Ambient Ionization & Miniature Mass Spectrometers for Trace Analysis of Explosives

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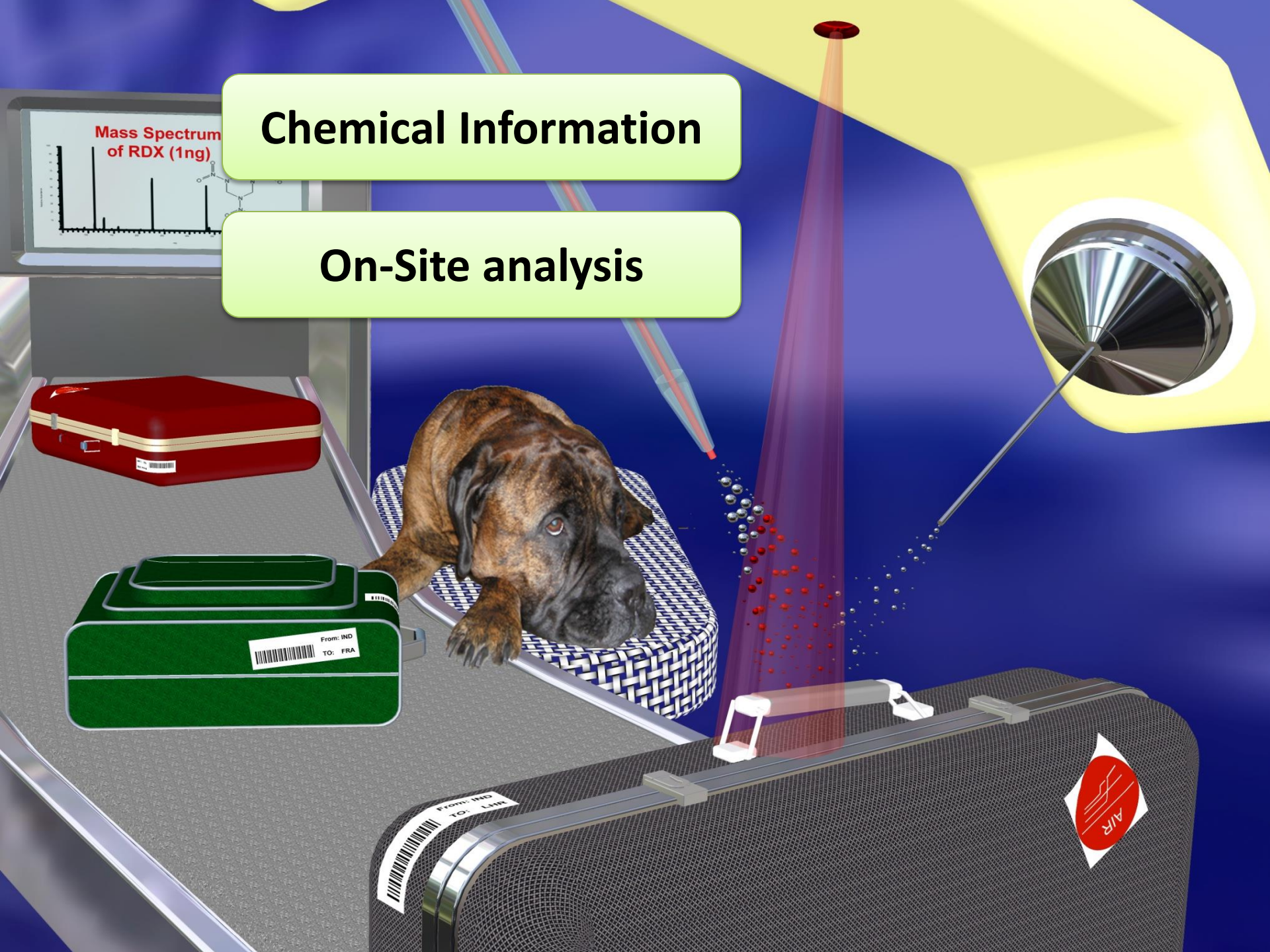
Presented by Ryan D. Espy


Chemical Information
On-Site analysis
Mass Spectrum
of RDX (1ng)
From: IND
TO: FRA
From: IND
TO: LHR
AIR

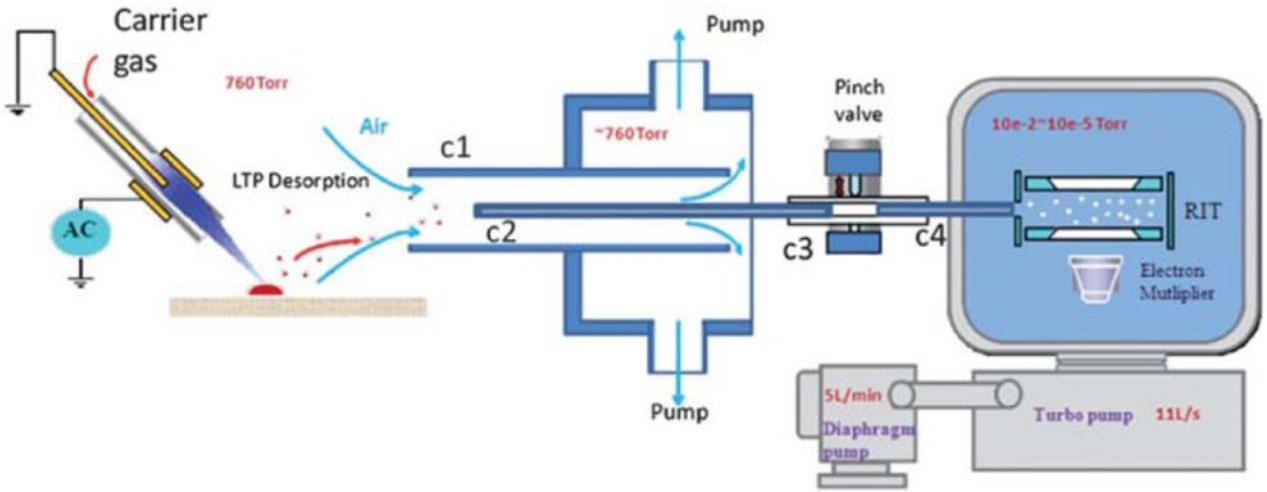
In-situ Analysis of Complex Materials

Ambient Ionization

1. No sample preparation
2. Ionization in open air
3. Rapid *in-situ* analysis

Miniature Mass Spectrometer

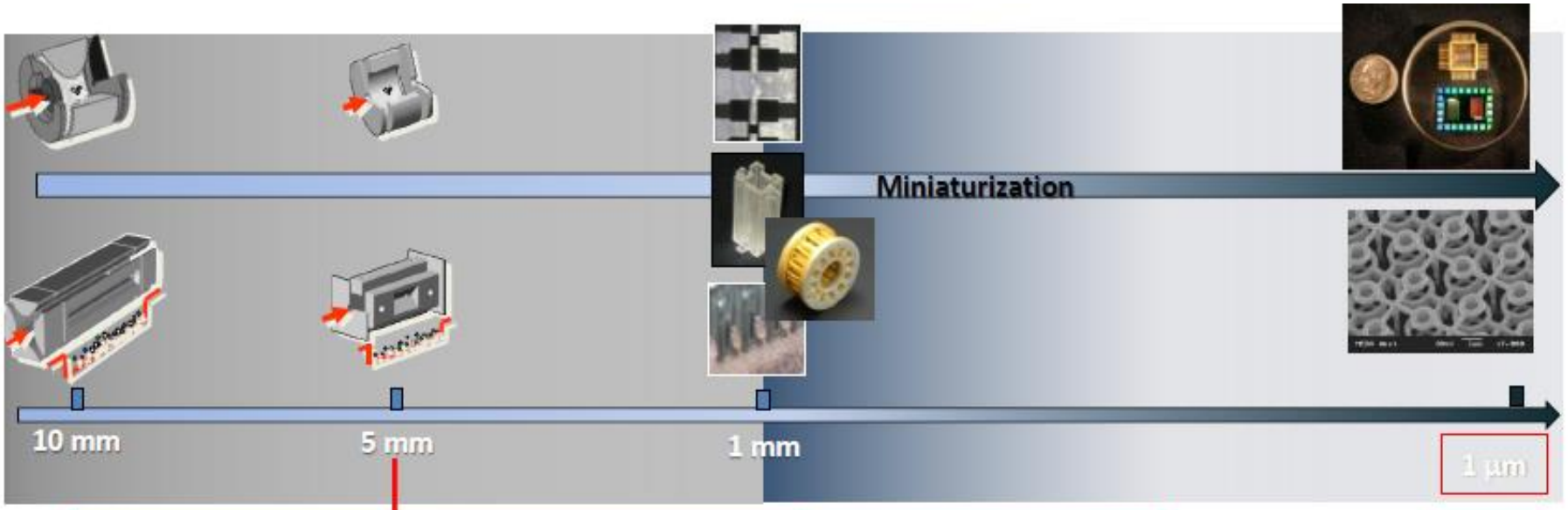
1. Mini fitted with ambient ionization
2. MS/MS capabilities
3. Small & large molecules



Miniaturization Mass Spectrometers

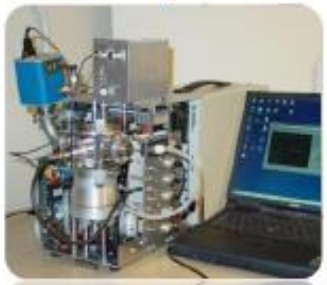
System	Self-sustainable Portable Systems						Portable Systems without rough pumping	
	Mini 10/11/12	ChemCube™ /ChemPack	Suitcase TOF	Griffin™ 824	Guardion-7™	IonCam™	Palm-portable MS	HAPSITE®
Developer	Purdue University	Microsaic Systems	Johns Hopkins Applied Physics Lab	Griffin Analytical Technologies, Inc.	Torion Technologies	OI Analytical	Samyang Chemical Co.	Inficon
Weight	10kg/4kg/15kg	9kg/14.9kg	N/A	22.7kg	11kg	19kg	1..5kg	18kg
Power	70W/30W/65W	45W	N/A	N/A	75W	150W	5W	<150W
Mass Analyzer	Rectilinear ion trap	Quadrupole mass filter	TOF	Cylindrical ion trap	Toroidal ion trap	Mattauch-Herzog sector	Cylindrical ion trap	Quadrupole mass filter
MS/MS	Yes	No	No	Yes	Yes	No	No	No
Sampling /Ionization	MIMS, direct leak, GDEI, APCI, ESI, DESI, LTP, PS, LS	SPME, EI	MALDI	SPME, MIMS, EI	SPME, mini GCEI	Direct gas leak EI, mini GCEI	Pulsed gas leak EI	GCEI
Mass range /Resolution	*m/z* 700, R = 700; *m/z* 1500, R = 750	*m/z* 600, R = 400; *m/z* 400, R = 200	*m/z* 70,000, R = 70	*m/z* 425, R = 400	*m/z* 500, R = 500	*m/z* 300, R = 300	*m/z* 300, R = 150	*m/z* 300, R = 300
System Photo								

Miniaturization of Ion Trap Mass Spectrometers



65 kg

25 kg



10 kg

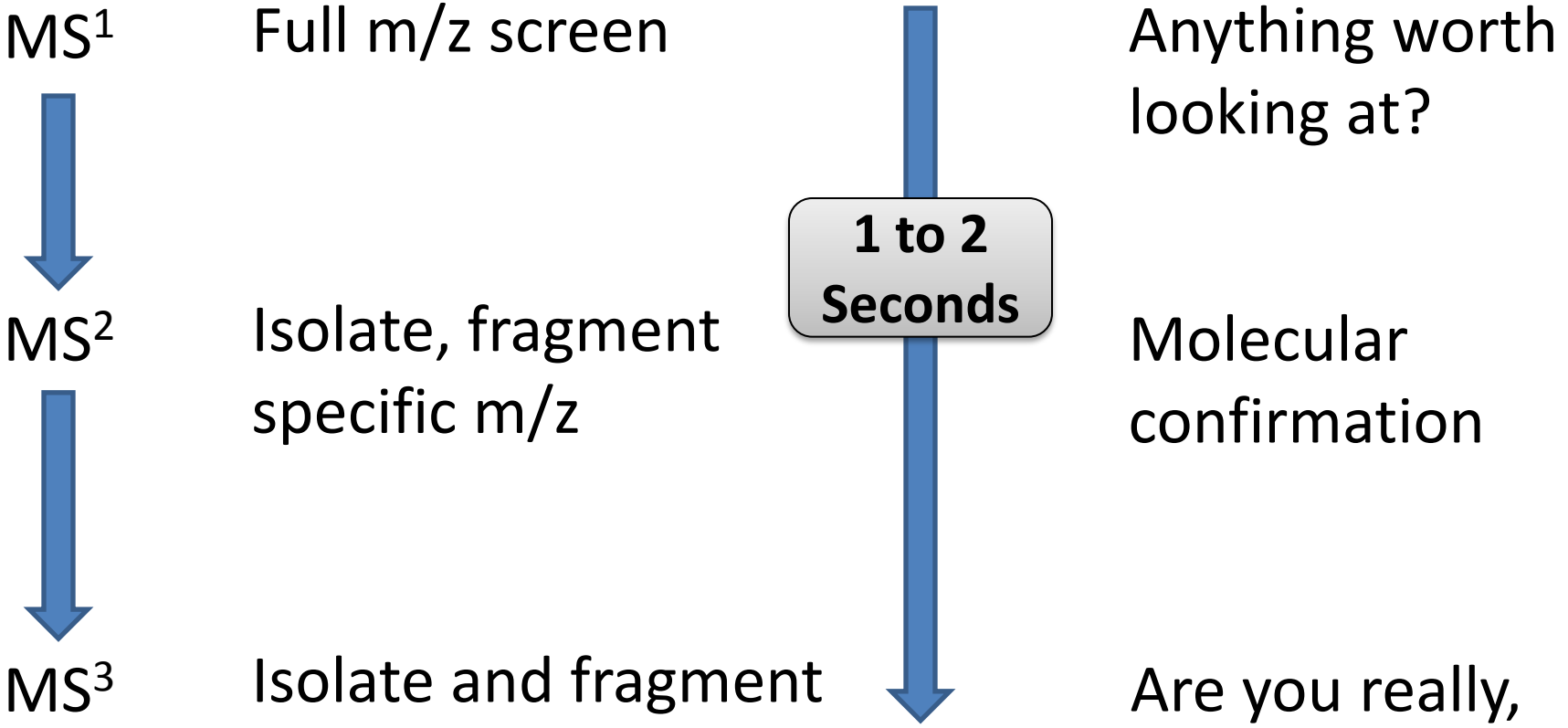
4 kg

100 g

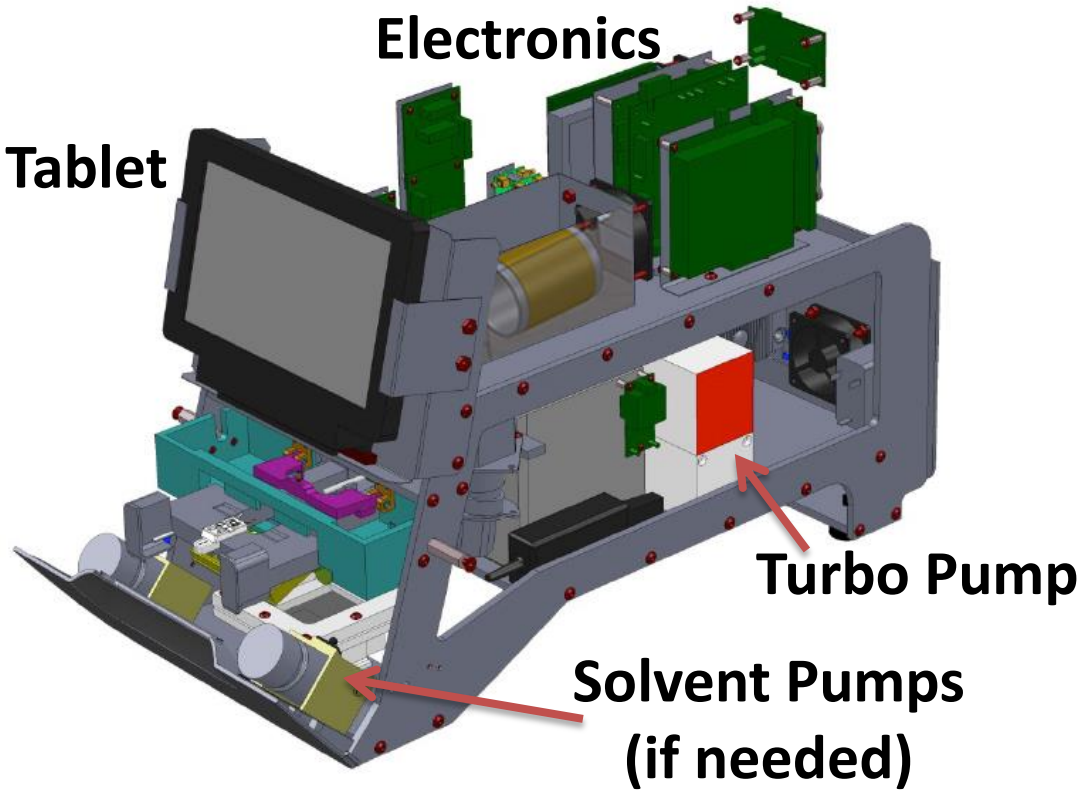
?

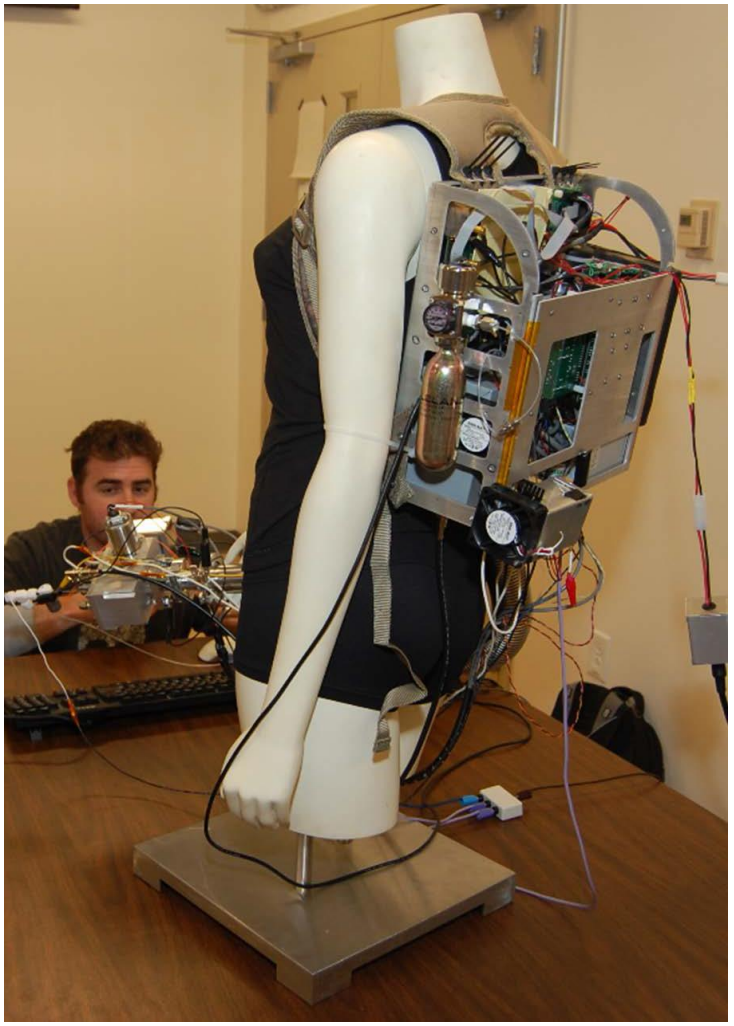
Tandem Mass Spectrometry

Structural information for enhanced selectivity = reducing false positives



Instrumentation: Mini/Portable MS for in-situ analysis





Multiple instrument configurations

-Wearable backpack w/ sampling head unit

11.3 kg (25 lbs)

-Desktop portable

15 kg (33 lbs)

Power consumption

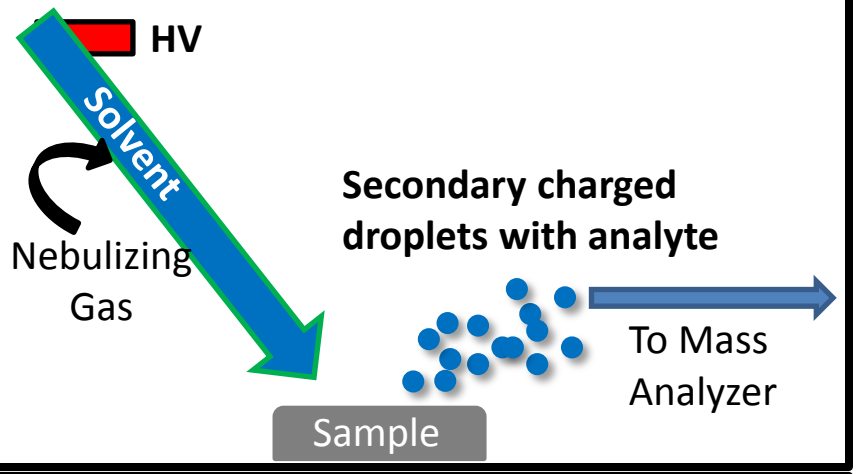
-65 W average; 144 W peak

-1.5 hrs on battery power

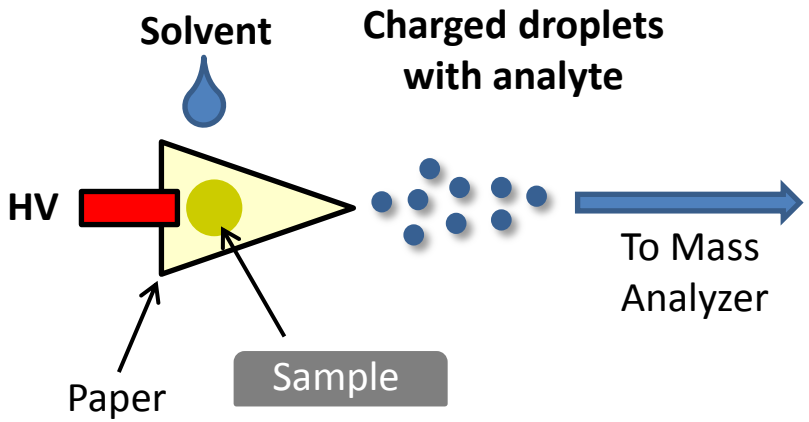
Four Ambient Ionization Methods

Ambient Ionization: Ionization of sample in its native state with transfer of ions not whole sample into MS

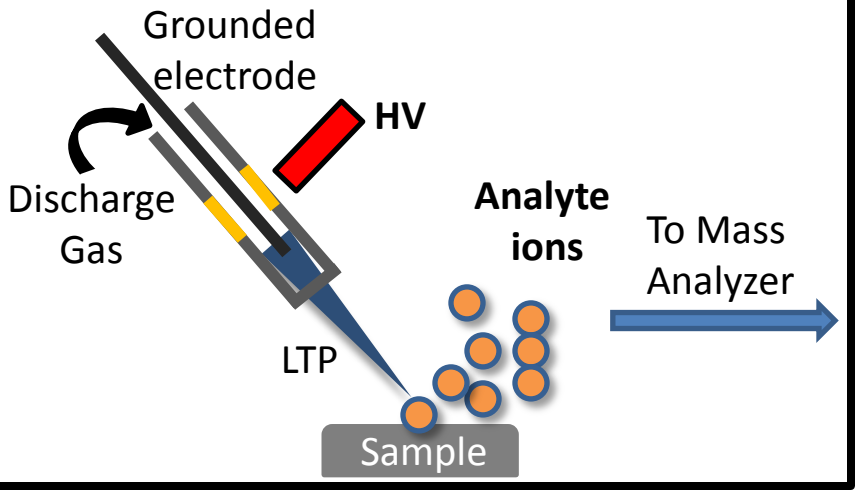
DESI [V, pneumatic, solvent]



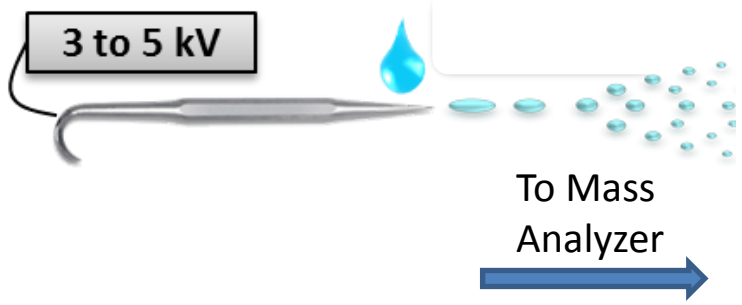
PAPER SPRAY [V, solvent]



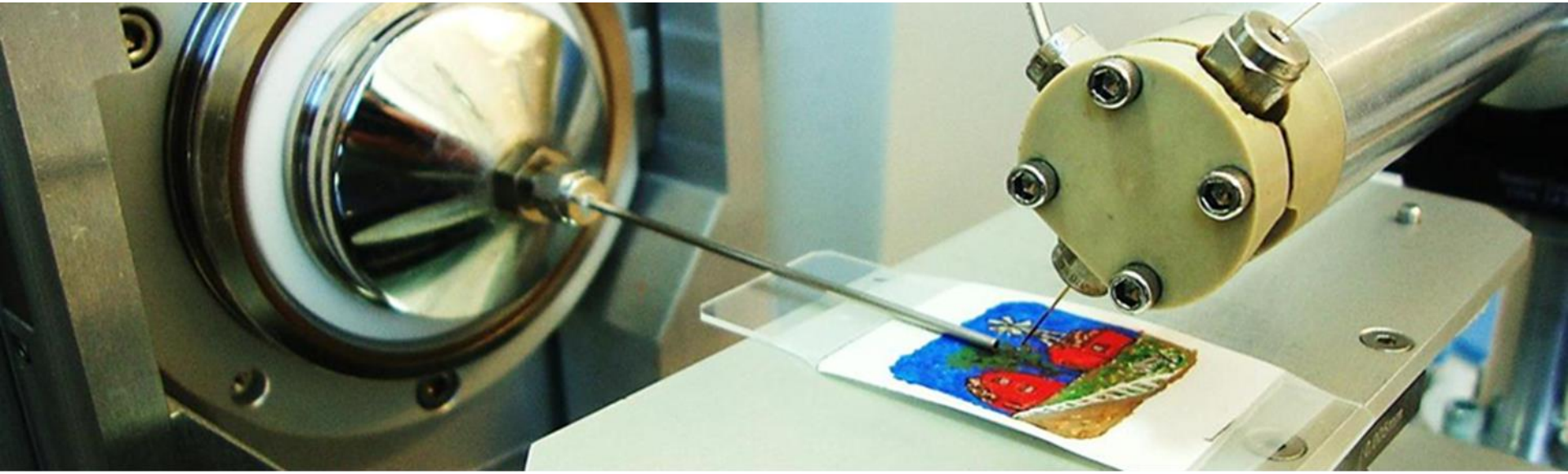
LTP [V, gas]

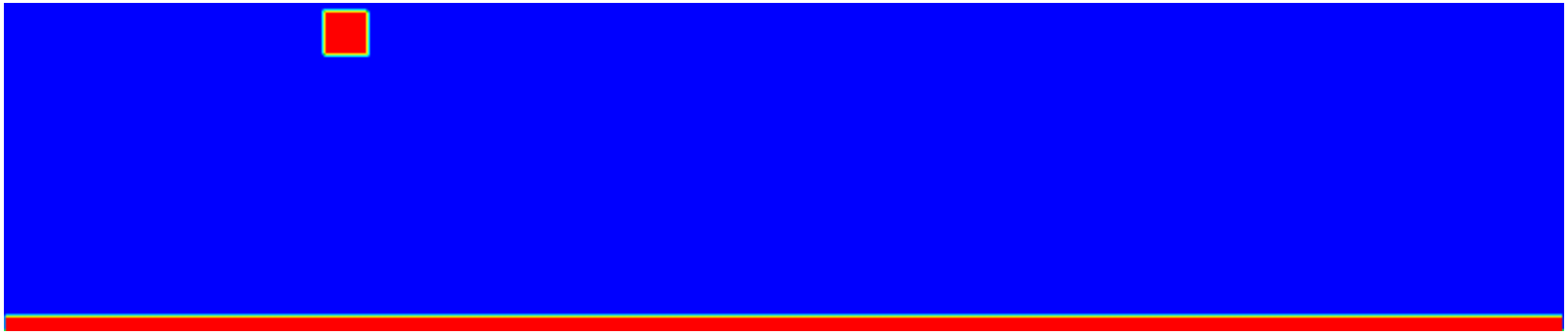


Touch SPRAY [V, solvent]



Desorption Electrospray Ionization





Fingerprint

DESI Imaging

Chemical Fingerprint

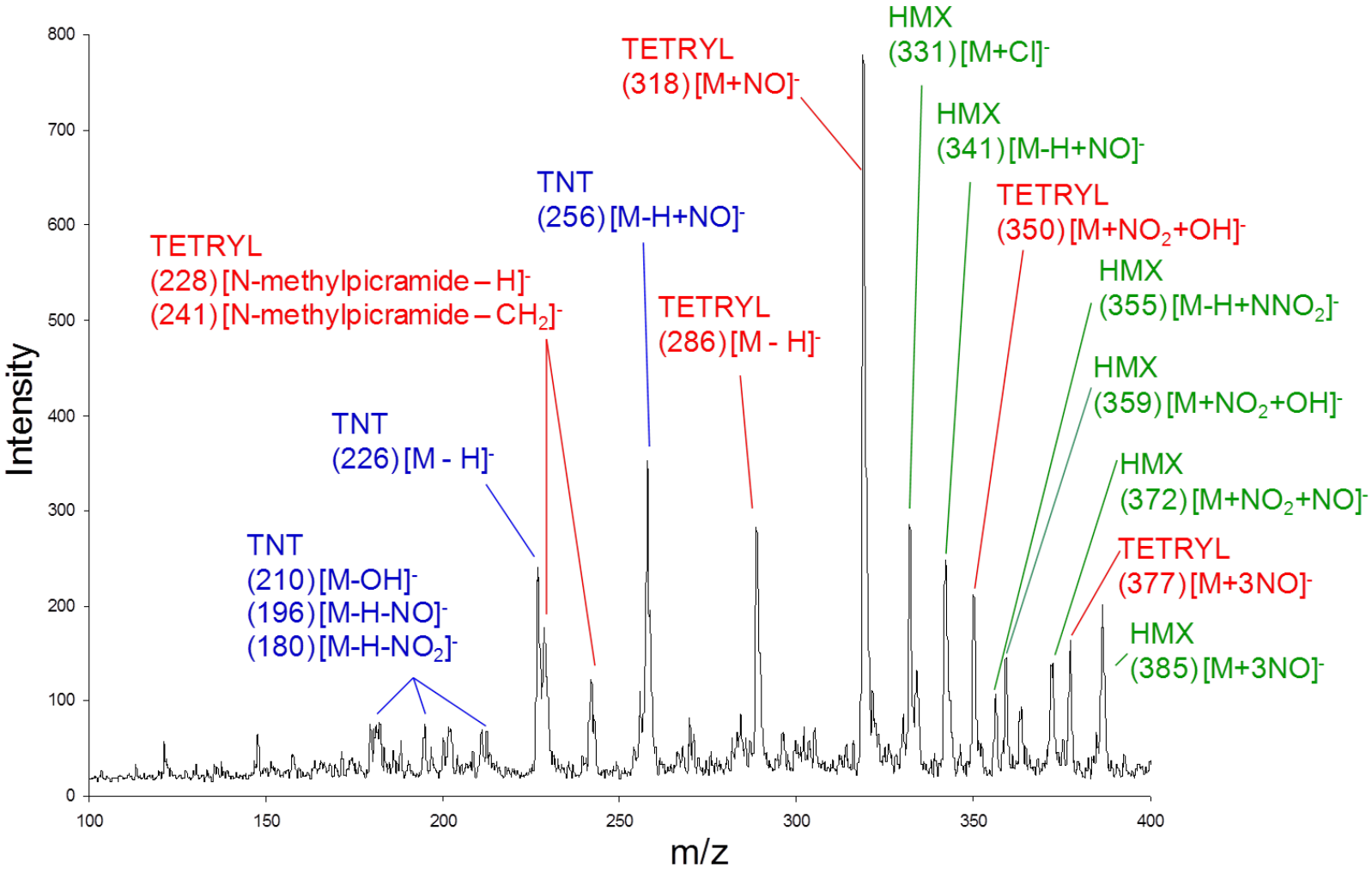
CSI:

CRIME SCENE INVESTIGATION

CRIME SCENE DO NOT CROSS CRIME SCENE DO NOT CROSS CRIME SCENE DO NOT CROSS

Ifa, DR et al, *Science*, 2008

Explosives mixture analysis: DESI

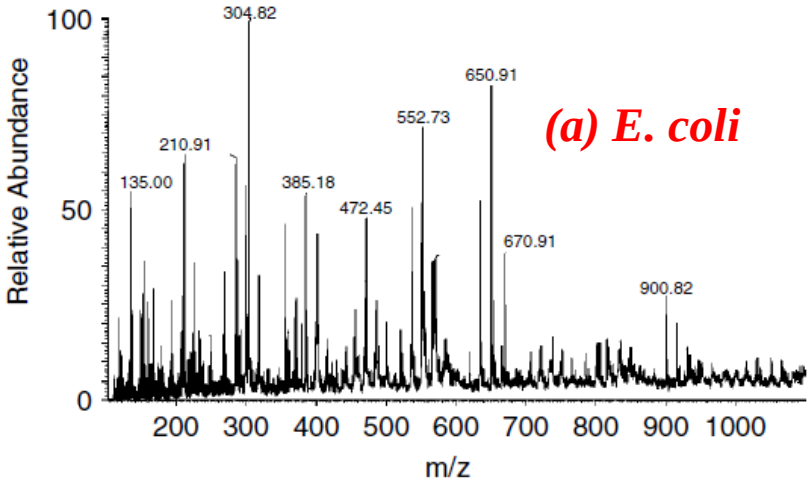


Mini 10 (10 scan average; 1 μg total amount, on 1cm^2 area)

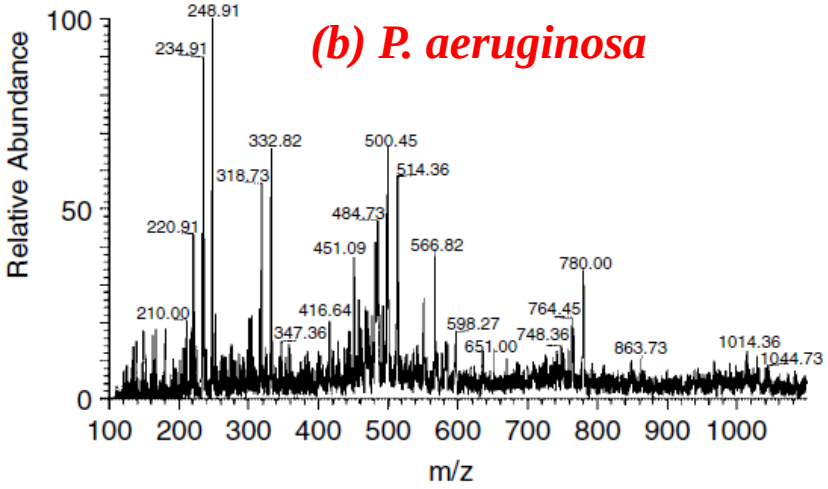
Nathan Sanders, Sameer Kothari, and Gary Salazar

Real-Time Microorganism Analysis by DESI

DESI-MS of freshly harvested cells dried on PTFE



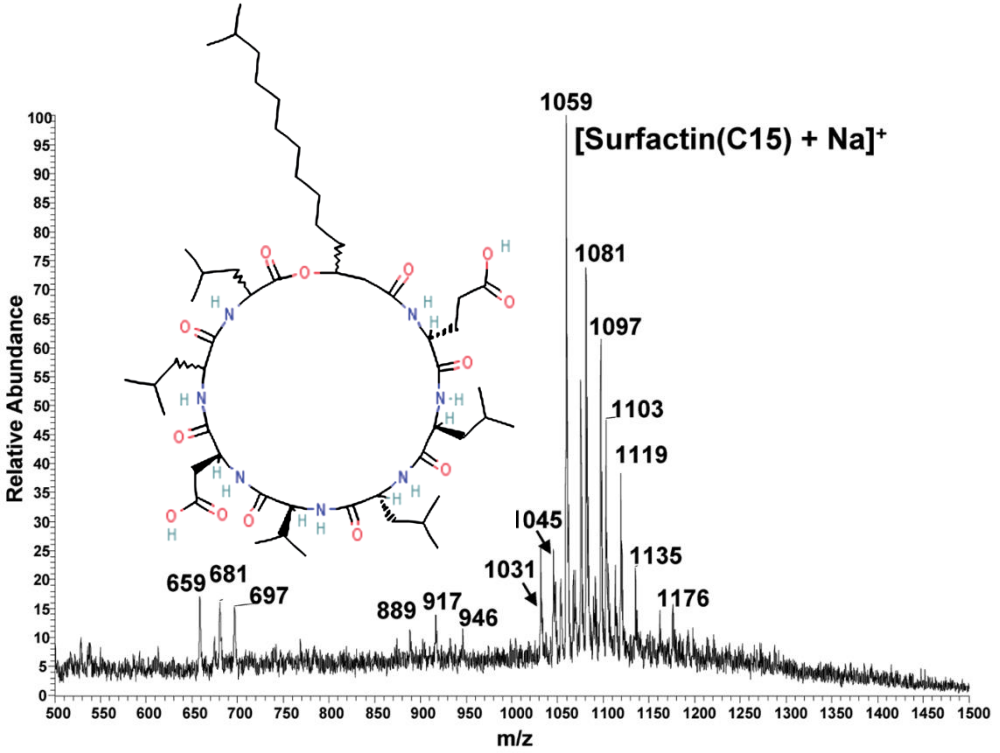
(a) E. coli



(b) P. aeruginosa

J. Mass Spectrom. 2005, 40, 1261-1275

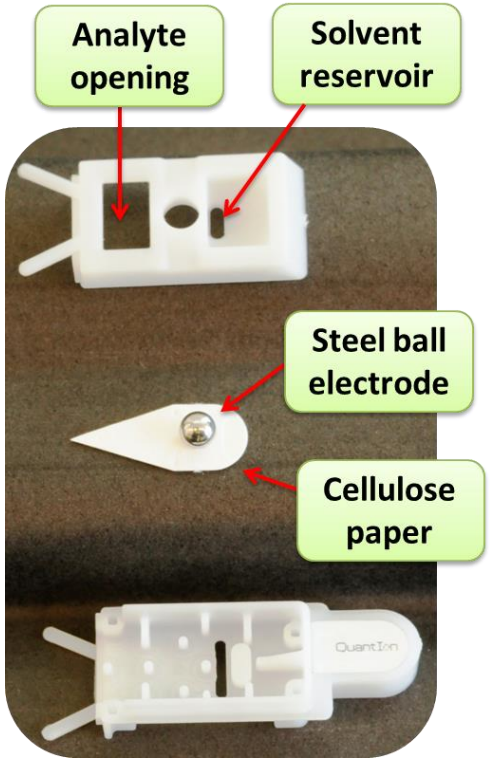
In vivo recognition of *Bacillus subtilis* by DESI-MS

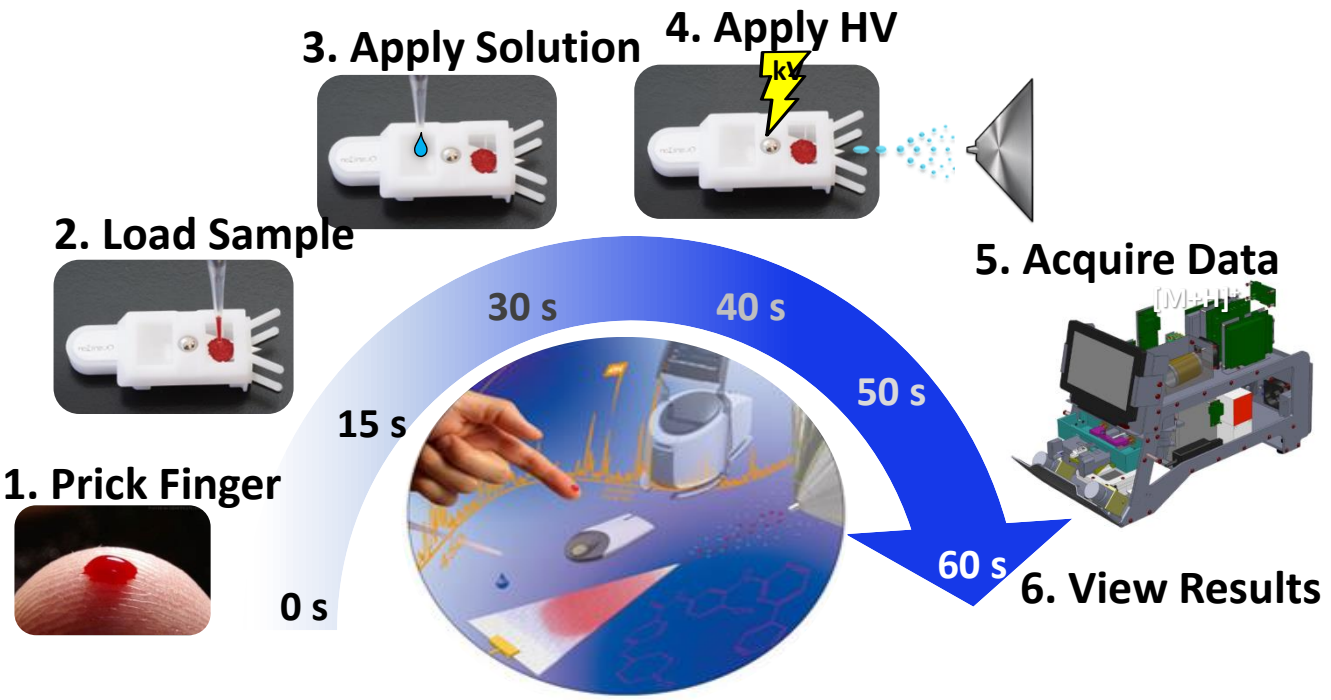


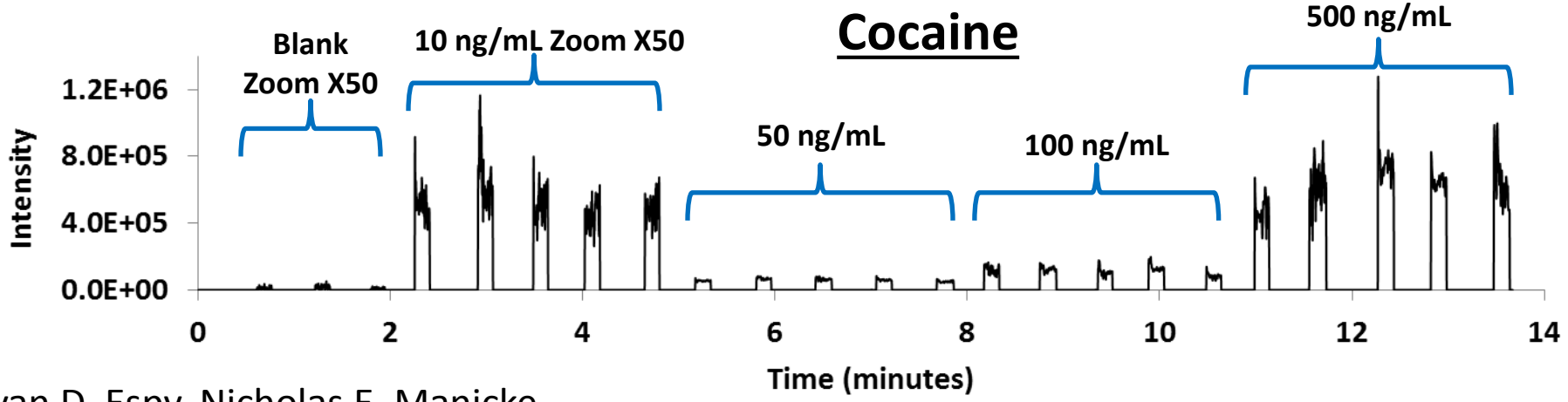
Bacillus subtilis as a biofilm growing on agar nutrient: simple, high quality mass spectra dominated in both the positive and negative ion modes by signals due to the cyclic lipopeptide, Surfactin.

Analyst. 2009, 134, 838-841

Paper Spray: Immediate Point-of-Care Analysis



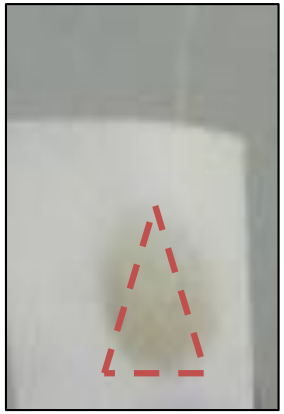




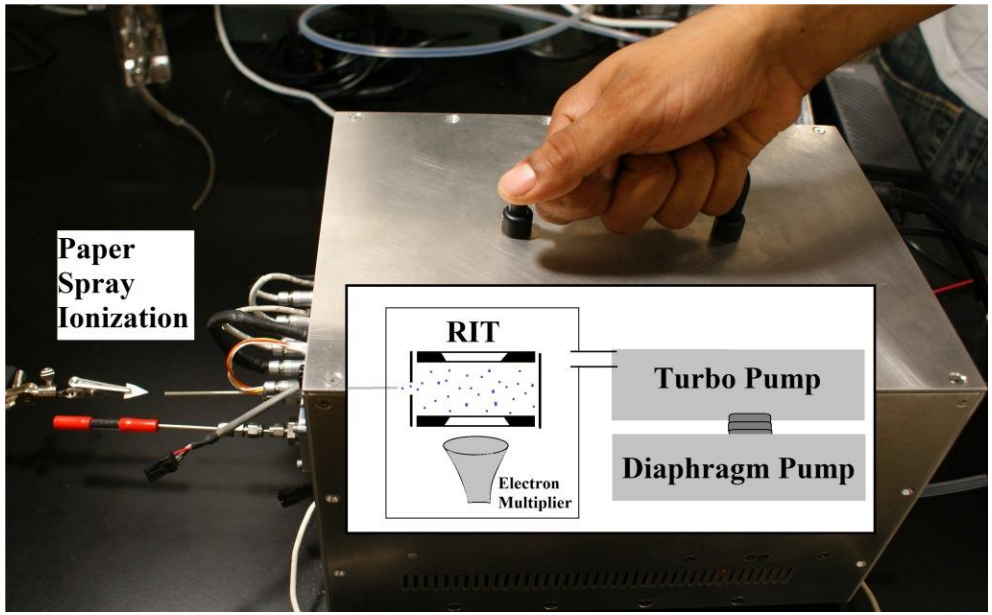
Ryan D. Espy, Nicholas E. Manicke

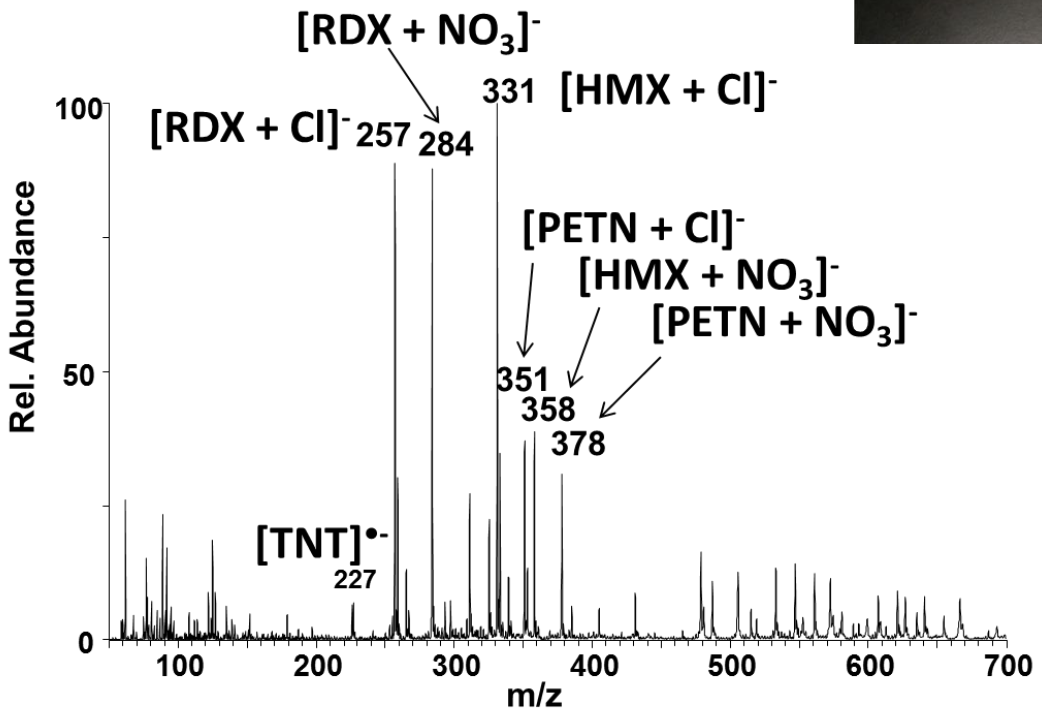
Paper Spray Surface Wiping

Wipe surface using paper



Cut paper into triangle

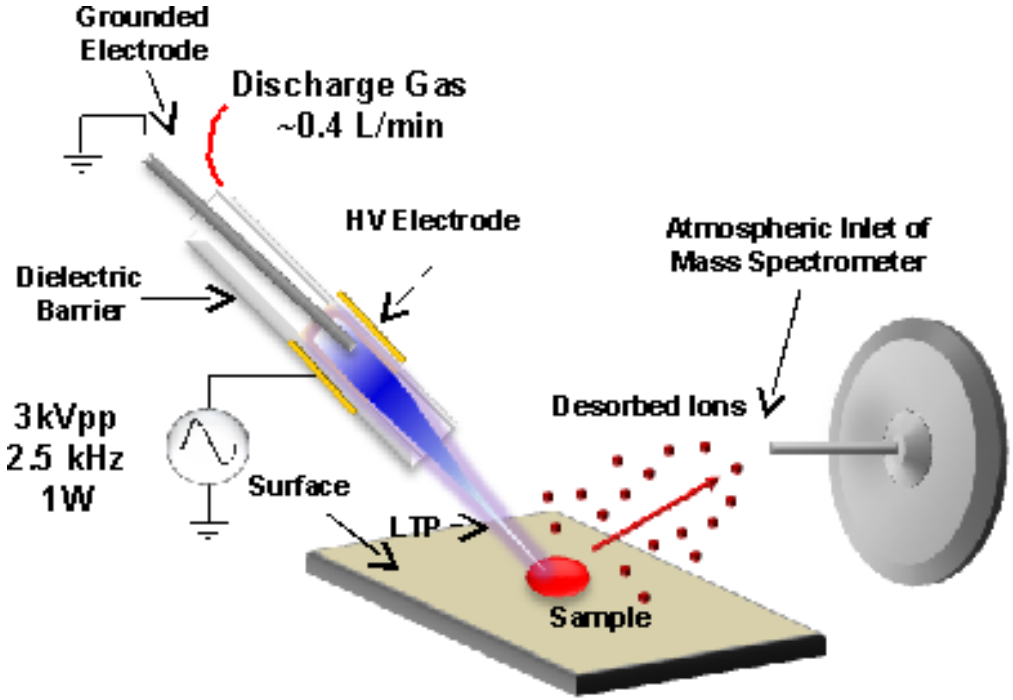




Paper Spray Mass Spectrometry of 50 ng each RDX, TNT, HMX, and PETN on Whatman filter paper with MeOH as a spray solvent at -5.0 kV.

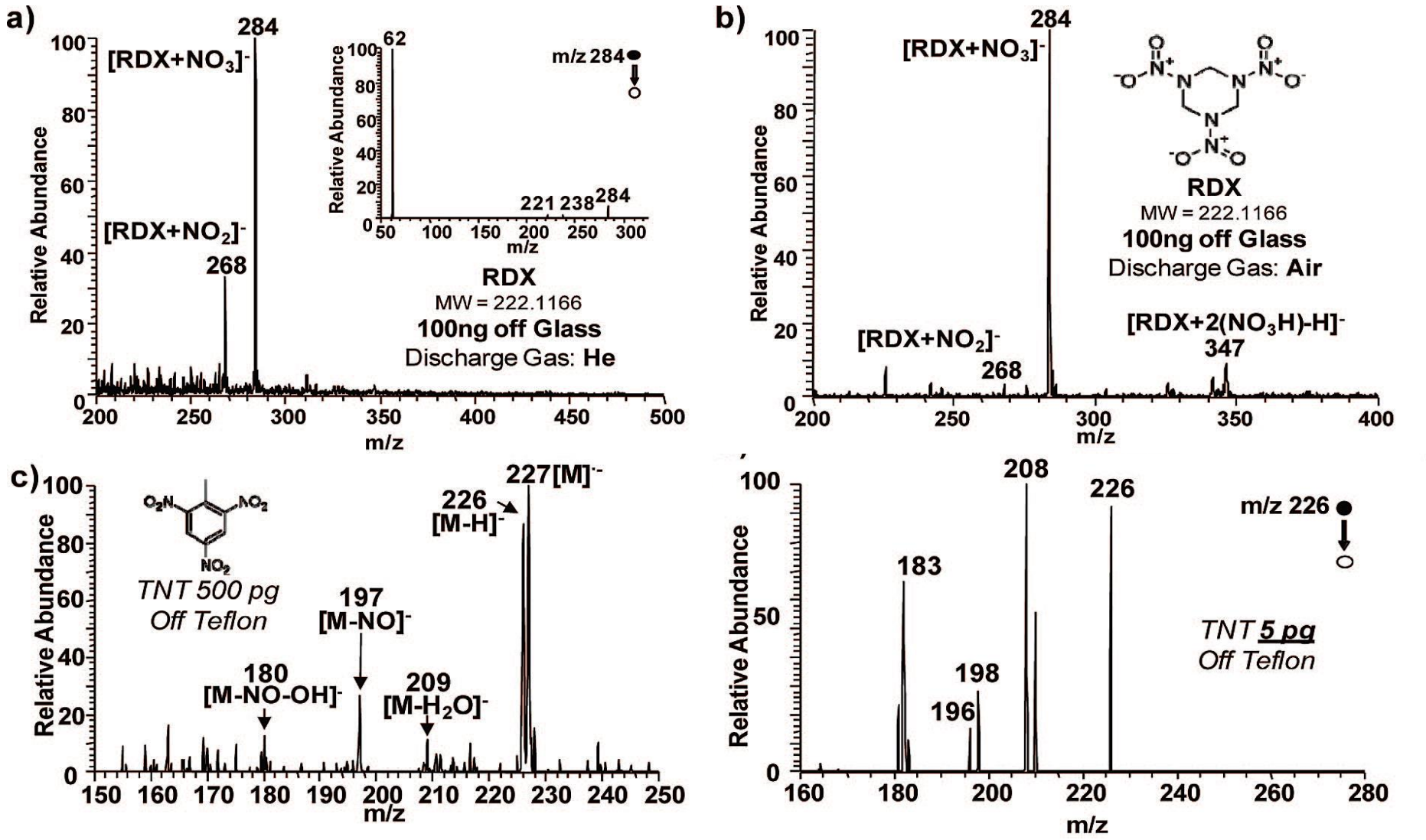
Ryan D. Espy

LTP Handheld Unit



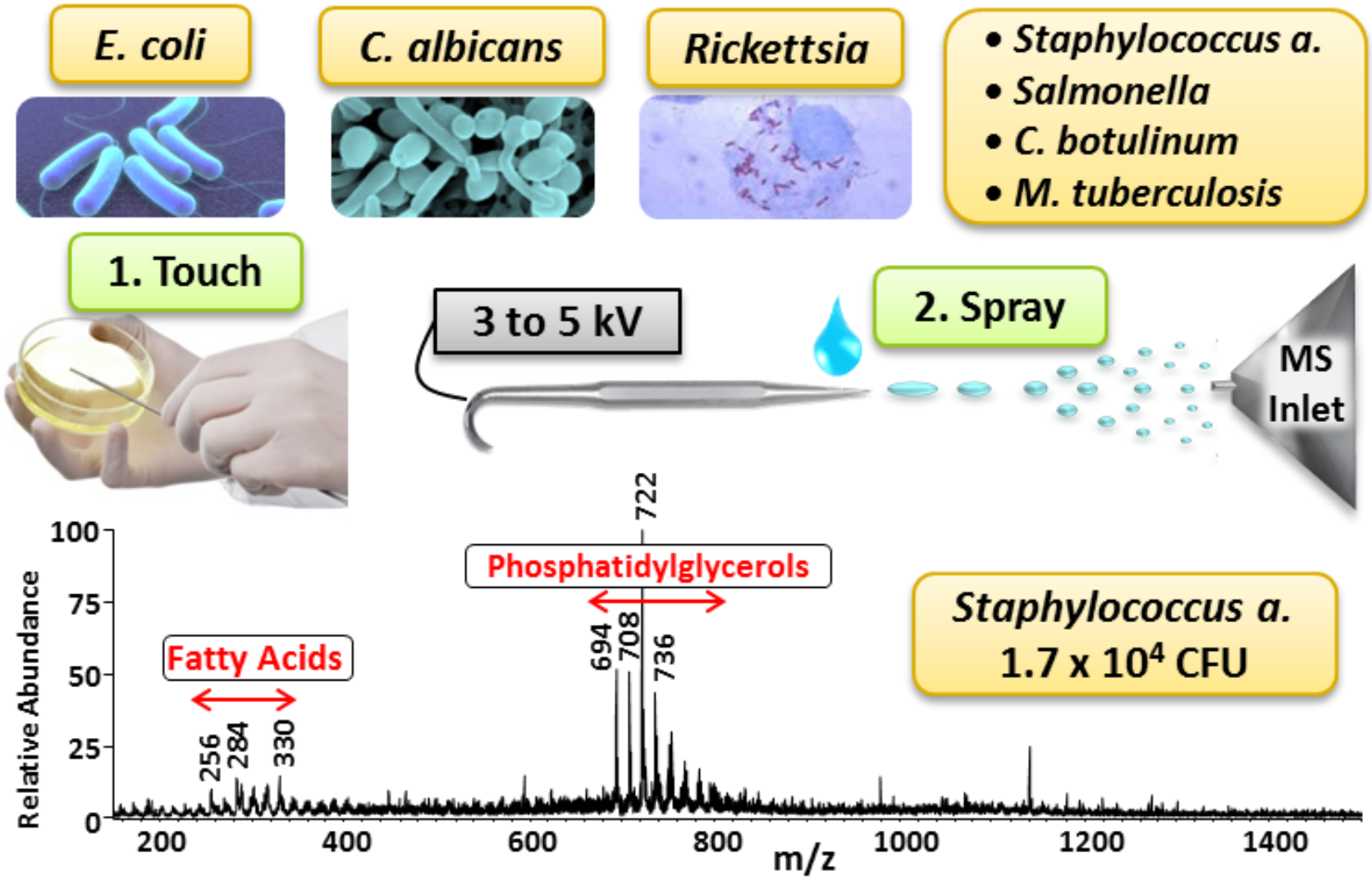
JS Wiley, JT Shelley, RG Cooks, *Anal. Chem.* **2013**, 85, 6545−6552

LTP Analysis of Explosives



JD Harper et al., *Anal. Chem.* **2008**, 80, 9097–9104

Touch Spray of Biologicals



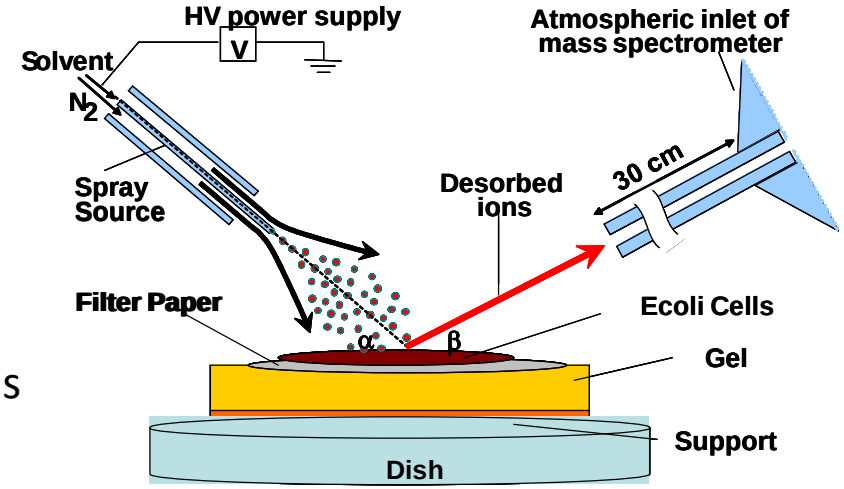
Ahmed Hamid, Alan K. Jarmusch, Kevin Kerian

Summary

Instrumentation

- Miniature/portable mass spectrometers
  - Backpack MS
  - Portable benchtop MS
- Ambient Ionization
  - Desorption Electrospray Ionization (DESI)
  - Low Temperature Plasma (LTP)
  - Paper Spray (PS)
  - Touch Spray (TS)

- ✓ No sample preparation
- ✓ Ionization in open air
- ✓ Rapid in-situ analysis



Applications

- In-situ, on-site analysis
  - Explosives
  - Microorganisms
  - Drugs in blood, urine, & other biofluids
  - Fingerprints
  - Cloth, skin, tissue, all surfaces!
- All varieties of molecules (small vs. large, polar vs. nonpolar)
- **Mini's not commercially available, but 20 are out for testing**