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Technical Report

Robustness Evaluation of the LCMS-8060NX with a Newly-Developed Ion Source, IonFocus™ Unit

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Abstract:

The LCMS-8060NX is the culmination of Shimadzu's expertise in triple quadrupole mass spectrometry, offering further improvements in ease of operation and robustness while achieving world-class sensitivity and measurement speed. The newly-developed IonFocus ion source unit efficiently introduces only ions into the mass spectrometer while removing unwanted solvents and contaminants. In addition, the LCMS-8060NX, equipped with new, more robust ion guides, the UF-Qarray™ II and the UF-Lens™ II, maintains outstanding data stability even under the harshest analytical conditions such as performing multiple consecutive analysis on biological samples.

Keywords: IonFocus, UF-Qarray II, UF-Lens II, robustness, LC-MS/MS

1. Introduction

The LCMS-8060NX is the culmination of Shimadzu's expertise in triple quadrupole mass spectrometry and brings further improvements in ease of operation and robustness while retaining the world-class sensitivity and measurement speed of the LCMS-8060.

Recent changes in working style and increasing pressure to reduce costs, combined with a more diverse range of demands placed on LC-MS systems, require highly efficient systems that are capable of delivering high-sensitivity performance yet are extremely robust and easy to operate. Therefore, we have developed a new proprietary ion source, the IonFocus unit (Patent No.: JP6593548, US10546740), which efficiently introduces only ions into the mass spectrometer while removing unwanted solvents. In addition, the LCMS-8060NX features new technology such as the UF-Qarray II and UF-Lens II ion guides, which have been re-designed by making their shape and applied voltage more resistant to contamination, thus minimizing system downtime and improving user efficiency.

This report describes these new technologies in detail and presents results from a performance evaluation where the LCMS-8060NX performed consecutive analyses under demanding analytical conditions.

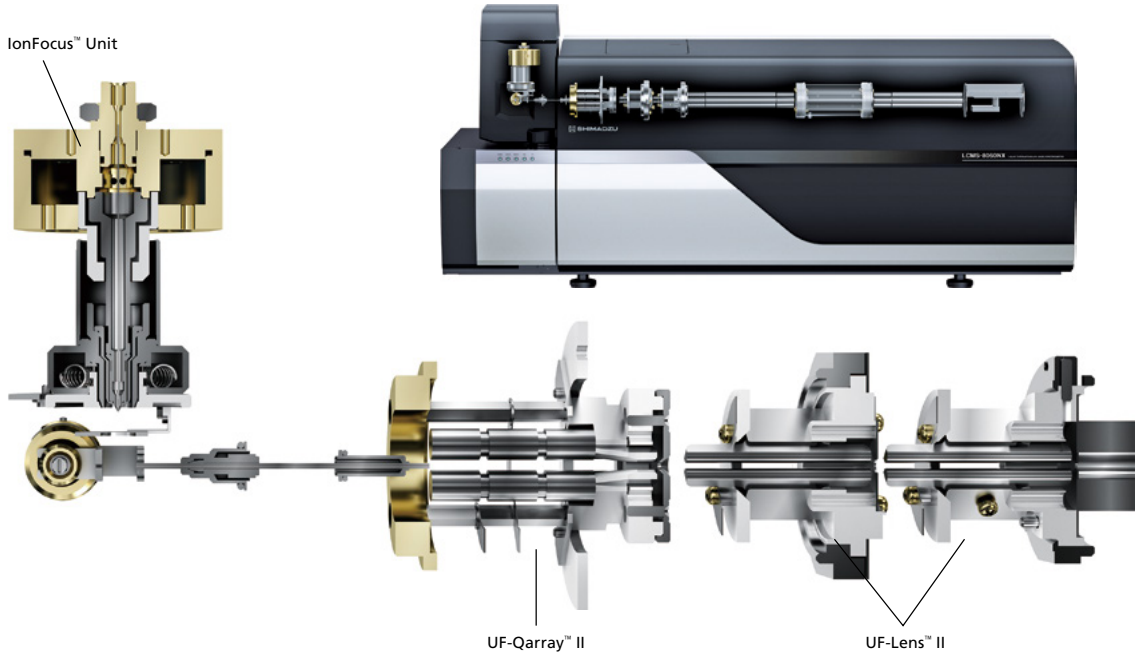


Fig. 1 LCMS-8060NX Triple Quadrupole Mass Spectrometer

1 Analytical & Measuring Instruments Division

2. IonFocus Unit

2-1. Concept

Electrospray ionization (ESI) is a widely used LC/MS ionization method that creates ions by spraying the sample through a thin tube while applying a high voltage and drying the resulting aerosol. Ions generated this way are injected into the system for mass separation, however, if inadequately dried solvents enter the system, the contamination can cause a decrease in system sensitivity.

Moving the ion spray away from the ion inlet port to mitigate contamination reduces the transmission of neutral particles that cause the contamination but also reduces the transmission of analyte ions and hence sensitivity, which has been a problem.

We therefore developed the IonFocus unit with focus electrodes at the ion source to control ion transport, as shown in Fig. 2. The IonFocus unit efficiently introduces only ions into the mass spectrometer while removing unwanted solvents and contaminants to achieve both high-sensitivity analysis and excellent system robustness.

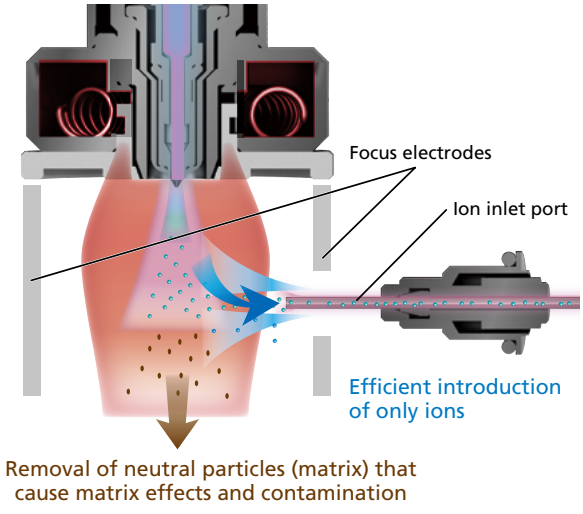


Fig. 2 IonFocus Unit Concept

2-2. Simulation Analysis

We used simulation technology to develop the IonFocus unit. Normally, the ion source operates at atmospheric pressure, and gas is used to assist sample aerosolization and drying, so ion movement is greatly influenced by the gas flow as well as the electric field. Therefore, we analyzed the gas flow in the ion spray unit using ANSYS® Fluent® simulation software. The results are shown in Fig. 3.

We also used simulation technology developed in-house to analyze the complex behavior of the ions in the gas flow when an electric field is applied. This allowed us to simulate ion behavior at atmospheric pressure, which has previously been difficult to achieve and investigate the effects of the shape of the focus electrodes and the applied voltage.

The combination of these simulation techniques makes it possible to study the design prior to prototyping and enables an extremely efficient development process.

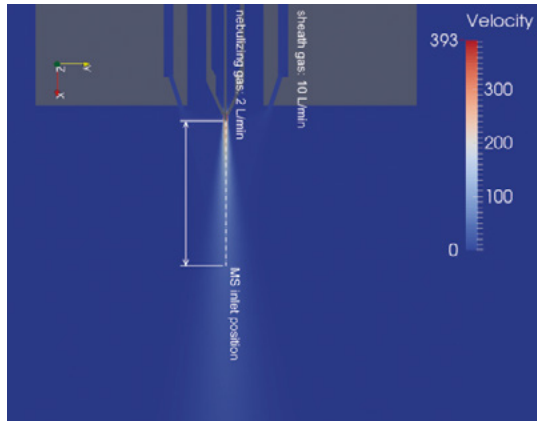


Fig. 3 Simulated Gas Flow in Ionization Region Simulated with ANSYS® Fluent®

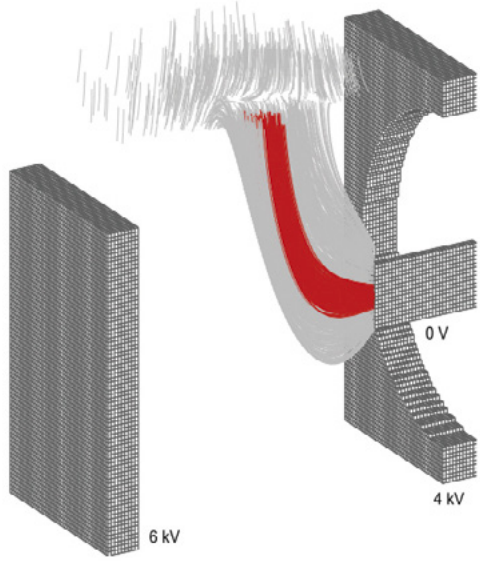


Fig. 4 Simulated Ion Trajectory under Influence of both Gas Flow and Electric Field

2-3. Optimization by Experimentation

After performing the simulations described above to narrow down the electrode shape to a number of candidates, prototypes were fabricated and installed on a system for testing.

These experiments involved adjusting physical parameters such as electrode internal diameter and distance between electrodes, as shown in Fig. 5, along with applied voltage and other parameters, then assessing the effects on ion transport and neutral particle removal as well as ease of maintenance and safety issues.

These optimizations resulted in the new IonFocus unit, which efficiently introduces only ions into the mass spectrometer while removing unwanted neutral particles.

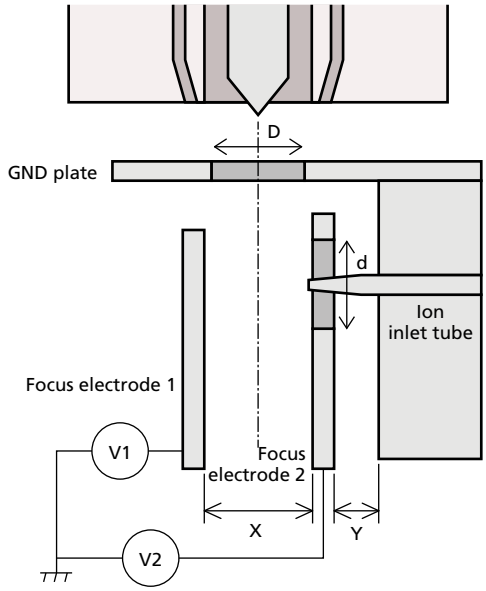


Fig. 5 Parameters Adjusted during Development of IonFocus Unit

3. UF-Qarray II and UF-Lens II

To further improve the robustness of the LCMS-8060NX, we also investigated the possibility of further improving the UF-Qarray ion guide, which combines high ion focusing power and excellent robustness (Patent No.: JP3379485, US6462338, and DE19941670), and the UF-Lens ion guide that can be maintained easily and without tools. Fig. 6 shows results obtained by simulating the sample gas flow in the UF-Qarray unit.

We repeatedly assessed where gas collides with the UF-Qarray, which areas are prone to contamination, and what component shapes are less prone to gas contamination. This allowed us to optimize component shapes and make further improvements in robustness. We also modified the voltage pattern applied by the UF-Lens II that provides the additional function of removing unwanted ions. These changes protect the quadrupole rods, which are the heart of the mass spectrometer, from contamination, reduce the maintenance frequency.

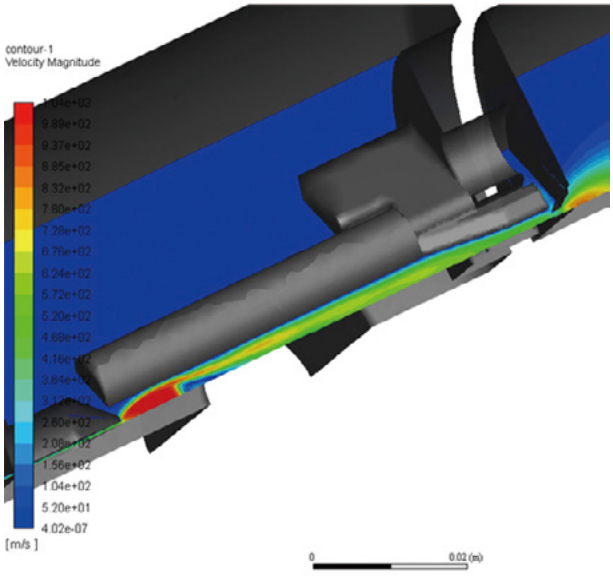


Fig. 6 Simulated Gas Flow in UF-Qarray II Unit

4. Maintaining High Sensitivity Even during Consecutive Analyses under Demanding Conditions

The excellent robustness of the LCMS-8060NX can be seen most clearly during consecutive analyses of samples of biological origin that tend to contaminate instruments. We performed the consecutive analyses of human blood plasma spiked with alprazolam on the LCMS-8060NX and plotted the resulting area values and area ratios (internal standard material: alprazolam-*d*5). To evaluate the robustness under even more demanding conditions, we performed a total of 15,000 consecutive analyses without using valves to remove impurities.

As shown in Fig. 7, the results were extremely stable, with an area value reproducibility of 1.79 %RSD and an area ratio reproducibility of 1.71 %RSD. Images of the ion source before and after the consecutive analysis are shown in Fig. 8. Although the entire ion source, including focus electrodes, is covered with a white contaminant, this did not affect the system's ability to transport ions.

This demonstrates the excellent stability of results with the LCMS-8060NX even during consecutive analyses of samples with large amounts of contaminants such as urine and blood plasma.

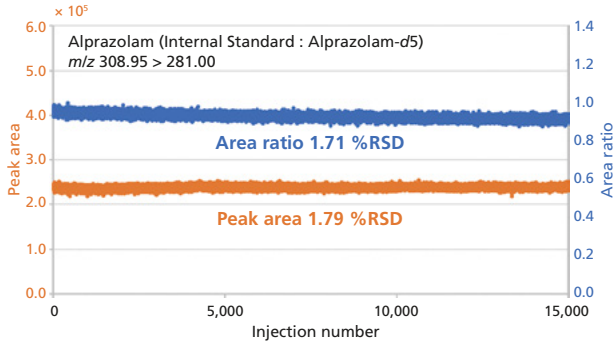
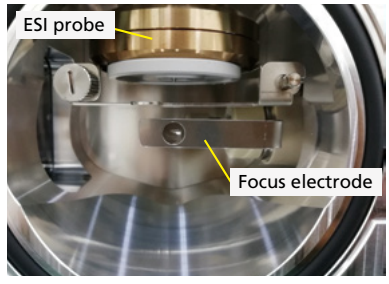
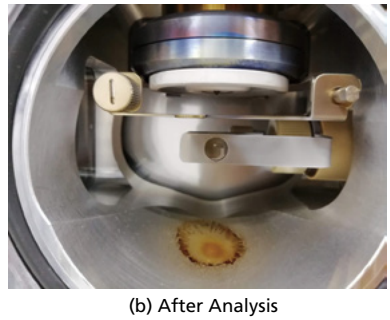


Fig. 7 Results from Consecutive Analyses of Alprazolam-Spiked Human Blood Plasma



(A) Before Analysis



(b) After Analysis

Fig. 8 Ion Source Contamination Before and After Consecutive Analyses

5. Conclusions

- The newly developed IonFocus ion source unit improves system robustness by efficiency introducing only ions into the mass spectrometer and removing unwanted neutral particles and contaminants.
- The UF-Qarray II is an updated version of the UF-Qarray Shimadzu's patented technology engineered to be resistant to contamination. The UF-Qarray II retains the high ion focusing power of its predecessor while making further improvements in robustness.
- A new applied voltage pattern allows the UF-Lens II to remove unwanted ions and protect the quadrupole rod from contamination.
- Equipped with these technologies that further improve robustness, the LCMS-8060NX delivers stable results even under demanding analytical conditions such as the continuous analysis of biological samples. By simplifying sample pretreatment and minimizing system downtime, the LCMS-8060NX contributes significantly to the efficiency of user workflows.

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