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Improving Quadrupole Performance with a Thin DC Only Quadrupole Prefilter: Achieving High Performance in Tandem Mass Spectrometers with Reduced Size

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Introduction

Prefilters enhance quadrupole sensitivity

Ion transmission efficiency at unit resolution can be enhanced by augmenting the fringe field region of a quadrupole mass filter. A conventional RF-only Brubaker prefilter modifies this fringe field region by applying the filtering RF to four quadrupole rods placed adjacent to the filtering quadrupole to create a delayed DC ramp. Alternatively, a similar enhancement of ion transmission efficiency can be achieved by partially cancelling the quadrupole DC field in the fringe field region, see Ref 1. This can be achieved by applying cancelling DC voltages (±W) to a thin quadrupole lens positioned directly before the filtering quadrupole, as shown in Figure 1.

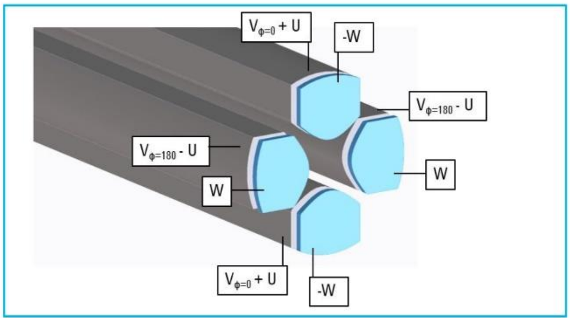

Figure 1. DC prefilter (blue) adjacent to a quadrupole. V and U are the filtering RF and DC voltages, respectively, applied to the quadrupole.

Here, we report the characterization of our thin DC-only prefilter, which is a key component in Agilent Technologies new reduced size triple quadrupole LC/MS system, the Ultivo (Figure 2). The size reduction between Brubaker prefilters and thin DC-only prefilters enables high performance within a compact instrument footprint.

Figure 2. Agilent's Ultivo triple quadrupole LC/MS.

Instrumentation

The DC prefilter is a key part of Agilent's Ultivo.

After ions are created in an atmospheric pressure ion source, they pass through a sampling capillary and skimmer before reaching a novel multipole ion guide called the Cyclone, as shown in Figures 3 and 5.

Figure 3. Simplified ion optics of Agilent Technologies Ultivo triple quadrupole LC/MS. DC pre- and postfilters shown in red. ±10 kV HED and electron multiplier not shown (right hand side).

The Cyclone ion guide compresses and collimates the ion beam using two superimposed twisted and tapered hexapoles that pass through several vacuum stages. The inner hexapole receives two out of phase (φ = 0° and 180°) RF voltages at 9 MHz, which allow transmission of low mass ions. One phase of 1 MHz RF voltage is applied to the short outer hexapole, which improves high mass transmission at the Cyclone entrance. The taper causes compression of the ion beam, and the twist enables a greater pressure drop over a shorter length by allowing smaller openings between the vacuum stages. A DC bias along the inner rods gently pulls the ions through the device. See Refs 2 and 3.

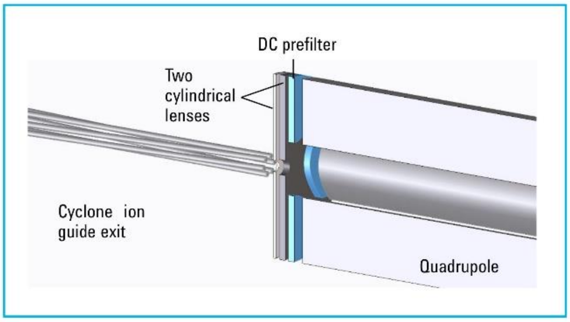

Figure 4. DC prefilter positioned between ion guide exit and quadrupole entrance

Upon exiting the Cyclone ion guide, the ions pass through two cylindrical lenses before reaching a DC prefilter (also called a Virtual prefilter) and entering the first quadrupole, as shown in Figure 4.

Instrumentation

A DC postfilter follows the first quadrupole. Two cylindrical lenses follow the MS1 postfilter and enable efficient ion injection into the Vortex collision cell shown in Figures 3 and 5.

The Vortex collision cell is made of a tapered and twisted hexapole surrounded by a shroud to contain nitrogen, the collision gas. The taper enables ion beam compression, and the twist reduces the gas flow out of the cell while maintaining a large opening to collect ions exiting MS1. A DC bias along the rods gently pulls the ions toward the second quadrupole. Two cylindrical lenses follow the vortex collision cell.

Figure 5. Cyclone ion guide (left) and Vortex collision cell with rods shown in blue.

The second filtering quadrupole is preceded by a DC prefilter. After MS2, the ions reach a detector assembly made of a cylindrical lens followed by a ± 10 kV high energy dynode and an electron multiplier.

Method

The DC prefilter was characterized using ion trajectory modelling and experiments.

Ion trajectory modelling was also used to characterize the performance of the DC pre- and postfilters. 3D models of MS1 were created in Simion test release version 8.1 in early access mode to enable multi-core parallel computations, see Ref 4. Simulated ions were generated in the low pressure exit of the Cyclone ion guide, where they were thermalized with a low pressure background gas. The ions passed through two cylindrical lenses before reaching the DC prefilter, the filtering quadrupole, a DC postfilter, two more cylindrical lenses, and finally a simulated ion detector (in place of the Vortex collision cell). The simulated quadrupole was tuned to yield approximately unit resolution (0.7 m/z FWHM), and the resulting simulated abundance and peak width were recorded during mass scans 3 m/z wide centered at 118, 622, 1222 Th. The percent of ions transmitted through the MS1 optics (abundance analogue) and peak width were recorded as a function of the two DC voltages applied simultaneously to both the pre- and postfilter.

Method

To experimentally characterize the DC pre- and postfilters, opposing elements of the DC prefilter were shorted together, and the resulting electrode pairs were connected to two ± 600 V DC voltage supplies. Resulting ion abundances and peak widths for Agilent Technologies ESI-L tuning mix ions (approx. m/z/: 118, 322, 622, 922, 1222) ionized using an Agilent JetStream ion source were recorded at various combinations of voltages applied to the DC prefilter. Performance of the MS1 DC prefilter, MS1 DC postfilter, and MS2 DC prefilter were investigated.

Results and Discussion

Ion trajectory modelling and experiments show ion transmission enhancement when cancelling DC voltages are applied to the DC-only prefilter.

The results of ion trajectory modelling through a simulated MS1 assembly with DC pre- and postfilters are shown in Figure 6.

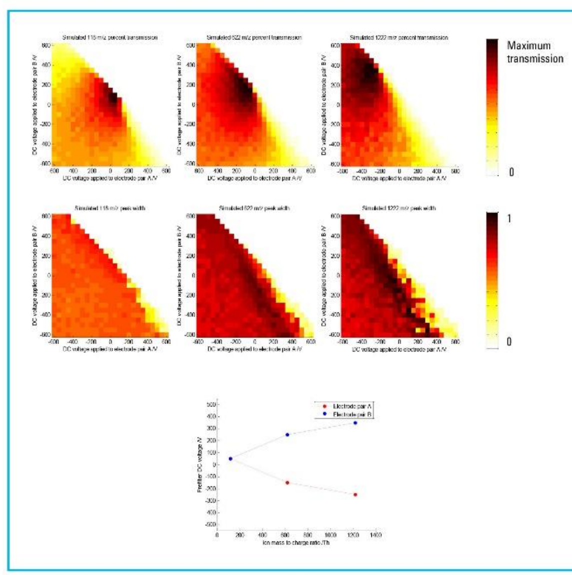

Figure 6. Simulated MS1 normalized percent ion transmission (upper) and peak FWHM (middle) as a function of two DC voltages applied simultaneously to the pre- and postfilter for ions of increasing m/z. The inset plot shows the voltages required to achieve maximum ion transmission for each m/z.

Results and Discussion

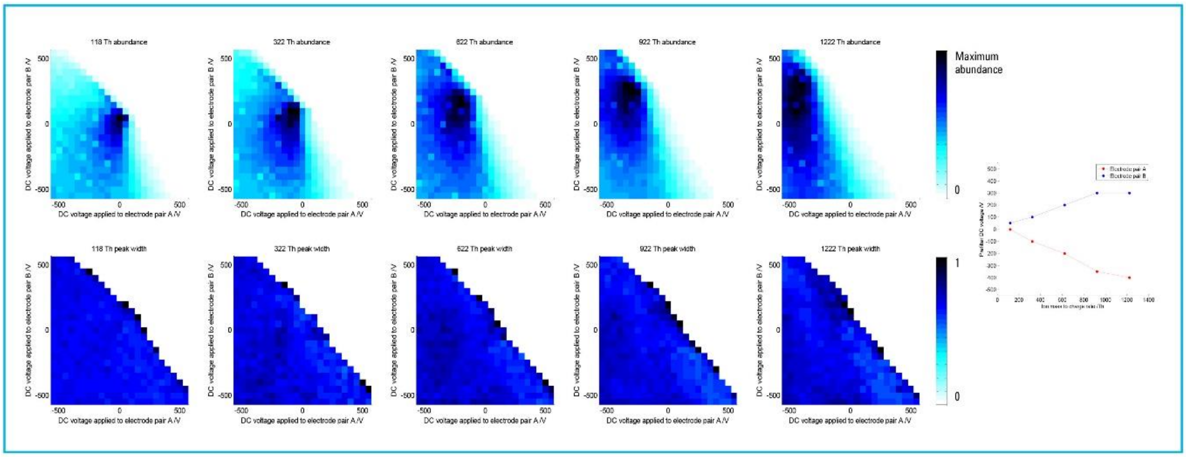

Figure 7. Experimental MS2 abundance (upper) and peak FWHM as a function of two DC prefilter voltages for ions of increasing m/z. The inset plot shows the voltages required to achieve maximum ion transmission for each m/z.

Maximum ion transmission is achieved when the DC applied to each prefilter element is the opposite polarity of the filtering DC applied to the quadrupole rod. Additionally, increasingly large DC voltages are required to maximize ion transmission as the ion m/z increases, as is shown in the inset plot. Minimal effect on peak width is observed as the pre- and postfilter voltages are changed indicating that the DC prefilter enhances the ion transmission efficiency without loss of resolution.

Figure 7 shows experimental results for the MS2 prefilter. These experimental results are similar to what was observed in the in the MS1 pre- and postfilter ion trajectory modelling shown in Figure 6. Maximum ion transmission is achieved when the DC applied to each prefilter element is opposite in polarity to the filtering DC applied to the quadrupole rod. Additionally, increasingly large DC voltages are required to maximize ion transmission as the ion m/z increases. Minimal effect on peak width is observed as the prefilter voltages are changed indicating that the DC prefilter enhances the ion transmission efficiency without loss of resolution.

Similar data were recorded for the MS1 prefilter and MS1 postfilter. The data are not presented here, but their performance shows similar trends to those presented.

Conclusions

Data presented here demonstrate that DC (Virtual) prefilters can be used to enhance ion transmission efficiency at unit resolution in a quadrupole mass filter by partially cancelling the DC field in the fringe field region. A primary advantage of the DC-only prefilters is their small size when compared to traditional Brubaker RF-only prefilters, which makes them an ideal component for miniaturized and small footprint instruments. These DC-only pre- and postfilters are a key component of Agilent's new reduced size yet high performance Ultivo triple quadrupole LC/MS.

References

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