Mass spectrometer robustness improvement with a quadrupole ion guide bandpass filter

SCIEX The Power of Precision

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ABSTRACT

This presentation describes a new quadrupole ion guide bandpass filter to create a controllable high mass cutoff. We have conducted a series of highly accelerated contamination workflows with different matrices to demonstrate that this bandpass filter is able to effectively reduce the contamination downstream of the ion guide and thus improve the mass spectrometer robustness.

INTRODUCTION

Mass windowing in an RF-only quadrupole ion guide can be achieved by adding a set of auxiliary electrodes where DC voltages are applied to produce a high m/z cut-off to effectively remove high m/z species and narrow the m/z range of ions transmitted downstream[1,2]. In our work, a short set of T-shaped auxiliary electrodes (T-bars) is placed within a quadrupole ion guide in the collisional focusing regime. The DC potentials applied on T-bars introduce an octopolar DC field which weakens the radial RF confinement of ions and destabilizes ion trajectories[3]. By adjusting the DC offset potential and the RF level applied to the Q0 ion optic, it was possible to create transmission windows with varying mass location and width.

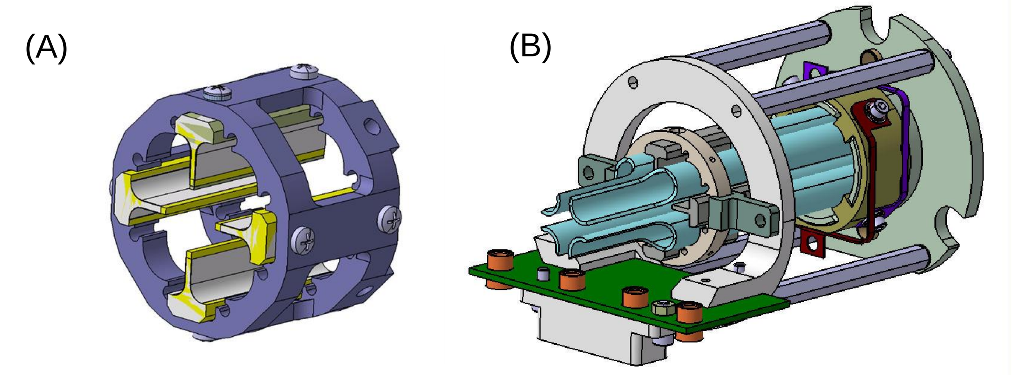


Figure 1. Illustrations of (A) T-bar assembly and (B) the assembly comprising T-bars on Q0 ion guide

Previous studies have demonstrated that charged contamination downstream of a Q0 ion guide (e.g. IQ1 lens and Q1) can lead to system performance degradation. This has motivated us to explore T-bar bandpass as a potential approach to reduce the ion current and protect downstream ion optics components, thus improving the overall instrument robustness. This work will demonstrate the results of our robustness tests using different matrices and show the capability of T-bars as a bandpass device to effectively control m/z windowing and reduce the contamination of downstream ion optics. A series of experiments were conducted with extracts of tea and arugula to determine the importance of bandpass location with regards to robustness improvement and subsequent experiments were conducted with extracts of cannabis.

MATERIALS AND METHODS

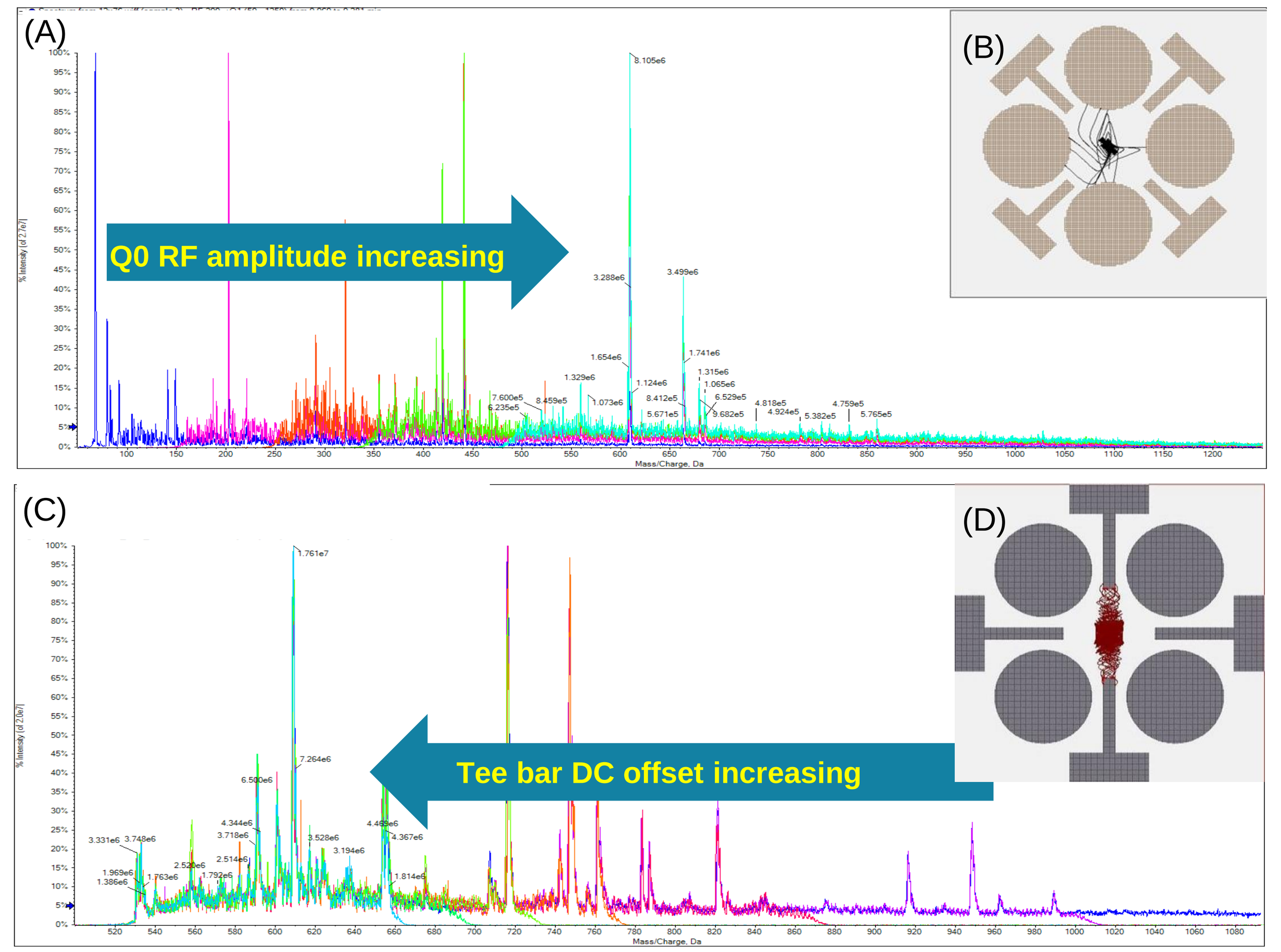
Mass spectrometer
Experiments were conducted on a modified research-grade mass spectrometer with a standard ESI source. A set of T-bar electrodes was assembled on a holder (Figure 1A) and placed within a Q0 quadrupole (Figure 1B). The RF voltage applied to the Q0 rods was provided by an external RF power supply, and the DC voltages applied on T-bars electrodes were provided by an external DC power supply with an output range of 0 to +/- 700 V. Both software and firmware were modified to enable direct control of T-bar voltages and parameter ramping.

Highly accelerated contamination experiments
Highly accelerated contamination experiments were conducted with a variety of matrices including extracts of tea and arugula matrix, diluted extra virgin olive oil, and extracts of cannabis. The sample preparation protocols were developed for each matrix. Solutions of reserpine and PPGs were used to baseline the instrument and measure performance. After contamination, instruments were cleaned following a standard protocol using SCIEX cleaning package.

RESULTS

T-bars/Q0 ion guide bandpass filter

Figure 2. A bandpass filter mechanism. (A) Low-mass cutoff (LMCO) is controlled by RF amplitude on Q0, and the cutoff shifts to higher m/z as RF amplitude on Q0 increases. (B) Low mass ions below LMCO are filtered to Q0 rods as shown in simulation. (C) High-mass cutoff (HMCO) is controlled by DC potentials applied to T-bar electrodes, and increasing the DC offset shifts the cutoff to a lower m/z. (D) High mass ions beyond HMCO are filtered to T-bar electrodes as shown in simulation.

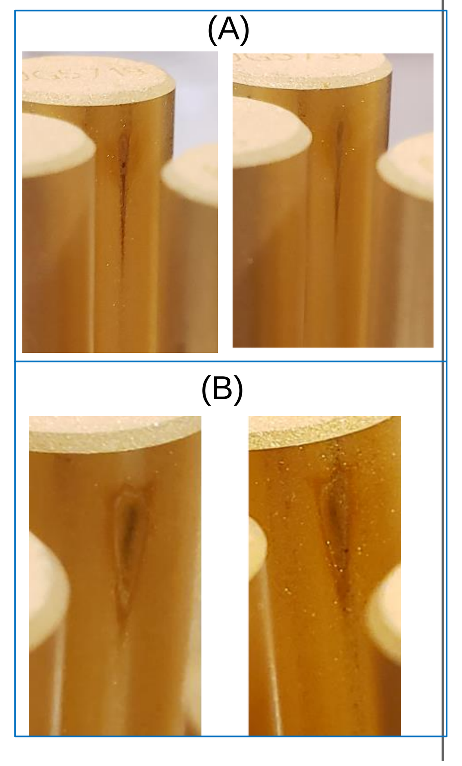


Tea/Arugula matrix highly accelerated contamination experiments

Configuration	Failure Point (mL Matrix)	Heavy Debris on Q1?	Heavy Debris on T-Bars?
(1). No T-Bar windowing	30 ml	Yes	No
(2). T-bar/Q0 Transmitting m/z 200-400	> 100 mL	No	Yes
(3). T-bar/Q0 Transmitting m/z 400-800	> 100 mL	No	Yes
(4). T-bar/Q0 Transmitting m/z > 720	40 ml	Yes	No
(5). T-bar/Q0 Transmitting m/z < 900	> 100 mL	No	Yes

Table 1. Robustness test results with tea/arugula extracts, under various bandpass window conditions. The solutions of tea/arugula extracts were continuously infused, and instrument performance was monitored following a protocol. "Failure point" means the amount of tea/arugula solutions infused when the instrument performance meets a stop criteria. In these test, the stop criteria for contamination was either >10% change in FWHM in a polarity switching test or >30% change in MRM signals in a polarity switching test. For this matrix, robustness can be improved by at least 3X by applying a high-mass cutoff using T-bars only. There is no need to create a low-mass cut-off.

Figure 3. Heavy debris observed on Q1 rods after (A) 30ml infusion with no T-bar windowing and (B) 40mL infusion with T-bar/Q0 transmitting ions of m/z >720.



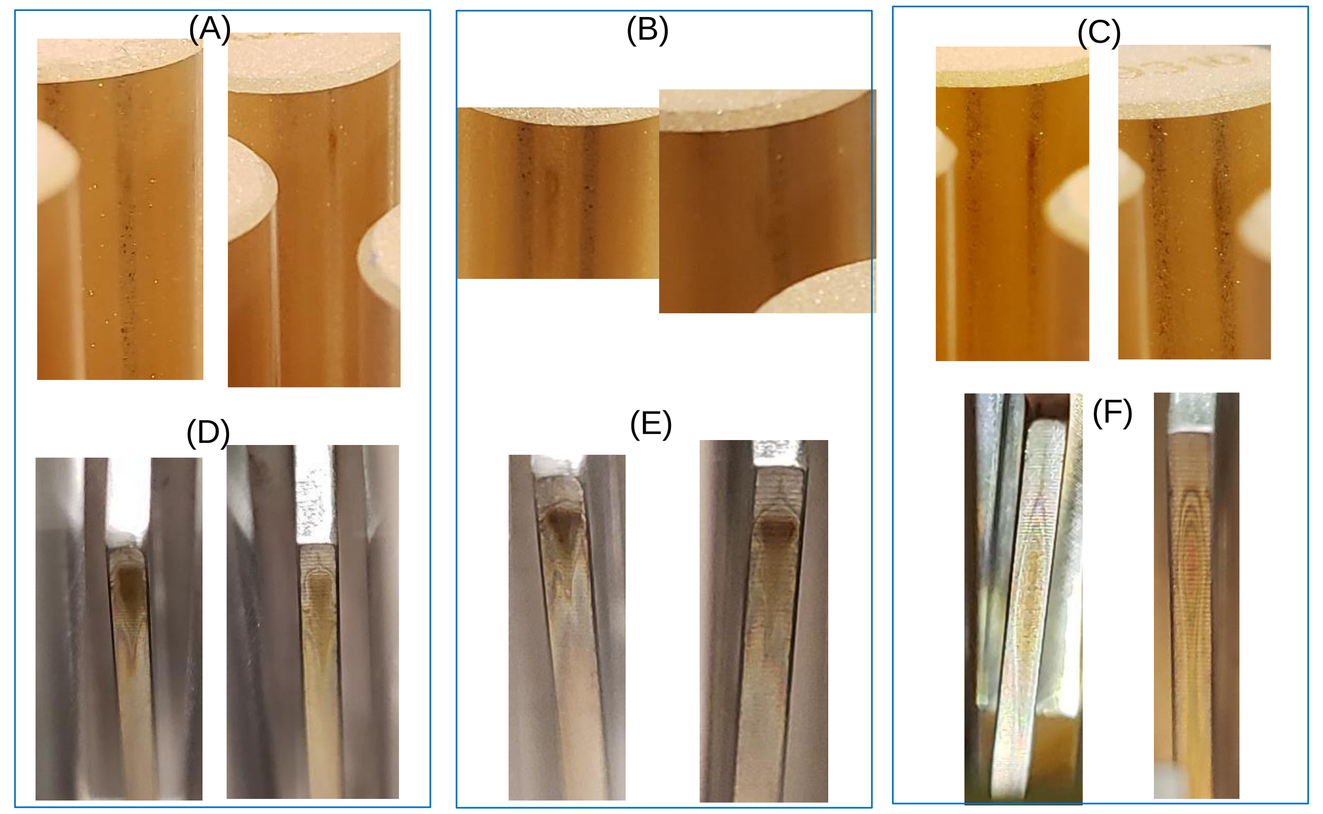


Figure 4. Clean Q1 rods observed after infusing 100 mL of tea/arugula matrix with (A) T-bars/Q0 transmitting m/z 200-400, (B) T-bar/Q0 transmitting m/z 400-800, and (C) T-bar/Q0 transmitting <m/z 900. The debris were observed on one pair of T-bar electrodes where filtered high-mass ions were deposited under three bandpass configurations respectively (D-F).

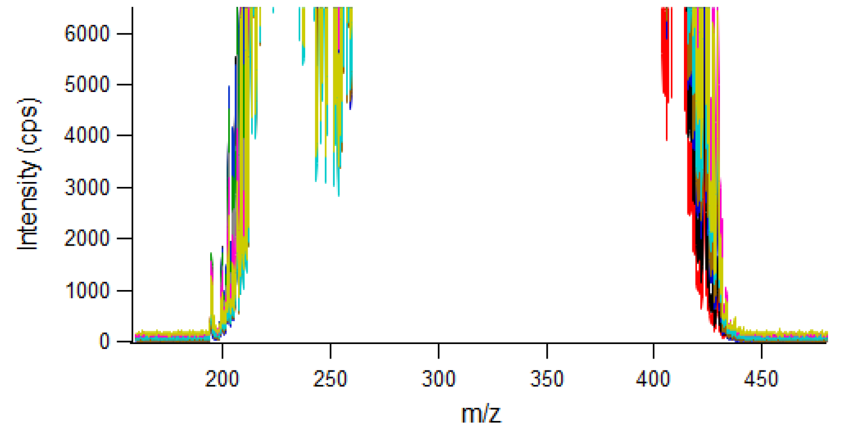


Figure 5. Overlay of Q1 windows transmitted in the 10 different overnight matrix infusions. Bandpass windows generated by T-bars did not shift when up to 100 mL of tea/arugula matrix was sprayed.

Olive oil highly accelerated contamination experiments

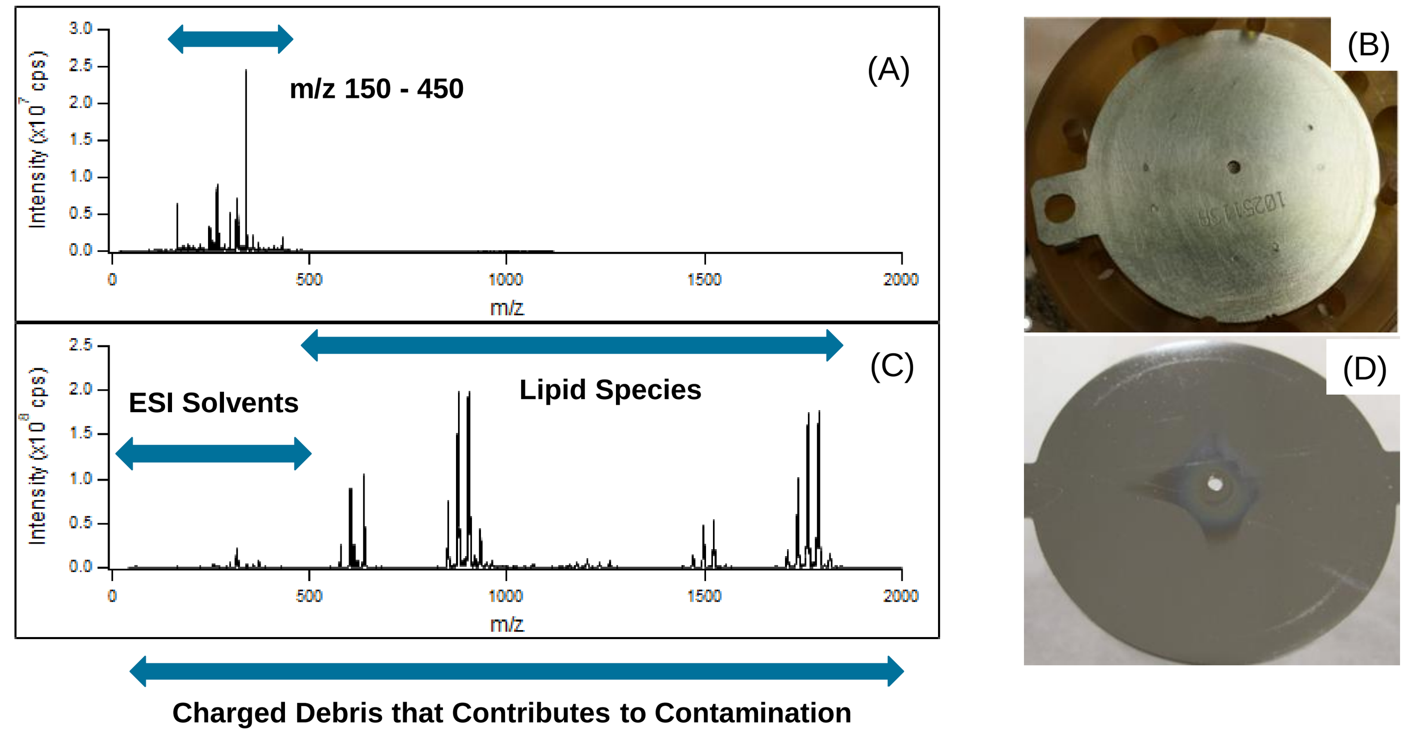


Figure 6. (A) Mass spectrum of olive oil matrix with T-bars bandpass applied to transmit ions with m/z 150- 450. (B) After 72 mL infusion, the IQ1 was clean with only faint deposit which is signs of low mass solvent passing through. The instrument performance can be recovered by cleaning ion optics upstream of Q0 only . (C) Mass spectrum of olive oil matrix without T-bar bandpass. (D) After 72 mL infusion, substantial debris was observed on the IQ1 lens, leading to signal reduction which requires cleaning to recover the system performance. In this test, using T-bars to reduce contamination on the IQ1 lens improved the robustness by at least 2x.

Cannabis highly accelerated contamination experiments

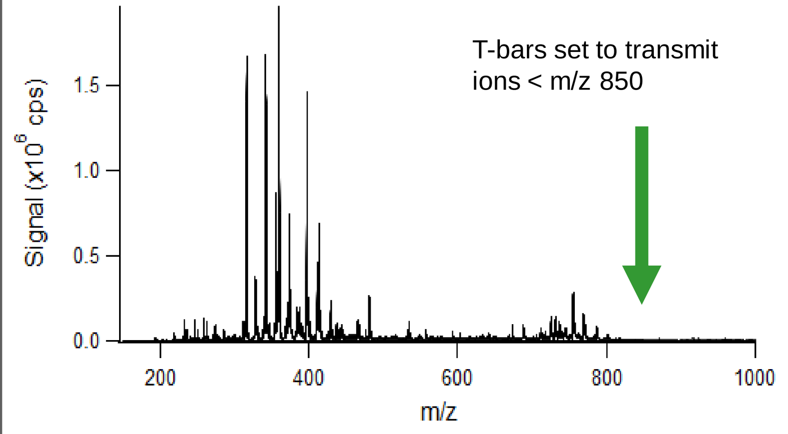


Figure 7. Mass spectrum of Cannabis matrix.

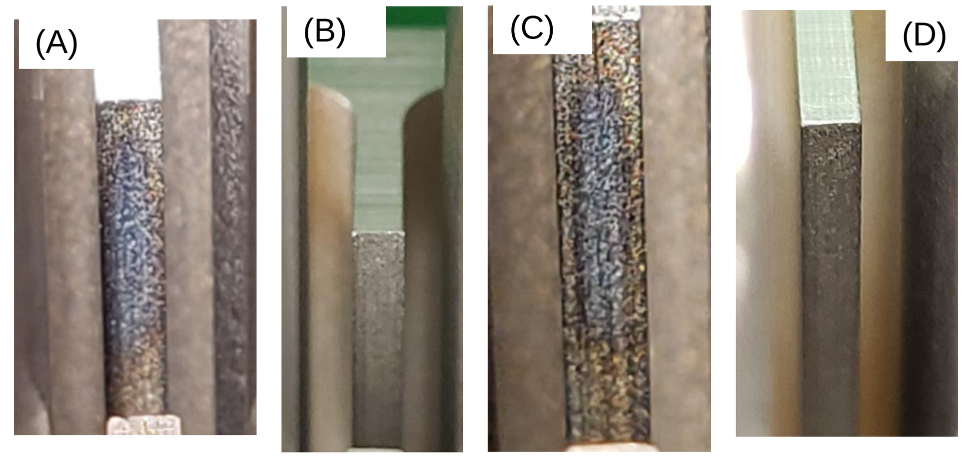
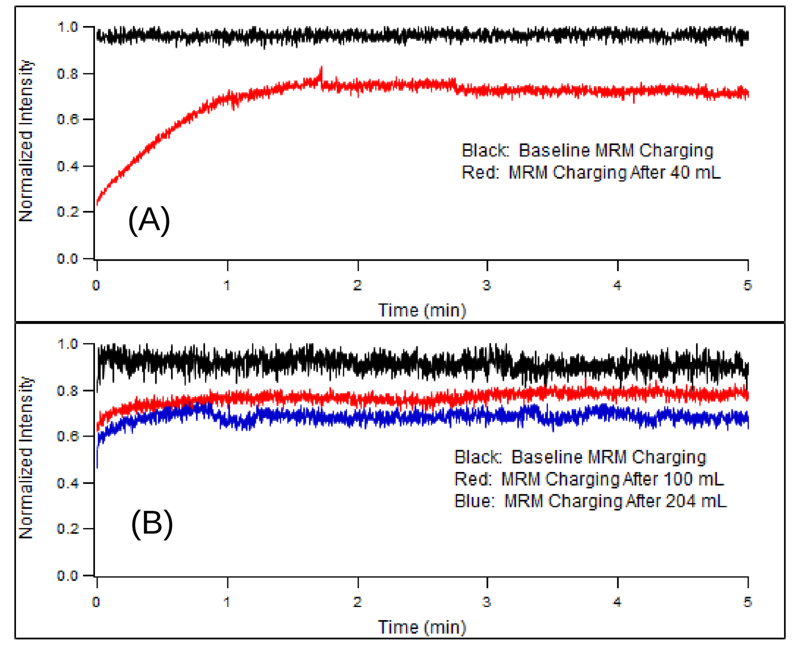


Figure 8. When the highly accelerated infusion test was conducted with the Q0 T-bars imposing a high m/z cut-off around m/z 850, the system was able to pass all tests with 204 mL of cannabis matrix infused. Very large build up of debris on one pair of T-bars (A,C) and this kept the Q1 cleaner for a longer period of time. As expected, the other pair of T-bars was clean (B,D). The Q0 T-bar mass window did not drift with up to 204 mL of matrix infusion.

Figure 9. When the highly accelerated infusion test was conducted without T-bar bandpass, the system failed an MRM charging test in 40 mL (Figure 9A). The black trace shows the MRM charging test prior to infusing cannabis extract and the red trace shows the charging tests after infusing 40 mL of cannabis extract without a Q0 bandpass, showing significant charging. When the bandpass was included, it was possible to spray 204 mL of cannabis matrix with no significant charging (Figure 9B for the baseline (black), charging test after 100 mL (red trace), and charging tests after 204 mL (blue trace).



The T-bars reduced contamination of Q1 and improved robustness by more than 5X.

CONCLUSIONS

A series of highly accelerated contamination workflows with different matrices were used to compare instrument robustness in back-to-back comparisons with the T-bar bandpass enabled and disabled. This novel Q0 bandpass device that allows for removal of high m/z ions clearly improves the instrument robustness and extends the cleaning interval for MS instruments by at least 2 – 5X. The unwanted high m/z species are deposited into T-bar electrodes and thus effectively prevent the contamination on downstream ion optics (e.g. IQ1 and Q1).

REFERENCES

1. Patent US10741378
2. Patent US20210327700
3. Loboda et. al. Eur. J. Mass Spectrom, 2000, 6, 531-536

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