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- Products
  - Sample Introduction
     Thermal Desorption

    - **Sorptive Extraction**
    - Solid-Phase Microextraction
    - Headspace
    - Multi-Mode Inlet
    - Sample Extraction and Enrichment
    - Sample Preparation Robots

  - Gas Chromatography.
     Flow Modulator for GCxGC
     Thermal Modulator FOR GCxGC
    - <u>Hyper-fast GC-TOF MS</u>
  - Mass Spectrometry
  - Time-Of-Flight Mass Spectrometry
    Hard & soft (Tandem) Ionisation

    Data Analysis Software
  - - Chemometrics Software
    - GC-MS Software
    - GCxGC Software
- <u>Techniques</u>
  - GCxGC (2D GC)
  - Time-of-Flight Mass Spectrometry (TOF MS)
- Applications
  - Biomarker Discovery
  - Cannabis Profiling
  - Flavours & Fragrances
  - Petrochemical Fingerprinting
  - Recycled Plastics
  - Odours & Emissions
  - Total Petroleum Hydrocarbons (TPH)
- Content Hub
  - Articles
  - Blog
  - Brochures
  - Case Studies
  - E-Books
  - Scientific Posters
  - <u>Training</u>
  - Webinars
  - White Papers
- Company
  - About Us
  - Company Video
  - Consultancy services
  - Employment Opportunities
  - Events
  - Meet the Team
  - News
- Contact Us

Search

- Products
  - Sample Introduction
    - Thermal Desorption
    - Sorptive Extraction
    - Solid-Phase Microextraction
    - Headspace
    - **Multi-Mode Inlet**
    - Sample Extraction and Enrichment
    - Sample Preparation Robots
  - Gas Chromatography
    - Flow Modulator for GCxGC
    - Thermal Modulator for GCxGC
    - Hyper-fast GC-TOF MS
  - Mass Spectrometry
    - <u>Time-Of-Flight Mass Spectrometry</u>
    - Hard & soft (Tandem) Ionisation
  - Data Analysis Software
    - Chemometrics Software
    - GC-MS Software
       GCxGC Software
- <u>Techniques</u>
  - o GCxGC (2D GC)
  - Time-of-Flight Mass Spectrometry (TOF MS)
- <u>Applications</u>
  - Biomarker Discovery
  - Cannabis Profiling
  - Flavours & Fragrances
  - Petrochemical Fingerprinting
  - Recycled Plastics
  - Odours & Emissions
  - o Total Petroleum Hydrocarbons (TPH)
- Content Hub
  - Articles
  - <u>Blog</u>
  - Brochures
  - Case Studies
  - E-Books
  - Scientific Posters
  - <u>Training</u>
  - Webinars
  - White Papers
- Company
  - About Us
  - Company Video
  - Consultancy services
  - Employment Opportunities
  - Events
  - Meet the Team
- News
- Contact Us

>

#### <u>Home</u>

What is Time-of-flight mass spectrometry (TOF MS)?

# What is Time-of-flight mass spectrometry (TOF MS)?

Time-of-flight mass spectrometry, commonly known as TOF MS, is a detection method for gas-phase ions that determines their mass-to-charge ratio (m/z) based on measuring how quickly they travel a known distance.

For the analysis of mixtures of relatively small organic molecules (boiling below about 550°C), TOF MS is commonly coupled with gas chromatography (GC), and this will be the focus of our discussion here.

# How does TOF MS work?

In TOF mass spectrometers, analyte molecules are given a positive charge, and are accelerated by an electric field of known strength. Ions with the same charge will all end up with the same kinetic energy, but those with a larger mass will travel more slowly, and so will arrive at the detector later.

This travel time from the ion source to the detector is what is measured in TOF MS, and it means that ions across the entire m/z range can be monitored in one run.



Ions are accelerated into the flight tube from the ion source with the same initial kinetic energy

Small ions travel faster than large ones, thereby separating the ions (by m/z) before they reach the detector

The multi-stage reflectron improves resolution by extending the flight path

The principle of operation of a TOF mass spectrometer (in this case SepSolve's BenchTOF2). The path taken by the ions is shown by the dotted red line.

# How does TOF MS differ from quadrupole MS?

Conventional single-quadrupole mass spectrometers work by scanning through the mass range, meaning that only ions with a specific mass-to-charge ratio will reach the detector at any one point in time; all other ions are discarded.

In contrast, TOF instruments simultaneously analyse all ions, making them far less wasteful of the sample, and so inherently more sensitive.

Another benefit is that, because they generate full-range spectra, they allow identification of **targets and unknowns** in the same run, which also makes **retrospective analysis** of data possible.

The sensitivity of quadrupoles can be boosted by using selected ion monitoring (SIM), but in this mode only target compounds can be monitored, meaning that full characterisation of the sample is not possible in a single run, and retrospective searching of data is impossible.

Instrument	Targets	Non-targets	Sensitivity
Single quadrupole MS (scan mode)	✓	✓	×
Single quadrupole MS (SIM mode)	✓	×	✓
Time-of-flight MS	✓	<b>✓</b>	✓

Time-of-flight MS provides highly-sensitive detection of targets and non-targets in a single run

#### What's the difference between orthogonal and axial acceleration?

In TOF MS instruments, two main methods are used to extract the ions from the ion source:

- Orthogonal acceleration ejects the ions at 90° to their ultimate flight path, using a continuous ion source and an ion repeller with a relatively small field (1–30 V) to eject ions from the source.
- Axial (or direct) acceleration, as employed in the BenchTOF2 system, maximises sensitivity by extracting packets of ions from the ion source in-line with the flight path using a more powerful pulsed electric field (typically greater than 300 V).

( ) onal acceleration is still used in many TOF MS instruments, but axial acceleration (as employed in <u>BenchTOF2</u>) offers better long-term stability, reducing the need for source maintenance, and so minimising downtime.

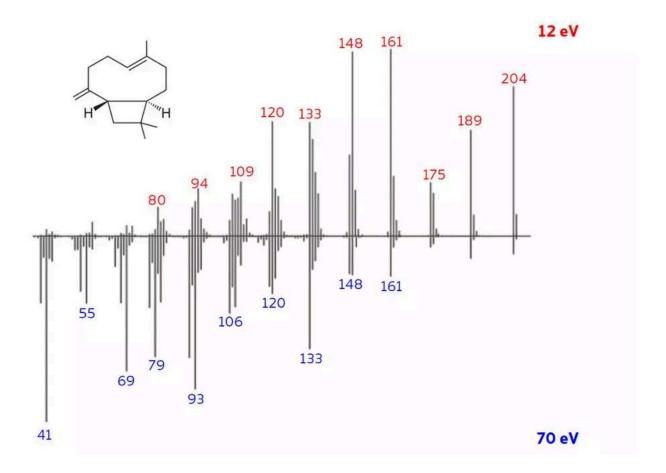
## Can you use soft ionisation methods with TOF MS?

In short, yes.

The majority of TOF MS systems used with GC employ 70 eV electron ionisation (EI), in which the accelerating voltage is set at 70 V. This so-called 'hard' ionisation is favoured because at this voltage, the energy transfer from the electrons to most organic molecules is at a maximum, and varies little with electron energy.

This results in good sensitivity and consistent mass spectra. However, at 70 eV, some molecules undergo extensive fragmentation, making the signal from the molecular ion very weak, and making it difficult to separate some ions from the background.

In addition, many isomers (such as terpenes and branched hydrocarbons) have very similar spectra at 70 eV, making it impossible to identify them confidently.



This pair of EI spectra acquired on BenchTOF2 show the extensive fragmentation of caryophyllene that occurs at 70 eV, and how this is resolved using soft ionisation at 12 eV – which thanks to the ion optics used, is achieved while maintaining sensitivity at acceptable levels.

To resolve these problems, soft ionisation at lower voltages can be used. Unfortunately, low-energy EI was historically unworkable because of the large drop in sensitivity caused by electron clustering around the filament. The other alternative, chemical ionisation (CI), requires a different ion source configuration, additional source pressurisation, and the use of reagent gases, making it very time-consuming to implement. Fortunately, these problems have now been circumvented by the availability of ion optics that initially use a high potential difference to accelerate the electrons away from the filament, but then reduce their energy before they arrive in the ion chamber.

For more information on how this works, <u>read our Technical note: Tandem Ionisation® – Revolutionary soft ionisation to enhance confidence in identification.</u>

## What are the applications of TOF MS?

The ability of TOF MS to allow target and non-target analyses on a single platform makes it a perfect detector to expand the scope of any GC application that would otherwise be carried out using a quadrupole instrument. In addition, the speed of TOF MS means that it can also be applied where fast GC run times are needed, making it ideal for GC×GC, as well as regular GC.

#### Applications of TOF MS include:



- Metabolomics
- Food
- Fragrances
- Petrochemical
- · Odours and emissions

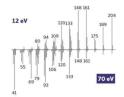
# Time-of-flight mass spectrometry products



<u>Time-of-flight Mass Spectrometry</u>

<u>Modern labs must constantly adapt to cope with new analytical challenges and ever-increasing workload, all the while improving data confidence and reducing associated costs. BenchTOF2 time-of-flight mass spectrometers address these challenges through enhanced performance in easy-to-use</u> workflows.

#### **Details**



#### Tandem Ionisation

Award-winning Tandem Ionisation® enables easy switching between hard and soft ionisation to generate complementary information about each component, increasing the dimensionality of your analysis and improving confidence in identification. **Details** 

# **Further reading**



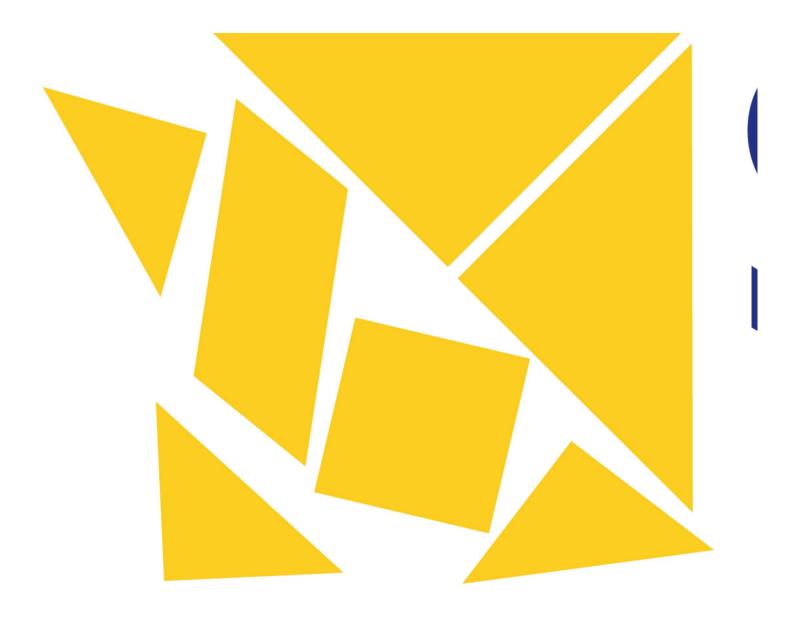


Why Choose a Time-Of-Flight Mass Spectrometer

In this technical note, we explore such advantages of TOF MS, specifically SepSolve's BenchTOF2™ instruments, with examples for both research and routine applications

<u>Details</u>





<u>Technical note: Tandem Ionisation – Revolutionary soft ionisation to enhance confidence in identification</u>

This technical note describes the use of Tandem Ionisation® for BenchTOF2™ mass spectrometers to acquire both hard (70 eV) and soft (10–20 eV) electron ionisation (EI) in a single analysis.

#### <u>Details</u>

## Get in touch

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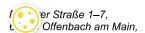
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