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Ion Transmission Characterization Through a Dual-Field Converging Multipole Ion Guide

Haopeng Wang, Laura L Pollum, Patrick M Batoon

Agilent Technologies, Inc., Santa Clara, CA

Introduction

Mass spectrometers coupled to liquid chromatographs (LC/MS) have been widely utilized for the identification and quantification of analytes in complex samples. Thanks to the highly efficient ion transmission through a dual-field converging multipole ion guide (Cyclone ion guide), it was possible to reduce the instrument footprint without sacrificing analytical performance. The Cyclone ion guide is the key component of Agilent Ultivo LC/MS Triple Quadrupole and Agilent LC/MSD iQ Single Quadrupole instruments.

Although many LC/MS applications are aimed at ions with high m/z ratios, the recent emergence of applications like pharmaceutical impurity detection (Nitrosamines) and emerging contaminants (PFAS/PFOA) calls for sensitive detection of ions with low m/z ratios. Here, the mass dependent ion transmission through Cyclone ion guide is evaluated. Specifically, the transmission of low m/z ions is evaluated and characterized.

Experimental

Cyclone ion guide

The Cyclone ion guide is between the skimmer and quadrupole mass filter. It expands through three pressure stages, with more than 1000-fold pressure reduction.

As shown in Figure 1, the ion guide consists of one set of inner hexapole and one set of outer hexapole. The inner hexapole is geometrically twisted and tapered, which enables phase space compression of ion beam. The outer hexapole is also twisted and tapered, covering the entrance half the ion guide.

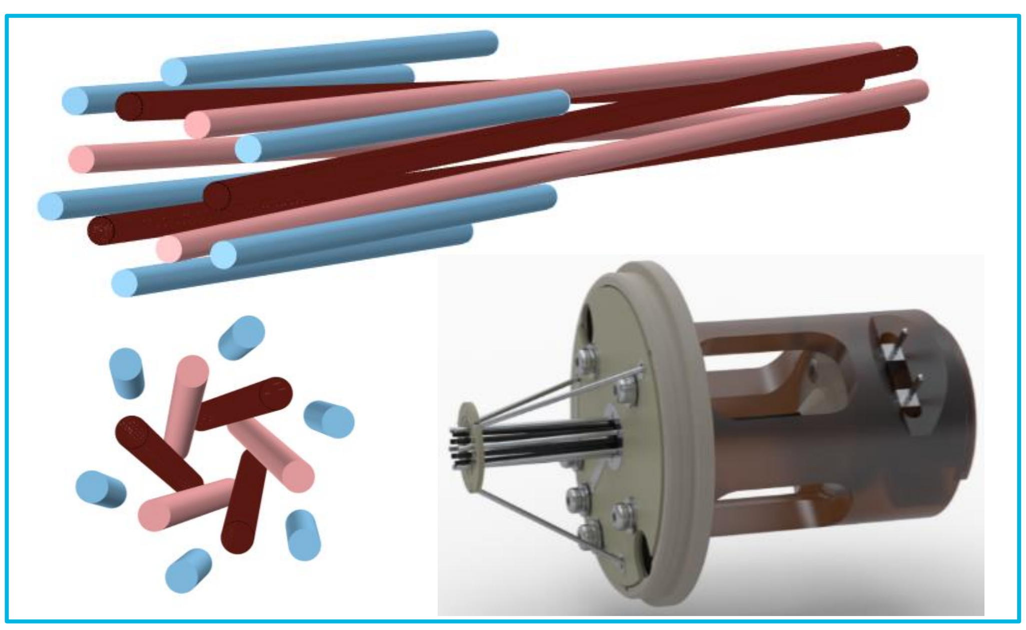

Figure 1. Cyclone ion guide electrodes, shown top and left. Outer rods are shown in blue. Inner rods are shown in pink and maroon. The full cyclone assembly is shown on the lower right.

Experimental

Variable frequency RF driver

Confining RF voltages are applied to both the inner hexapole and the outer hexapole on the Cyclone ion guide. As shown in Figure 2, applying two opposing phases of RF voltage to the inner rods produce a hexapole field. Applying an additional single phase RF voltage to the outer rods creates a dodecapolar field at the entrance of the ion guide.

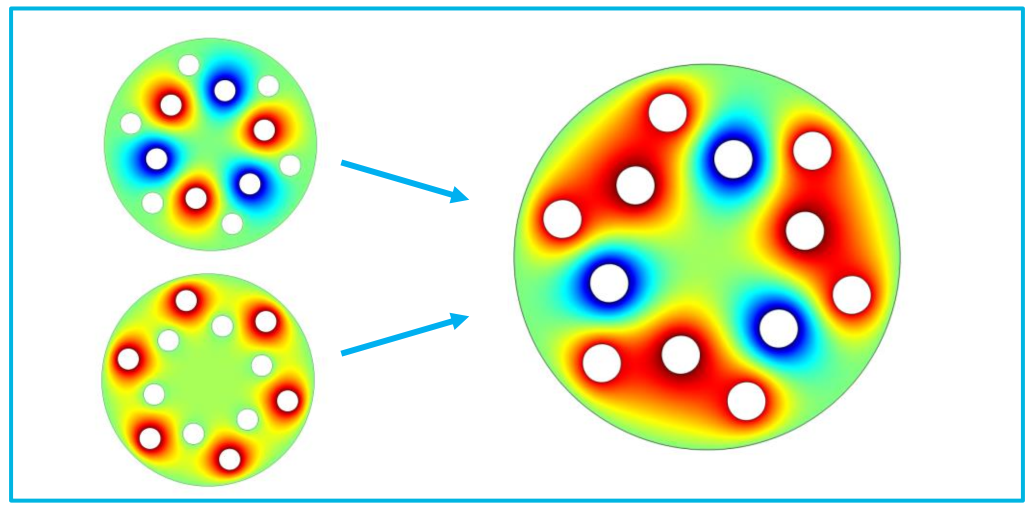

Figure 2. Electric potential within cyclone rod structure at one RF phase. Red is positive potential and blue is negative potential.

The Cyclone ion guide is driven by variable frequency RF voltage generators. The variable frequency drivers each consist of a signal generator and broadband power amplifier driving a tunable LC resonant voltage step-up circuit. During operation, the signal generator is set to the chosen frequency and then the resonant circuit is manually tuned to that same frequency to efficiently generate the required voltage.

Ion transmission characterization

Ion transmission through Cyclone ion guide was characterized experimentally on Agilent LC/MSD iQ Single Quadrupole mass spectrometer. Trace amount of potassium acetate was spiked into Agilent ESI-L tuning mix to provide stable ions with low m/z ratio. Chemicals are introduced using the built-in Calibrant Delivering System and ions are generated with electrospray ion source.

Abundance of ions (with m/z 39, 118, 322, 622, 922, and 1222) at unit resolution are recorded as function of the amplitude of RF voltages on both inner hexapole and outer hexapole. In addition, the frequency of RF voltage on inner hexapole is also evaluated.

Simulation

The gas flow and ion transmission through the Cyclone ion guide is simulated by Computational Fluid Dynamic (CFD) and SimIon, respectively.

Results and Discussion

Appropriate inner and outer RF voltages enables efficient transmission of ions through cycle ion guide for most applications.

Previous investigations suggested applying 9 MHz RF voltages on Cyclone inner rods and applying 1 MHz RF voltages on Cyclone outer rods provide high transmission efficient for ions between m/z 100 and 1500. Figure 3 shows the ion abundance as function of the amplitude of inner RF and outer RF.

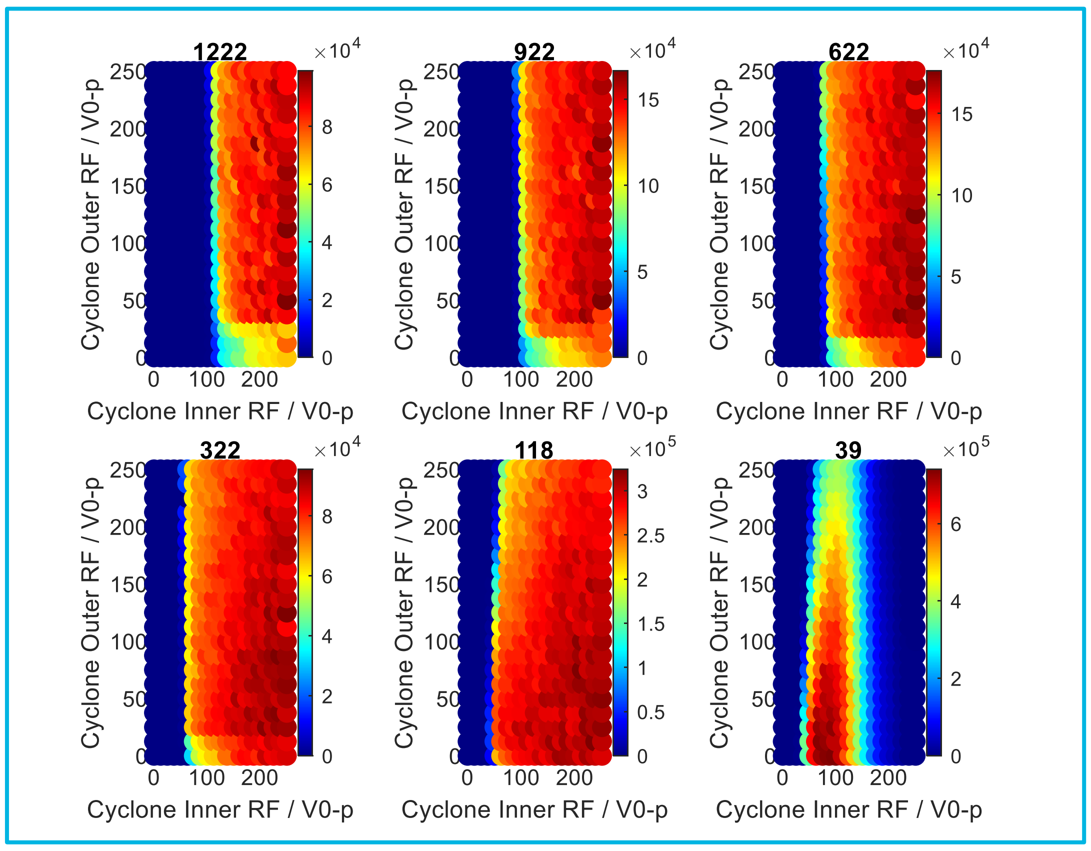

Figure 3. Ion abundance as a function of inner and outer RF amplitudes in cyclone ion guide. Deep red is maximum abundance and deep blue is zero signal.

As shown in Figure 3, high ion transmission efficiency is achieved when sufficient pseudo-potential is created by combination of RF amplitudes applied to the inner and outer rods. For ions with m/z above 100, single pair of RF amplitudes can provide highly efficient ion transmission. This feature of Cyclone ion guide simplifies the optimization and operation of the instrument.

Applications aiming at low m/z (<100) ions may benefit from different operating parameters.

Ion with m/z below 100 behaves slightly different. When high RF amplitude is applied to either inner rods or outer rods, the ions are not able to overcome the non-adiabatic pseudo-potential resulting in loss of ions. This can be seen from both experimental and theoretical results.

In order to enhance transmission of low m/z ions, a different set of operating parameters might be necessary. As show in Figure 5, with lower RF amplitude applied to inner rods, the abundance of m/z 39 can improve more than 100%. However, the enhanced transmission of m/z 39 is accompanied by reduction of other higher m/z ions.

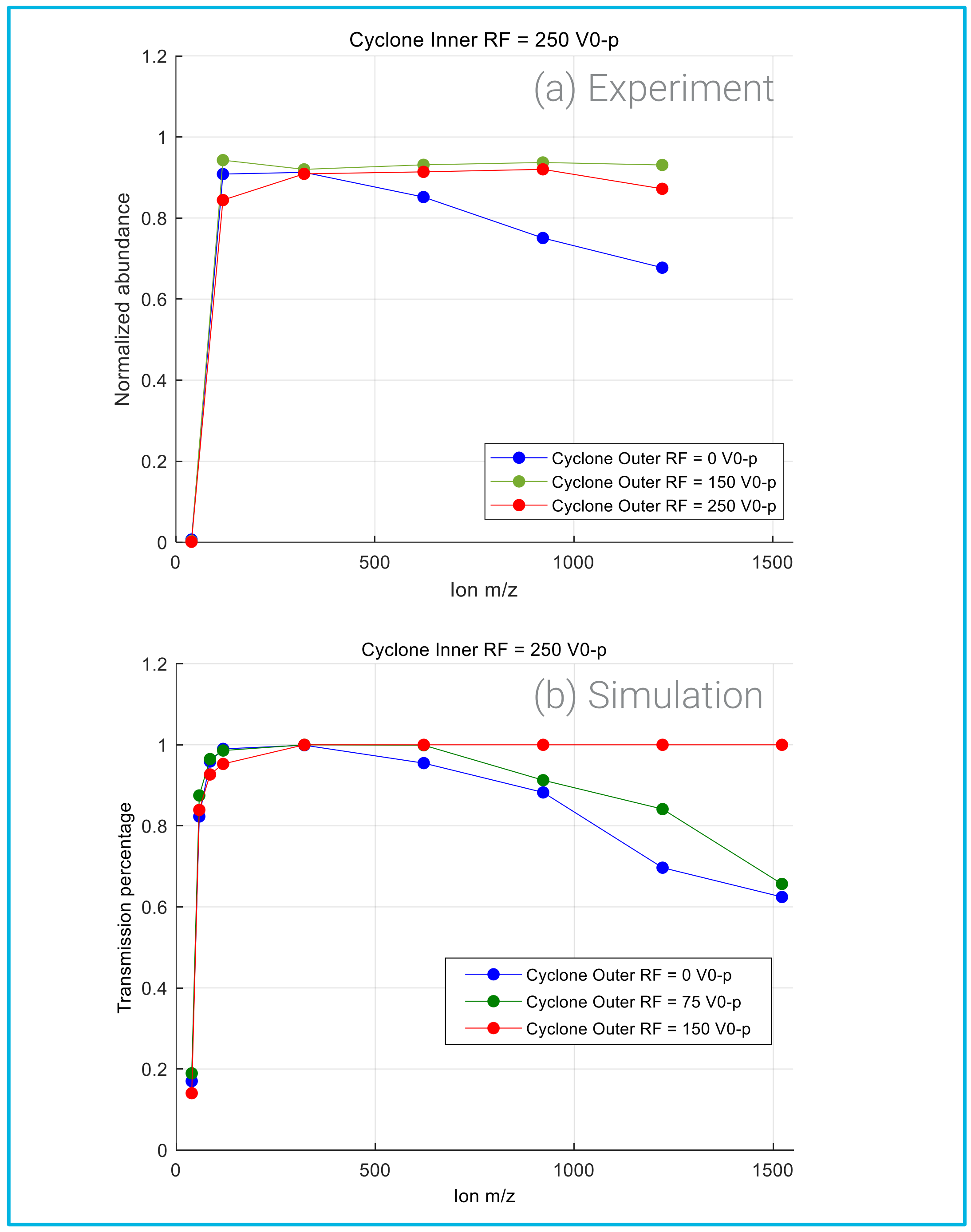

Figure 4. Mass dependent Ion transmission at selected RF amplitude based on experimental results and simulation. (Acknowledgement to Kenneth R. Newton for providing the simulation data.)

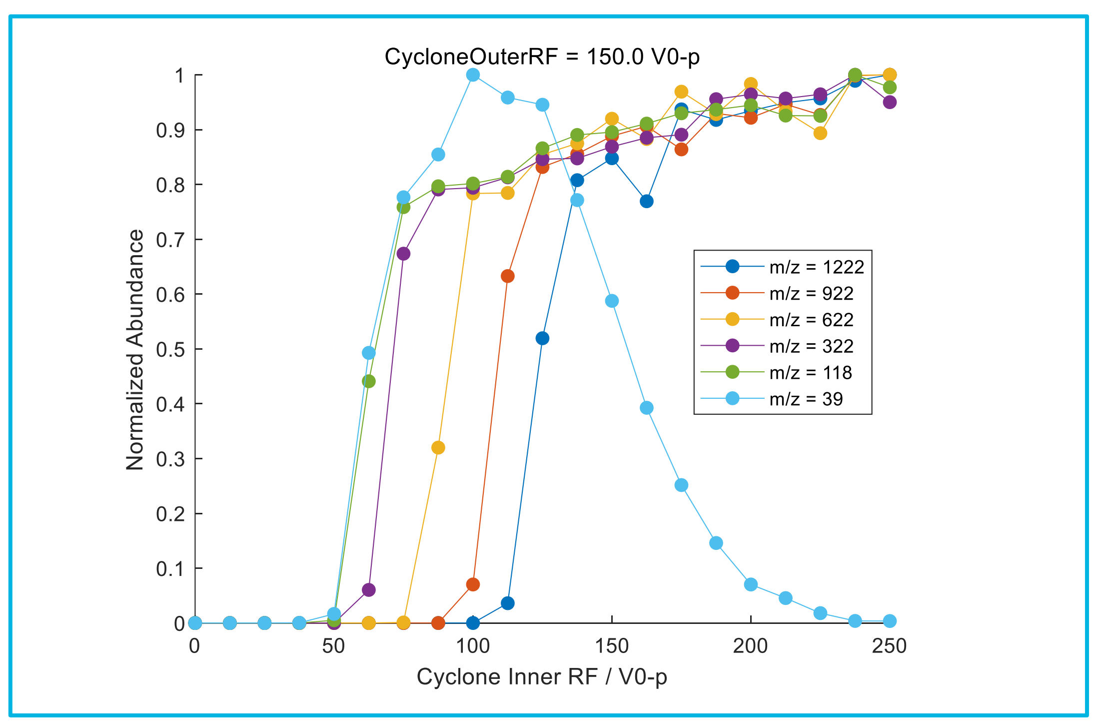

Figure 5. Ion abundance as function of RF amplitude applied on the inner rods.

Results and Discussion

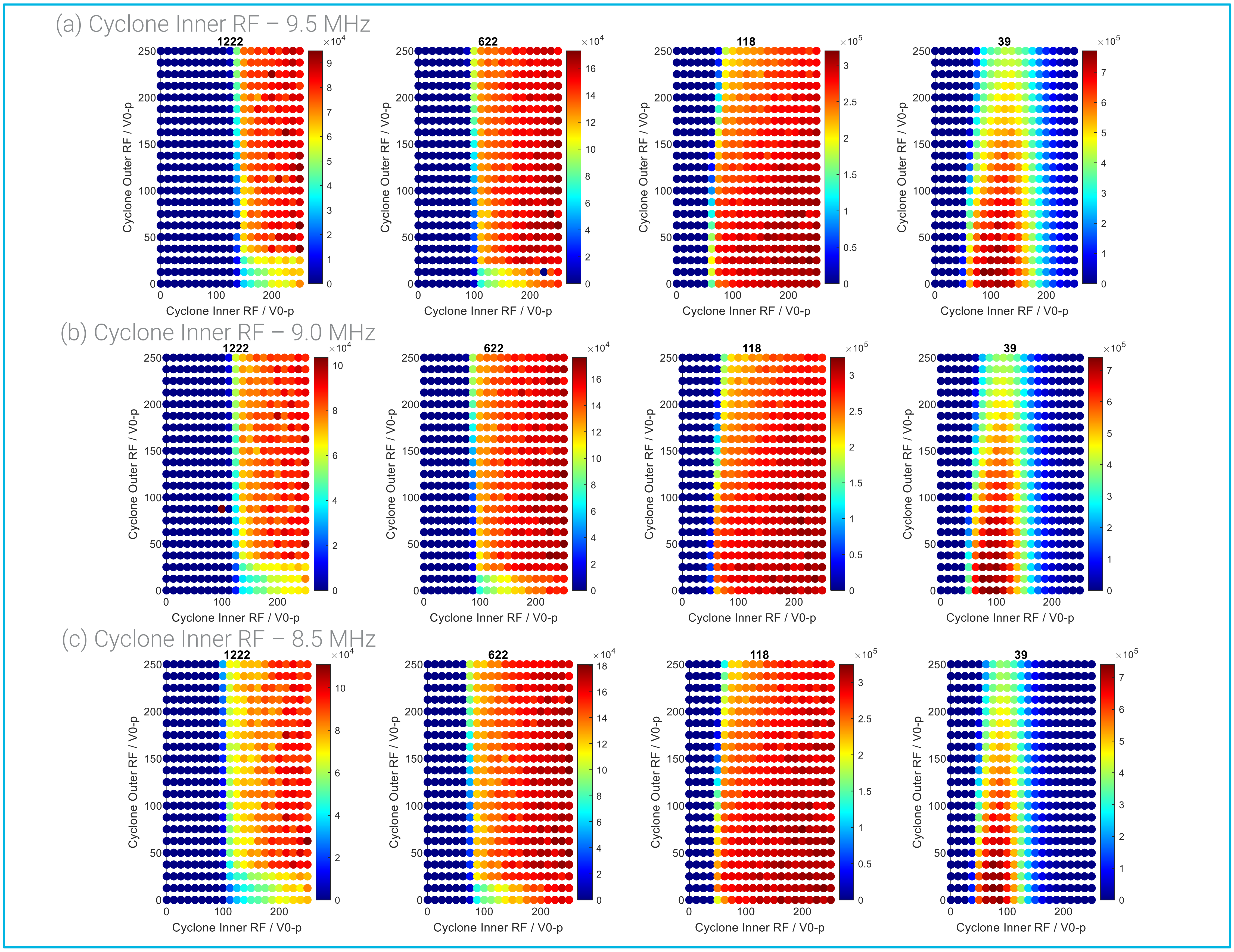

Figure 6. Ion abundance as a function of inner (at frequency of 9.5 MHz, 9.0 MHz and 8.5 MHz) and outer (at frequency of 1.0 MHz) RF amplitude in cyclone ion guide. Deep red is maximum abundance and deep blue is zero signal.

Transmission of low m/z ions could benefit from RF voltages with different frequency.

The combination of 9 MHz on inner rods and 1 MHz on outer rods was selected based on transmission of ions above m/z 100. Figure 6 shows at higher frequency (9.5 MHz), transmission of low m/z ions is improved with high RF amplitude. However, it's still challenging to find one set of optimal across the entire mass range.

Application based tuning and optimization could greatly improve the versatility of the instrument.

Conclusions

- Cyclone ion guide allows reduction of instrument size without sacrificing performance.
- Application based tuning could further improve instrument performance for selected applications.

References

Bertsch JL, Newton KR, Howard L. US Patent No. 9,449,804 B2. Sep. 20, 2016.

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