

Nov 2024, SCION Instruments, Applications Department, V.1

What is mass spectrometry?

Mass spectrometry (MS) measures the mass to charge ratio (m/z) of one or more compounds present within a sample. The measurements that are produced from the mass spectrometer can be used to calculate the molecular weight of the components of a sample. Mass spectrometry is often used to identify unknown compounds by their molecular weight and by fragmentation pattern to quantify known compounds and determine structure as well as chemical properties of molecules.



Figure 1 Inside of the Mass Spectrometer

All mass spectrometers are comprised of at least four parts, the transferline, the ionization source, the quads and the ion detector (figure 1). These four parts are all in a vacuum chamber, to ensure a friction free environment for the ions to 'float' through.

Transferline

The column goes into the heated transferline (figure 2) through the repeller into the source. The transferline is made with dual heaters for fast heating. The repeller holds and aligns the source in place.



Figure 2 Transferline

How does ionization work in mass spectrometry?

At the ionization source, the gas-phase molecules are ionized and converted into ions and fragments by electrons generated from the filament. The reflector behind the filament makes sure that the ions go in the right direction. The generated ions are accelerated towards the quads using the repeller and the ions are focused by the lenses (figure 3).



Figure 3 Inside of the source

There are different methods of ionization such as Electron Ionization (El), Chemical Ionization (Cl). The most common mechanism used is El, a technique that often results in significant fragmentation of sample molecules.

Another technique, Chemical Ionization (CI), uses a softer ionization method that produces less fragmentation. Which is beneficial for analysing larger, more complex molecules with simpler spectra.

Quads

After ionization the ions are separated using the quads. The ions are first separated using the Quad 0 (Q0) after this they are separated with the Quad 1 (Q1).

The Q0 is particularly designed to improve the accuracy and robustness of the SQ (pre-filtering). Using the Q0 as pre-filtering keeps the main quad (Q1) clean this reduces interference.

Because the Q0 is curved on an 90 degree angle the noise is reduced, the neutrals you don't want are deflected out of the quad. This separation improves the mass stability.

At SCION Instruments we also have a premium heated Q0 available with He-Gas (figure 4). Adding He gas will improve the overall sensitivity.

Technical Note How does the SCION Instruments 8700 Single Quad Mass Spectrometer work?



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Figure 4 Q0, He on/He off

In the Q1 the ions with specific m/z ratios are filtered. Ions that are outside the m/z range are lost in the quad, mass filtering.

The Q1 or mass filters, consist of four rods with a lens-free path design which are separated into three parts. The pre filter ion guide, the mass filter and the post ion filter ion guide (figure 5).



Figure 5 Q1

An ion has a unique mass and charge ratio (m/z). The four rods create an electric field. The ions 'float' through the middle of this field. By determining the correct parameters for the RF (Radio Frequency) and DC (Direct Current) voltages only ions with a specific m/z ratio will be stable and 'float' through the Q1 and pass to the detector. Other ions will be deflected and removed.

The DC voltage provides a constant electric field that helps in stabilizing the ion trajectories. The RF voltage creates an oscillating electric field by alternating at a high frequency, this helps filtering the ions based on their m/z ratio.



Figure 6 filtering ions in Q1

This specific combination allows the quad to selectively filter the ions (figure 6), making this a powerful tool for the SCION Instruments mass spectrometer.

Ion detector

The separated ions will arrive at the detector the detector sends a signal that will be detected in the software. SCION Instruments uses an electron multiplier detector with Extended Dynamic Range (EDR).

Different scan modes

Fullscan, measures all the ions in a chosen mass range. Using Fullscan is best for identifying new/unknown components. This results in a spectrum of a specific compound. The library search in MSWS is a useful tool with Fullscan measurements to find the corresponding compound.

Selected Ion Monitoring (SIM) measures only selected/chosen masses this goes from one mass to another mass. SIM mode is usually used when you have known compounds with their corresponding masses. SIM will give a higher sensitivity and a lower noise result because it will only look for that specific mass.

Why should you choose for the SCION 8700 SQ-MS?

These are the main reasons why you should choose the SCION 8700 SQ-MS.

- The SCION SQ-MS has a lens free lon path this increases sensitivity by reducing ion losses, leading to more accurate quantification and identification. No lenses or apertures to contaminate this means easier for use.
- The SCION SQ-MS has an Extended Dynamic Range (EDR), enables optimal detection in every scan, accommodating both trace components and highabundance compounds in the same run. Accurate quantitation and reliable library search results.
- 3. The SCION SQ-MS has a high capacity turbopump (400 L/s) which is the fastest pump down speed on the market, improving productivity in high-throughput environments.
- 4. The SCION SQ-MS 'Multi-curve' design 90° curved Q0 and 90° off-axis detector reduces the neutral noise and gives ultra-high sensitivity (S/N).
- 5. The SCION SQ-MS Q0 with helium active focusing provides added sensitivity in applications.