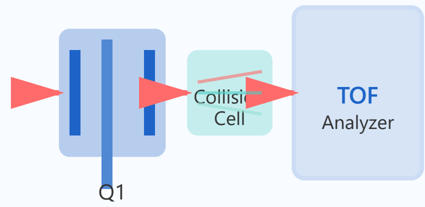
Common Applications

- Structural elucidation of unknown compounds
- Post-translational modification analysis in proteins
- High-throughput quantitative proteomics
- Natural product characterization and dereplication
- Glycomics and complex carbohydrate analysis
- Small molecule sequencing and de novo identification



3D Ion Trap

Hybrid Q-TOF



Alternative Hybrids

- Q-Orbitrap
- Triple Quadrupole
- Ion Trap-Orbitrap
- Q-Ion Trap

Performance Comparison

Analyzer Type	Resolution	Mass Accuracy	Mass Range	Scan Speed	Sensitivity
Quadrupole	Unit (1 Da)	0.1 Da	Up to 4,000 Da	Very Fast	High
TOF	10,000-40,000	2-5 ppm	Unlimited	Very Fast	Medium-High
Orbitrap	>100,000	<1 ppm	Up to 6,000 Da	Medium	High
Ion Trap	1,000-4,000	0.1-0.3 Da	Up to 6,000 Da	Fast	Very High