

High Performance Ion Mobility Spectrometry – An Ideal Field Analytical Instrument

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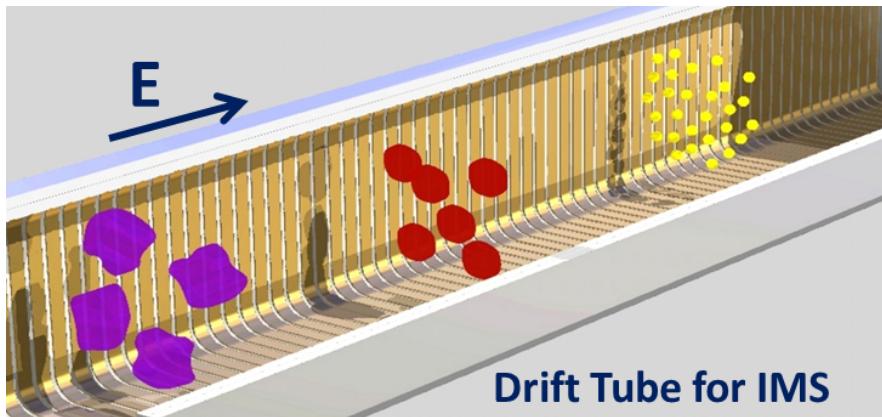
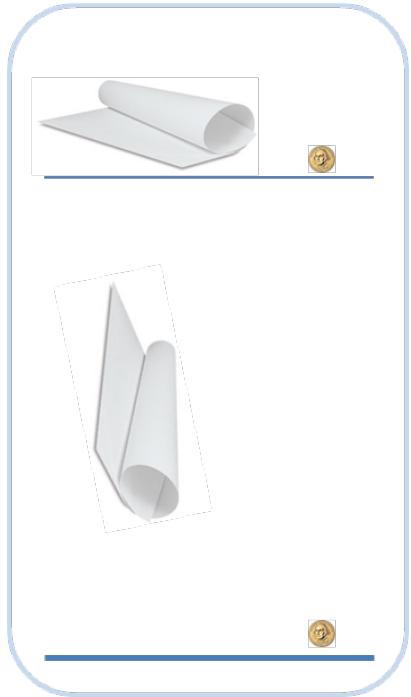


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HPIMS™

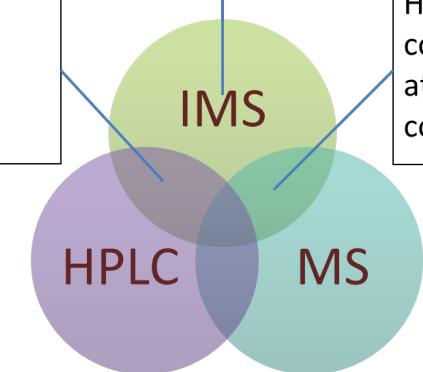
Ion Mobility Spectrometry

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Ion mobility based separation relates to gas phase size, shape, and stereo-structure

Interaction based separation rely on analyte and drift media properties



High speed m/z correlated separation at low instrument cost with portability

$$v = KE \Rightarrow \frac{L}{t_d} = K \frac{V}{L} \Rightarrow K = \frac{L^2}{V t_d}$$

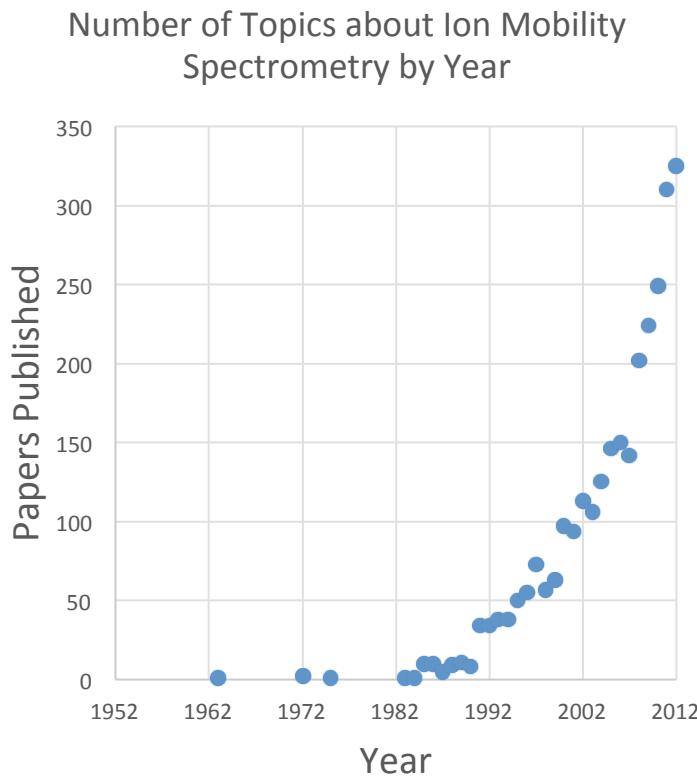
$$K = \frac{3}{16N} \left(\frac{2\pi}{\mu kT} \right)^{1/2} \frac{q}{\Omega} \quad \mu = \frac{mM}{(m+M)}$$

$$t_d = \frac{16N}{3} \left(\frac{\mu kT}{2\pi} \right)^{1/2} \frac{L^2}{V} \frac{\Omega}{q} \Rightarrow t_d \propto \frac{\Omega \mu^{1/2}}{q}$$

In Instrumentation Field IMS Adoption is Accelerating

"Ion Mobility...A prevailing theme at ASMS this year"

JP Morgan, "ASMS 2013 Final Thoughts"



Waters Synapt G2



Excellims MA3100
with Thermo Orbitrap



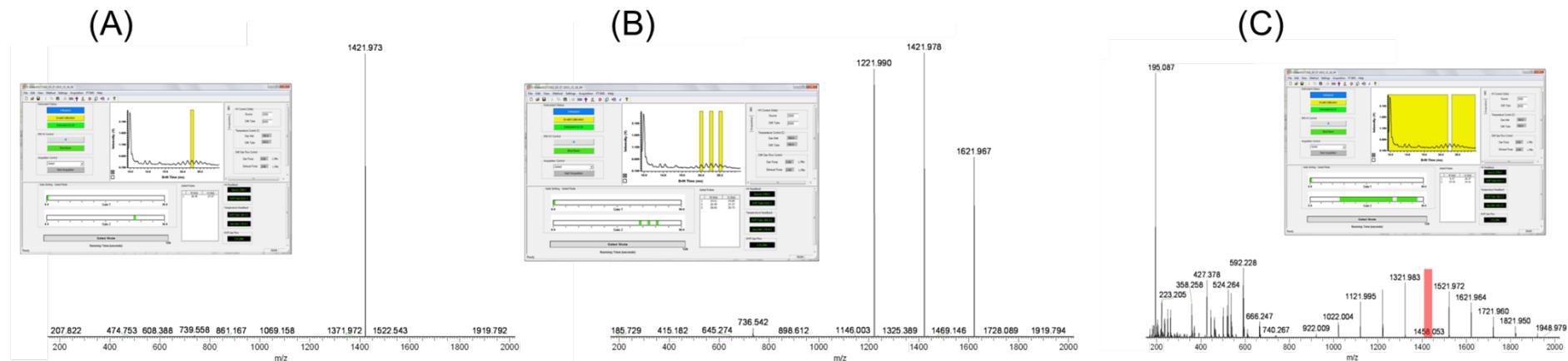
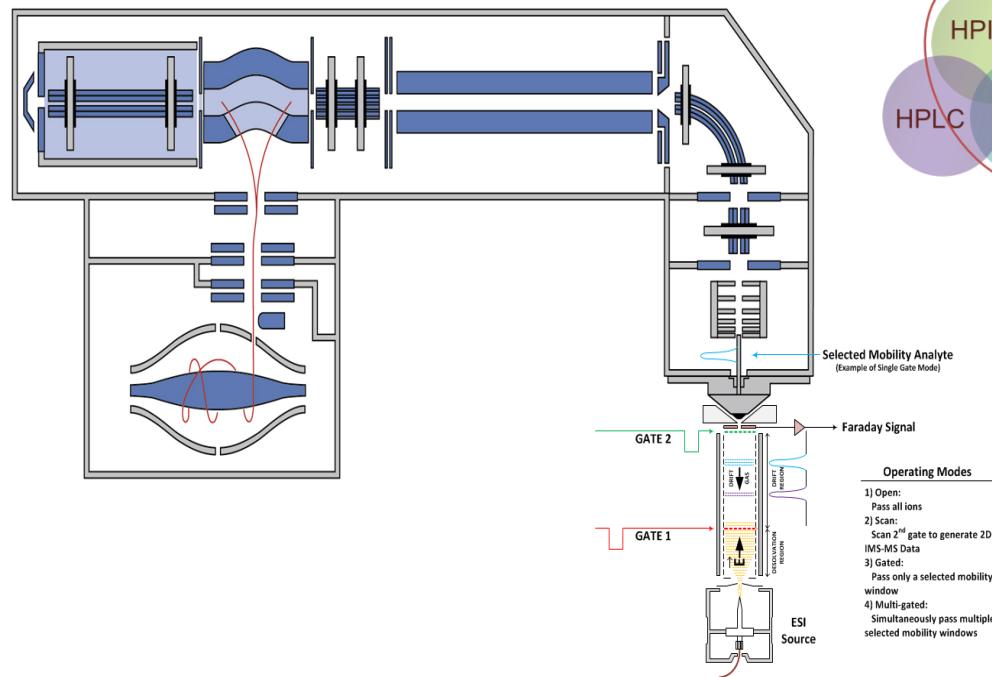
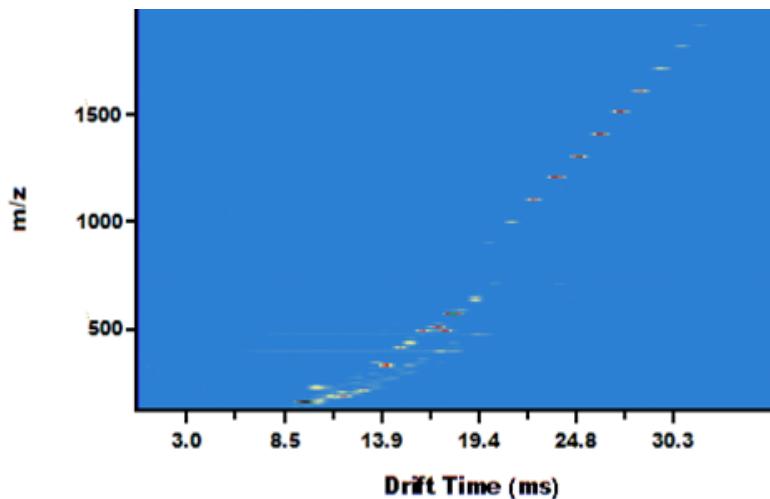
Agilent 6560



AB Sciex Seletion

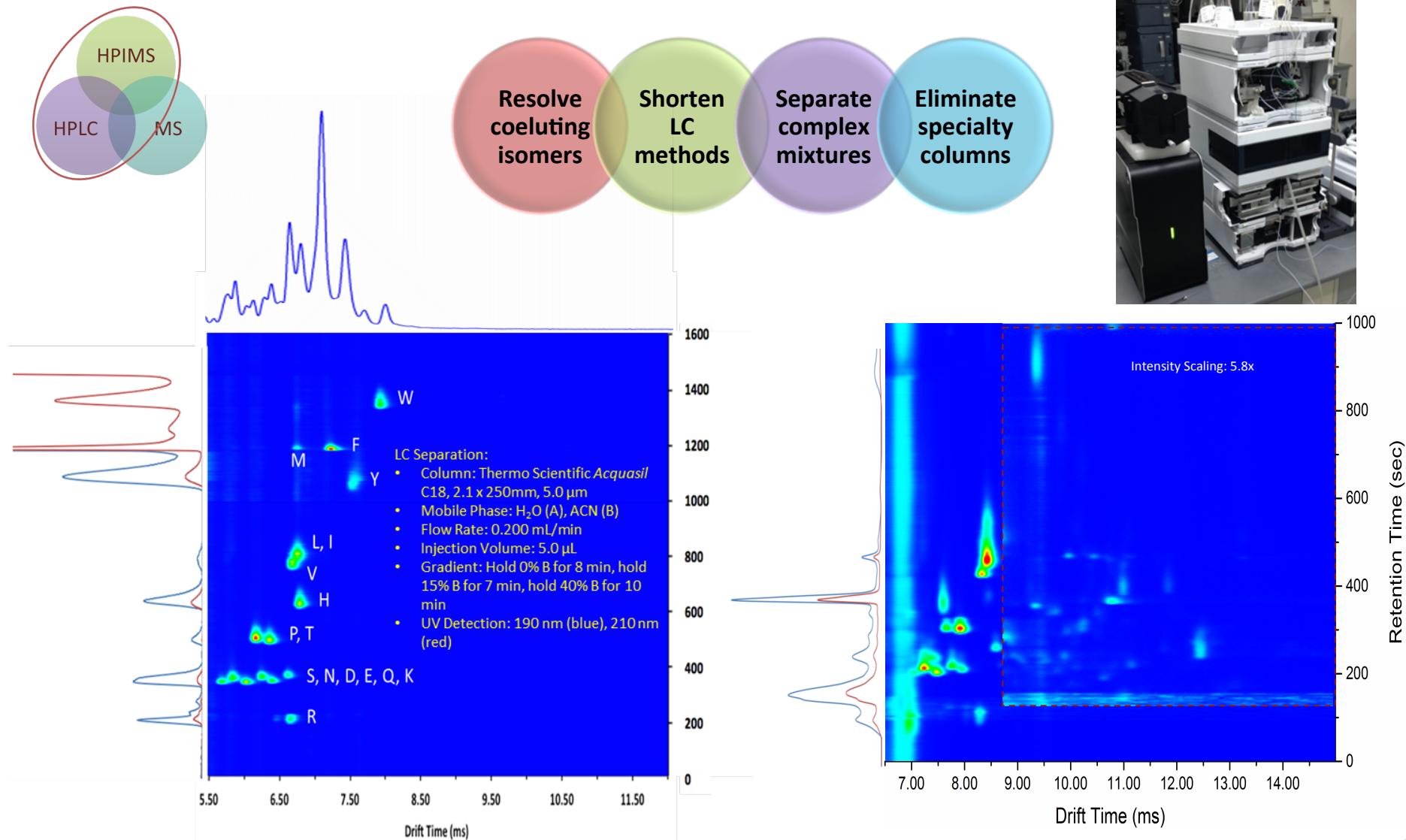
Hyphenated IMS-MS

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Hyphenated HPLC-IMS

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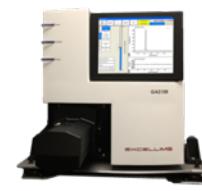
Bring Spectrometers toward the Analytical Targets



Resolution 450,000

Resolution 1000
unit mass

Resolution 250



Resolution 70-120



Resolution 35

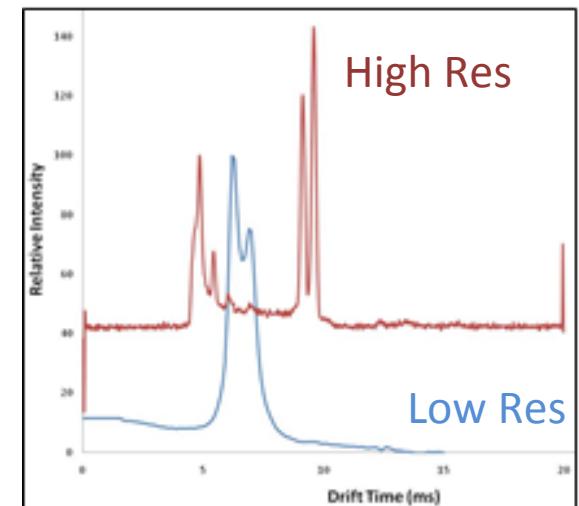


Resolution 15

*m/z measurement
Vacuum measurement
Reduced performance
in field-use*

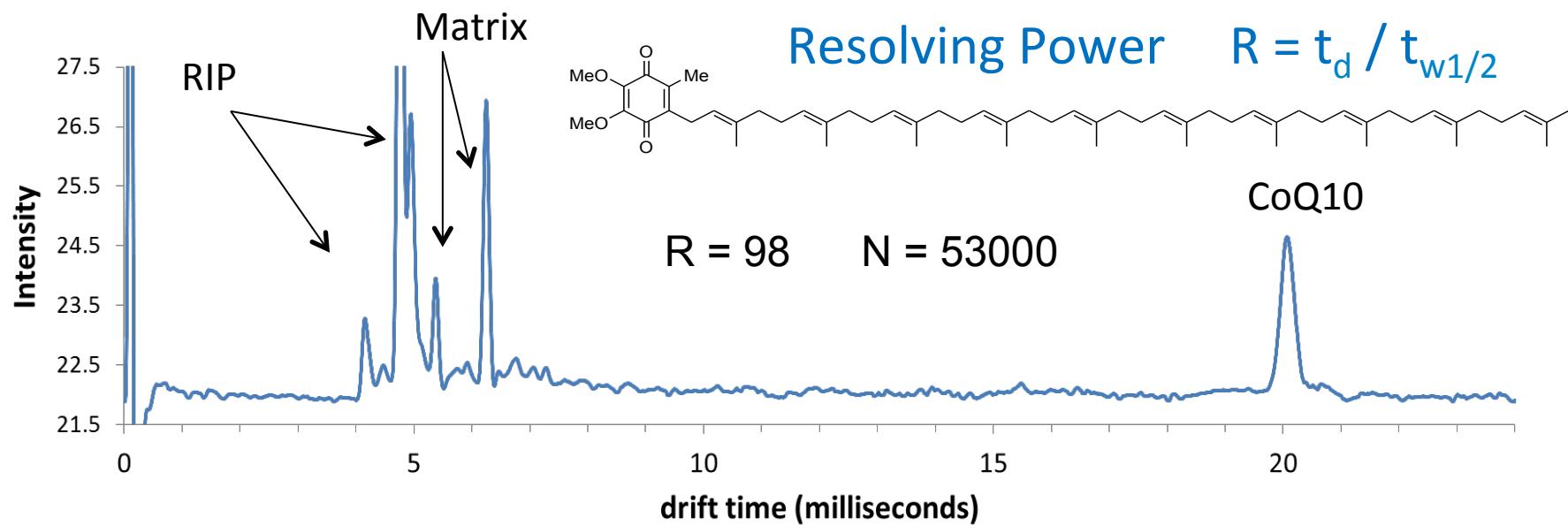
*Size measurement
Ambient pressure
Easiest field-use
Improved performance*

For targeted field analysis, IMS has superior advantages because of its robustness and no vacuum required



Standalone

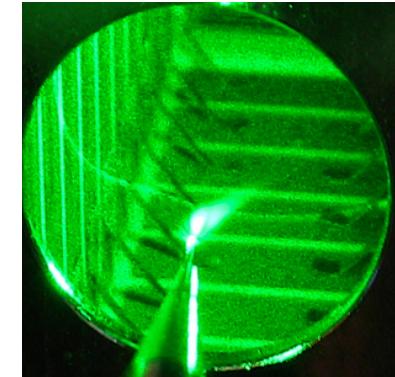
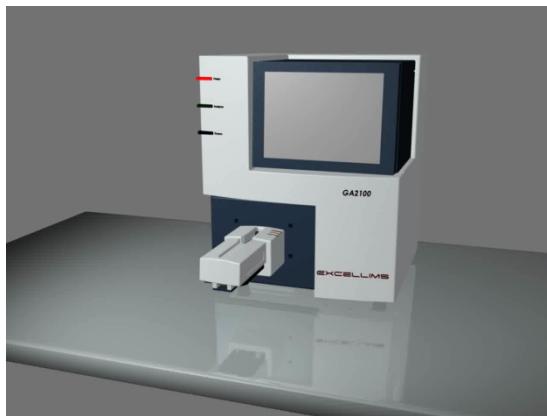
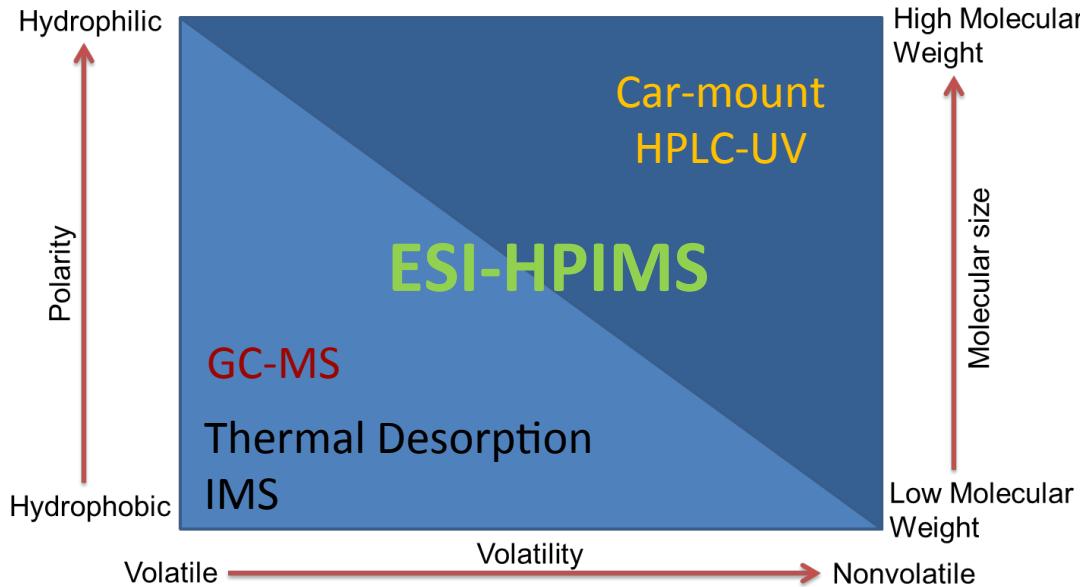
High Performance Ion Mobility Spectrometry



	(U)HPLC	GC	Conventional IMS	HPIIMS
Resolving Power (R)	65	145	30	70-120
Analysis Time	3 min	20 min	10 sec	10 sec

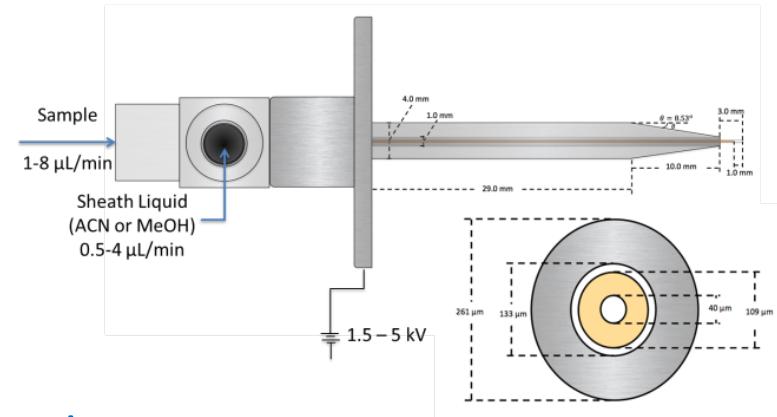
HPIMS For Field Analysis

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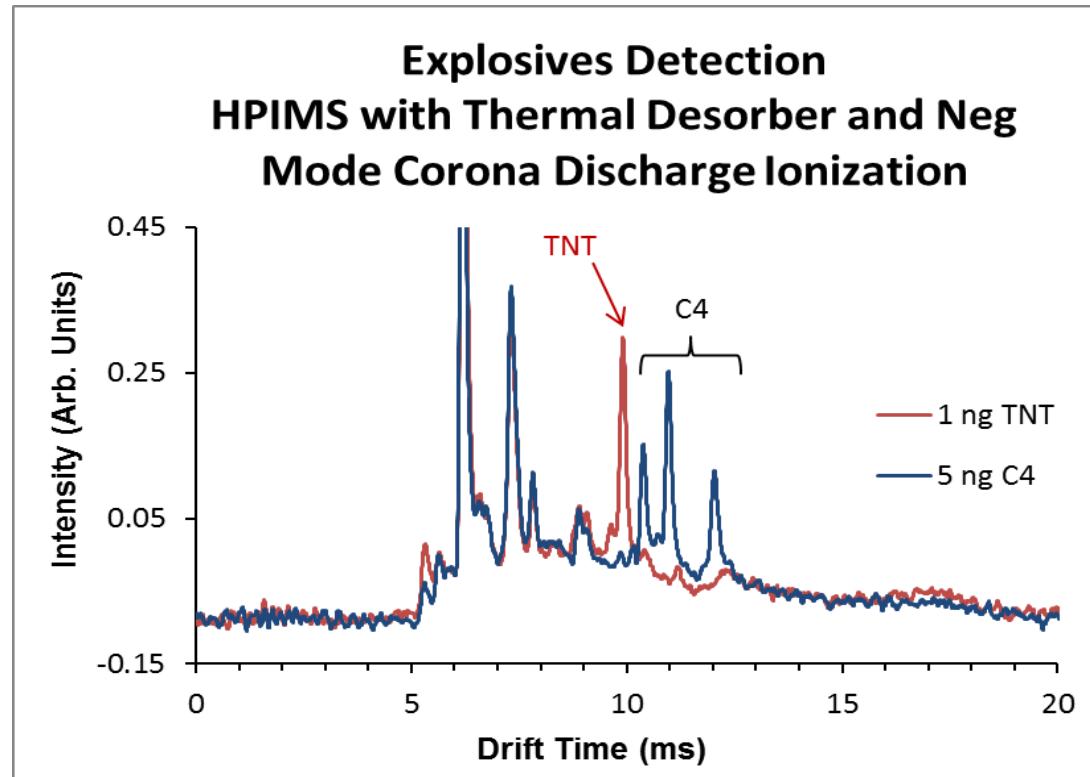
ESI Spraying Tip

Electrospray Source

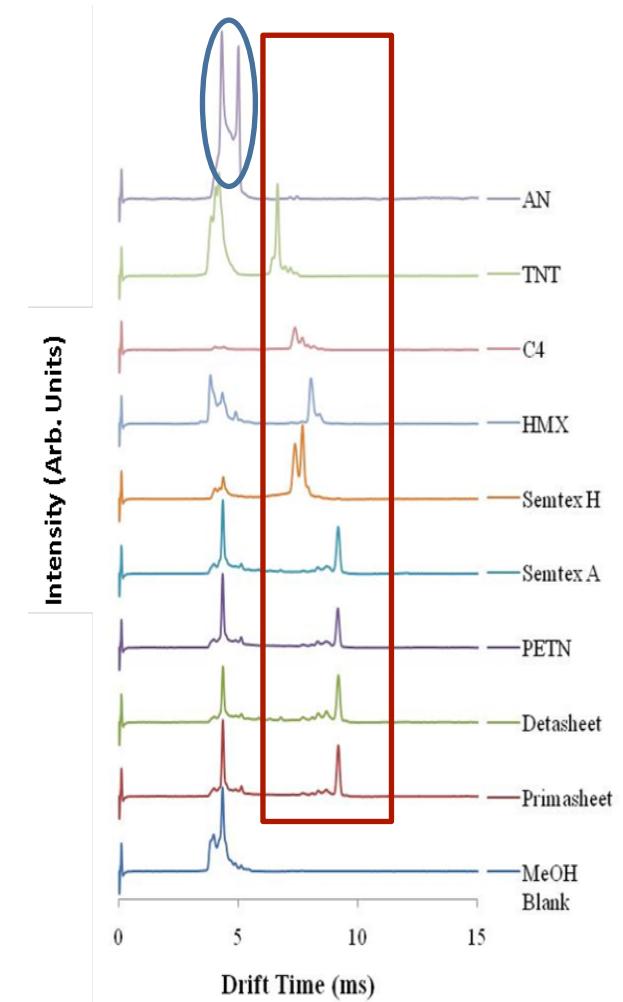


One Step Liquid Sample Analysis - Directspray Ionization

HPIMS for Explosive Detection



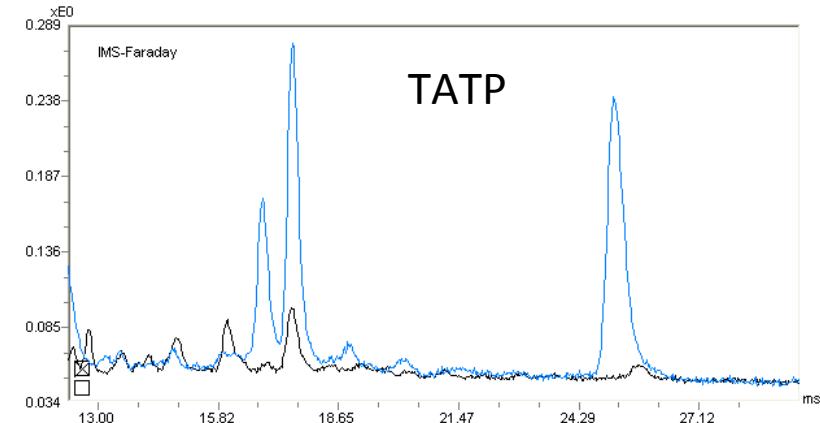
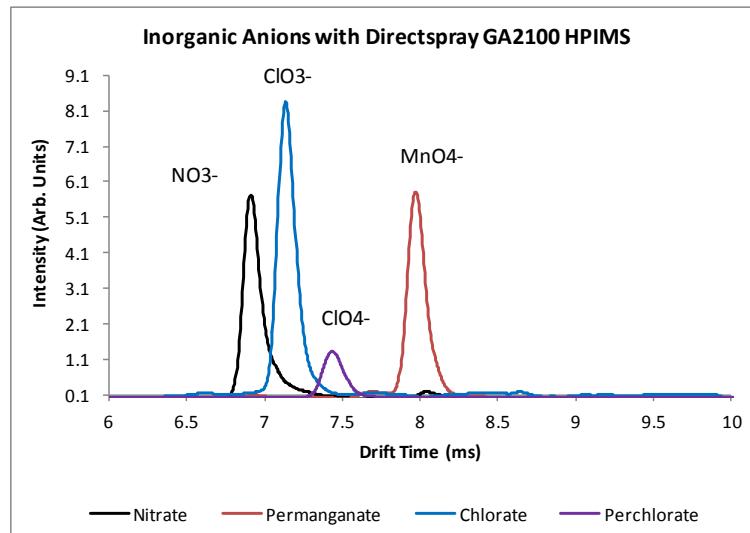
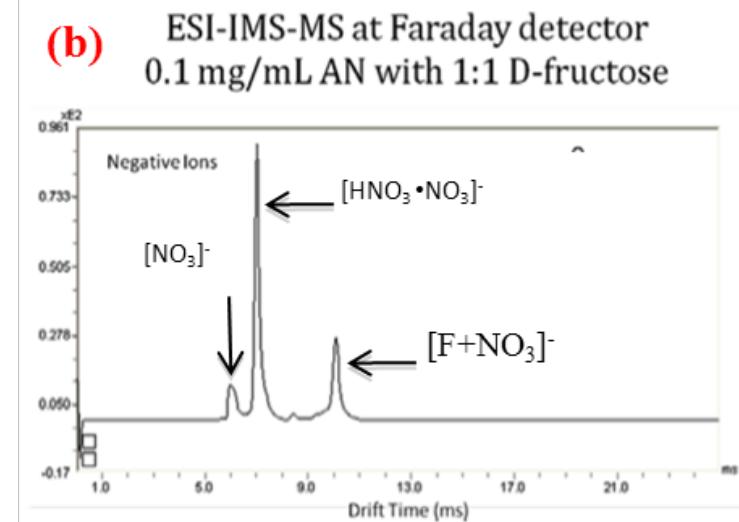
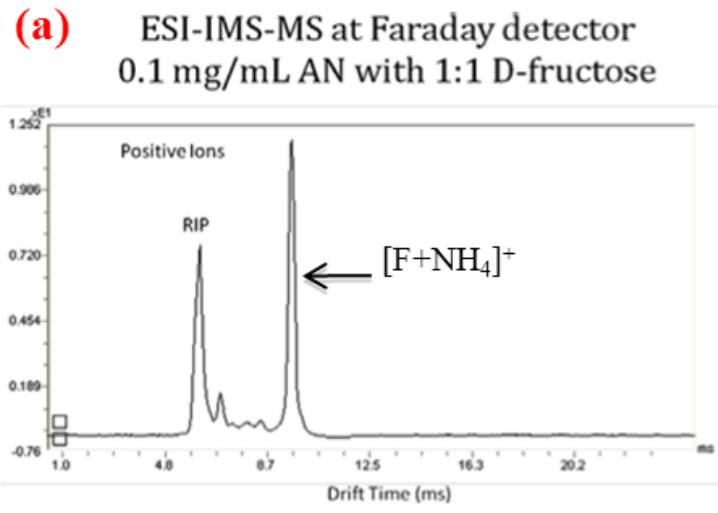
1ng TNT and 5 ng C4 using CDI-TD and HPIMS



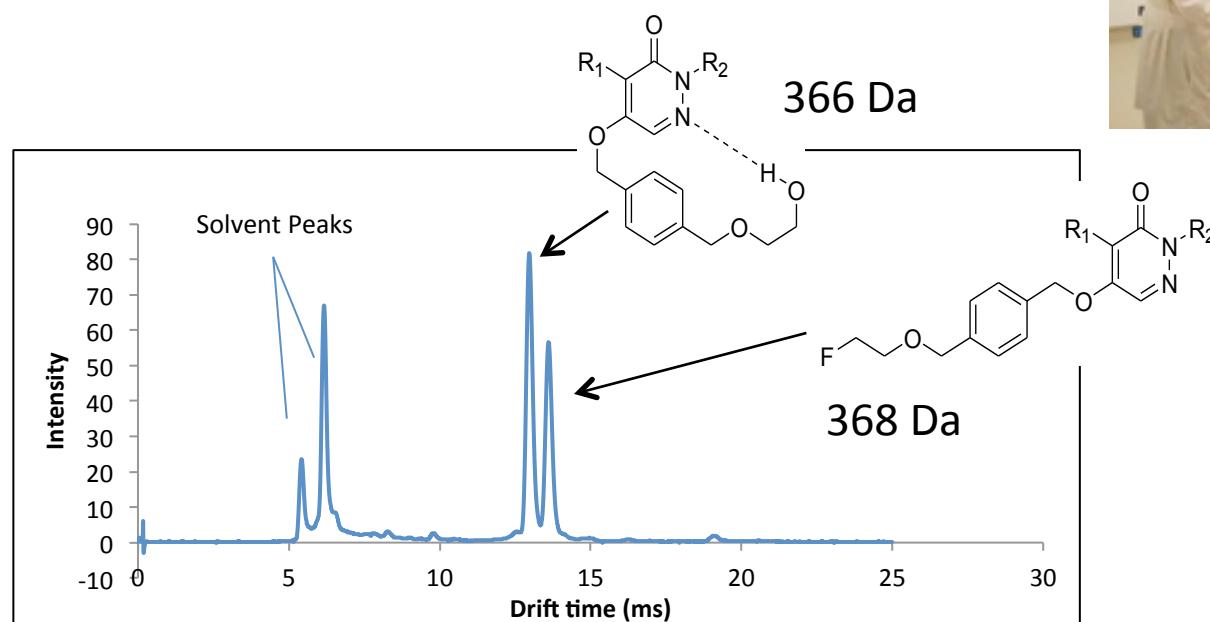
ESI-HPIMS: C. Wu and co-workers, *IJMS*, 2010, 298, 64.

ESI-HPIMS Enables Detection of HME and Inorganic Explosives

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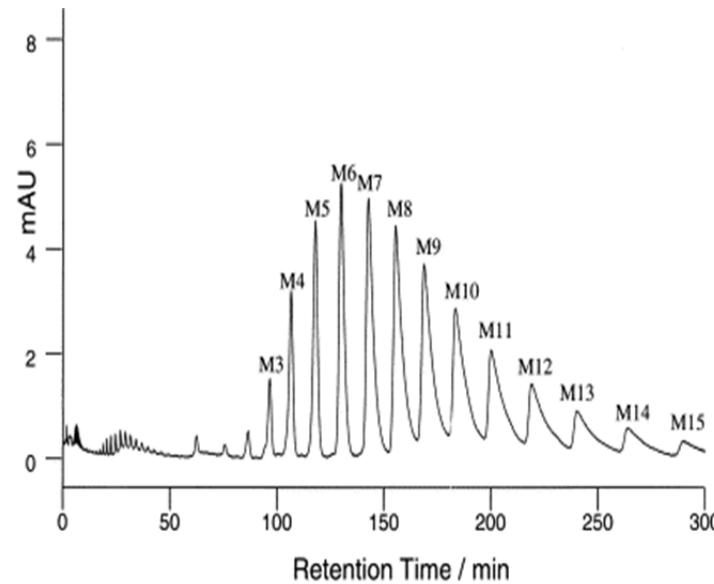


Reaction Monitoring – Radiopharmacy

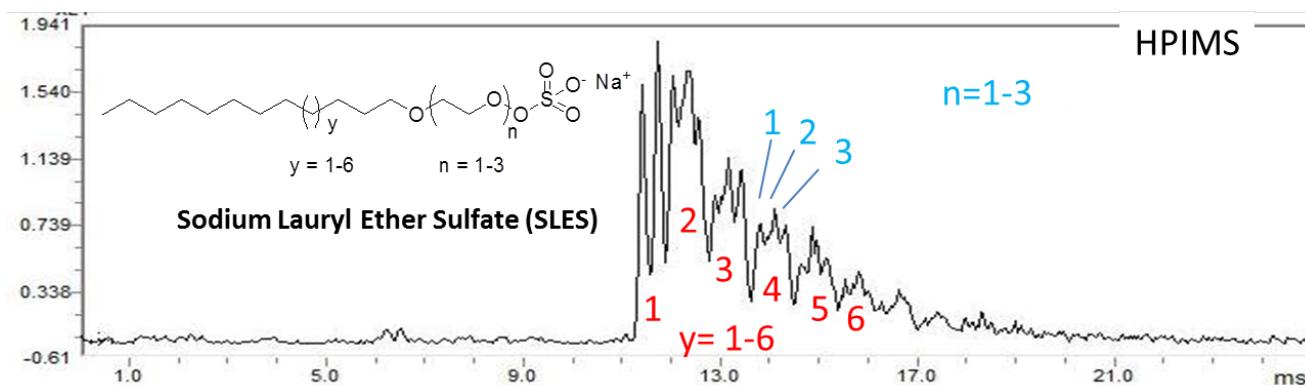
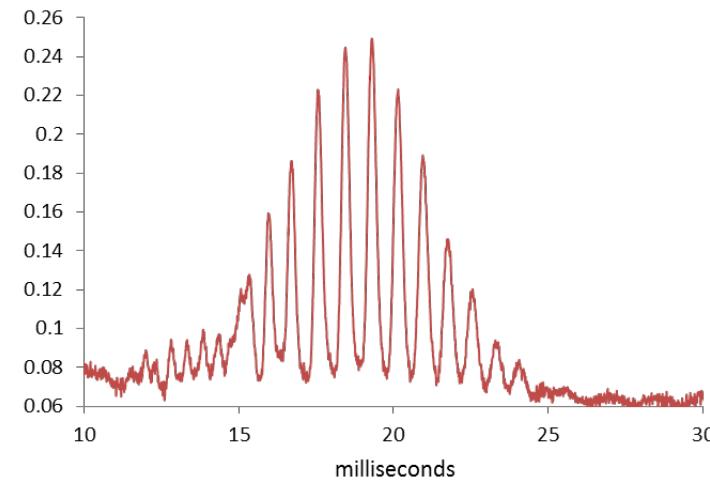


- Constrained versus straight geometry identified in the gas phase
- 2 amu difference in OH-compound compared to a F-compound shows baseline separation due to hydrogen bonding interaction

Process Monitoring – Surfactants



Journal of Chromatography A
Volume 852, Issue 2, 13 August 1999, Pages 475–485



Cleaning Validation

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Swab Recovery

Parameters	HPLC	ESI-HPIMS	Commercial IMS
Recovery (%)	84.5	83.4	Not detectable
Precision RSD (%)	2.1	8.0	Not detectable
Total analysis time per run	~12 min	< 1 min	NA

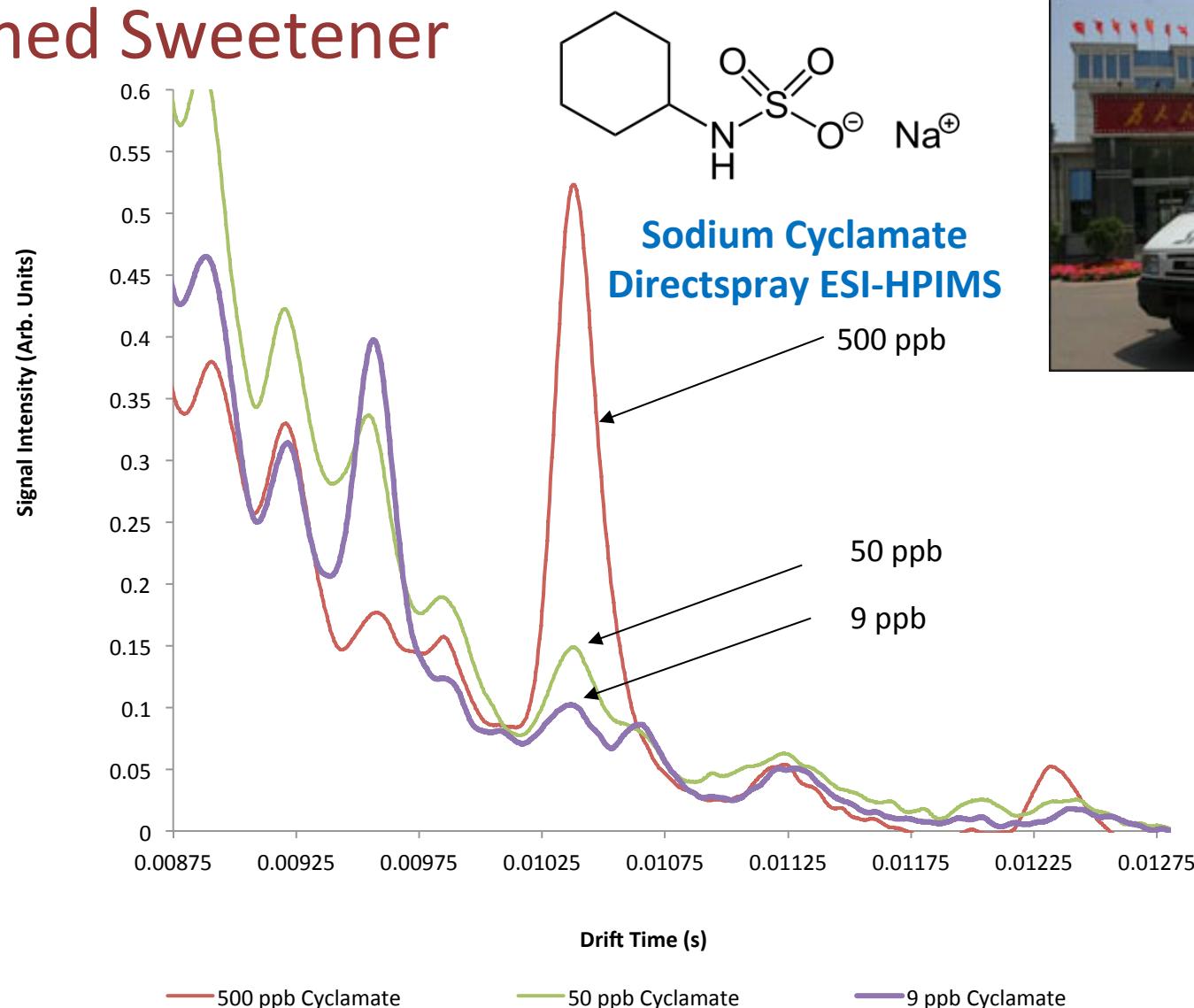
- Spike level: 1.66 µg/cm²
- Results from HPLC and ESI-HPIMS analysis are comparable



- Speed is critical
- At line analysis is desirable

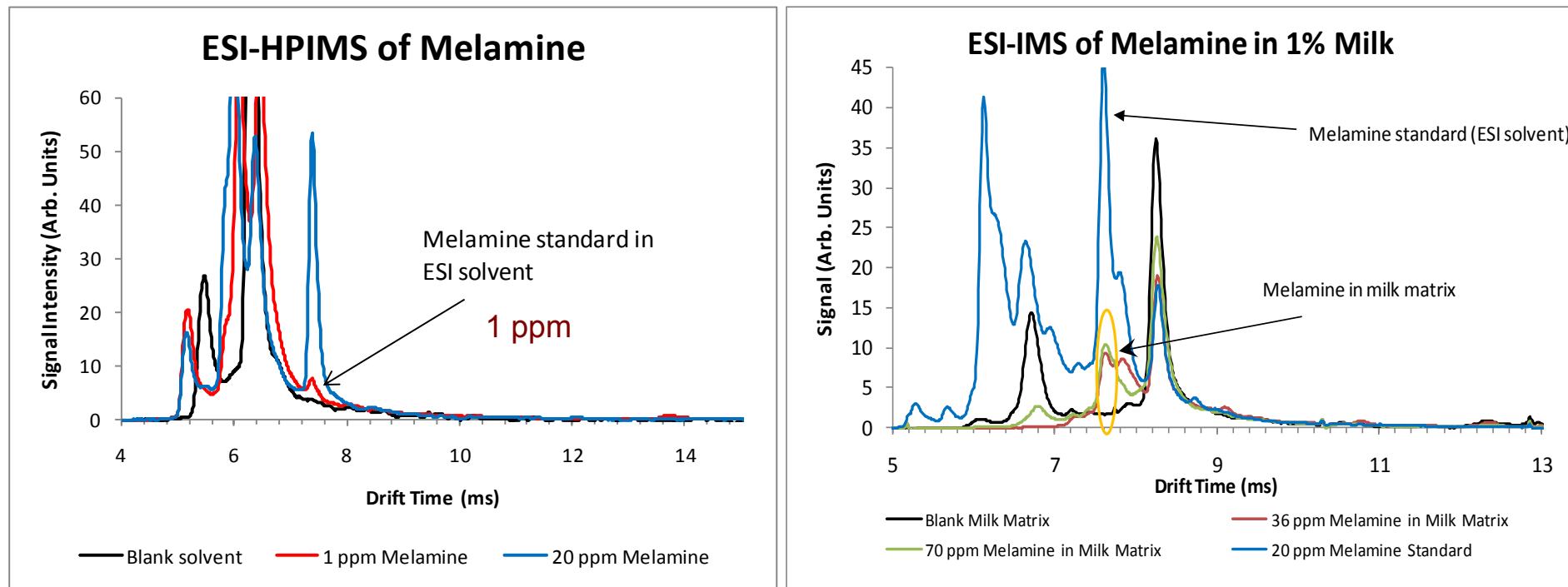
Food Safety Inspection Banned Sweetener

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Directspray Milk Sample Melamine Detection

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Simplified sample prep:

- Denatured 1 mL of 1% milk with 5 mL of 1M acetic acid (aq)
- Filtered with 0.45 m nylon syringe filter
- Add 1 mL methanol and analyzed both spiked and unspiked

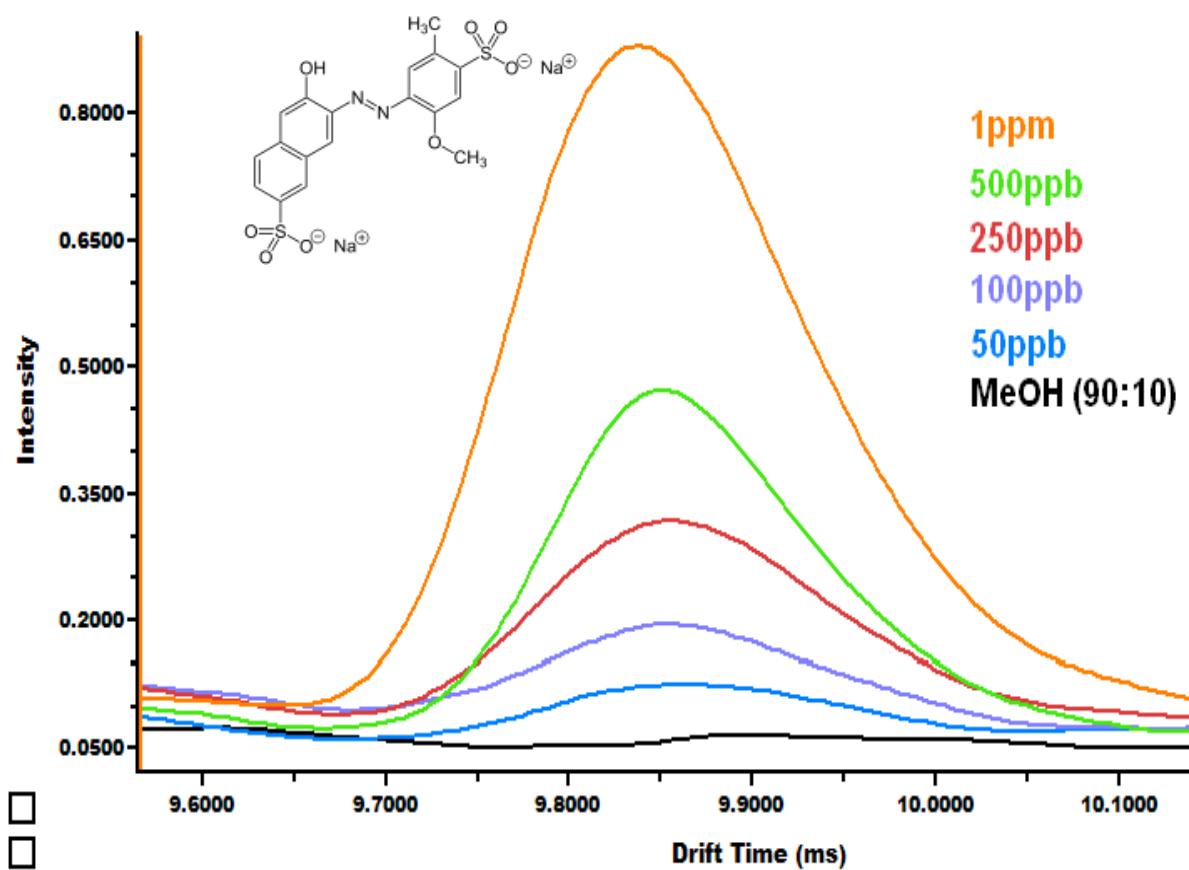
36 ppm of melamine detected with good signal-to-noise in milk

- Lower concentrations should be detectable

Food Safety Inspection

Food Dye

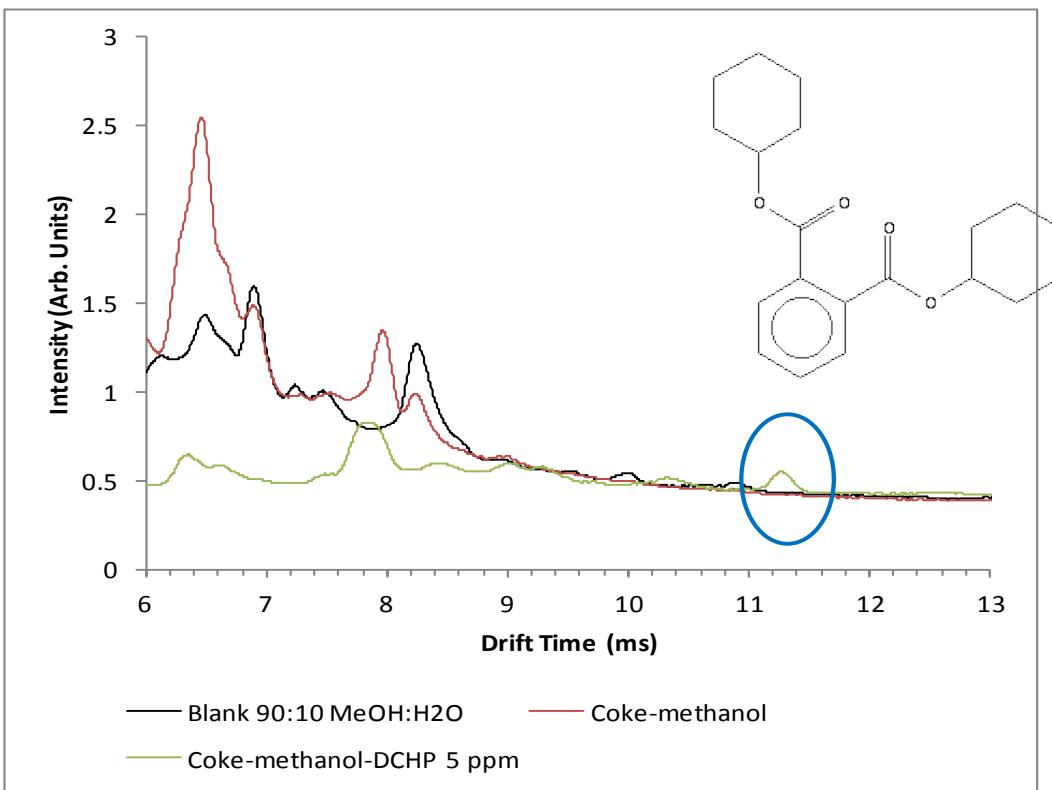
Allura Red AC



- Negative ion mode with air drift gas
- Detect anion of salt
- 170°C IMS temperature
- Can detect 50 ppb

Food Safety Inspection Coca-Cola – spiked with DCHP

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Use a simplified sample preparation and detect phthalate spiked into an actual beverage sample

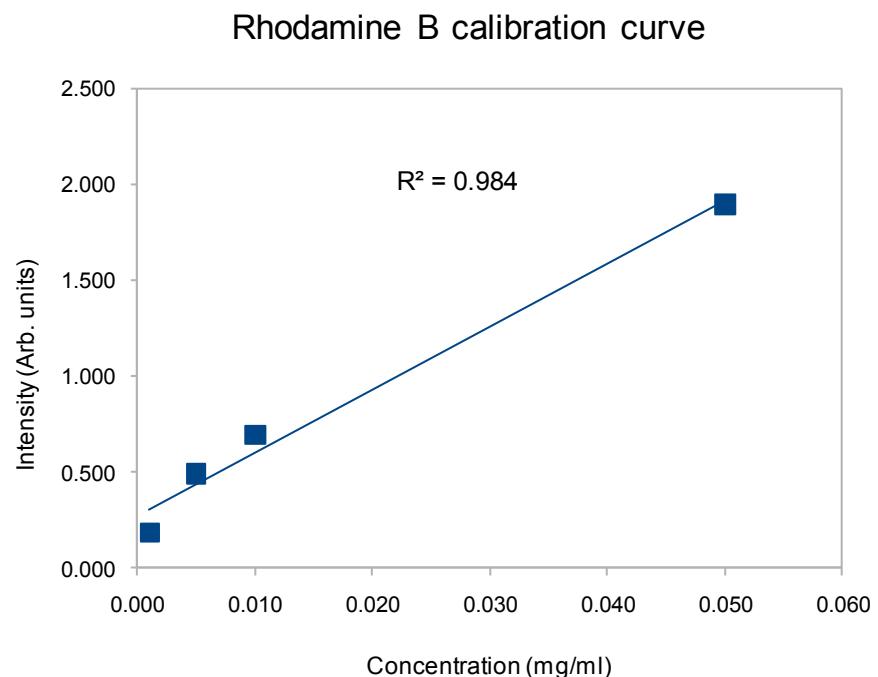
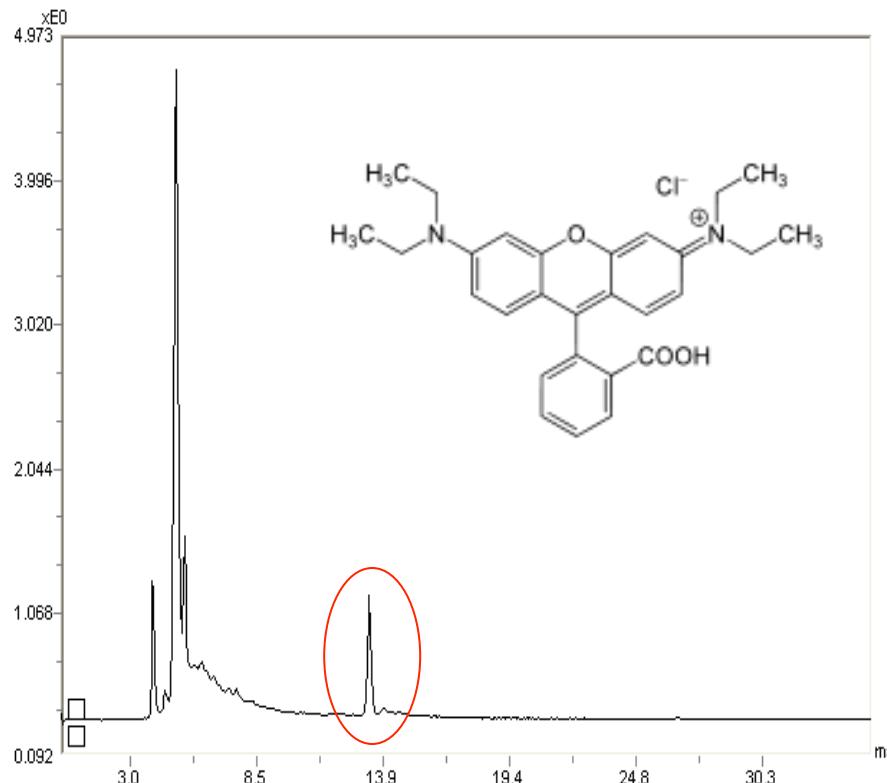
Black: Blank – MeOH/water(90:10)

Red: Coke/MeOH (90:10)

Green: Coke/MeOH/DCHP(5 ppm)

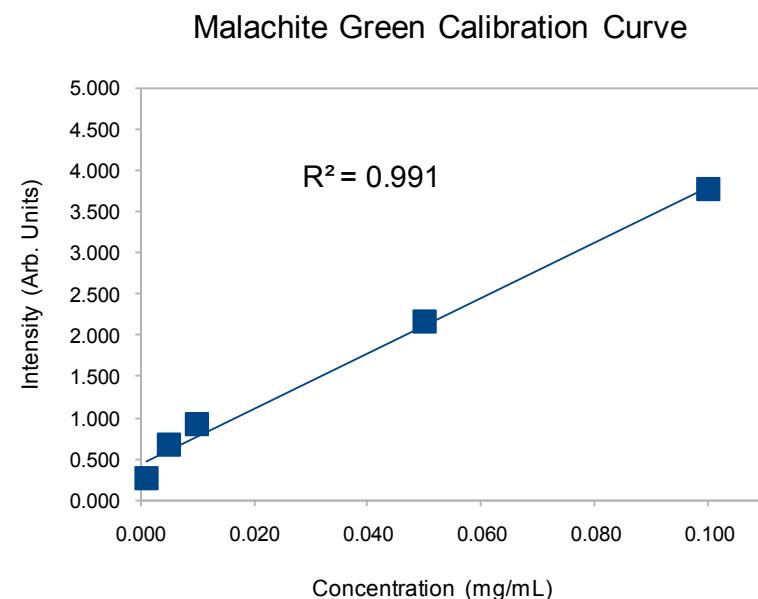
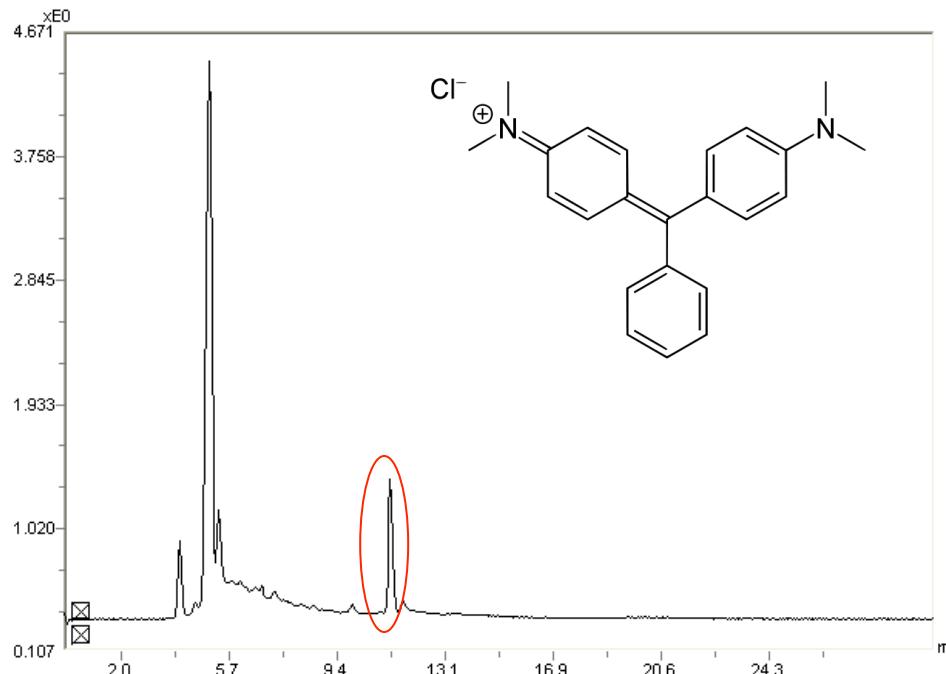
- Diluted Coca-cola 9:1 with methanol both spiked and unspiked
- Can detect 5 ppm in the cola
- Factor of 30 lower than the current accepted method can detect

Rhodamine B – Illegal Food Dye



- Lowest conc. detected with GA2100 (ESI solvent) = 50 ppb
- Sciex published method <100 ppb with LC-MS

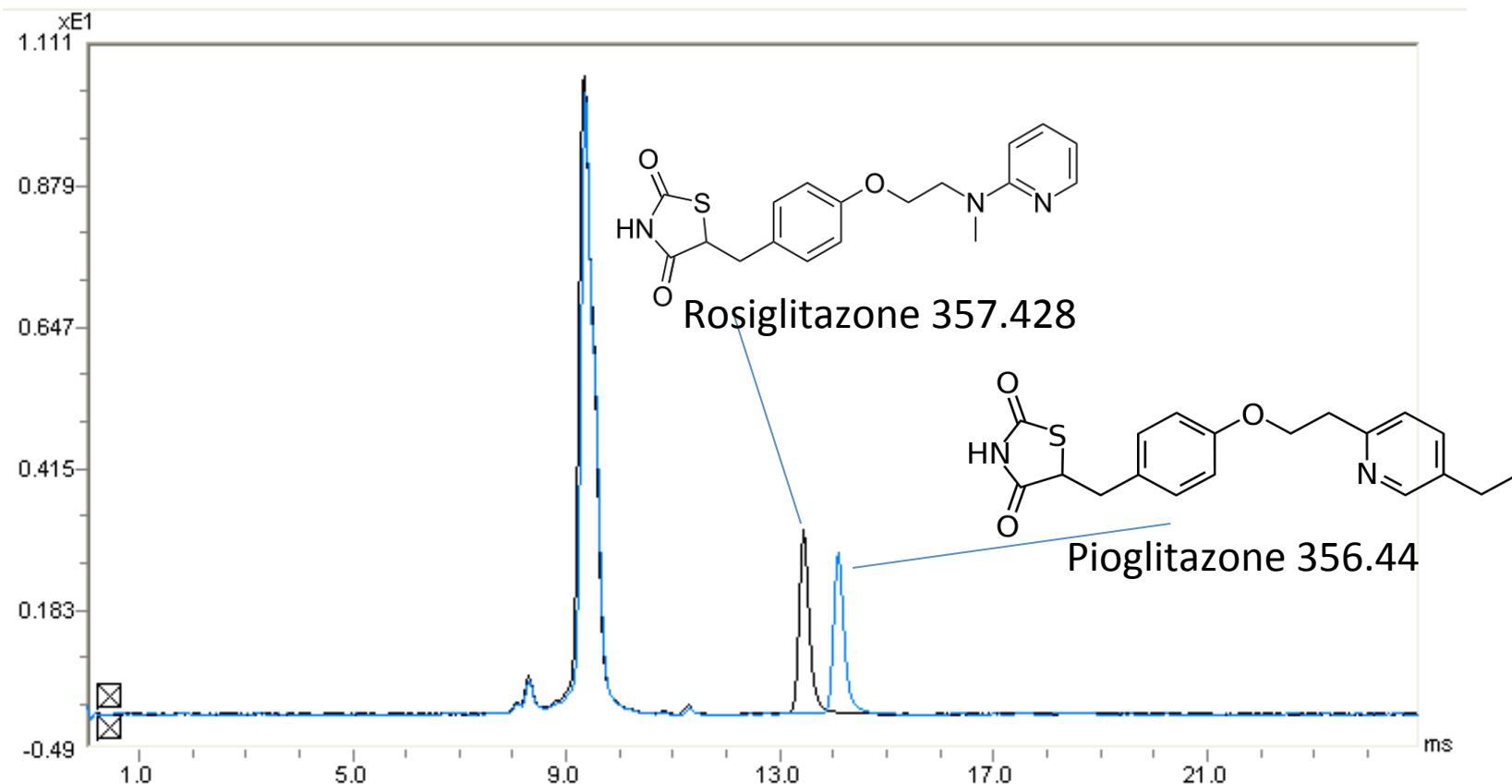
Malachite Green – Aquaculture By-product



- Lowest conc. detected (ESI solvent) with GA2100 ~ 100 ppb
- Two-order of magnitude linear response range

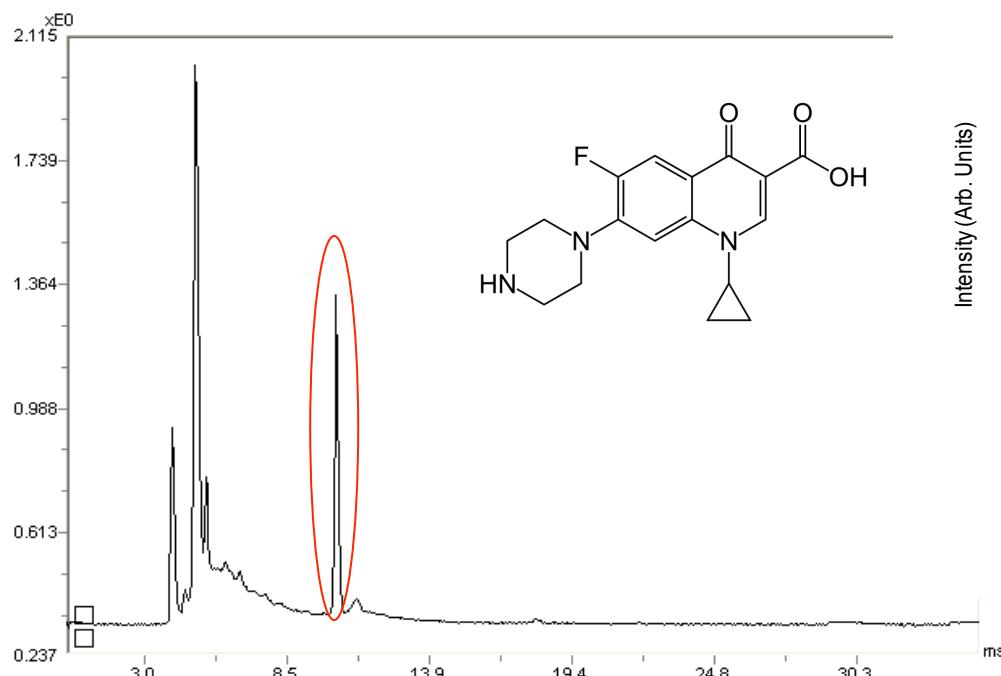
Drug Safety Inspection

Herb Medicine Additives – Prescription Drugs

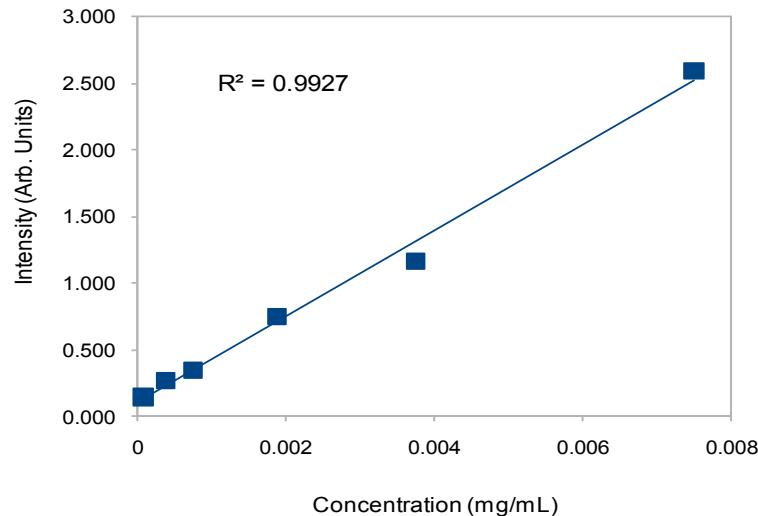


Ciprofloxacin – Antibiotic Residue

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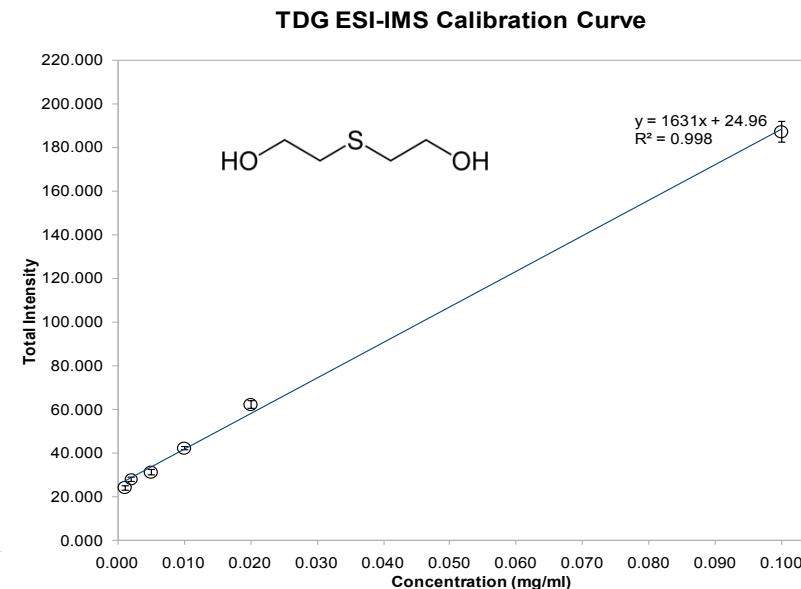
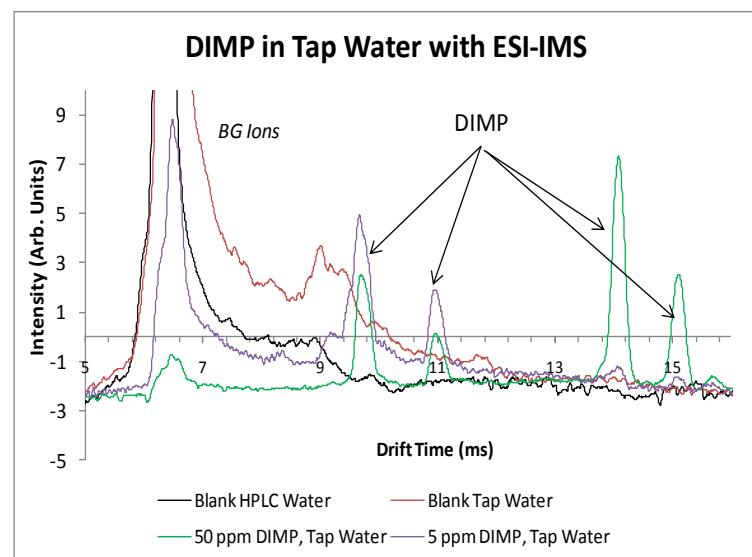
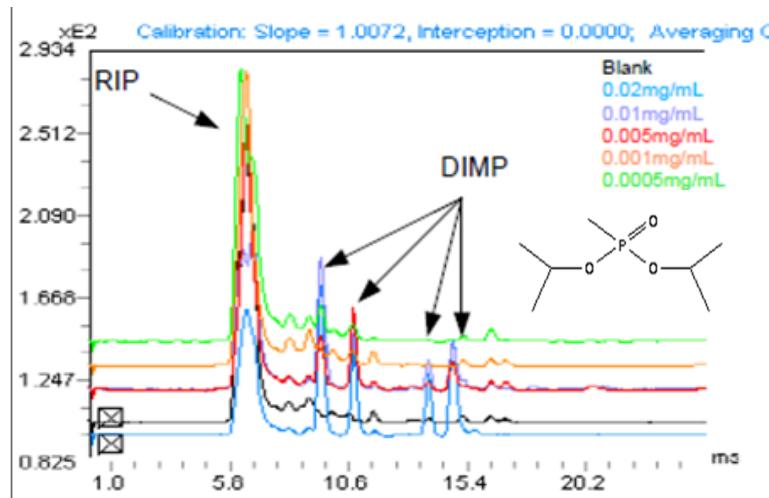
Ciprofloxacin Calibration curve



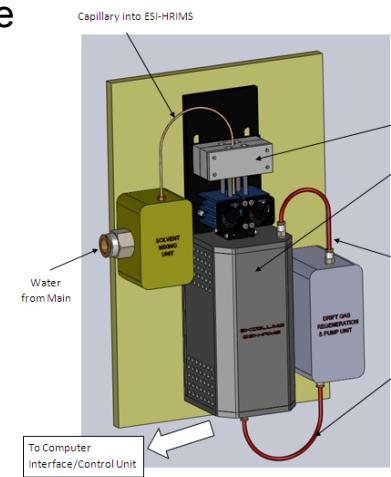
- Lowest concentration detected (in ESI solvent) = 75 ppb
- Two order of magnitude linear response

ESI-HPIMS for Online Water Analysis

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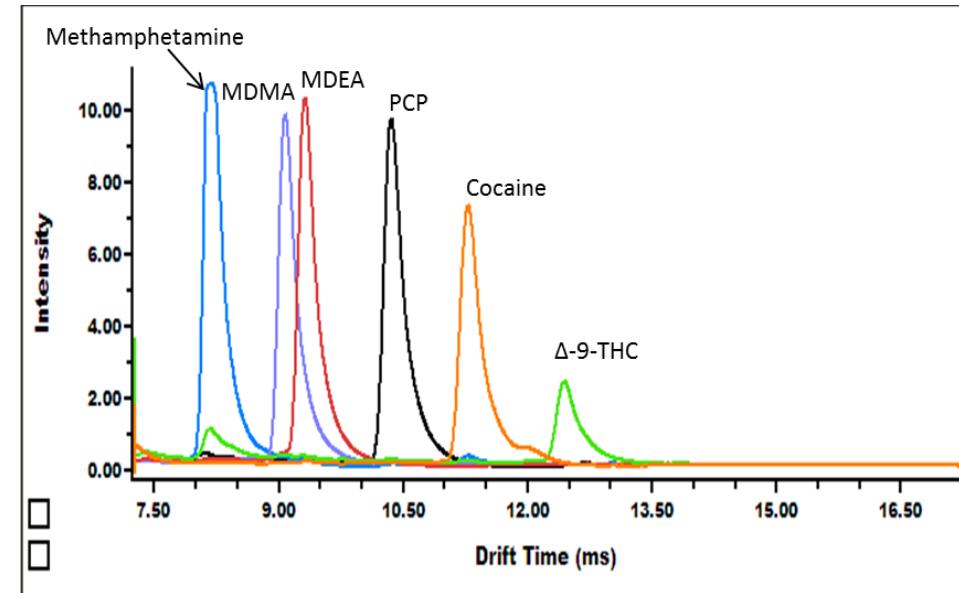
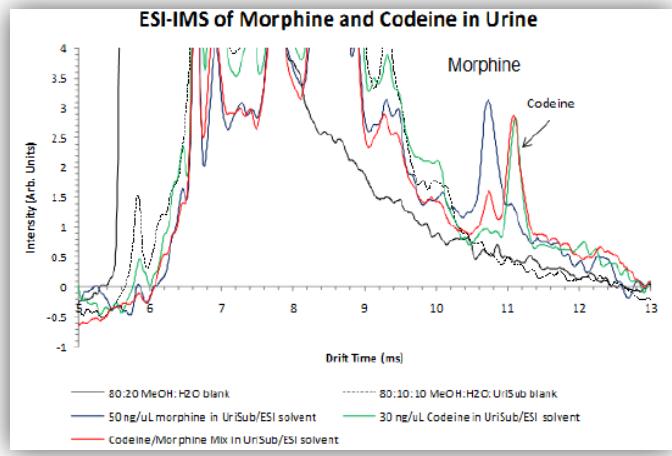
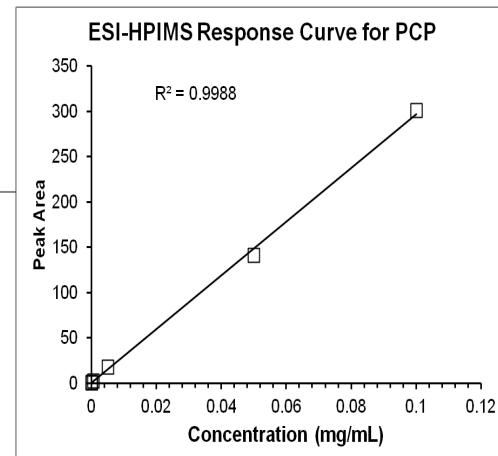
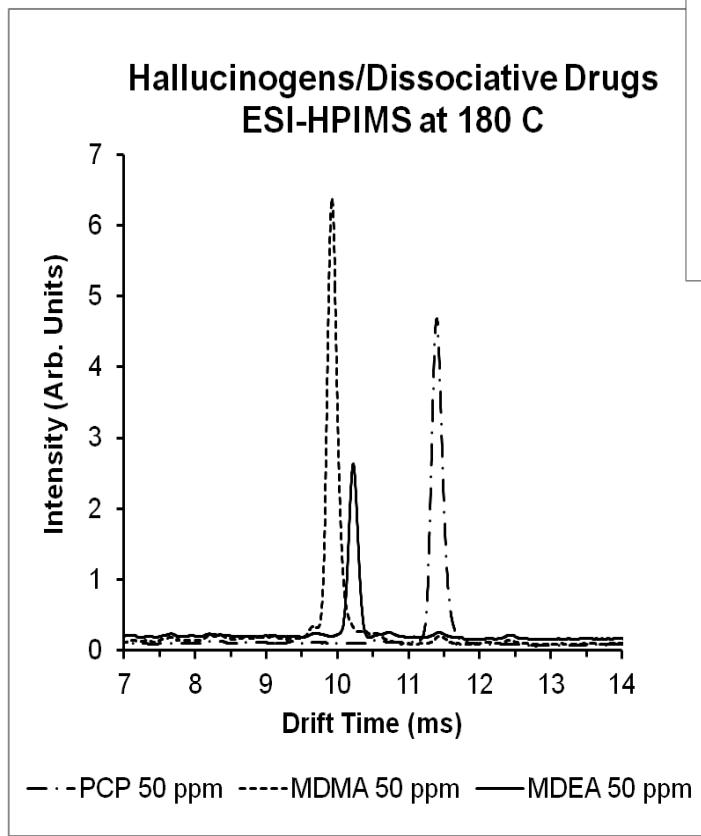


Thiodiglycol (TDG) Response Curve ESI-HPIMS



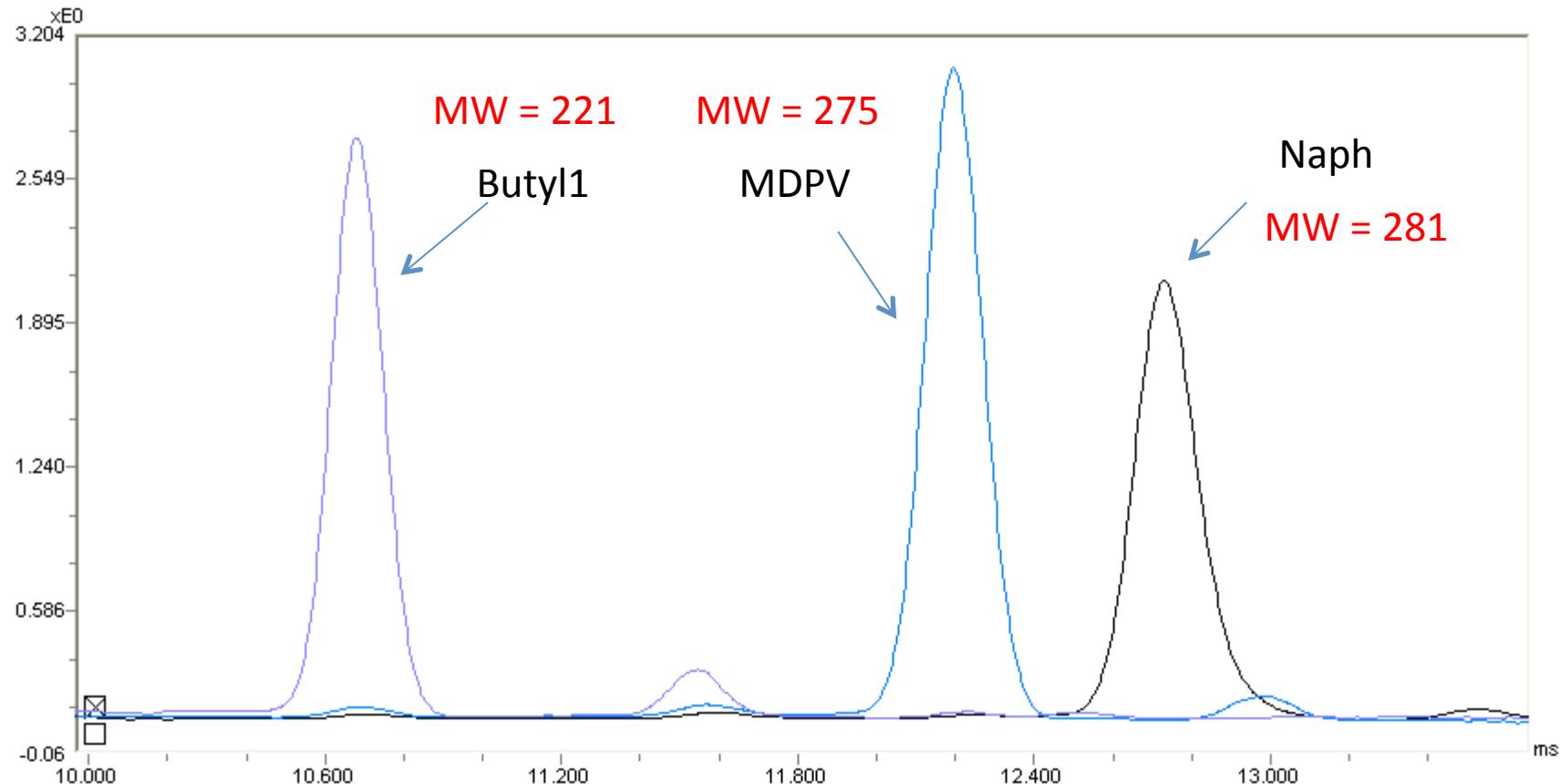
Controlled Substances – Improve Throughput of Forensics Labs

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Controlled Substances – Bath Salts

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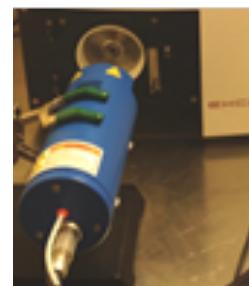
Future Developments

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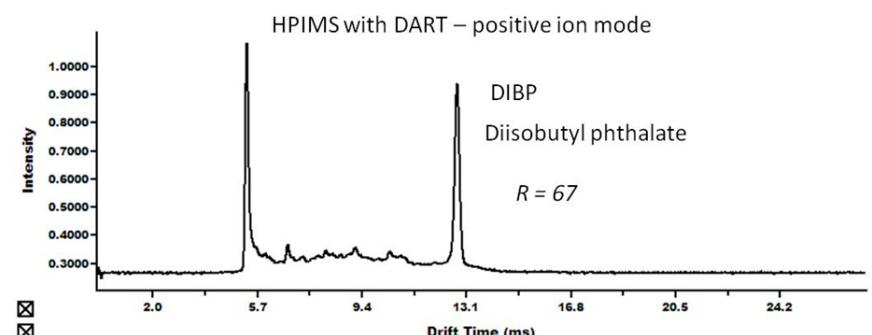
- Reduce Car-mount system to handheld size without compromising performance
- New sample introduction enable direct analysis
- Rapid sample preparation method development



HPIMS from Car-mount to Handheld



DART Ionization
for direct sample introduction



Acknowledgement:

DHS: HSHQDC-09-C-00110

EPA: EP-D-10-025

FDA: 1R43FD003502



Thank you.

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