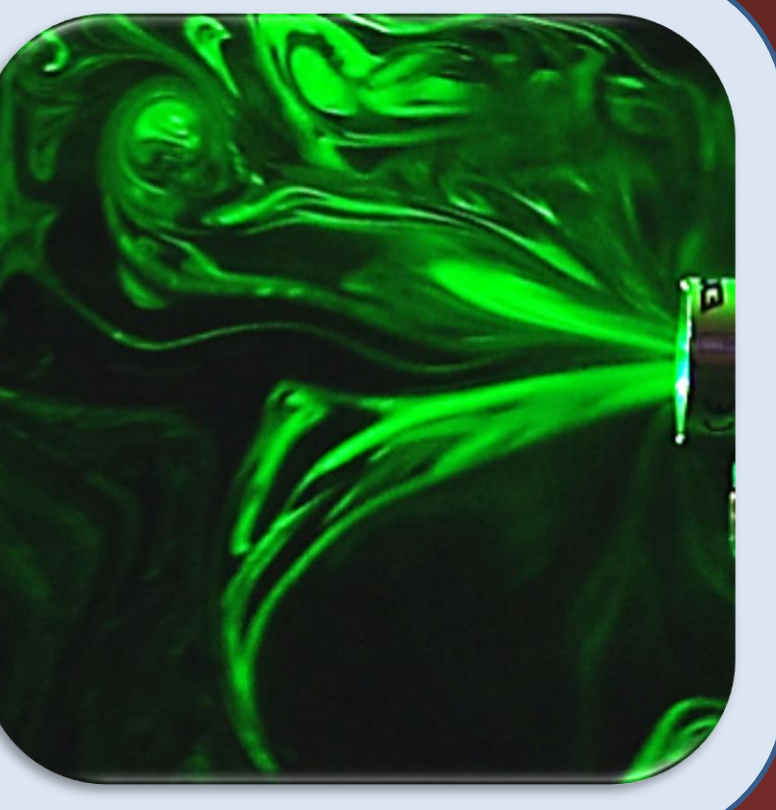


# Non-Proximate Sampling of Vapors and Aerosols for Real-Time Chemical Detection with Venturi-assisted Entrainment and Ionization Mass Spectrometry

**NIST**  
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## Overview

### Purpose

- Develop systems for the real-time chemical detection of remotely sampled vapors and aerosols – targeting clandestine narcotics laboratories, homemade explosives, and chemical weapons
- Explore platforms to enhance aerodynamic reach of the collection system and efficient transport/ionization for mass spectrometry (MS) analysis
- Explore alternative configurations – continuous facility monitoring and swipe sampling infrared thermal desorption

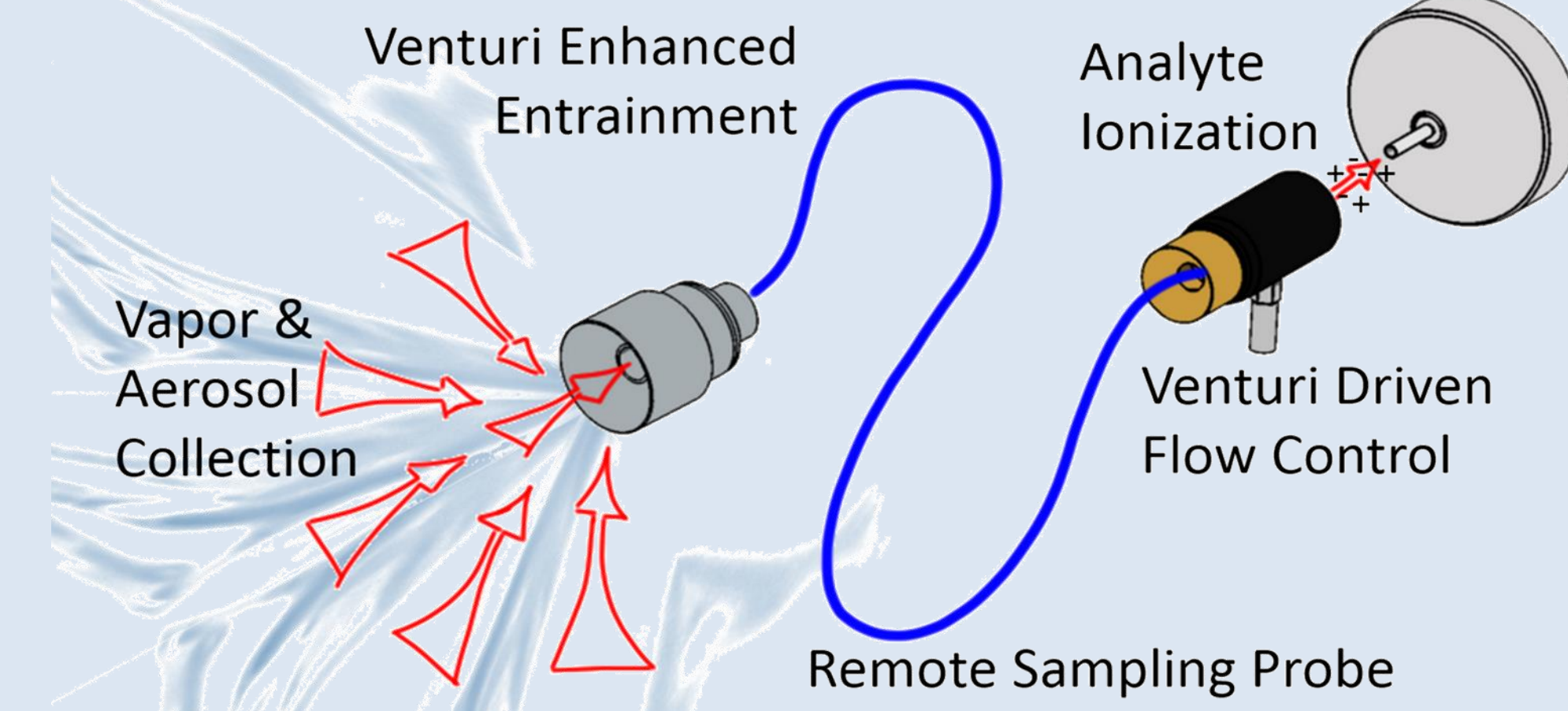
### Methods

- Develop the Venturi-assisted ENtrainment and Ionization (VENTI) platform for efficient collection, transport, and MS detection
  - Incorporate Venturi & Coanda effects in robust air amplifier components
  - No moving parts and requires only a pressurized gas to generate flow control and collection and transport of analytes
- Utilize probe lengths of 0.5m, 1.0m, 2.5m, and 10.5m for non-proximate collection of vapors, aerosols, and dust particulate
- Incorporate real-time atmospheric pressure chemical ionization by transport through a corona discharge region
- Investigate alternative configurations for facility monitoring (no remote probe) and swipe sampling thermal desorption (short wave infrared emission)

### Results

- VENTI demonstrated 3-fold enhancement in aerodynamic reach and collection over simple suction:
  - MS experiments, laser-light sheet visualization, and schlieren imaging
- Transport through 2.5m probe: residence times on order of  $10^{-2}$ s to  $10^{-1}$ s & Reynolds numbers on the order of  $10^3$  to  $10^4$
- Volatile chemical vapors (single  $\mu\text{mol}_{\text{analyte}}/\text{mol}_{\text{air}}$ ), explosive vapors (100's of  $\mu\text{mol}_{\text{explosive}}/\text{mol}_{\text{air}}$  samples), and explosive, narcotic, and mustard gas surrogate aerosols (20  $\mu\text{L}$  plumes)
- Continuous facility monitoring of 90 m<sup>2</sup> (570,000 L) room for 60-minutes
  - Chemical vapors and mustard gas surrogate detection within minutes
- Pulsed broad spectrum infrared thermal desorption of swipe samples
  - Efficient desorption and trace detection of volatile and non-volatile explosives and narcotics

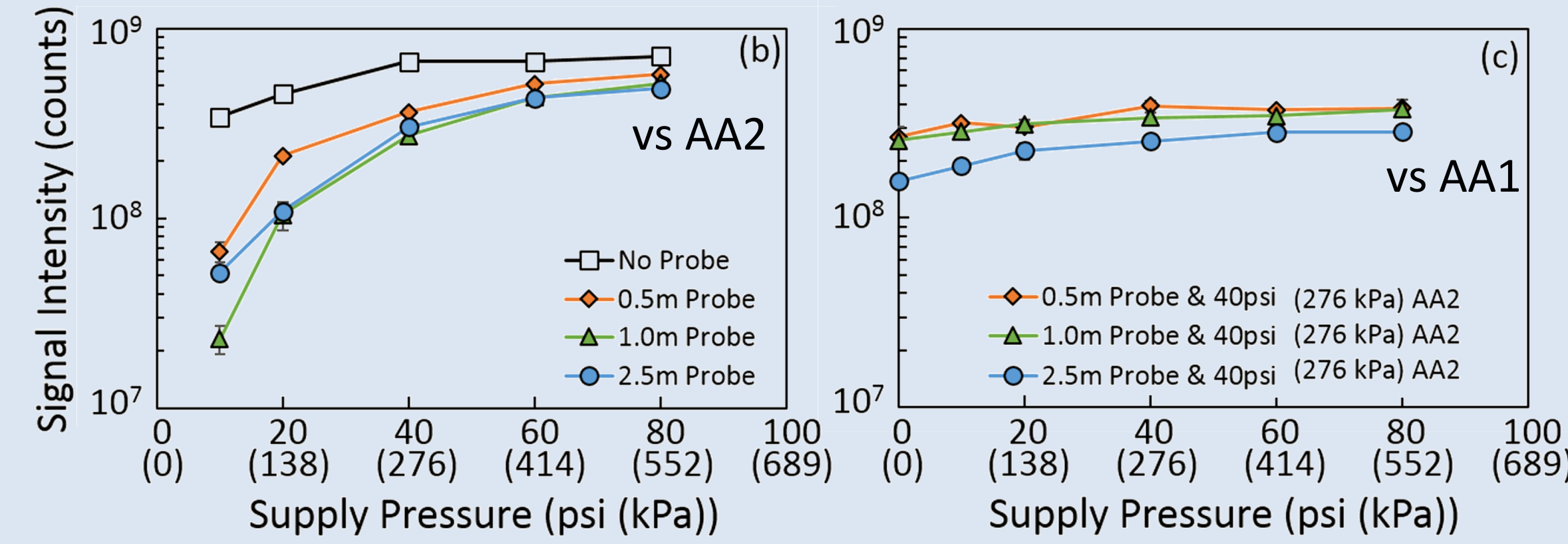
## VENTI Remote Vapor Sampling



Two air amplifier components for entraining/collection vapors (AA1) and generating transport flow from remote collection to ionization region & inlet (AA2)
 

- Probes 0.5m to 2.5m – flow rates on the order of 10's L/min, Re  $10^3$  to  $10^4$ , and residence times  $10^{-2}$ s to  $10^{-1}$ s

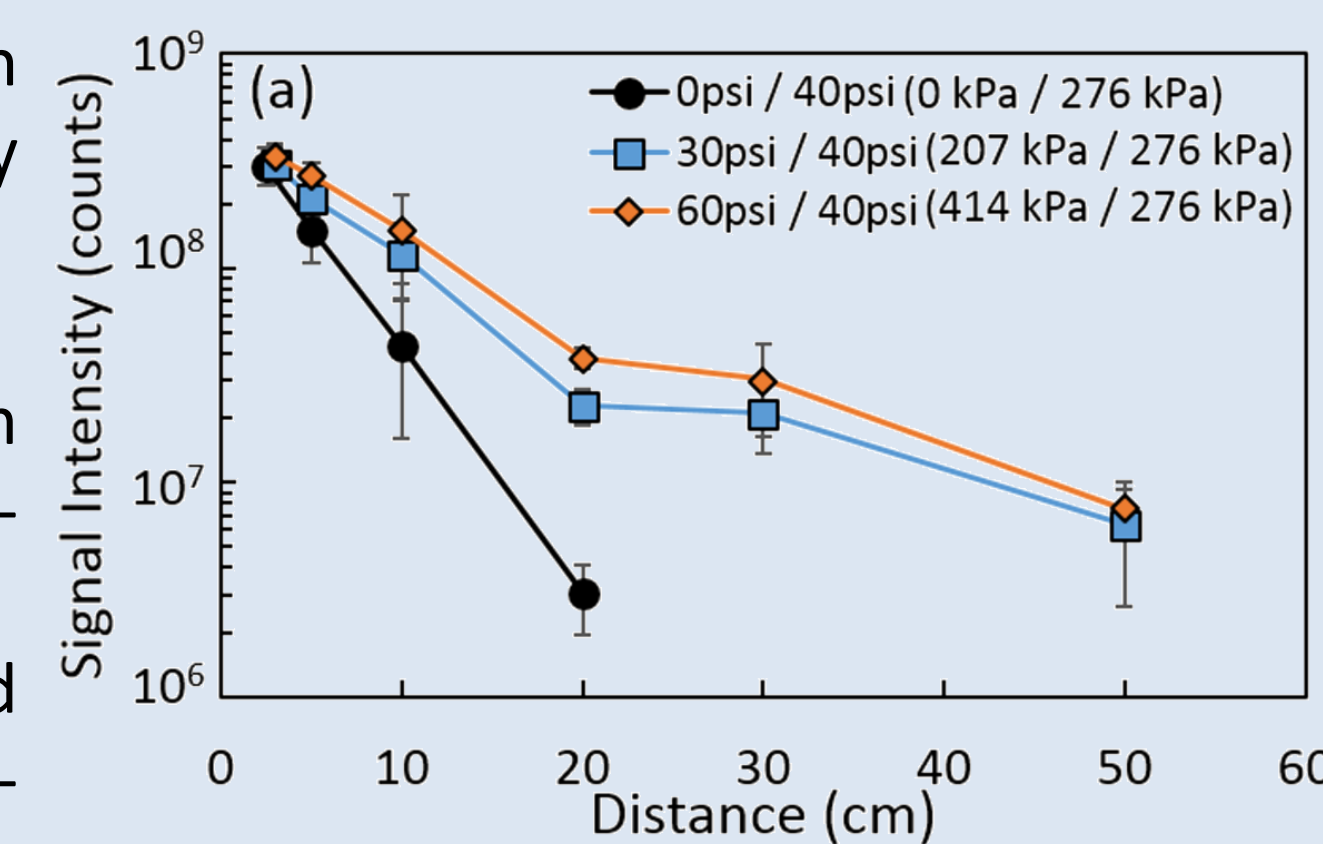
- MS response as a function of AA1 and AA2 supply pressures
- Sampling ethanol from 20mL vials for 30s durations – monitoring the dimer ( $m/z$  93 [2M+H]<sup>+</sup>)



## Enhanced Aerodynamic Reach

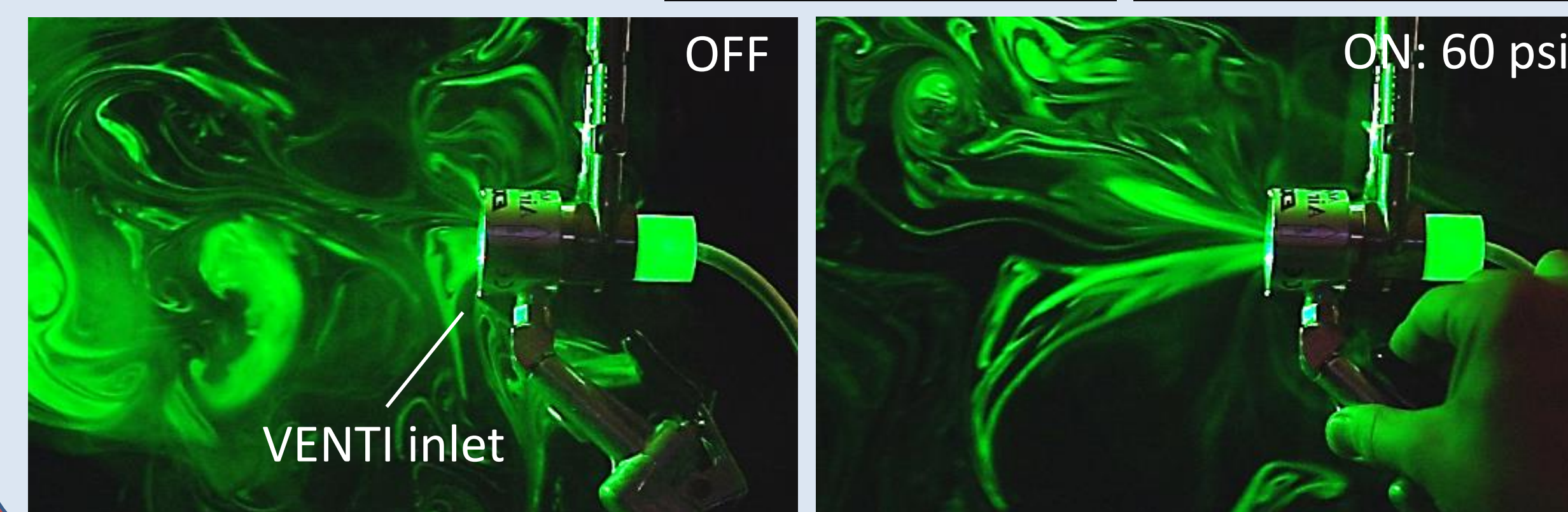
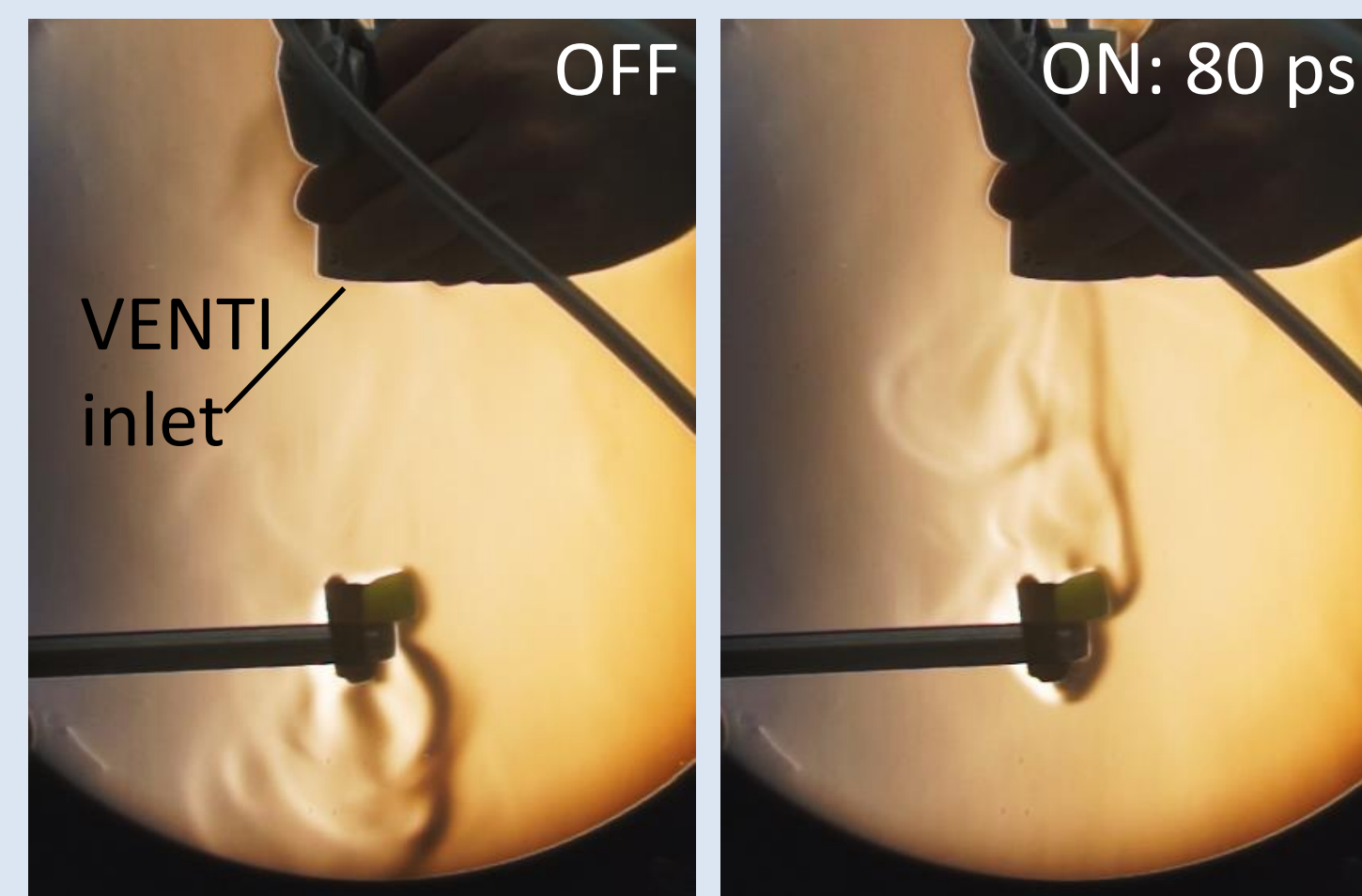
Aerodynamic reach: distance at which target vapors can be aerodynamically entrained into the detection system
 

- 60s ethanol vapor sampling periods
- 10-fold increase in signal at 20cm stand-off distance with Venturi-assisted entrainment
- Aerodynamic reach increase beyond 50cm (in 60s sampling period), ~3-fold increase



Enhanced aerodynamic reach corroborated with schlieren imaging of acetone vapor and laser-sheet flow visualization of cinematic fog

- Schlieren: 0psi / 40psi vs 80psi / 40psi
- Laser-sheet: 0psi / 20psi vs 60psi / 20psi

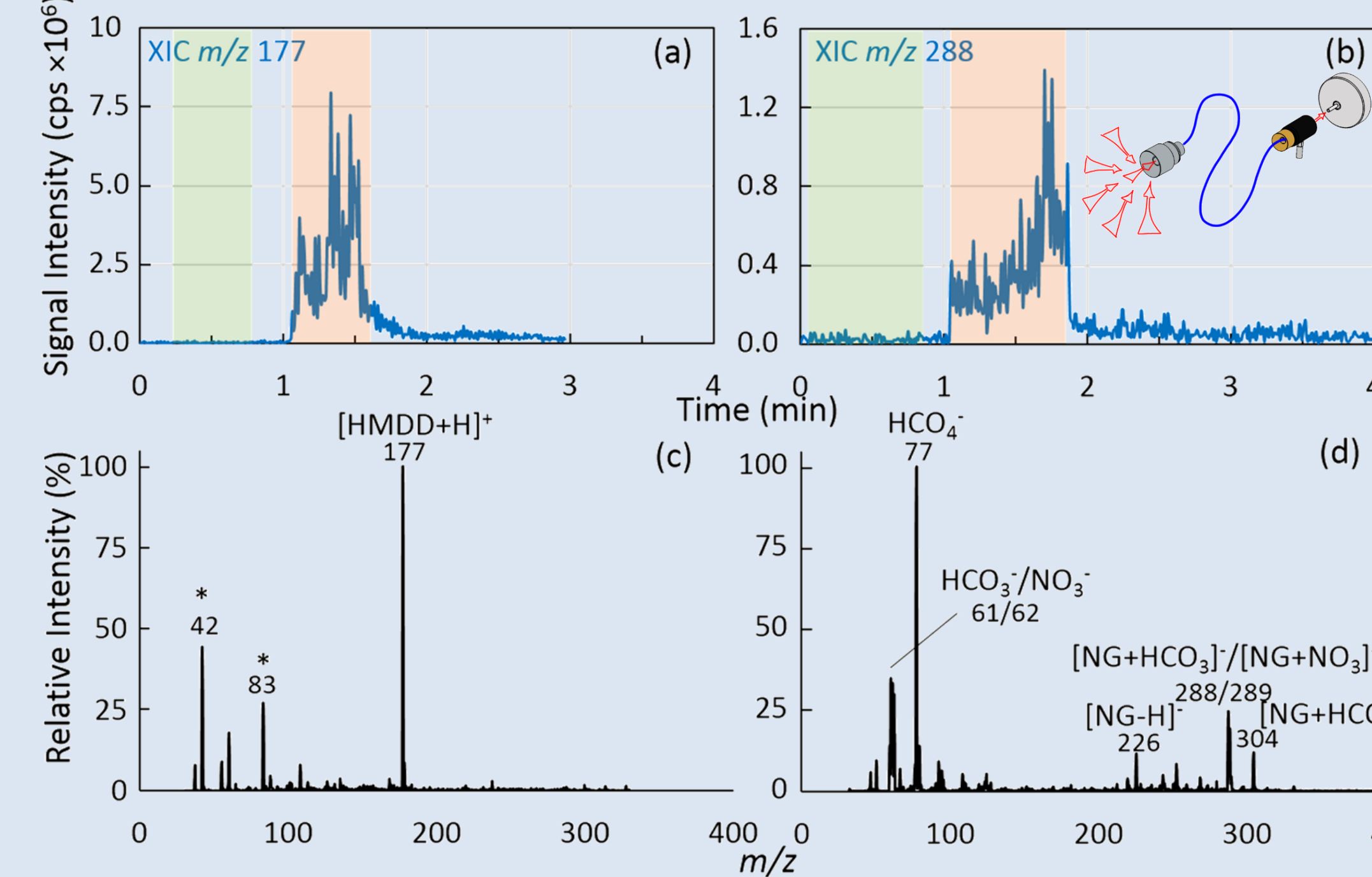


## Vapor Detection

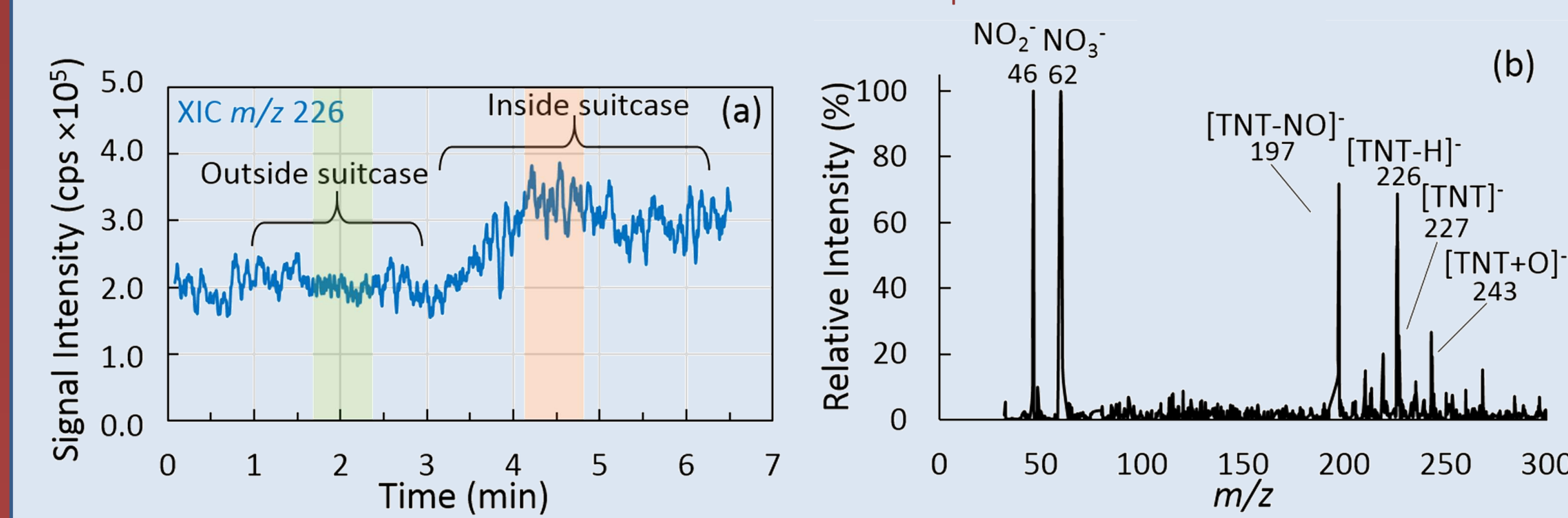
Vapor detection demonstrated for: organic solvents, a mustard gas analogue (methyl salicylate), peroxide-based, nitrate ester, and nitroaromatic explosives.

- 40 $\mu\text{g}$  to 400 $\mu\text{g}$  solution deposited and solvent allowed to evaporate
- Sample vials capped and volatilize for 45-minute period.
- Samples collected with 1.0m probe for AA1/AA2 of 60psi / 40psi at a stand-off distance of approximately 5 cm
- Detection of select relatively volatile explosives: HMDD, EGDN, DNT, NG
- Assuming no losses and equilibrium with surroundings: 100's of  $\mu\text{mol}_{\text{explosive}}/\text{mol}_{\text{air}}$  down to 100's of  $\text{nmol}_{\text{explosive}}/\text{mol}_{\text{air}}$

Extracted ion chromatograms and background subtracted mass spectra for HMDD and NG (orange and green boxes represent extracted and background spectra)



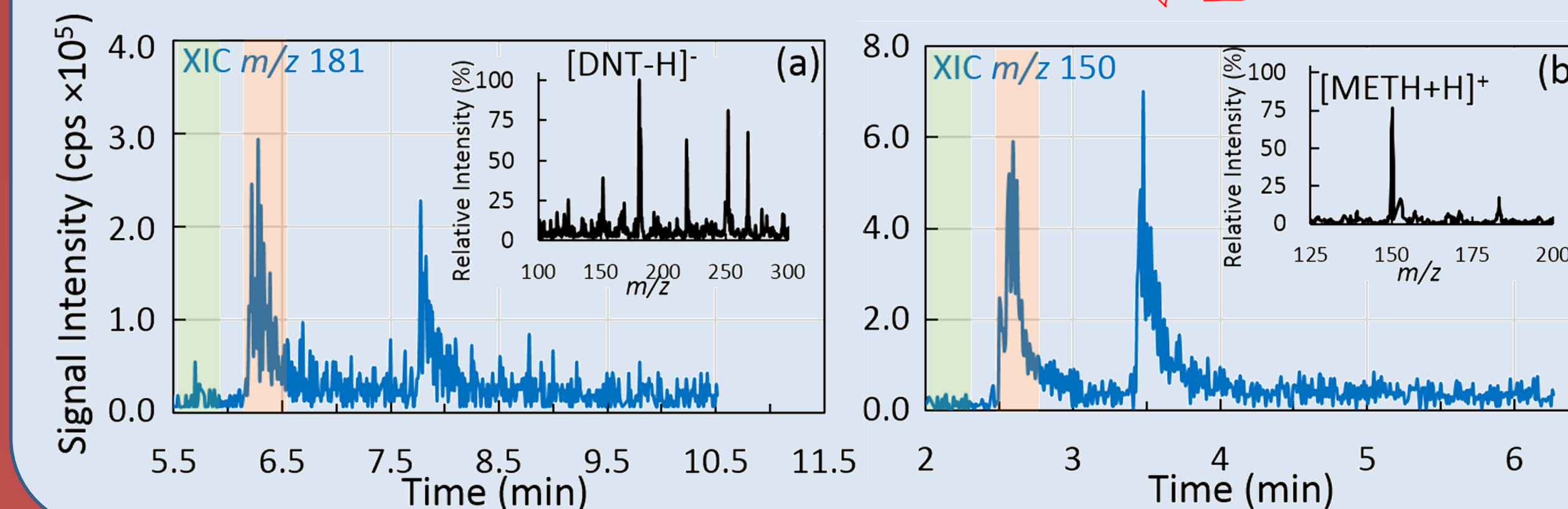
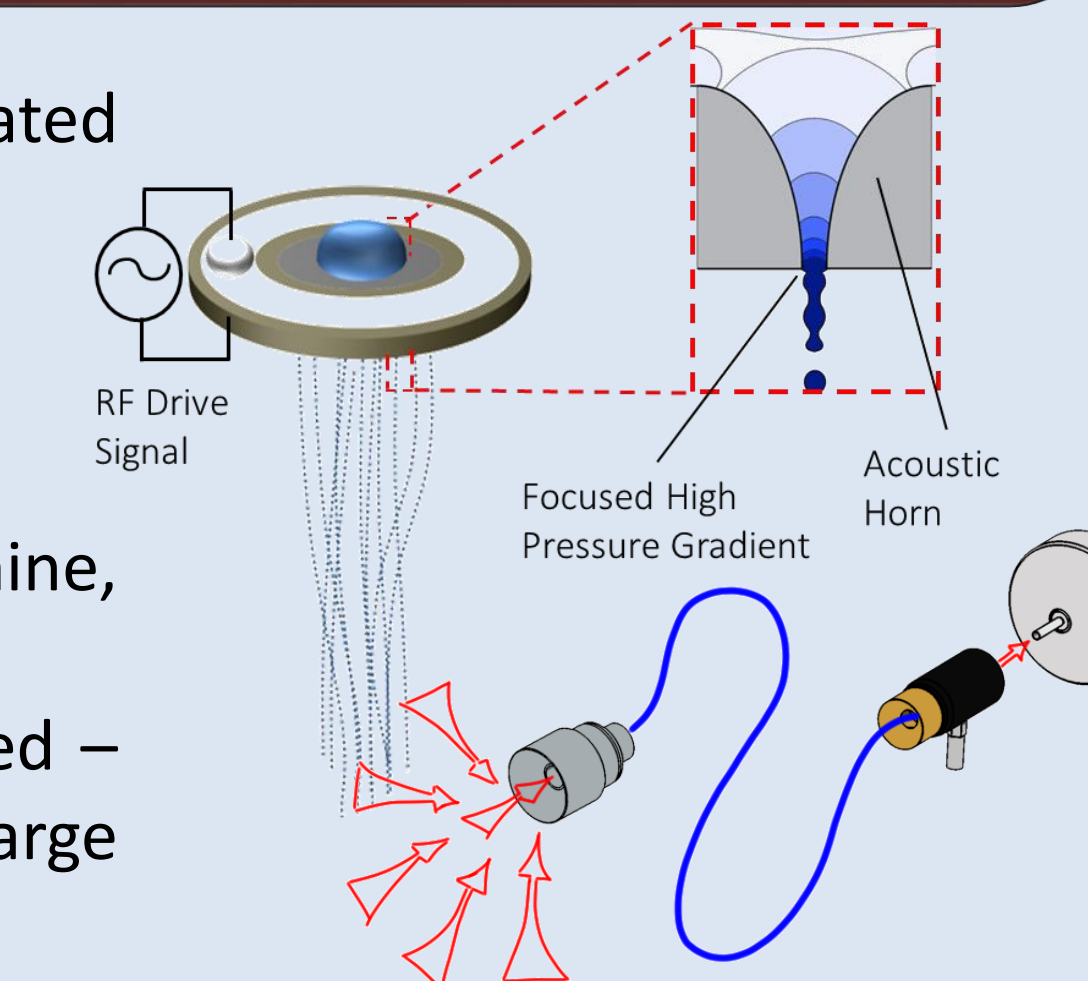
TNT flake K9 training aid (5g) in a "stash tin" within a zipped shut 23L carry on suitcase for 2.5 hours: detection of ~ 10 nmol<sub>explosive</sub>/mol<sub>air</sub> (2.5m probe)



## Aerosol Detection

Discrete 10 $\mu\text{L}$  to 20 $\mu\text{L}$  aerosol plumes generated with ultrasonic nebulizer (190kHz, 20V<sub>pp</sub>)
 

- Order of single micron diameter drops
- VENTI collection from ~20cm away
- 2.5m probe, AA1/AA2 of 60psi/60psi
- Demonstrated for DNT, methamphetamine, MDMA, and methyl salicylate
- TNT dust particulate aerosol also detected – desorption/etching through the discharge component

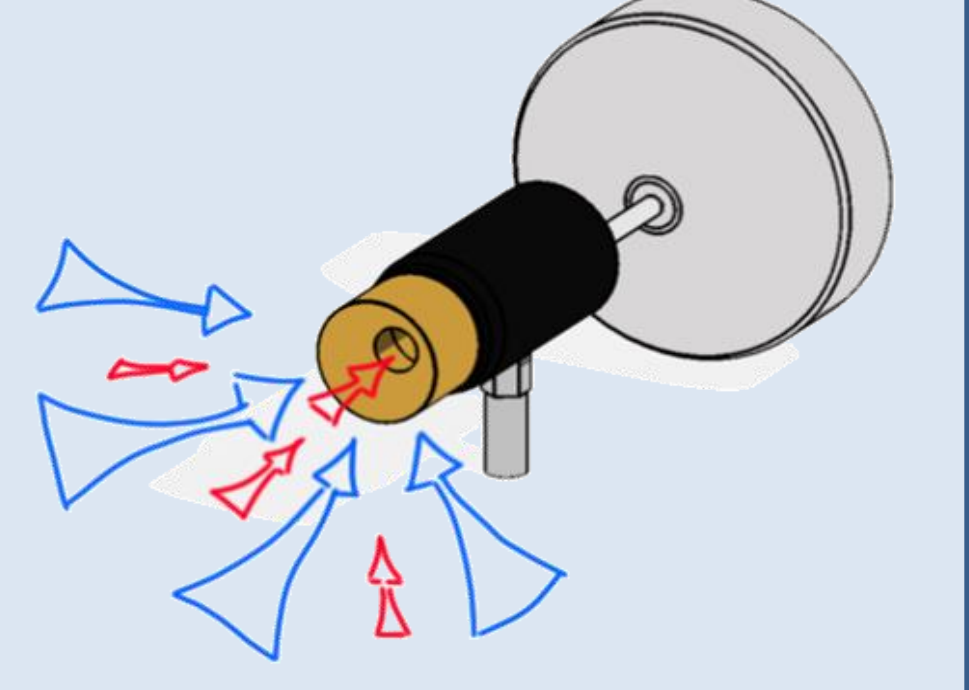
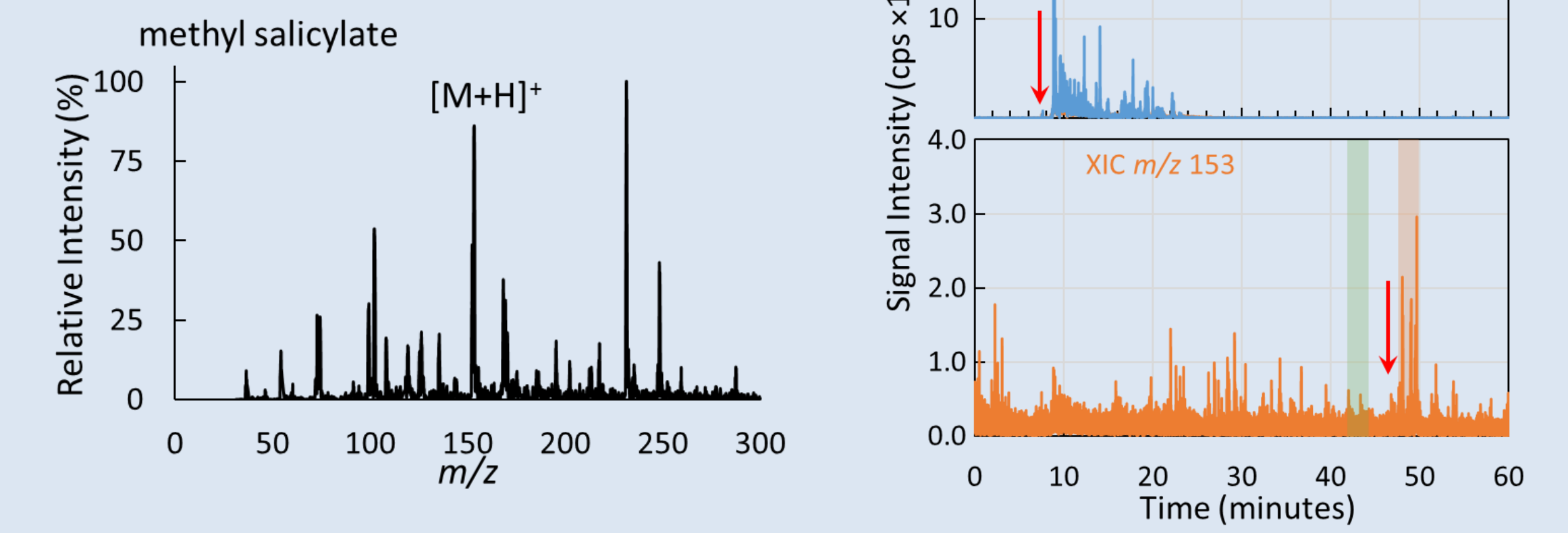


## Alternative Configurations

### Real-Time Facility Monitoring

Monitoring of a large laboratory (~ 90 m<sup>2</sup> / 570,000L) without the sampling probe
 

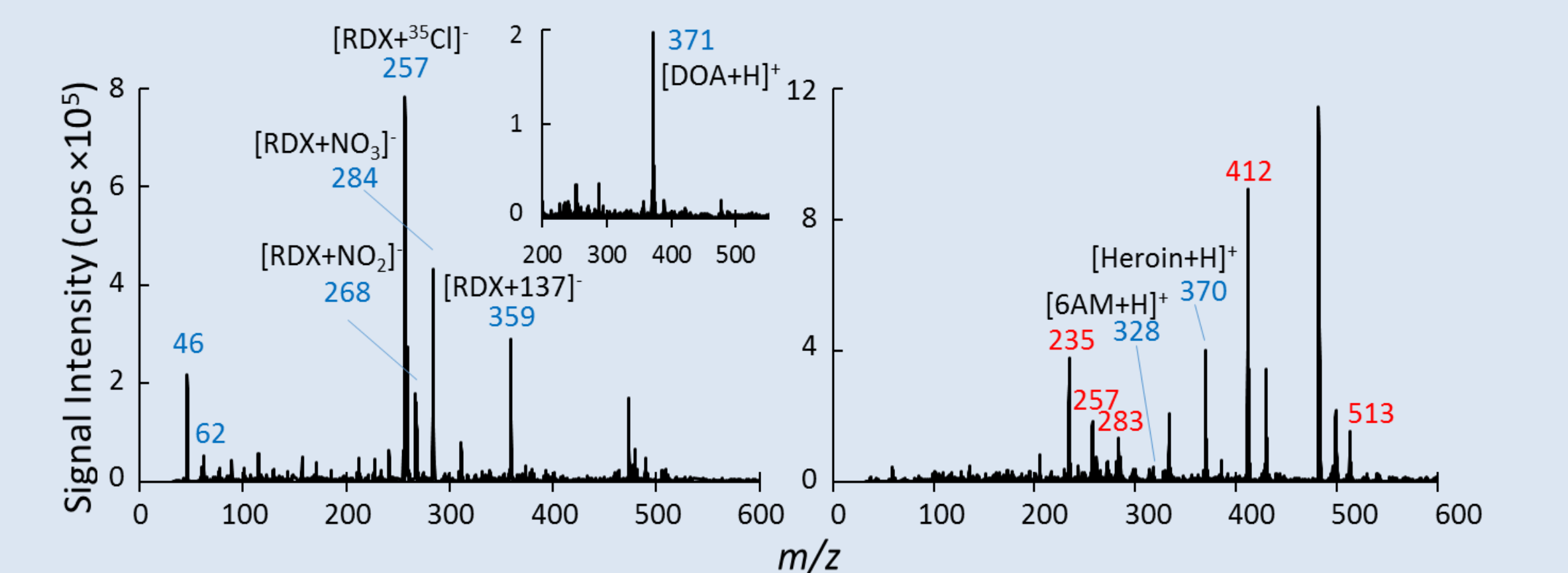
- 60-minute monitoring period
- Ethanol squirt-bottle glassware rinse, ~ 3.2m behind the VENTI-MS system
- Methyl salicylate - 100  $\mu\text{L}$  (mustard gas surrogate) deposited ~ 3m away
- Both detected within 2 minutes (transport time)



### Pulsed Broad Spectrum Infrared Thermal Desorption

Filament-based infrared (IR) emitters offer tunable broad spectrum emission, rapid response times (~1s), temporally discrete (pulsed) emission durations, and reduced costs (requiring only a power supply) and infrastructure requirements

- Trace (ng) level detection of narcotics and explosives
- Complex samples: plastic-bonded explosives (C-4) and exogenous narcotics collected from synthetic latent fingerprints



## Conclusions

VENTI demonstrated efficient and real-time entrainment, collection, transport, and mass spectrometric detection of remotely sampled vapors and aerosols
 

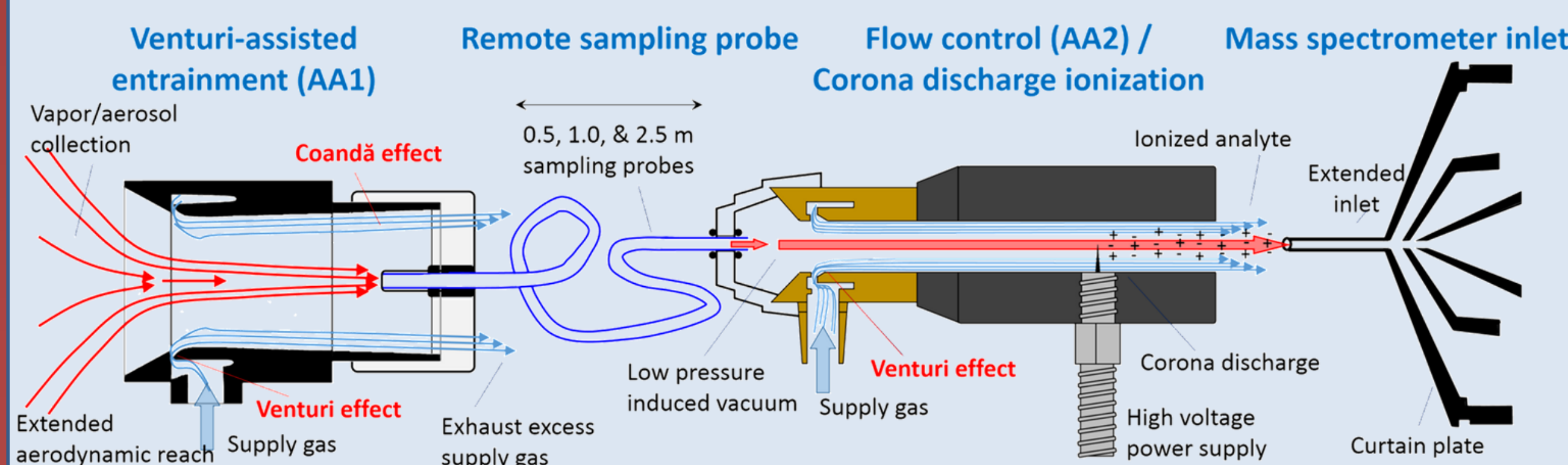
- Unlocking large volume scanning: cargo, bulk commercial transportation
- Efficient entrainment enables continuous real-time facility monitoring
- Alternative configurations also enable swipe based sampling using pulsed infrared emission for thermal desorption
- Complementary to the widely deployed swipe-based trace residue and particulate collection/detection techniques

### Acknowledgements

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Certain commercial products are identified in order to adequately specify the procedure; this does not imply endorsement or recommendation by NIST, nor does it imply that such products are necessarily the best available for the purpose.

## Venturi-assisted ENTrainment & Ionization



### VENTI-MS

- Air amplifier components with no moving parts, driven by pressurized gas
- Venturi Effect: exploited to generate low pressure vacuum inducing entrainment and bulk flow into the device
- Coanda Effect: high velocity supply gas flows along device walls, returning to the environment, preferentially collecting analyte at the end of probe
- Atmospheric pressure chemical ionization through corona discharge
- Sciex 4000 QTrap triple-quadrupole mass spectrometer with extended inlet

