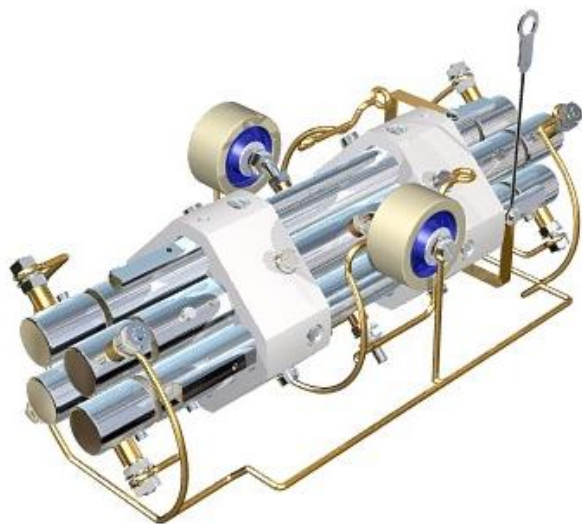


Quadrupole Assembly

Part Number:	700004180	Where Used:	Xevo TQ MS / Xevo TQ-S / Xevo TQ-XS
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Functional description



- The instrument contains two quadrupole mass filter assemblies, MS1 and MS2.
- They allow the transmission of selected ions according to their mass-to-charge ratio.
- For given DC and RF voltages, only ions of a certain mass-to-charge ratio pass through the quadrupole.
- The same RF is stepped down and applied to the pre-filters, the DC is stopped by the capacitor, and the pre-filter DC voltages are supplied by the lens control PCB.

CAUTION: *Always wear chemical-resistant, powder-free gloves when handling any of the critically cleaned analyzer components.*

WARNING: *The optic can be contaminated with biohazardous and/or toxic materials. Always wear chemical-resistant, powder-free gloves when handling the optic.*

Location

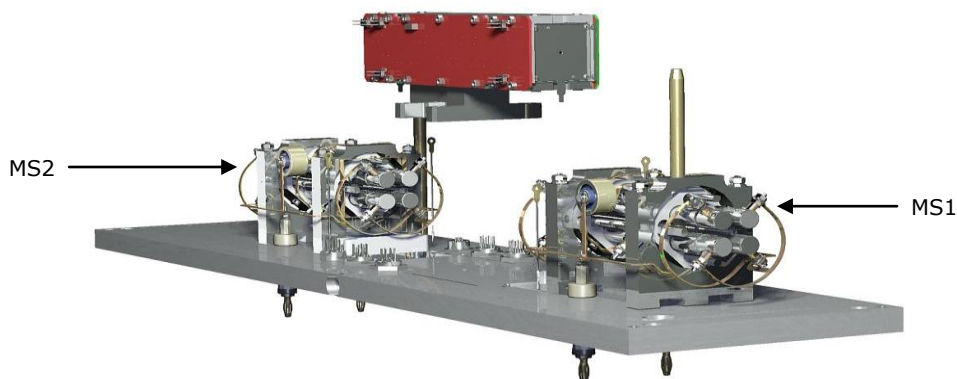
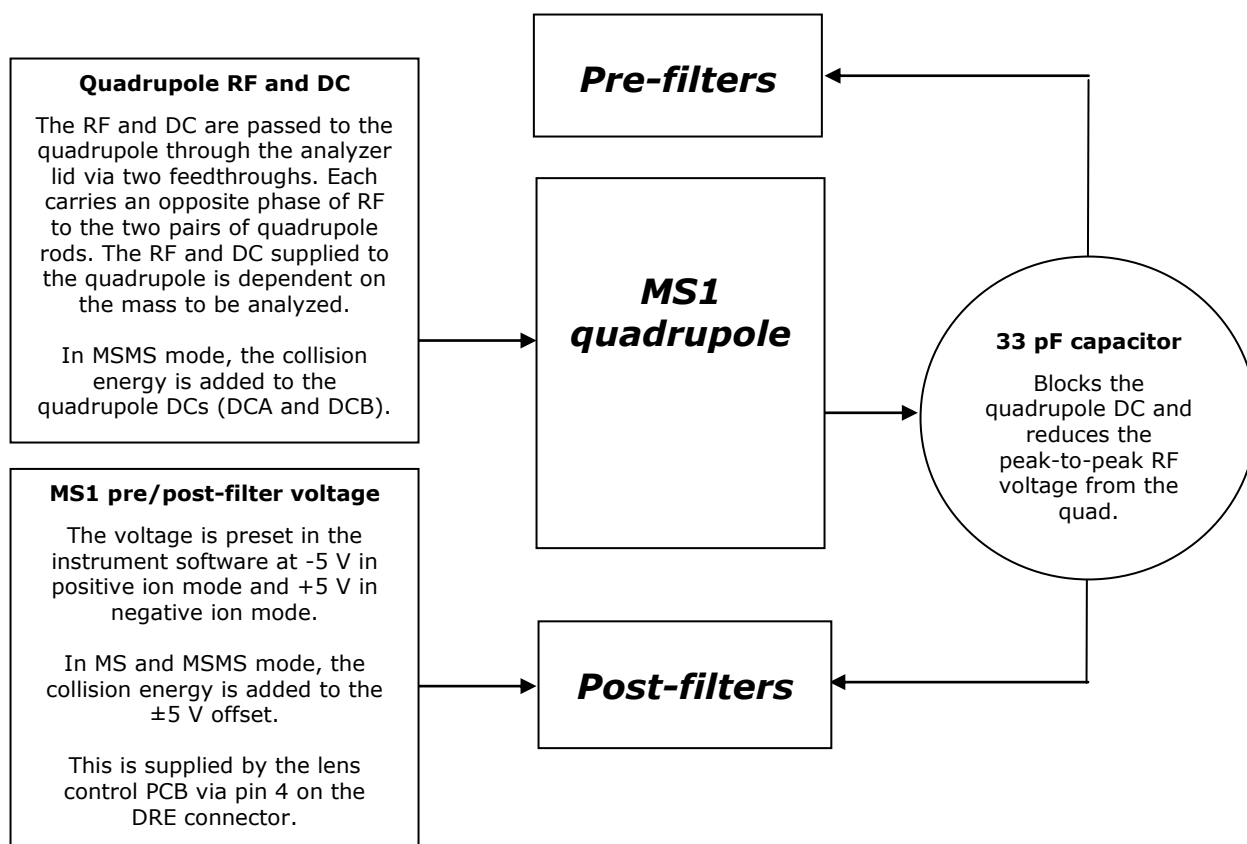


Figure 1 - Location of the quadrupoles on the lid assembly

Inputs/outputs

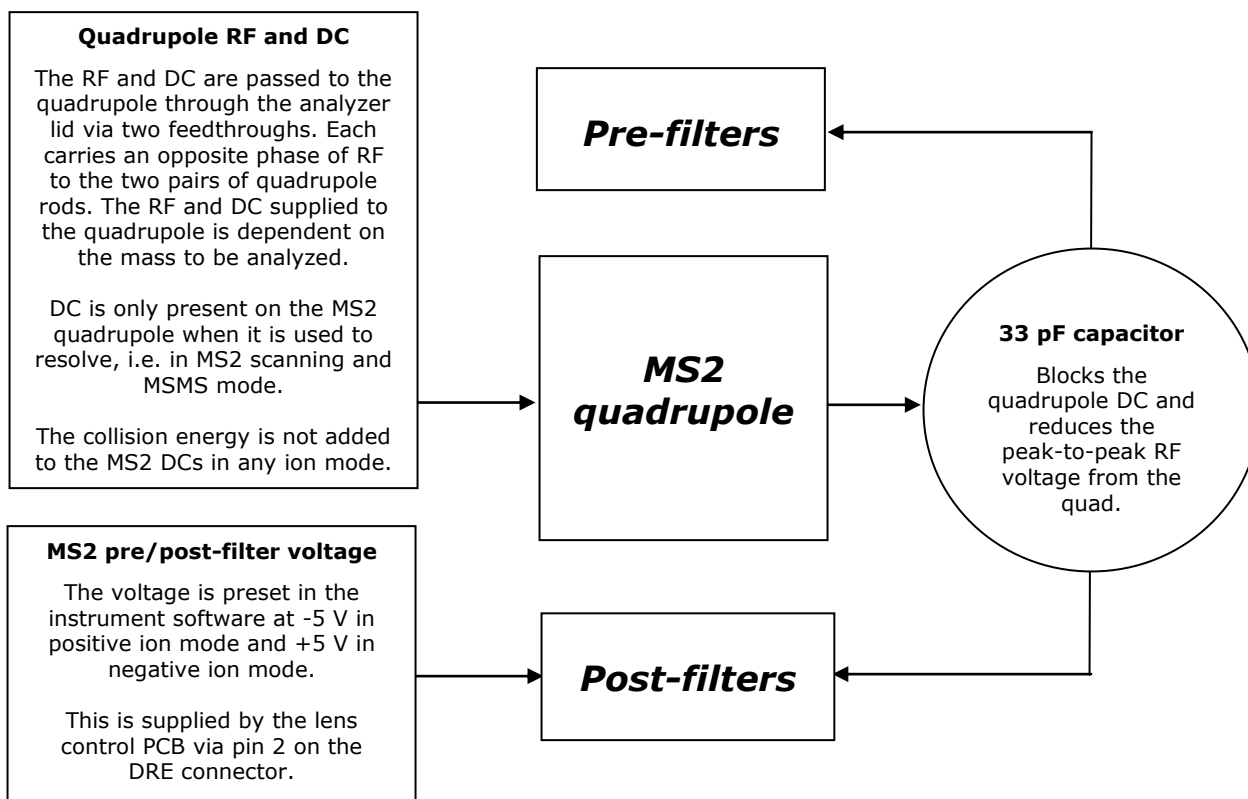
MS1 quadrupole



NOTE:

The collision gas must not be switched on for an MS1 scan [MS1 Scan]. This is the only scan mode that operates with no collision gas and must only be used for diagnostic purposes.

MS2 quadrupole

**NOTE:**

The collision gas must be on all of the time for an MS2 scan [MS Scan]. This is a fundamental difference between Xevo instruments and the legacy Quattro products. This functionality enables the instrument to switch very quickly from MS to MSMS within the time scale of a chromatographic peak.

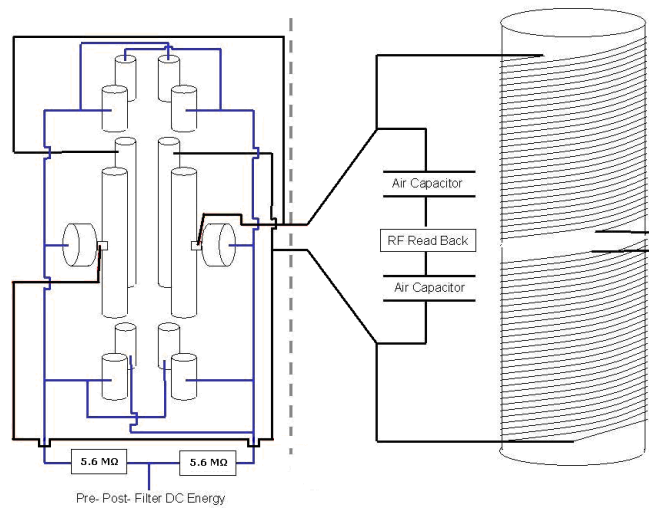


Figure 2 - Quadrupole circuit showing feedthroughs from RF generator

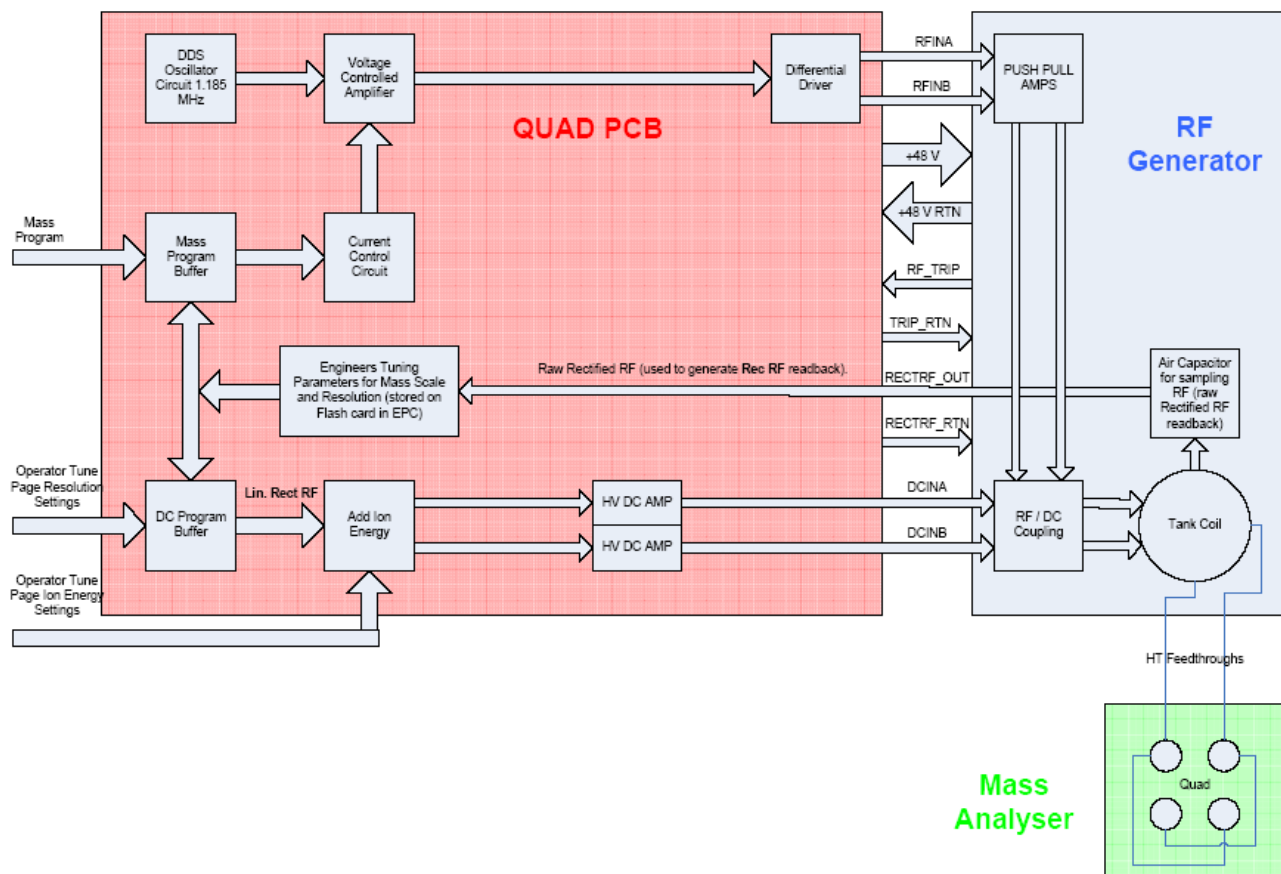


Figure 3 - Relationship between the quadrupole, RF generator, and dual quad PCB

Diagnostic procedures

CAUTION: *The quadrupole RF voltage align procedure must be performed if the analyzer has been opened.*

If a new quadrupole is fitted, set up the mass scale and resolution as described in the relevant manual:

- [Xevo TQ MS Installation Manual](#) (p/n 715001890)
- [Xevo TQ-S Installation Manual](#) (p/n 715002461)
- [Xevo TQ-XS Installation Manual](#) (p/n 715005249)

RF breakdown test

The RF breakdown test uses the photomultiplier tube on the detector to check if there is any arcing present within the analyzer.

1. Switch off any LC flow to the source to stop the ion beam.
2. Set desolvation temperature to **30 °C**.
3. Set the ion counting threshold to **0**.
4. Switch the capillary voltage to **0** and switch the ion energies fully negative.
5. Open a single window full mass range with a gain of **x10000**.
6. Re-initialize the baseline.
7. If RF breakdown is present, the baseline will rise towards the high mass when the RF voltage is at a maximum.

NOTE: *If RF breakdown is confirmed with this test, it suggests that the analyzer internal quad wiring is in close proximity to ground, facilitating an arc.*

8. To determine if the RF breakdown is in MS2, open a Daughter Scan window, set the following parameters, and check if the baseline rises towards high mass:

- Set Mass **2**
- Mass **1010**
- Span **2000**
- Gain **10,000**

9. To determine if the RF breakdown is in MS1, open a Parent Scan window, set the following parameters, and check if the baseline rises towards high mass:

- Set Mass **2**
- Mass **1010**
- Span **2000**
- Gain **1000**

10. Reset the ion counting threshold to **25**.

11. Re-initialize the baseline.

12. If RF breakdown is present, open the analyzer lid and inspect all of the wiring for its proximity to the analyzer lid or other conductive surfaces.

NOTE: *This test cannot be used to confirm if RF breakdown is occurring within the RF generator because no arcing will be visible to the photomultiplier tube.*

13. Open a single mass window at full mass, 2040 Da with zero span to give a rectified RF readback of $\sim 10 \pm 0.1$ V.

NOTE: *If this value fluctuates or is lower, it suggests a problem with the RF generator (assuming the quadrupole RF voltage align procedure has been performed).*

Cleaning the quadrupole rods and pre-filters

1. Vent the instrument.
2. Remove the analyzer lid assembly and place on a clean surface.
3. Inspect the quadrupole rods for ion burn without removing or disturbing them.

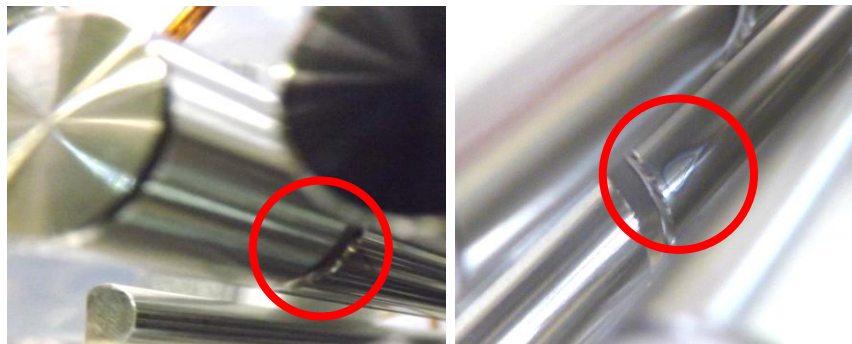


Figure 4 - Examples of ion burn

NOTE: There is no need to remove the collision cell or pre-filters from the lid to clean the quadrupole rods and pre-filters.

NOTE: The quadrupole rods and pre-filters are cleaned using lapping film, which is part of the Performance Maintenance Kit for the relevant instrument.

4. Cut the lapping film into eight strips approximately 8 cm long and 1 cm wide.
5. Position the lapping film around one quadrupole like a belt; use plastic tweezers to feed it through if necessary.
6. Hold each end of the lapping film strip and abrade any ion burn by alternately pushing and pulling the strip ([cleaning video](#)).

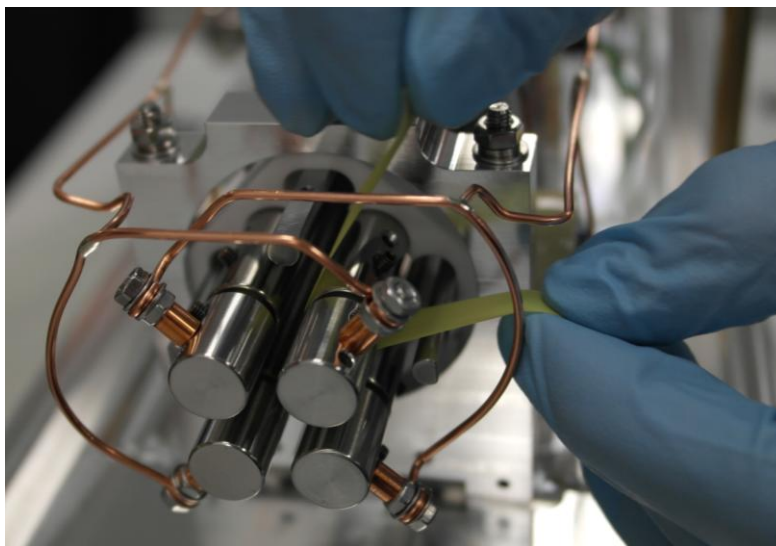


Figure 5 - Quadrupole rod cleaning

7. Clean the first 1 to 2 cm of quadrupole rod immediately after the pre-filter, ensuring that the lapping film is angled to make the correct contact with any affected area.

NOTE: *Any ion burn should be removed very easily after a few cycles.*

8. Use the same technique on the other three quadrupole rods using a new piece of lapping film for each rod.
9. Use the same technique to abrade all four pre-filters.
10. Once all four quadrupole rods and pre-filters have been cleaned of any ion burn, blow nitrogen through the whole quadrupole assembly.

CAUTION: *To avoid damage, do not clean the quadrupole rods with solvents.*

11. Visually check all connections and ensure RF wires are not touching. If the quad wiring has been bent out of the way for cleaning, re-inspect the wiring to ensure it is at least 5 mm away from anything it could short to, this includes the surfaces of the analyzer lid or other wiring.
12. Refit the analyzer lid assembly.
13. Pump down the instrument for at least two hours and ensure that ultimate vacuum is reached.
14. Perform the RF generator alignment procedure and ensure that the mass scale and resolution are correct, as described in the relevant installation manual.
15. Repeat the charging test, as described in the relevant PM technical reference.

CAUTION: *The "RF breakdown test" on page 5 must be performed once the instrument has been beam checked and pumped down.*

Replacing the ceramic rods

The following materials are required for this procedure:

- Chemical-resistant powder-free gloves
- 5.5-mm wrench
- 1.5-mm hex Allen wrench

CAUTION: *Always wear chemical-resistant, powder-free gloves while performing this procedure.*

1. Remove the analyzer lid assembly and place on a clean surface.

2. Use the 5.5-mm wrench to unscrew and remove the nut from one of the pre-filter rods, then remove the washers and quad wiring.

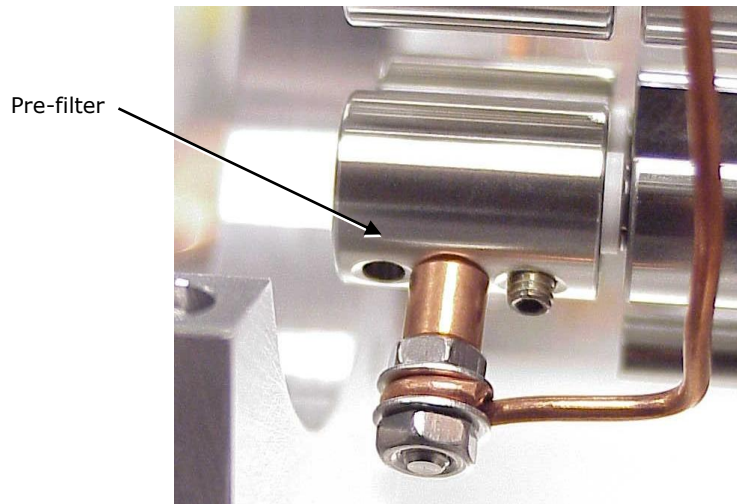


Figure 6 - Pre-filter fittings

3. Use the 1.5-mm hex Allen wrench to loosen the grub screw on the pre-filter and gently remove the pre-filter from the ceramic rod.

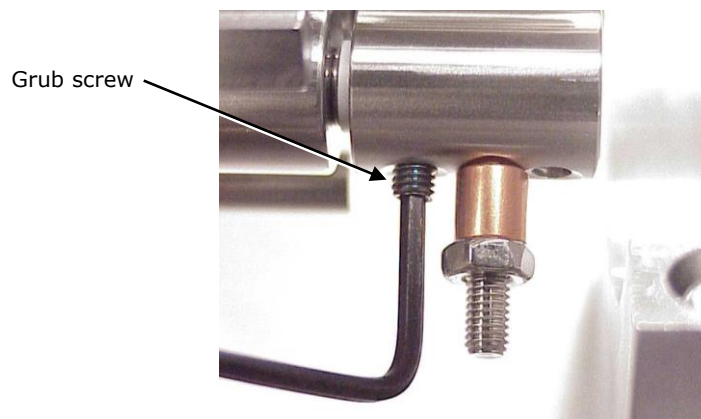


Figure 7 - Removing the pre-filter

4. Remove the ceramic spacer and spring ring on the ceramic rod.

CAUTION: *Record the position of the flat surface of the ceramic rod before removal so that the new rod is fitted with the flat side in the same position.*

5. Replace the ceramic rod.

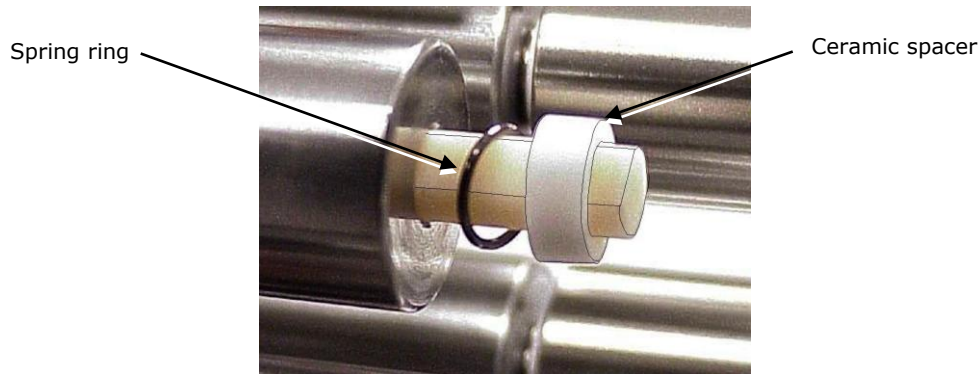


Figure 8 - Ceramic rod

Refitting the pre-filters

1. Refit the spring ring and the ceramic spacer onto the ceramic rod.
2. Refit the pre-filter onto the ceramic rod and gently compress the spring ring until the pre-filter does not move any closer to the quad.

CAUTION: *The ceramic rod has a flattened surface. Tighten the grub screw onto this surface to ensure that the fittings on the pre-filter align with those on the quad. Do not over-tighten, as the ceramic rod will crack with too much pressure.*

3. Use the 1.5-mm hex Allen wrench to tighten the grub screw onto the ceramic rod.

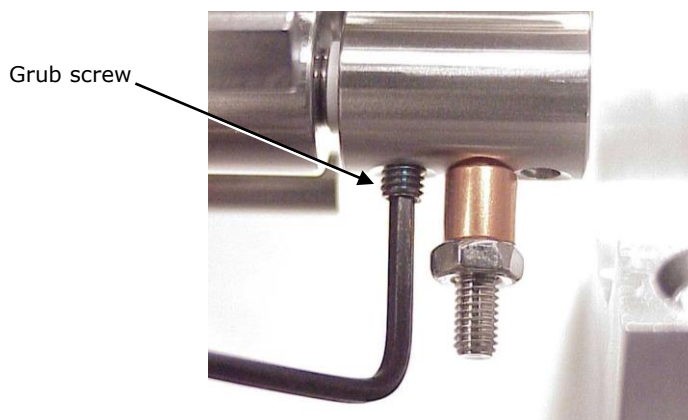


Figure 9 - Refitting the pre-filter

4. Refit the quad wiring, washers, and 5.5-mm nut to the threaded rod.

Definition of peak shapes

This section is a guide to the most common quadrupole faults and how to assess whether an unusual peak shape is acceptable or not.

Table 1: Peak shapes

Name	Symptom	Possible Causes
RF breakdown	Baseline rises towards higher masses.	• Quad wiring position. Check that any RF wiring is a minimum of 5 mm from ground, for example, the lid, or the analyzer housing when the lid is fitted. • Loose RF connections, particularly on: • feedthroughs • connections to the quadrupoles • connections to the capacitors • connections to the pre/post-filters • connections to the hexapole • Dust/scratches/stains on the quadrupole rods • Faulty quad capacitors. To check, swap the MS1 and MS2 capacitors over.
Poor peak switching performance	When switching between low and high masses, one or more of the peaks suffers a significant (>20%) drop in intensity.	• Dirty source ion guide. Inspect the ion guide and clean if necessary. • Loose air capacitors in the RF generator • Same as RF breakdown
Poor full mass test performance	When performing the Full Mass Test there is a significant (>50%) difference between the initial and final beam intensity.	• Dust/scratches/stains on the pre-filter rods and/or quadrupole rods
Poor peak shape	Peak shape exhibits one or more of the following: • precursor • shoulder • splitting	• Incorrect ion energy setup • Ion energy spread problems • Swap DC voltages - this may however simply shift the problem to the opposite ion mode • Dust/scratches/stains on the quadrupole rods • Misalignment of the quadrupole rods and/or optical rail assembly • Incorrect ion optic voltages • Dirty hexapoles/source ion transfer lens Refer to the "Assessing Quad Peak Shapes" section
Poor quad quality performance	In order to obtain adequate resolution, the resolution parameters have to be increased beyond their normal values and the ion energy reduced below its normal value. This in turn leads to poor peak intensity	• Same as poor peak shape
Poor high mass peak performance	No beam apparent at high masses (>1700 Da) or no apparent resolution	• High mass resolution parameter set too high • Ion energy set too low • Incorrect linearity setup • Degraded/incorrect sample • Same as poor peak shape • Miss-aligned RF generator • Poor vacuum

Ion energy optimization and DC balance

Using the correct value for ion energy is essential for quadrupole performance.

- Value too low - ions do not have enough energy to reach the end of the quadrupole and as a result the sensitivity of the instrument suffers.
- Value too high - ions travel through the quadrupole so quickly that the resolving capability is diminished.

Use the following procedure to ensure that the optimum balance between sensitivity and resolution is achieved.

CAUTION: *Ensure that the correct gas cell parameters are used for MS2 ion energy optimization for MS scan or SIR. Failure to do this will result in incorrect optimum ion energy.*

The DC balance must be adjusted if the quadrupole, RF generator, or dual quad PCB is replaced, or the instrument parameters have been lost from the Flash ROM.

A new ion energy setup procedure means that the DC balance is no longer applied in the traditional manner. Set the MS1 and MS2 DC balance to 0 at the start of the procedure. QP setup solution must be infused for this procedure at a flow rate of 10 µL/min.

This method optimizes the ion energy required for low mass transmission so that the low mass ions do not become distorted. The DC balance (ion energy ramp with mass) is then optimized for the transfer of high mass ions.

The source ion energy slider can then be adjusted to optimize transmission for different experiments; the DC balance offset is adjusted for the entire mass range.

MS1 ion energy optimum (positive mode)

1. Ensure that the MS1 DC balance has been set to **0**.
2. Ensure that the collision energy is set at **5 V** (normal MS1 optimal value).
3. Ensure that the entrance and exit lenses have been set to **30 V** (normal MS1 optimal value).
4. Open one MS1 scan mass window on **59 Da** with a span of **3**.
5. Set the Source Tune page MS1 ion energy so that the 59 Da peak intensity has been optimized.
6. Set the "gain" of the window so that the peak only just reaches the top of the window.
7. Reduce the ion energy until the peak intensity is less <10%, but >5%.
8. Add **0.5 V** to the current ion energy value. This is the optimal low mass ion energy.
9. Ensure that the top of the peak is not distorted or has "chicken head" sub-peaks.
10. Record the optimal low mass ion energy for MS1.
11. Open a second MS1 scan mass window on **2034.62 Da** with a span of **3**.
12. Using the best peak shape DC polarity found on page 17, set the MS1 DC balance in the Resolution Tune page so that the 2034.62 Da peak intensity is optimized.
13. Set the "gain" of the window so that the peak only just reaches the top of the window.

14. Depending on the DC polarity, reduce or increase the DC balance until the peak intensity is <10%, but >5%.
15. Restore the peak intensity using DC balance until 0.5 V has been restored onto the DC balance.

NOTE: *This may mean that 0.5 V is subtracted or added to the 5% value depending on the instrument. The beam intensity must increase as the 0.5 V is restored to the ion energy. This is the optimal high mass ion energy.*

16. Input the DC balance value for MS1.

MS2 ion energy optimum (positive mode)

1. Ensure that the MS2 DC balance has been set to **0**.
2. Ensure that the collision energy is set at **5 V** (normal MS2 optimal value).
3. Ensure that the collision gas icon is on, and that the flow rate is set to 0.15 mL/min.
4. Ensure that the entrance and exit lenses have been set to **2 V** (normal MS2 optimal value).
5. Open one MS scan mass window on **59 Da** with a span of **3**.
6. Set the Source Tune page MS2 ion energy so that the 59 Da peak intensity has been optimized.
7. Set the "gain" of the window so that the peak only just reaches the top of the window.
8. Reduce the MS2 ion energy until the peak intensity is at 10%.
9. Add **1.0 V** to the current ion energy value. This is the optimal low mass ion energy.
10. Ensure that the top of the peak is not distorted or has "chicken head" sub-peaks.
11. Record the optimal low mass ion energy for MS2.
12. Open a second MS scan mass window on **2034.62 Da** with a span of **3**.
13. Using the best peak shape DC polarity, set the MS2 DC balance in the Resolution Tune page so that the 2034.62 Da peak intensity has been optimized.

CAUTION: *If the DC balance will exceed ± 3 V, contact GSS.*

14. Set the "gain" of the window so that the peak only just reaches the top of the window.
15. Depending on the DC polarity, reduce or increase the MS2 DC balance until the peak intensity is <15%, but >10%.
16. Restore the peak intensity using MS2 DC balance until 1.0 V has been restored onto the DC balance.

NOTE: *This may mean that 1.0 V is subtracted or added to the 10% value depending on the instrument. The beam intensity must increase as the 1.0 V is restored to the ion energy. This is the optimal high mass ion energy.*

17. Input the DC balance value for MS2.

Assessing quad peak shapes

To ensure that quadrupoles are fit for purpose and that their peak shapes are assessed against objective criteria, definitions of peak shape abnormalities are given below. In addition, the method of assessment is shown - decreasing span and increasing gain almost certainly show some deviation from an ideal peak shape. The method described helps judge if this deviation is acceptable or not. It is also important that the peak shape is not dominated by large amounts of electronic or probe noise.

NOTE: *Peak shapes in negative can be assessed on m/z 554.3 and 255, using QP leucine enkephalin set-up solution.*

Precursors

Precursors (imperfections on the low mass side of peaks) seen on quadrupole instruments are due to distortions in the electric field generated by the source and/or analyzer components. These distortions adversely affect the trajectory of the ions as they move through the instrument, ultimately leading to poor peak shape. These distortions can be due to a number of problems but the most common are due to contamination of the quadrupole rods, pre-filters, post-filters, or hexapole. In some instances they have been traced to dirty sources.

Precursors typically appear as bumps on the side of peaks approximately 0.1 Da to the side. However, they can appear up to 1 Da away from the main peak. Although they appear unsightly, the main reason they need prompt identification and rectification is that there is a possibility during an acquisition that the instrument will identify them as separate peaks. This in turn can cause further problems, particularly with regard to calibration.

Postcursors

Postcursors (imperfections on the high mass side) will not be apparent at optimum ion energies, though it is normal for them to form as the ion energy is increased. This is particularly apparent on quadrupoles with very good resolution in single quads and the MS1 position of triple quads.

Examples of precursors and postcursors

Postcursors are nodes in the oscillation of ions through the quad. At higher ion energies, ions travel faster through the quad. Nodes are present which are harmonics of the main oscillation. A quad with good resolution will display these as postcursors.

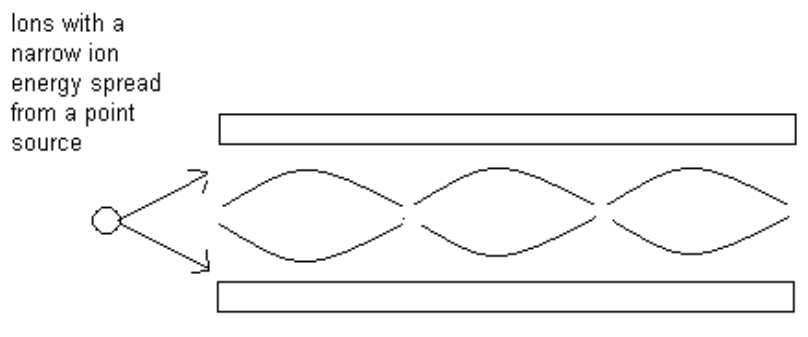


Figure 10 - Ions transiting the quad at higher ion energies

If the source of the ions has a higher energy spread (i.e. they pass through a collision cell with no gas in it), the nodes are smeared and are not visible on the peak.

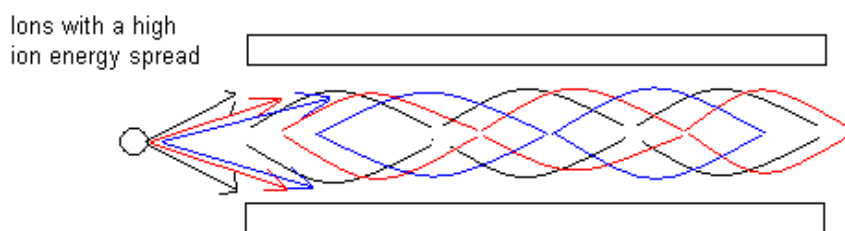
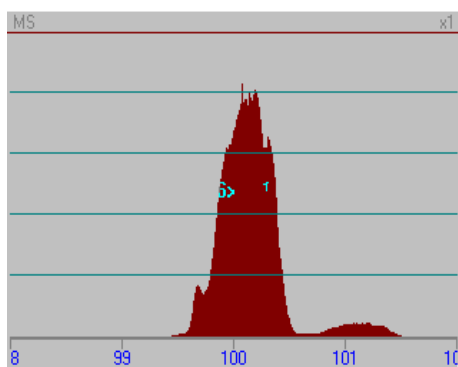


Figure 11 - Ions transiting the quad at high ion energy

Peak example 1 below shows a classic precursor (Figure 12).

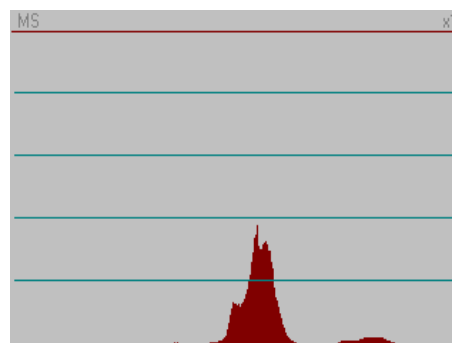
By observing the Tune page and increasing the resolution parameters it can be seen that the precursor moves to a higher mass with the main peak. When the resolution parameters are increased, the intensity of the precursor decreases at a different rate to that of the main peak, as seen in peak example 2 (Figure 12).

The same rules apply to postcursors; when the resolution is increased, they move with the main peak and their rate of decrease of intensity is different to that of the main peak.



Peak example 1

A typical example of a precursor.



Peak example 2

The same peak but with increased resolution. Note that the precursor has moved up the mass scale with the main peak. Its relative decrease in intensity is also much less than that of the main peak.

Figure 12 - Precursor examples

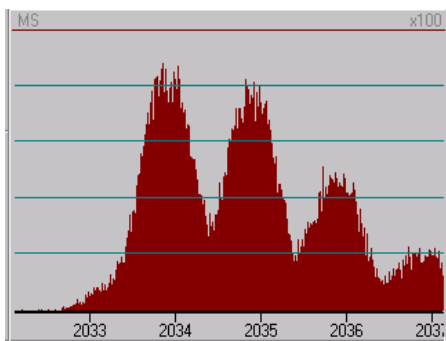
Precursors and postcursors also tend to be more apparent at higher values of ion energy. For a quadrupole to pass, precursors must not be present when the ion energy is increased to 0.6 V above the optimum value.

Precursors can manifest themselves in other less distinct forms. One of these is in the form of a shoulder, either on the low mass side or the high mass side of the peak. These are simply pre or postcursors that are much closer to the centre of the main peak. When the precursor or postcursor is particularly intense and lies close to the centre of the main peak, it may appear that the top of the peak is split. With this splitting, the main body of the peak may appear normal in shape but the top is split into two or more distinct peaks.

In either of these two cases, diagnosis may be made easier by increasing the resolution parameters or decreasing the ion energy.

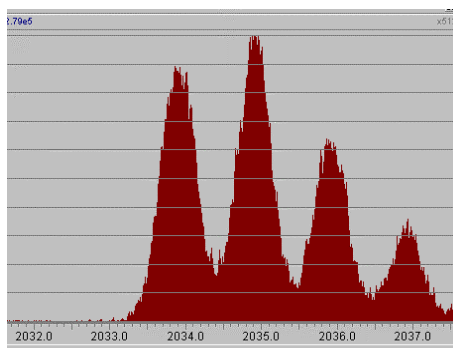
Precursors can also be seen as a sloping front or leading edge at the base of the peak, as shown in peak example 3 ([Figure 13](#)). Typically this form is seen on high mass peaks such as the one at 2034.63 Da.

Although this form is unlikely to be identified as a separate peak by the instrument, it does adversely affect the resolution capabilities of the instrument. As a result, it also requires prompt identification and rectification.



Peak example 3

A high mass peak showing a sloping front or leading edge. Note the poor resolution between the isotope peaks. This sort of peak shape is unacceptable and must be rectified.



Peak example 4

A high mass peak showing good peak shape and resolution. Note the symmetrical shape without any form of leading edge or shoulder.

Figure 13 - Precursor examples

Peak assessment examples

The abnormality on 1080 is too small to cause problems.

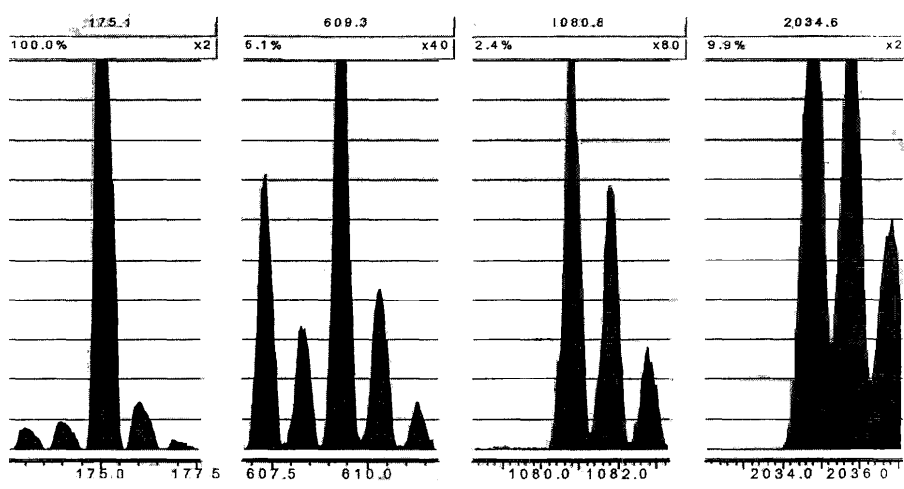


Figure 15 - Acceptable peak shapes

Pimple is too narrow for the data system to mistake for a real peak.

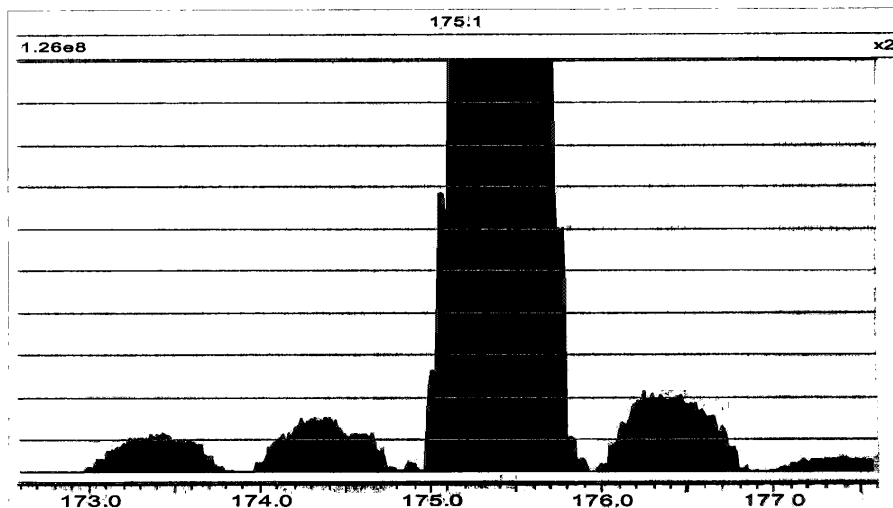


Figure 16 - Acceptable pimple precursor near 175

The precursor visible on the 175 peak is unacceptable.

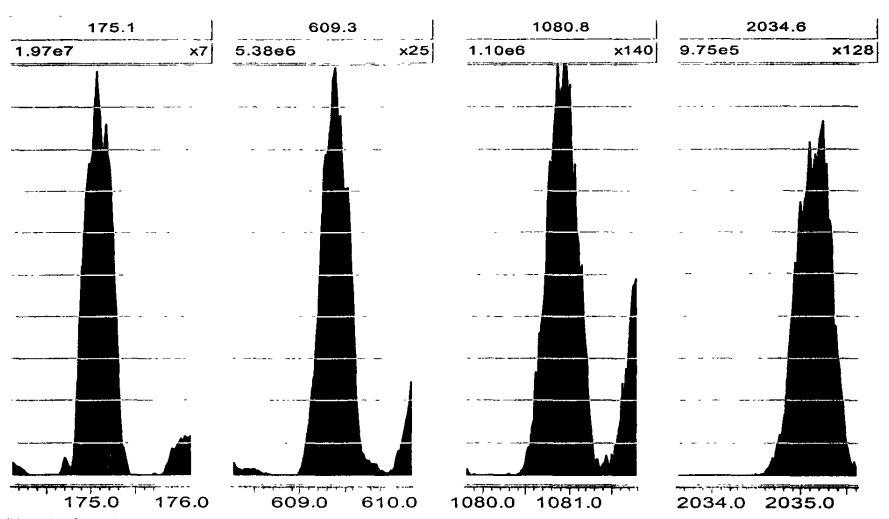


Figure 17 - Unacceptable peak shapes

The precursor on 609 and the leading edge on 2034 are unacceptable.

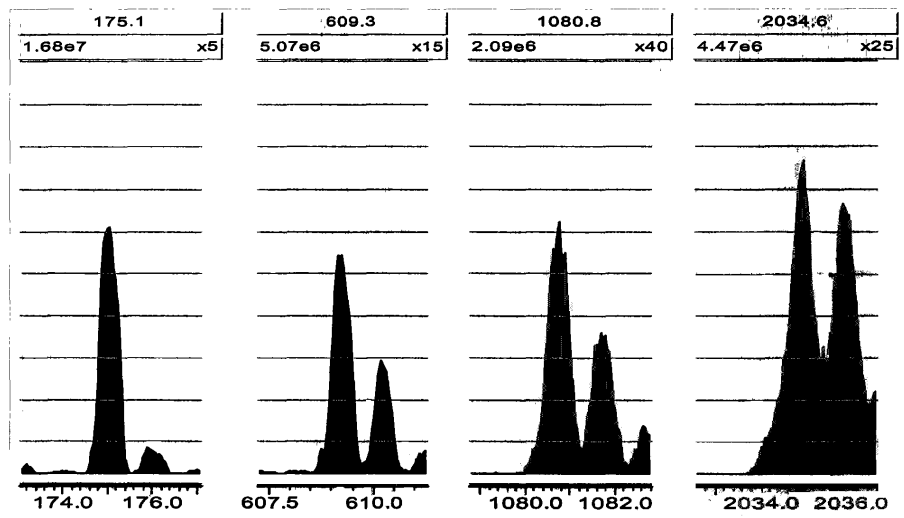


Figure 18 - Unacceptable peak shapes

Example of resolved precursors on 609, 1080, and 2034.

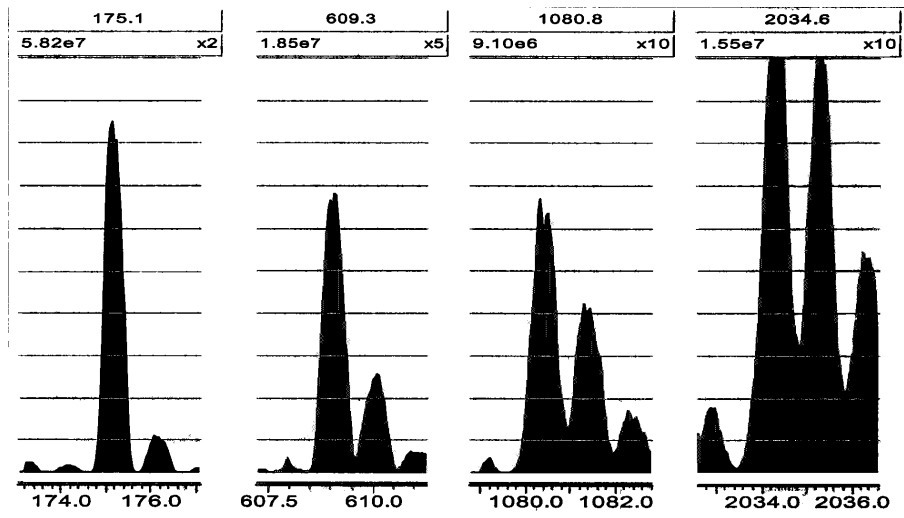


Figure 19 - Unacceptable precursors

Unacceptable precursors on 609 and 1080.

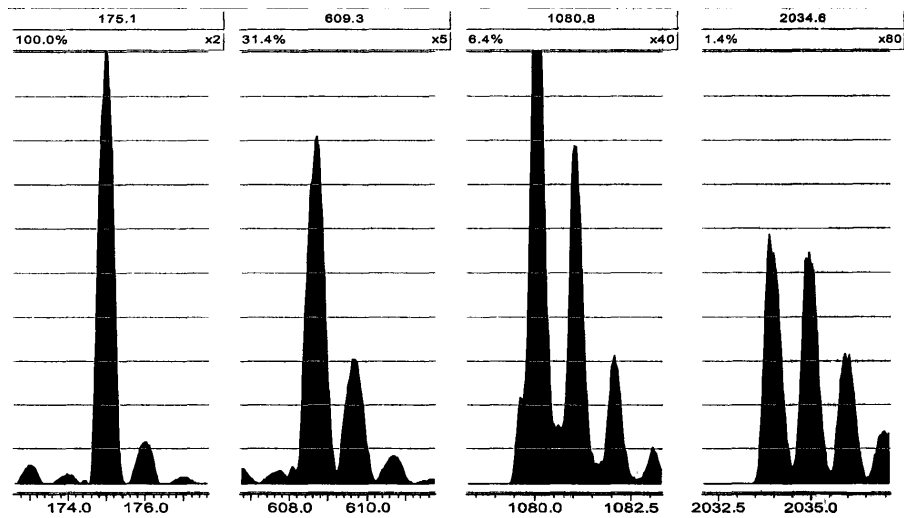


Figure 20 - Unacceptable precursors

Gross precursors.

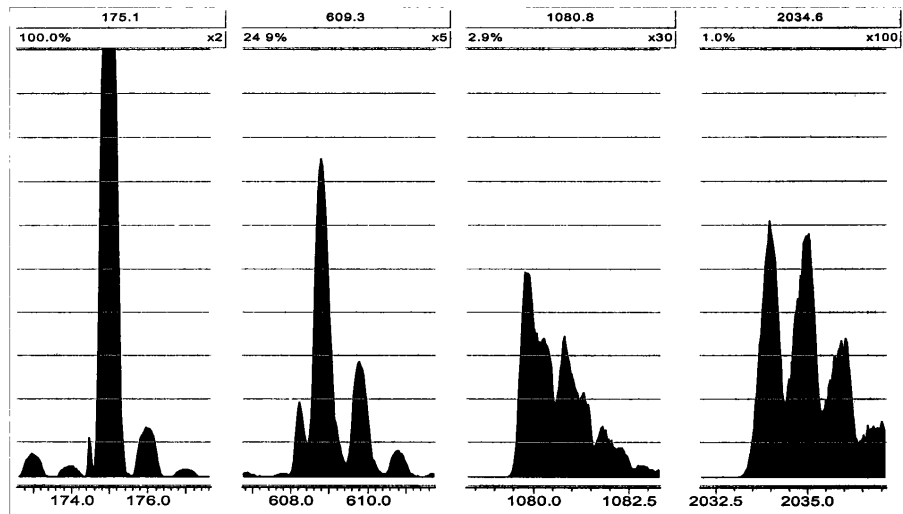


Figure 21 - Unacceptable precursors

The 1080 peak was assessed as having a "postcursor".

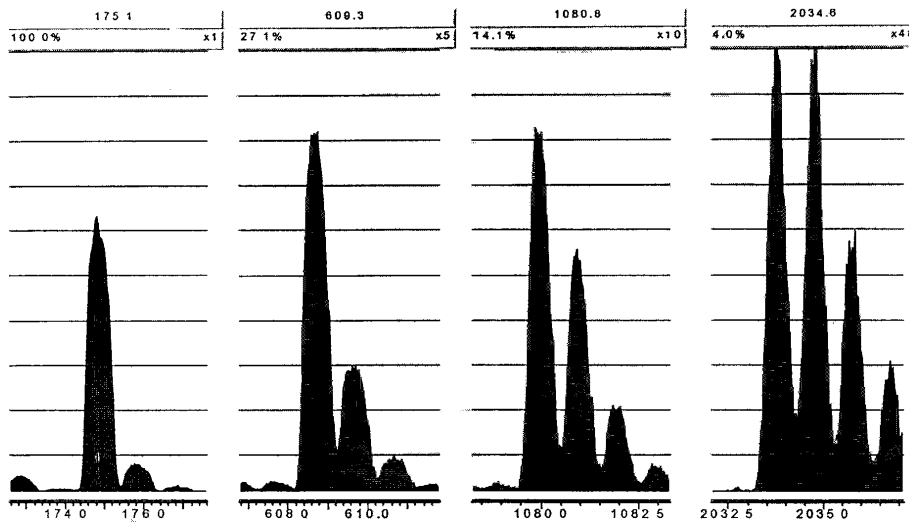


Figure 22 - Acceptable peak shapes

Great care is required when assessing the negative ion peak shape. This example is too weak to assess the peak shape from the hardcopy.

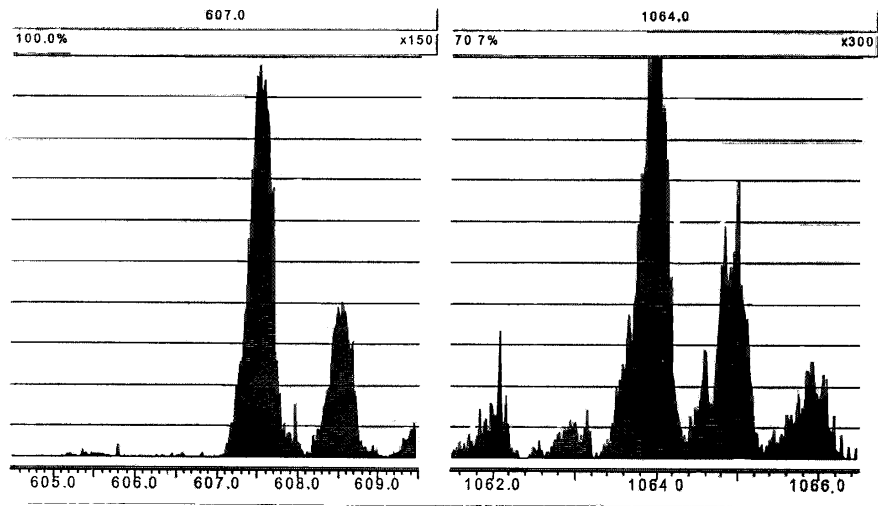


Figure 23 - Negative ion peak shape

The shoulder must be less than 10% of peak height at optimum +0.6 V ion energy. This is >20% at optimum ion energy.

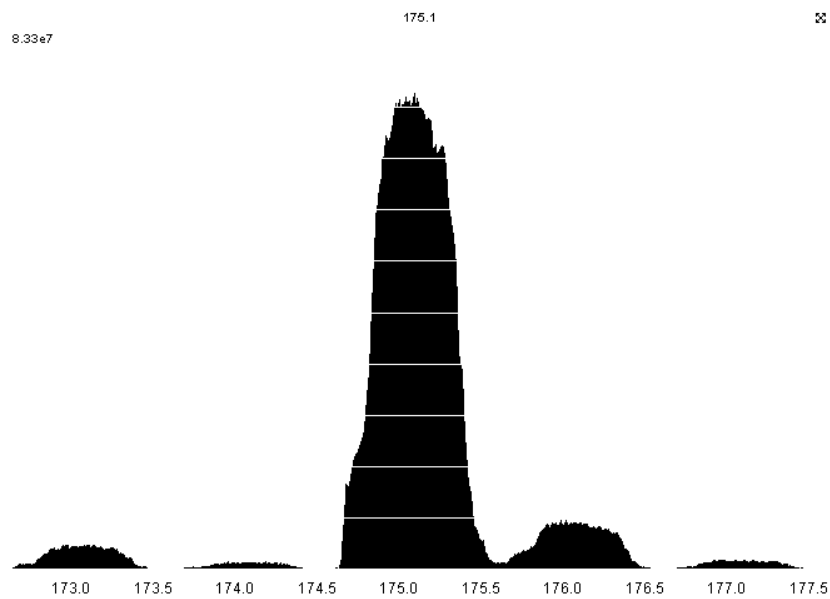


Figure 24 - Unacceptable shoulder