Visualization and Optimization of Various Ambient Ionization Source, Direct Sample Analysis, Conditions Using Schlieren Photography.

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1 Introduction

Ambient ionization sources often require the optimization of various parameters in order to obtain an adequate spectrum. Depending on the type of source, the variable conditions can include discharge voltage, source temperature, sheath gas pressure and composition. Schlieren photography allows visualization of transparent phenomenon based on a change in refractive index through which light is passing. The sheath gas has a different refractive index than the surrounding air. The different refractive index allows the sheath gas to be visualized with Schlieren photography. Presented are Schlieren photographs of various source and experimental conditions along with subsequent spectra resulting from each configuration.

2 Instrument Parameters

The DSA ion source was attached to a PerkinElmer SQ 300 mass spectrometer. Images were taken using either a Pentax K10, Canon Powershot A620 or EOS Rebel T2i digital camera. The mirror used was a commercial grade spherical concave mirror with a diameter of 15 cm and a focal length of 150 cm. The mirror was placed directly behind the DSA with the camera placed at twice the focal length. A very bright LED flashlight, focused through a pinhole cover, was directed slightly off axis at the mirror, focusing the light back through the sheath gas stream to the camera.

3 Experimental Setup

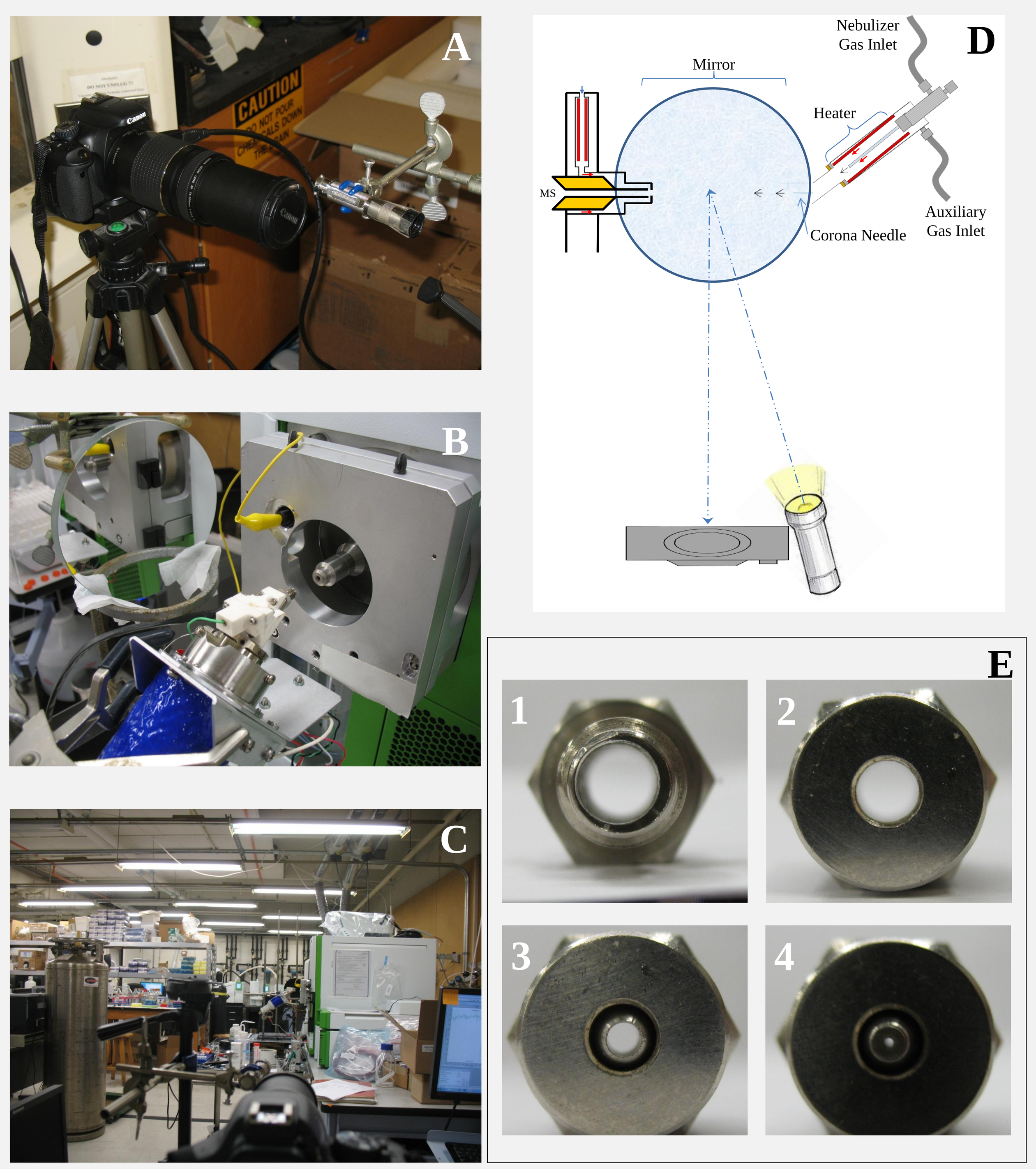


Figure 1. A) Camera and flashlight arrangement. **B)** DSA attached to SQ 300. **C)** Sightline of camera to instrument in Schlieren setup. **D)** Schematic of the DSA ionization source and Schlieren experimental setup.
E) Nozzles used: 1= 4.8mm i.d., 2= 3.2mm i.d., 3=1.5mm i.d., 4=0.5mm i.d.

4 Nozzle Size vs. Reagent Ion Spectra

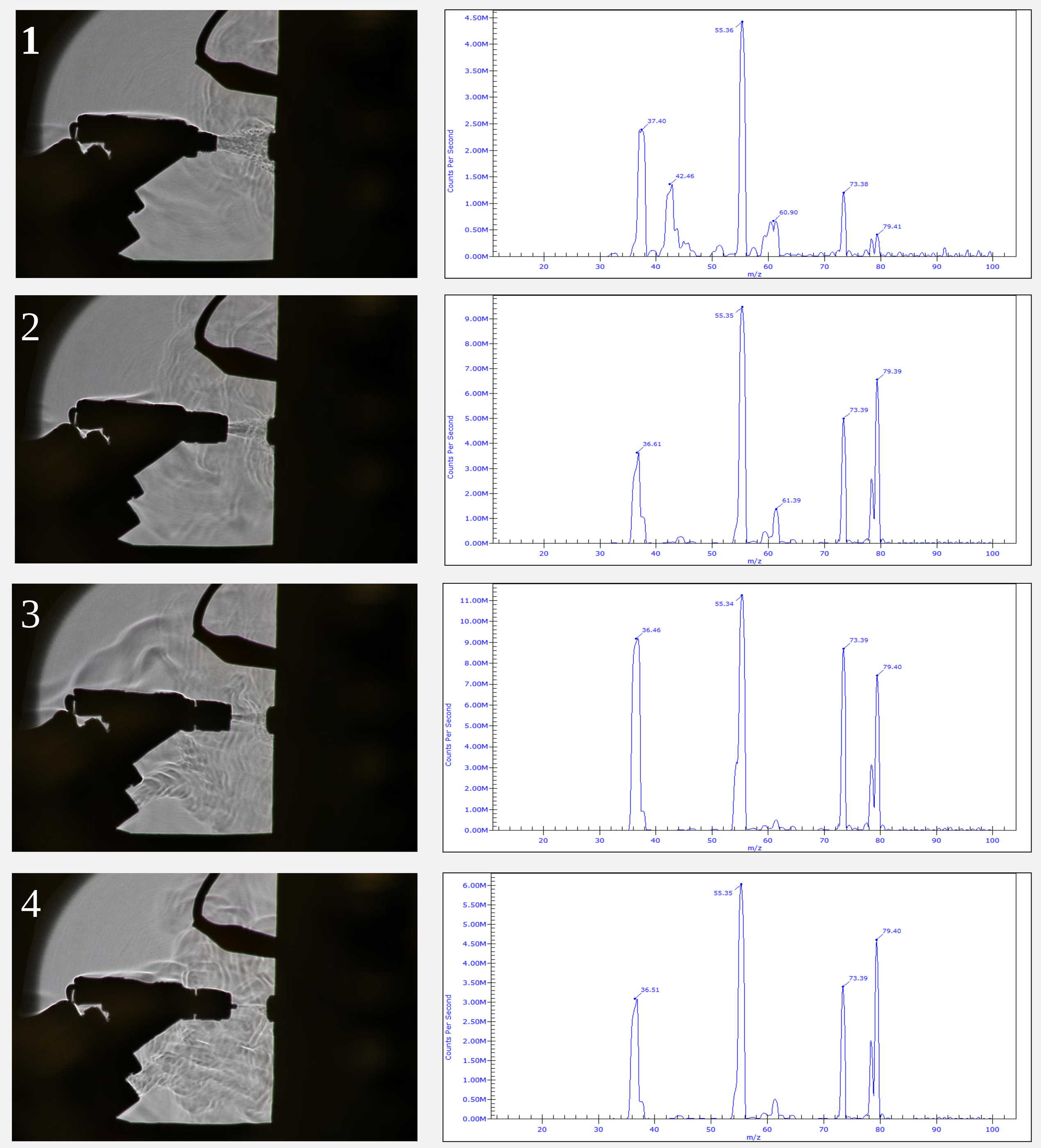


Figure 2. Schlieren images of the DSA with each of the four nozzles attached. Shown to the right of each image is the corresponding reagent ion spectra produced by this source configuration.

5 Caffeine vs. Rhodamine Dye

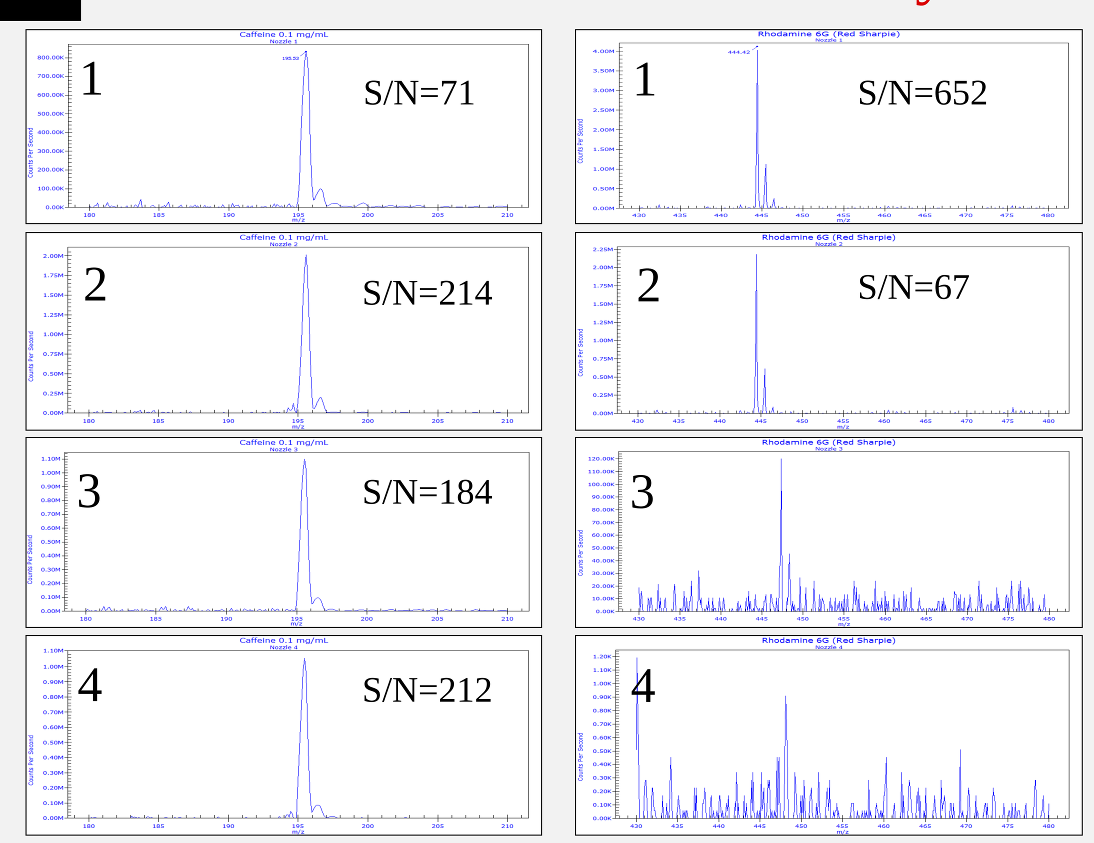


Figure 3. Spectra of two different species, caffeine and a rhodamine dye from a red permanent marker. Each spectra was taken with each of the four different nozzles shown in Figure 1.

6 DSA Position vs. Reagent Ion Spectra

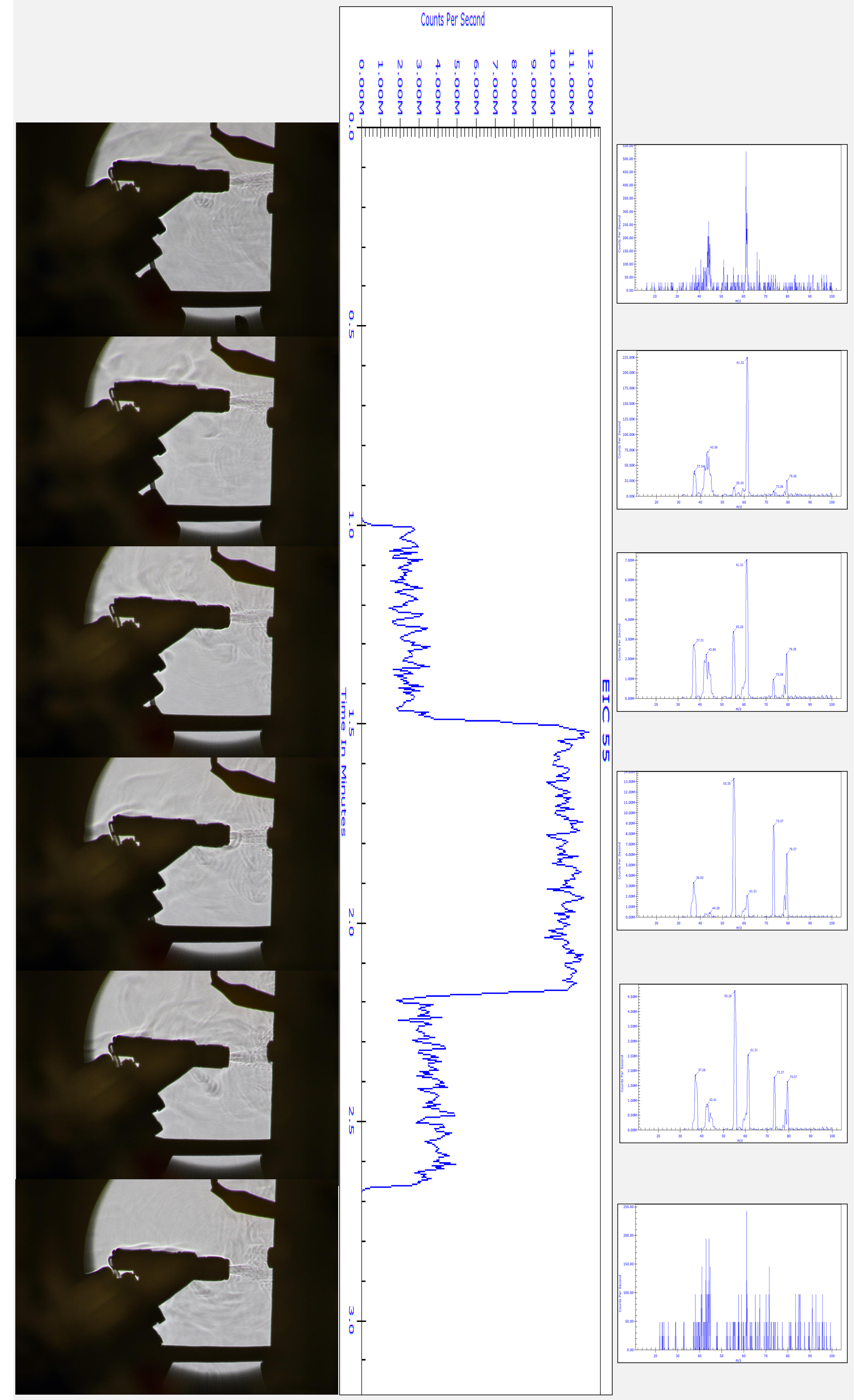
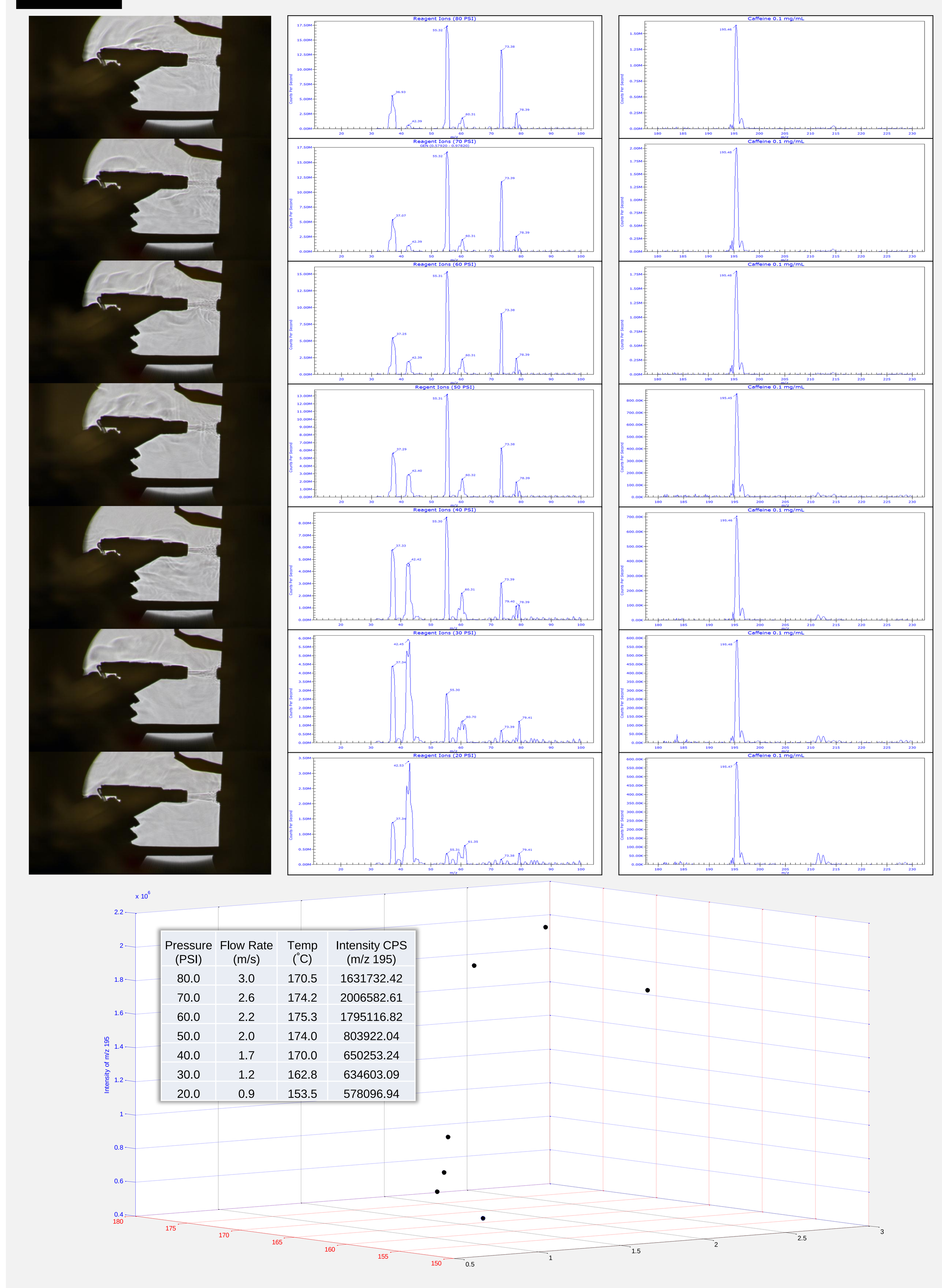


Figure 4. Schlieren images of the DSA with nozzle 2 attached. The DSA was passed vertically in front of the inlet of the mass spectrometer. Highest reagent ion intensity was observed when the DSA was oriented directly at the inlet. An EIC of m/z 55, $[(H_2O)_3H^+]$, is shown in the center. Corresponding spectra at each point are shown on the right hand side. The Schlieren photographs show a wide gas stream at reaching the inlet. Despite the wide stream, the majority of the reagent ions are grouped in the center of the gas stream.

7 Effect of Flow Rate on Ionization



Pressure (PSI)	Flow Rate (m/s)	Temp (°C)	Intensity CPS (m/z 195)
80.0	3.0	170.5	1631732.42
70.0	2.6	174.2	2006582.61
60.0	2.2	175.3	1795116.82
50.0	2.0	174.0	803922.04
40.0	1.7	170.0	650253.24
30.0	1.2	162.8	634603.09
20.0	0.9	153.5	578096.94

Figure 5. Shown above are Schlieren photographs of the DSA with nozzle 2 attached. Nitrogen pressure was reduced from 80 to 20 PSI from top to bottom. Corresponding reagent ion and caffeine spectra are shown to the right. Gas flow rates, measured temperature and caffeine ion intensity are shown in the Table embedded in the chart. The chart shows a plot of the measured temperature and flow rate versus caffeine ion intensity. The temperature was measured at the point where the sample is placed. The DSA heater was held at a constant 300 C. The variation in temperature is due to the changing flow rate. From the plot, the best conditions were found to be a flow rate of 2.6 m/s and subsequently a temperature of 174 C.

8 Conclusion

Schlieren photography allows for visualization of the invisible. This relatively simple and inexpensive experimental setup makes Schlieren photography a useful tool in the study of ambient mass spectrometry sources such as the DSA. It was observed that nozzle size can play an important role in the ionization efficiency of different compounds. The largest nozzle provided the best signal for the rhodamine dye sample while a smaller more focused nozzle provided the best signal for the caffeine standard. Sheath gas flow rate is an important consideration in these experiments. The flow rate affects gas temperature, ionization as well as ion transport. Going forward we would like to use Schlieren photography to probe and optimize different experimental configurations.

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