

Technical Report

Development of UF-Qarray™ RF Ion Guide with Improved Ion Focusing Capability

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Abstract:

Shimadzu's patented Qarray is a high frequency quadrupole ion guide designed to enhance ion focusing and minimize contamination. By further optimizing the ion guide geometry in the UF-Qarray design, the LCMS-8060 delivers higher sensitivity and improved robustness.

Keywords: UF-Qarray, ion guide, ion focusing capability, robustness, LC/MS/MS

1. Introduction

The LCMS-8060 is a triple quadrupole mass spectrometer that brings together Shimadzu's proprietary UF (ultra fast/ultra focusing) high-speed, high-sensitivity mass spectrometry technologies to deliver the world's highest sensitivity levels and unrivaled high-speed capability. To maximize sensitivity, without changing the proven robustness and minimal noise characteristics of the Qarray patented technology (patent numbers JP3379485, US6462338, and DE19941670), the LCMS-8060 required a new way of thinking in developing ion transfer optics that would work with a larger ion sampling orifice.

The result is the UF-Qarray ion guide technology, an innovative technology that achieves precise ion focusing despite higher gas flows from a larger sampling orifice. This groundbreaking design radically increases ion signal intensities while minimizing neutral noise resulting in performance far exceeding that of previous generations of LC/MS/MS systems.

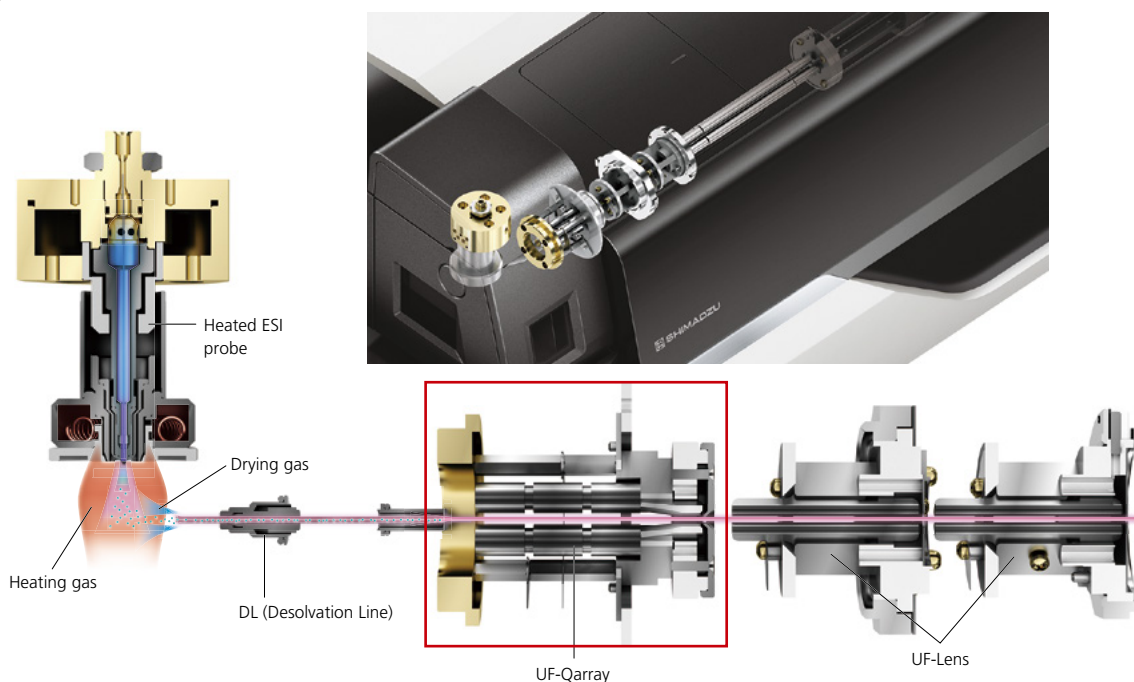


Fig. 1 LCMS-8060 Triple Quadrupole Mass Spectrometer and UF-Qarray Technology

2. Design

2-1. Simulation Study

To optimize the design of the new UF-Qarray a number of simulation studies were carefully considered using unique technologies developed by Shimadzu. Two simulation platforms were used to model increased gas flows and ion behavior in the first-stage low-vacuum region. FLUENT® software was used to determine a pole shape that would improve ion focusing with higher gas flows and an enhanced

pumping configuration. Optdesign® modelling software analysed the complex behavior of ion trajectories as a voltage is applied to the expanded ion cloud. Both simulation technologies significantly accelerated the development of an ion guide optimized for higher ion production and better focusing.

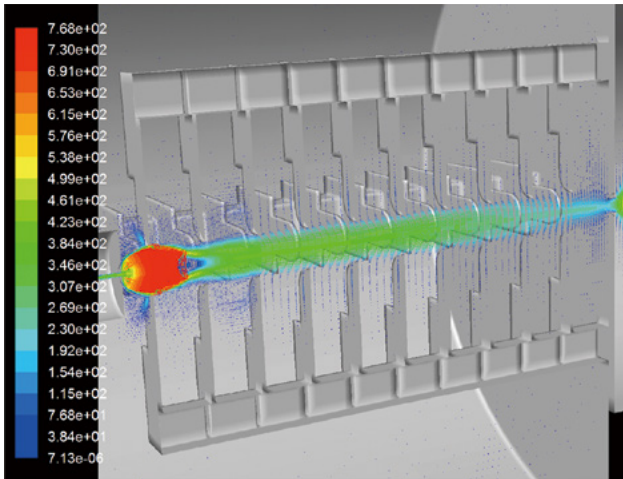


Fig. 2 Gas Flow Simulation Results Using FLUENT®

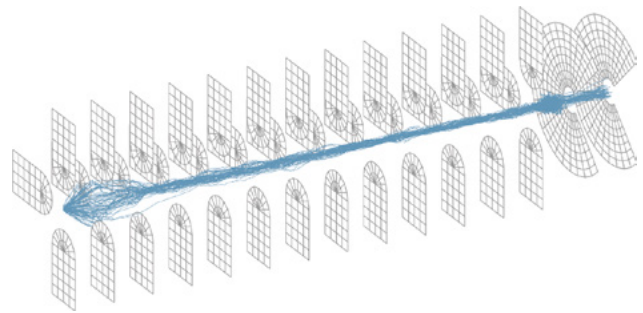


Fig. 3 Ion Trajectory Simulation Results Using Optdesign®

2-2. Optimization by Experiment

Using FLUENT® and Optdesign® simulation models several prototypes were developed for testing. The pole shape was optimized by varying physical parameters such as the inscribed circle radius, pole length (Fig. 4) and the applied voltage field. This iterative process carefully considered each change and its influence on noise and robustness.

The final optimized design resulted in a UF-Qarray pole geometry that ejected neutral noise and achieved a higher ion focusing capability without compromising the recognized stability and robustness of previous Qarray designs.

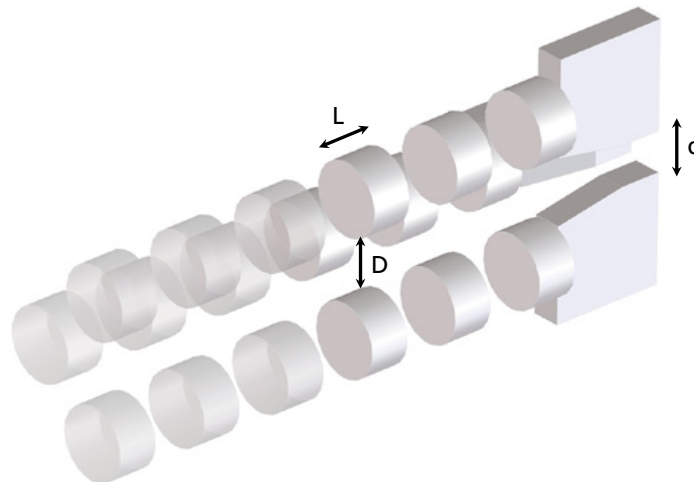


Fig. 4 Examples of Parameters Varied During UF-Qarray Development

3. UF-Qarray Effectiveness

3-1. Improved Ion Focusing Capability

As an example of the increased ion signal intensity provided by UF-Qarray technology, results from analyzing three pesticide components (fenoxaprop-ethyl, clofentezine, and triclopyr) are shown. A comparison of results obtained using an LCMS-8060 system equipped with UF-Qarray technology and an LCMS-8050 system equipped with previous Qarray technology is provided for each component.

Fig. 5 (a) shows that the LCMS-8060 signal intensity is over three times higher than the LCMS-8050.

However, as shown in Fig. 5 (b), the corresponding increase in baseline noise for the LCMS-8060 is minimal. This is due to the precise ion focusing capability of the UF-Qarray, ions from the ion source are transferred to the quadrupole mass analysers guided by the applied electric fields and neutral noise is dynamically ejected from the ion pathway.

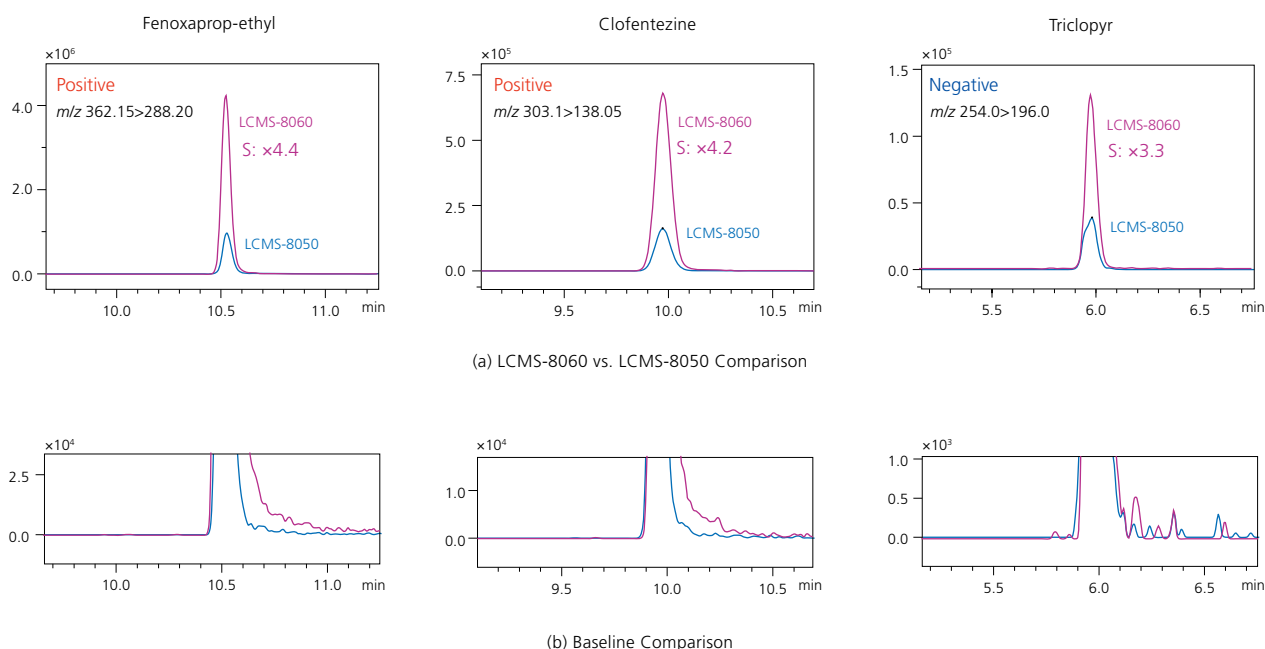


Fig. 5 MRM Chromatograms of Three Pesticide Components (at 100 pg/mL)

3-2. Improved Robustness

Another advantage of the enhanced ion focusing capability of the UF-Qarray design is improved robustness. Contamination due to ions is markedly reduced because ions travel closer to the center and farther from the ion guide poles. UF-Qarray involves unique technology that offers both higher sensitivity and higher robustness, which dramatically improves the reliability and accuracy of data measured at extremely low concentrations.

Data that indicates the superior robustness of the LCMS-8060 system

equipped with UF-Qarray technology is shown in Fig. 6. It is a plot of area and area ratio values measured by continuous acquisition from human plasma spiked with alprazolam (with alprazolam-d5 internal standard). Data was analyzed 400 times a day for six days, for a total of 2400 measurements.

As part of the robustness test the system was vented to model transient power failures or changes in sample workflows with no effect on baseline noise levels.

As indicated in Fig. 7, ion signal intensity was stable even after 2400 consecutive analyses.

The summary data in Table 1 indicates same-day variations in peak area values were typically 5%RSD and same-day variations in peak area ratio values were less than 3.5%RSD (using a deuterated internal standard). Day-to-day variations were less than 3%RSD and stopping

analysis and shutting OFF the vacuum had no effect on signal intensity or noise.

The UF-Qarray technology built into the LCMS-8060 delivers exceptional data stability for routine, high throughput applications demanding the highest sensitivity in complex matrices.

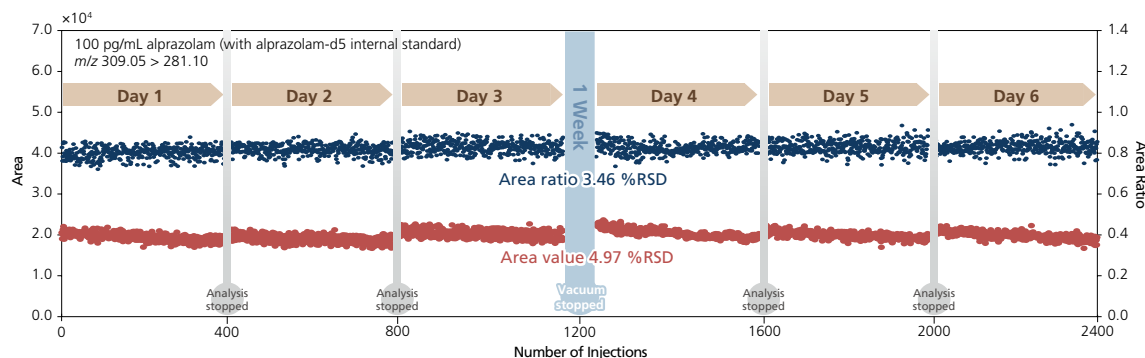


Fig. 6 Results from Continuous Analysis from Human Blood Plasma Spiked with Alprazolam

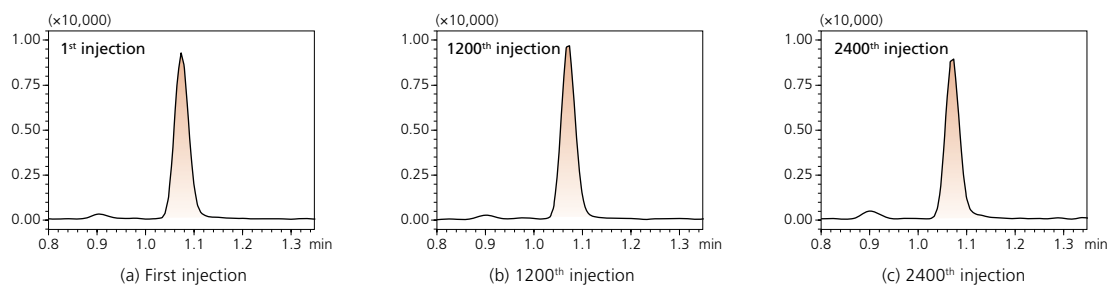


Fig. 7 MRM Chromatograms of Alprazolam (Added to Blood Plasma)

Table 1 Same-Day and Day-to-Day Variations from Human Blood Plasma Spiked with Alprazolam

Compound	Same-Day Variations (%RSD)						Day-to-Day Variations (%RSD)		
	Day 1	Day 2	Day 3	Day 4	Day 5	Day 6	First 3 Days	Last 3 Days	6 Days
Alprazolam	5.04	4.94	5.06	5.38	4.55	4.83	3.19	1.63	2.74
Alprazolam-d5 (ISTD)	5.04	4.68	5.48	5.31	4.26	4.91	2.62	1.89	2.18
Area Ratio (Alprazolam/Alprazolam-d5)	3.48	3.11	3.48	3.44	3.71	3.54	1.79	0.26	1.40

4. Conclusion

- The new UF-Qarray with an optimized ion guide design dramatically increases ion focusing capability and delivers high sensitivity with a minimal noise increase.
- The UF-Qarray offers superior robustness while still retaining the contamination resistance of Shimadzu's existing patented Qarray technology.
- The LCMS-8060 equipped with UF-Qarray offers the world's highest sensitivity levels and three times higher sensitivity than the existing LCMS-8050 model.

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