

# Actionable GC/MS analysis in the field, NOW!



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## Breakthroughs Happen

# Gas Chromatography / Mass Spectrometry

GC/MS is the  
'gold standard' of  
chemical  
identification and  
quantitation

- High sensitivity (addresses false negatives)
- High selectivity (addresses false positives)
- Identification of unknowns
- Orthogonal techniques
- Broad range of chemical species and matrices
  - Volatiles
  - Semivolatiles
  - Gas/liquid/solid samples
- But.. GC/MS instruments are typically tethered to the laboratory; requires "taking samples to the analysis"
  - Power
  - Support utilities
  - Sample preparation

# Rationale for taking the analysis to the sample

Faster is  
better  
when it  
comes to  
sample  
analysis

- TIME CRITICAL, ACTIONABLE DATA
  - Rapid identification in support of public health or safety
    - Risk assessment for emergency responders
    - Utility protection (e.g. water supplies)
  - Real-time decisions
    - Airport screening
    - Guide further sampling activities in contamination site extent and remediation.
- SAMPLE INTEGRITY
  - Intermittent or variable sample concentrations
  - Unstable or degradable samples
  - Quantitative analysis degradation due to volatile sample loss
  - Chain of custody
- COST
- And sometimes you just can't bring back a sample...

# Historical Drivers for Field Portable MS

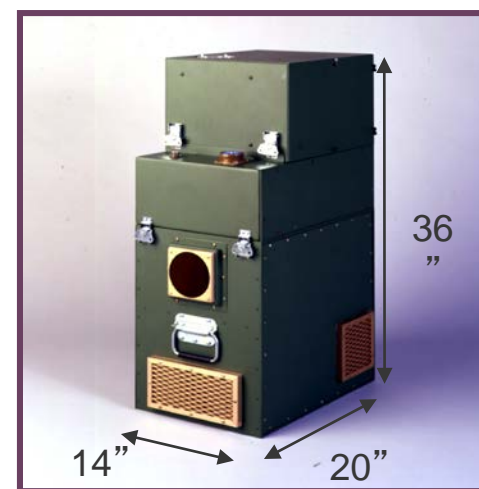
1970's

- NASA: Viking Mars Lander



1980's

- US Dept of Defense: Chem/Bio MS Systems



# The US Military's Next Fieldable Chem-Bio Detection “Vehicle”





# Application Drivers – Security/First Responders/Safety

- Military
- Emergency response
- Process monitoring & control
- Law enforcement/Forensics
- National security
- Ports, Airports, Buildings, Mail, Major Events
- Drug Interdiction/monitoring
- Hazardous site cleanup
- Agriculture
- Food safety
- Medicine
- Fugitive emissions



# Application Drivers – Science and Exploration

- Planetary science
- Astrobiology
- Geology
- Vulcanology
- Oceanography
- Field biology
- Archeology
- Arctic Sciences
- Atmospheric studies



“I have met the enemy..... and he is us”





# Field Portability Challenges

Developing a miniature GC/MS is more than simply miniaturizing the analyzer.

- Very small MS analyzers have very limited performance as many desirable features/capabilities of GC/MS are lost during miniaturization. Analytical performance must be maintained.
- Small, field-portable systems need to be ruggedized and hardened to physical shock and variable environmental conditions.
- Power and heat management becomes crucial.
- Often, sample handling and preparation are the limiting factors – especially in complex environments/applications.
  - Simple sample prep capability required
- A new generation of non-GC/MS expert operators needs to be supported with simple operation and data analysis

**OUR GOAL => to develop a fieldable, portable mass spectrometry system..... with laboratory-class capabilities**

# TRIDION™-9 Field Portable GC/MS System

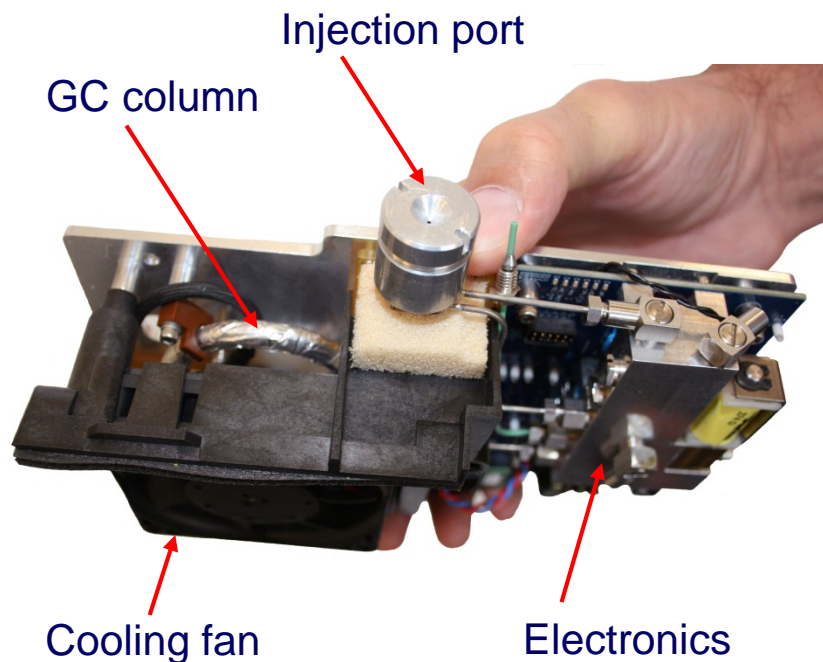


- **Dimensions:** 38 cm x 39 cm x 23 cm
- **Weight:** <14.5 kg or 32 lbs (including battery)
- **Power:** Peak ~120 W; Average ~ 60 W
- **Sample Introduction:** SPME or Direct Liquid
- **GC:** MXT-5, 5 m x 0.1 mm x 0.4  $\mu$ m
- **Temperature Programmable GC**
- **Electronic Pressure Control**
- **Ion Trap:** Toroidal Ion Trap MS
- **Electron Ionization:** Internal~70eV
- **Vacuum:** turbo molecular/diaphragm pump
- **Ion Trap Heater:** 150°C– 180°C
- **Mass Range:** 45 to 500 Daltons
- **Resolution:** Amplitude Scanning
  - 0.43 at m/z 134 (n-butylbenzene)
  - 0.53 at m/z 284/286 (hexachlorobenzene)

# Miniaturizing the GC



Conventional Laboratory GC

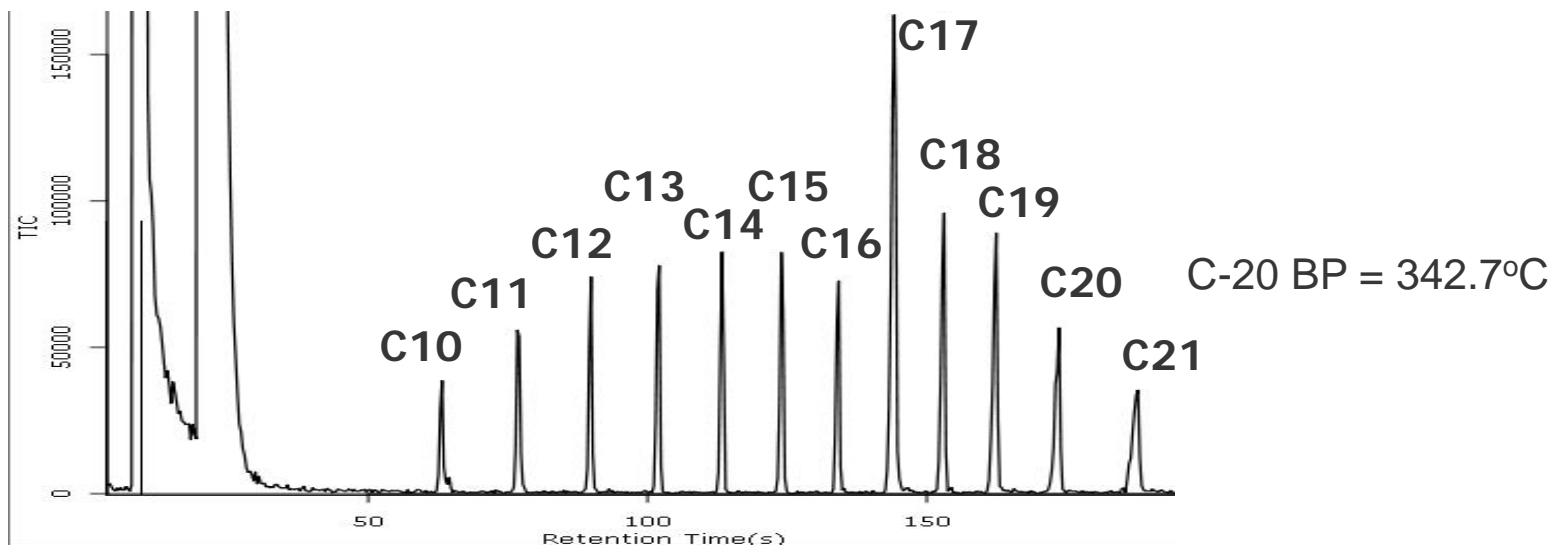
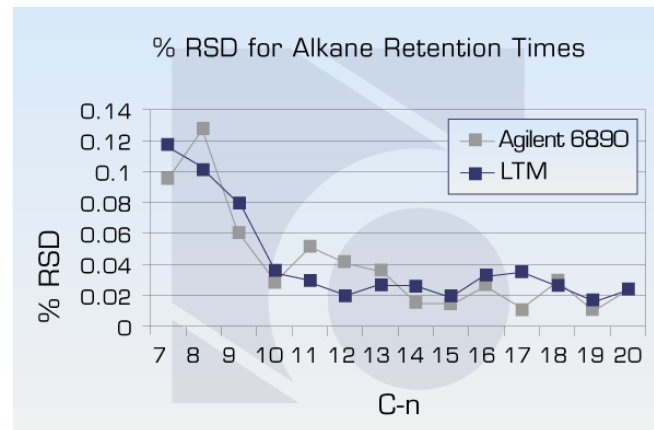
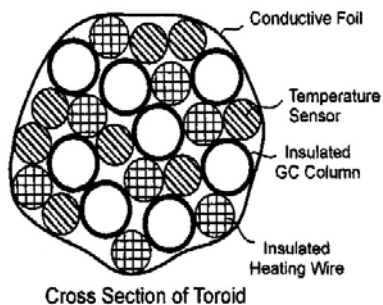
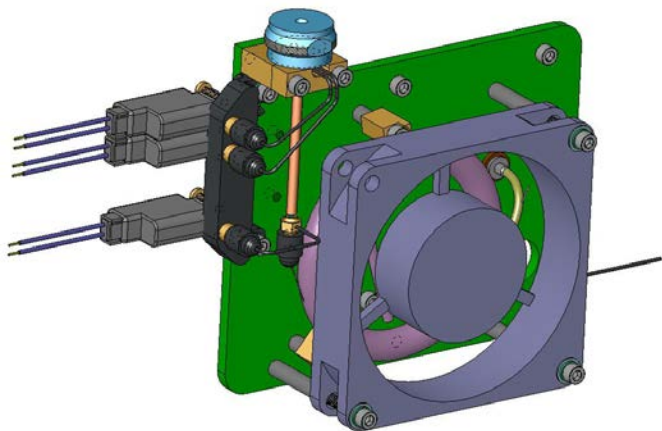


TRIDION™-9 GC

“Lab data is not as good as you think and field data is better than you think.”

*John Fitzgerald, Massachusetts DEP*

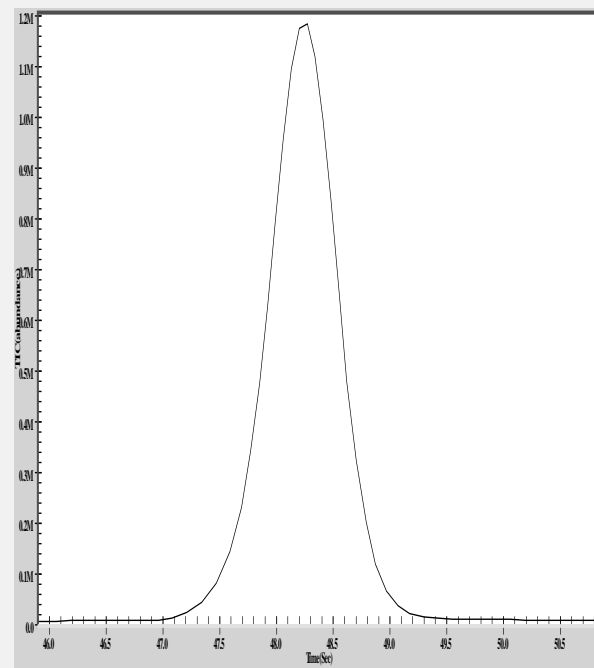
# Low Thermal Mass Gas Chromatograph





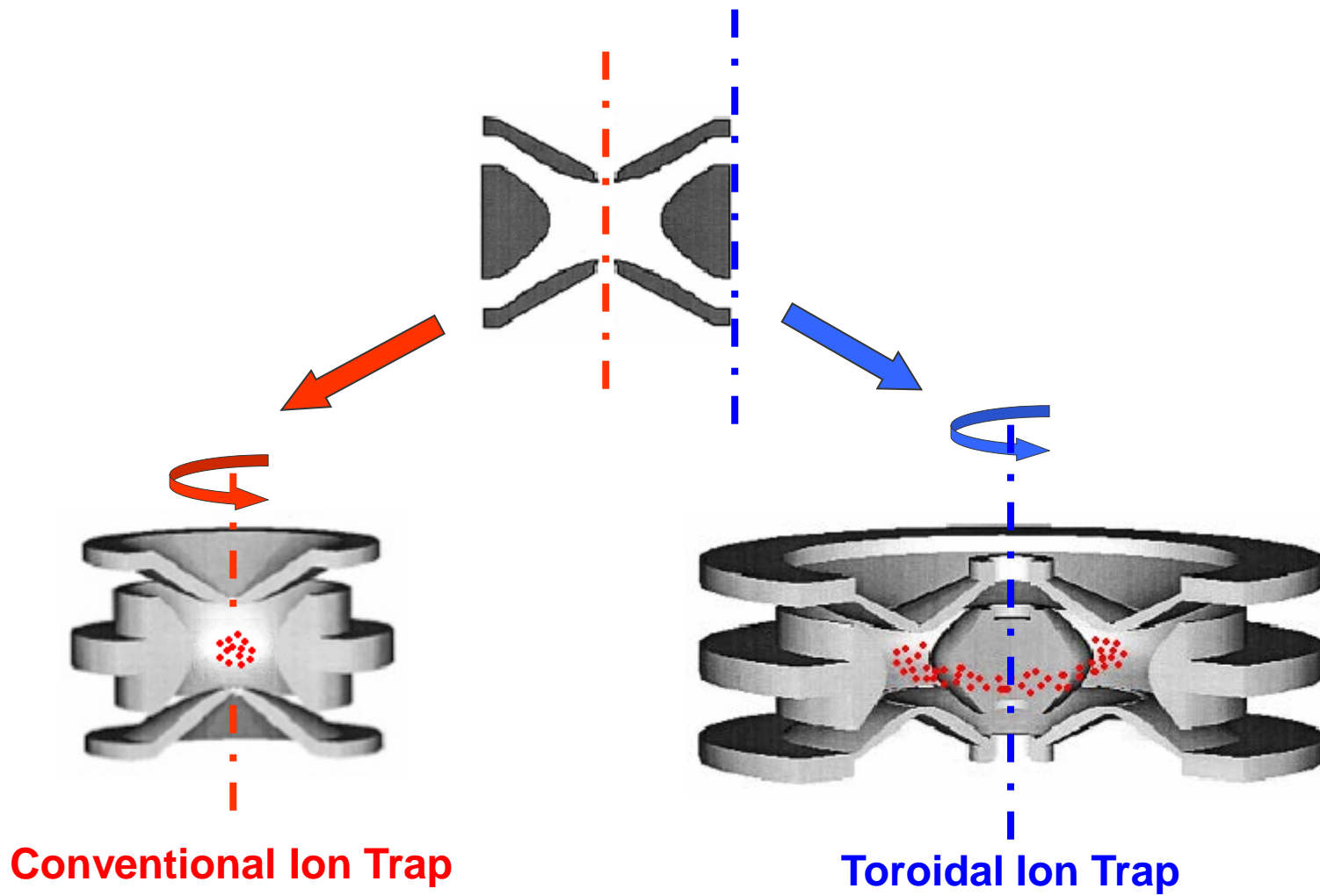
# GUARDION High-speed, High-resolution GC

- Metal Capillary GC Column
  - Type: MXT<sup>®</sup>-5 (DB-5)
  - Dimensions: 5 m x 0.1mm x 0.4 $\mu$ m d<sub>f</sub>
- Helium Carrier Gas
  - ~ 0.3 mL column flow
  - Provides better separation than N<sub>2</sub>
  - Electronic Pressure Control
    - Improves RT reproducibility
- Temperature Programming
  - Column temperature range 50 - 300°C
  - Up to 2.5°C/sec ramp rate
  - Cool-down in approx. 2 minutes at 22°C ambient temperature
- Fast Analysis
  - 2-3 minute analysis



# Miniaturizing the Mass Analyzer

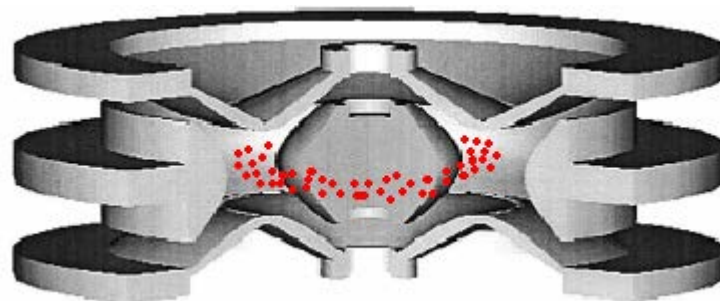
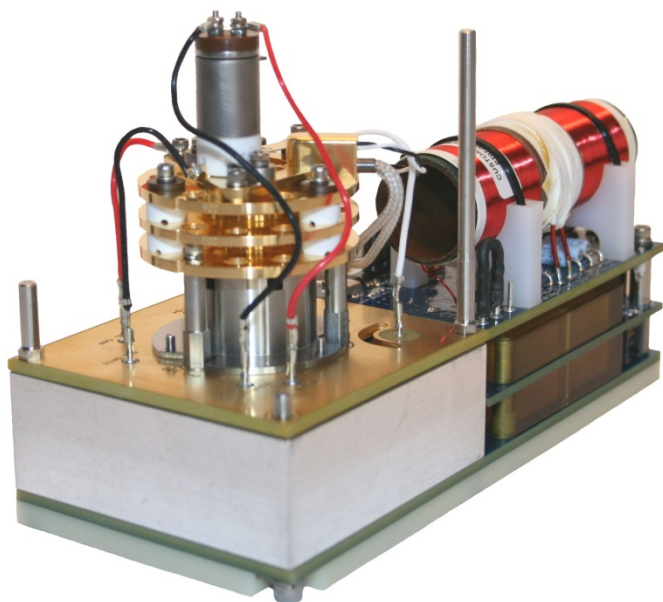
## Ion Traps - Traditional 3D/Cylindrical vs Toroidal



## Advantages of Toroidal RF Ion Trap Mass Analyzer

- Single mass analysis volume (compared to arrayed miniature cylindrical ion traps)
  - All ions experience the same trapping/mass analysis field
  - Easier coupling to ionization and detection optics
- Compact geometry (compared to linear ion traps of similar storage capacity)
  - Easier to eject ions from a circle than a line into the electron multiplier
- Homogenous field (compared to linear ion traps)
  - No end effects. All spatial positions within mass analyzer are equivalent

## Miniaturizing the Mass Analyzer (cont'd)



Miniature toroidal ion  
trap

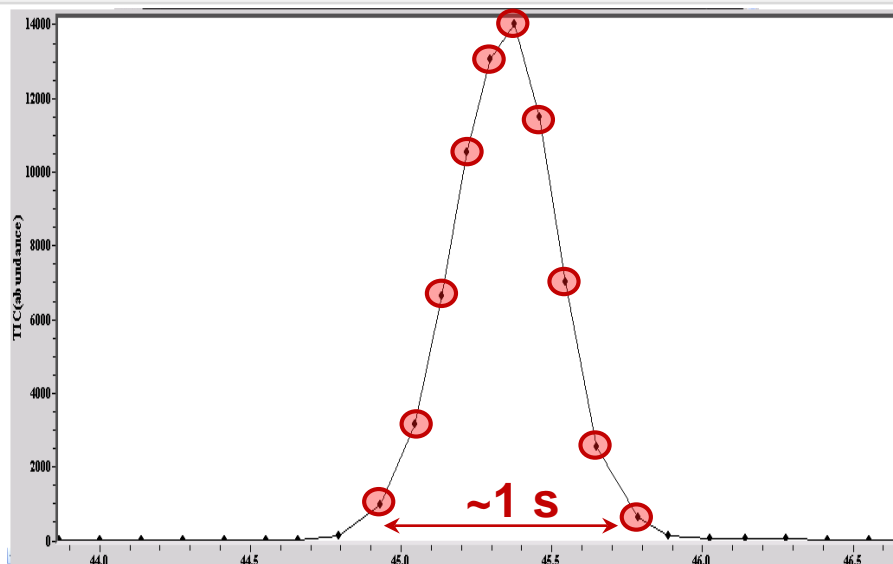
$$r_o = 2 \text{ mm}$$

$$\text{Trapping } V_{\text{max}} = \sim 2 \text{ kV}_{\text{p-p}}$$

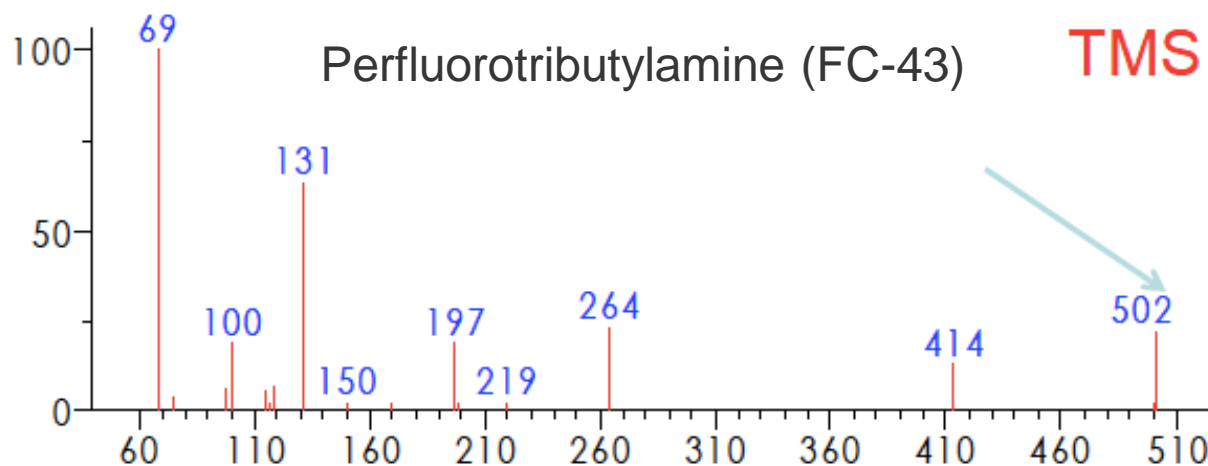


# MS Performance: Figures-of-Merit

- Scan speed:  
~10 scans/s

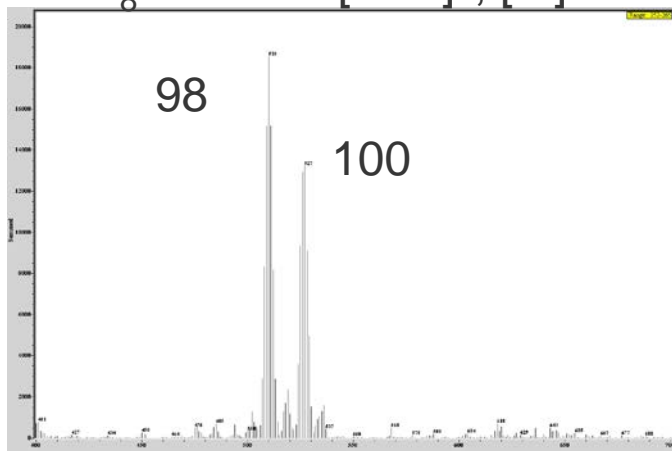


- Mass Range:  
43 - > 500 da.

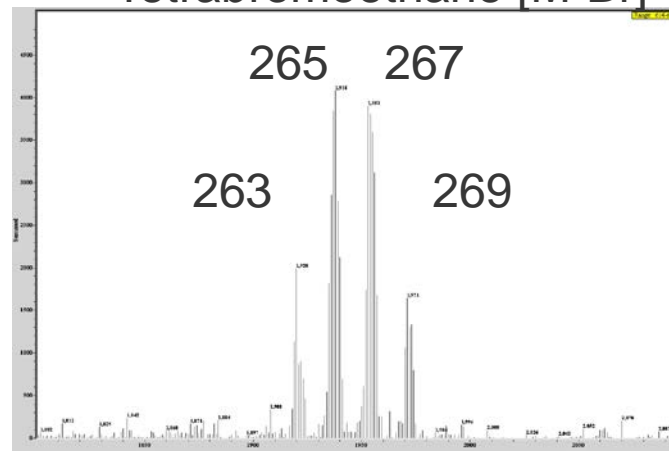


# Mass Resolution Performance

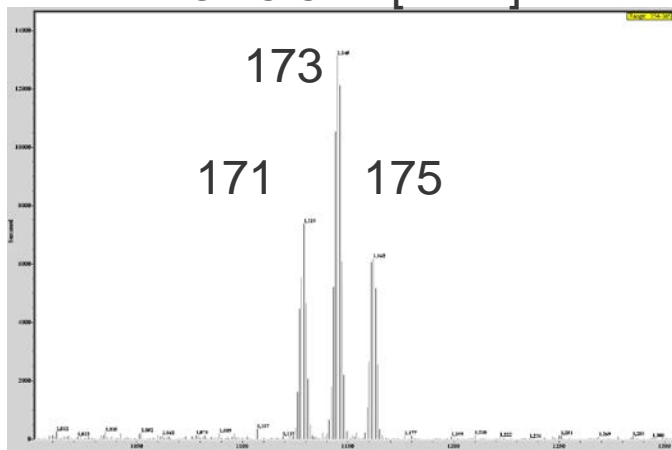
$d_8$ -toluene  $[M-H]^+$ ,  $[M]^+$



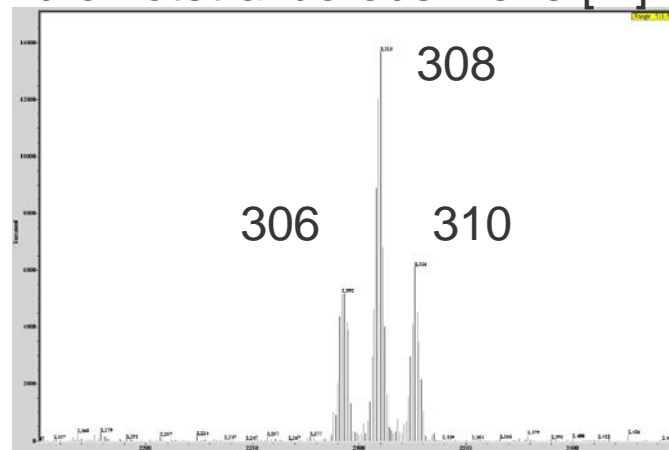
Tetrabromoethane  $[M-Br]^+$



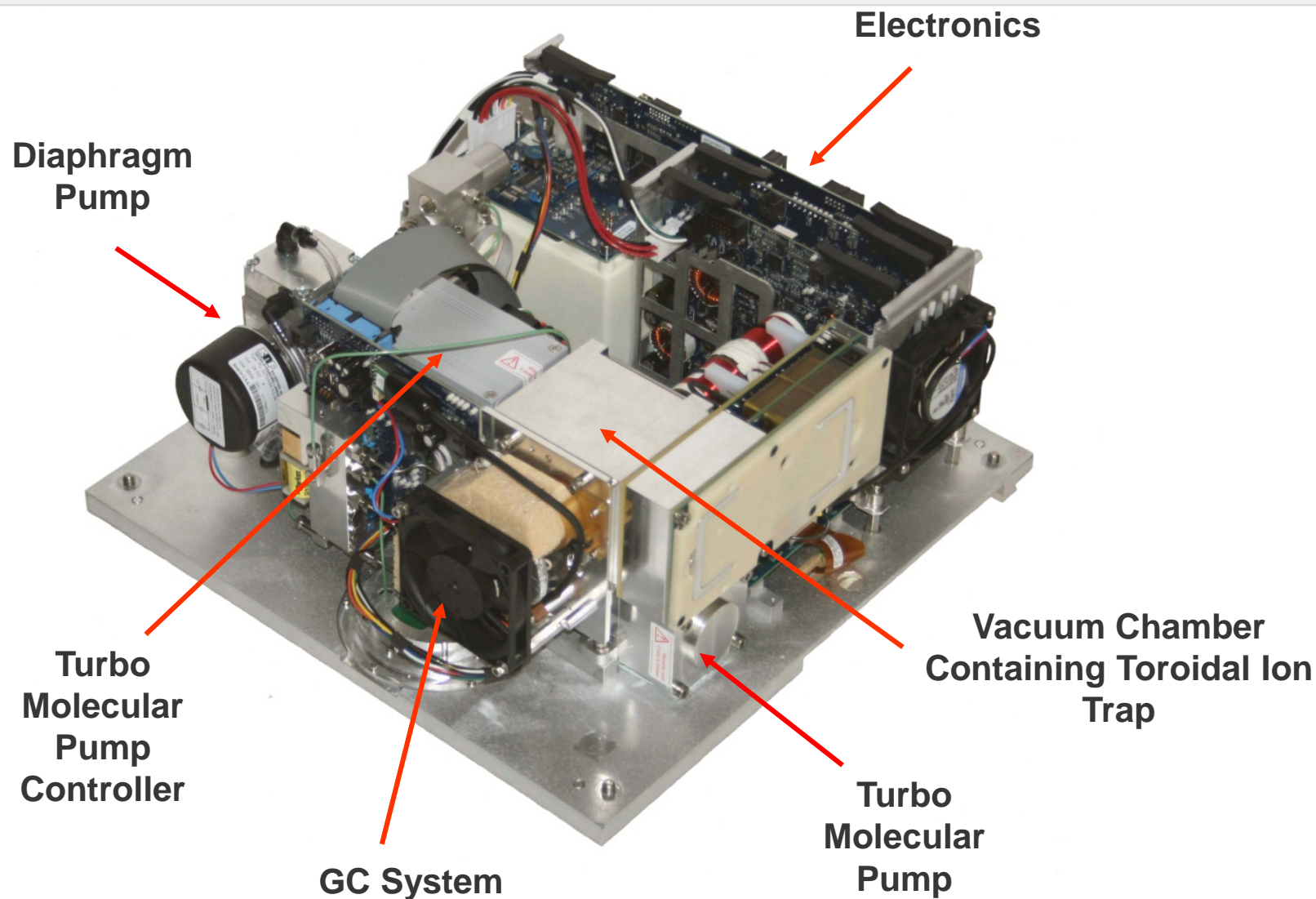
Bromoform  $[M-Br]^+$



Dibromotetrafluorobenzene  $[M]^+$



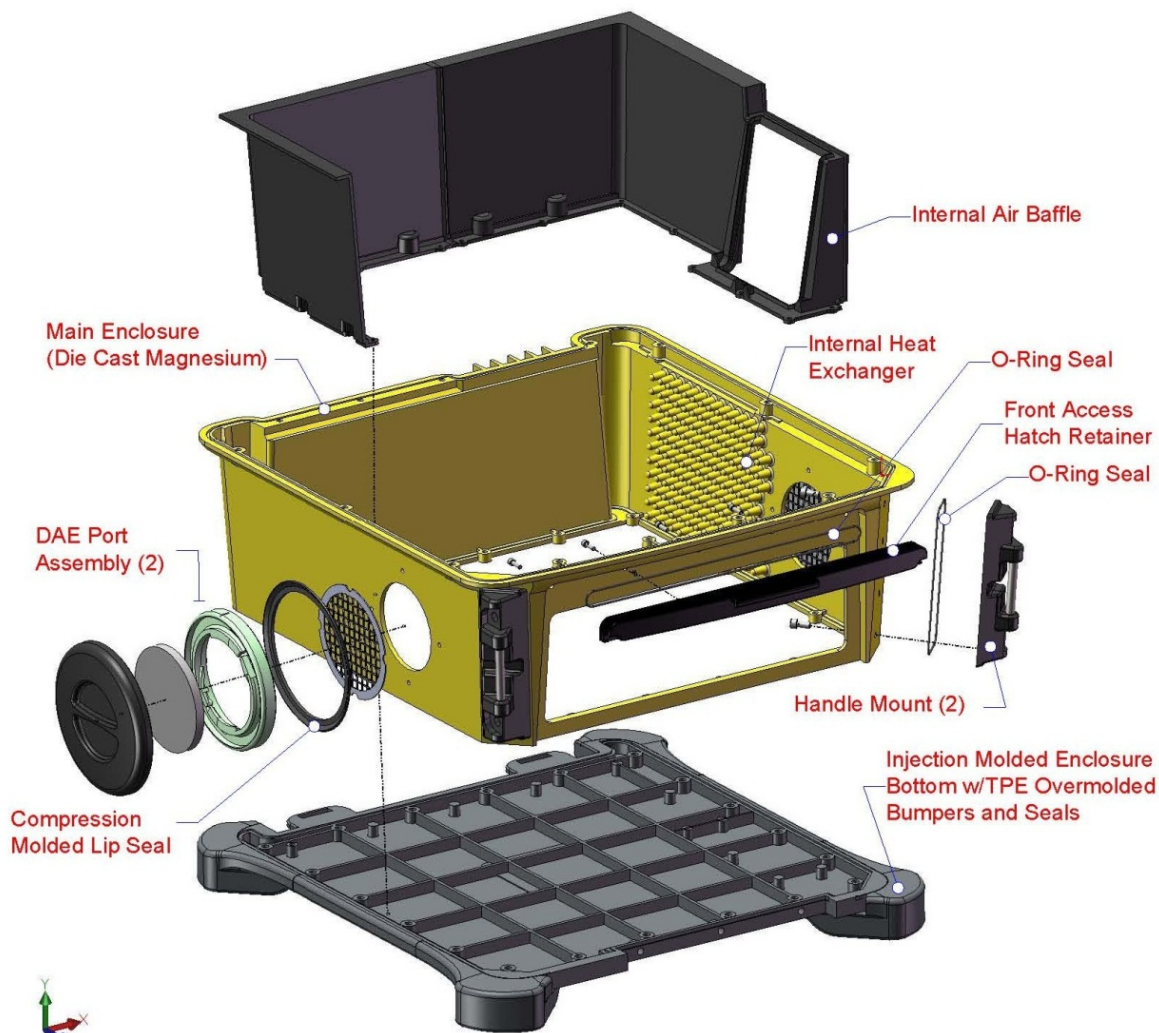
## “Under the Hood”



# Chassis Design

- Enclosure

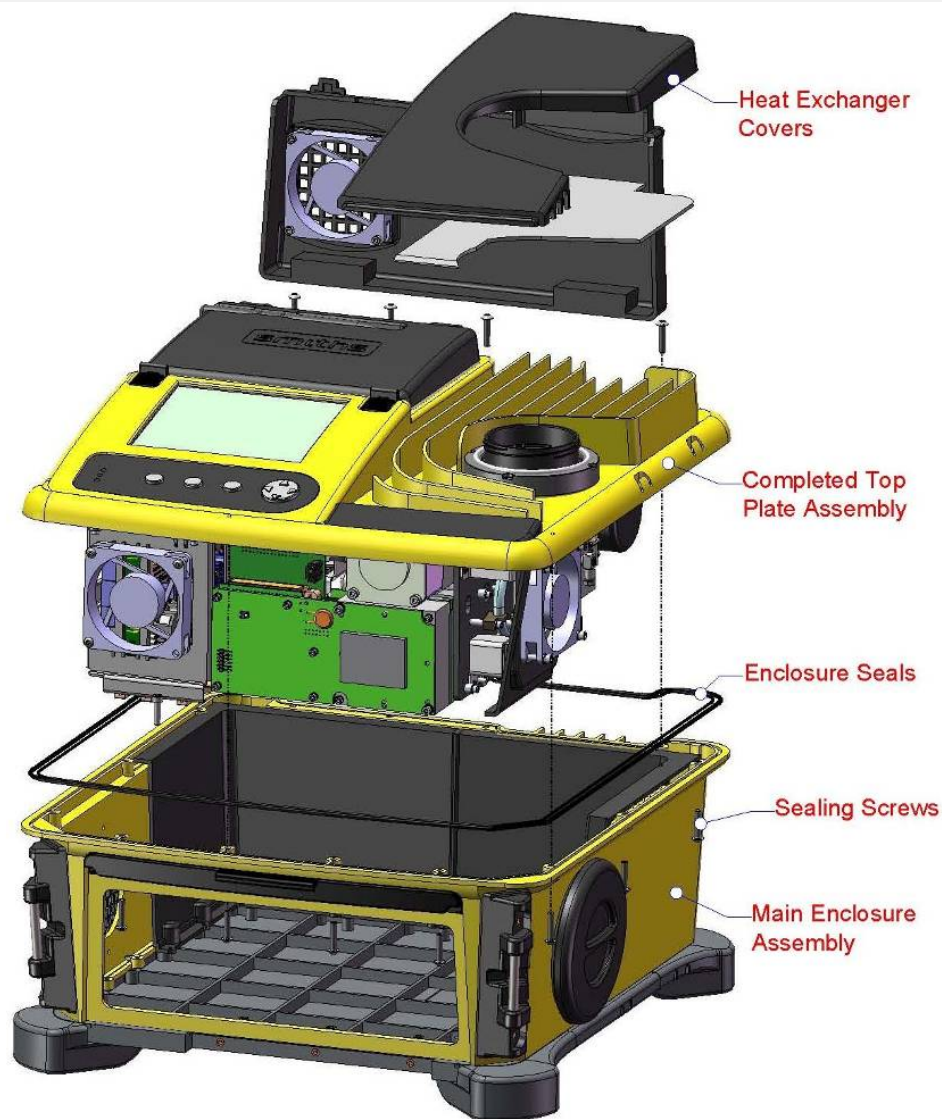
- Die cast magnesium to reduce weight
- Integrally cast internal heat exchanger improves heat transfer
- Internal air baffle interfaces with column fan shroud to control column cooling air source
- EMI coating on inner surface of enclosure bottom





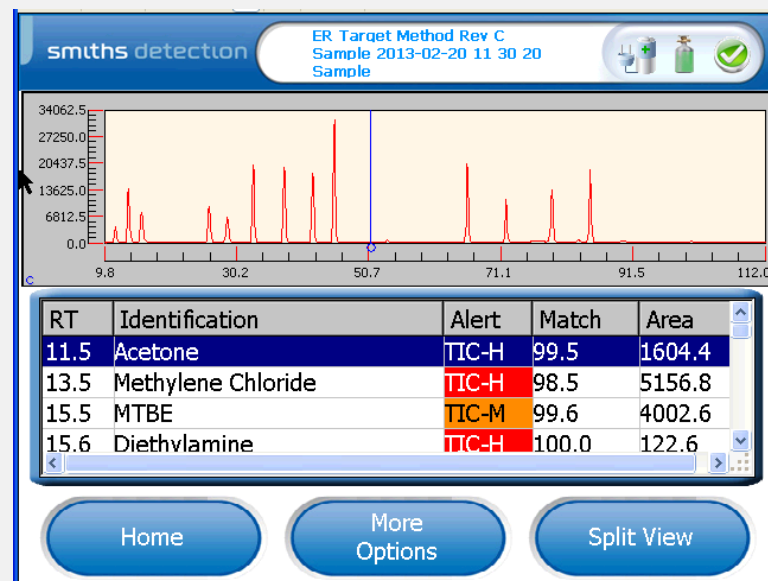
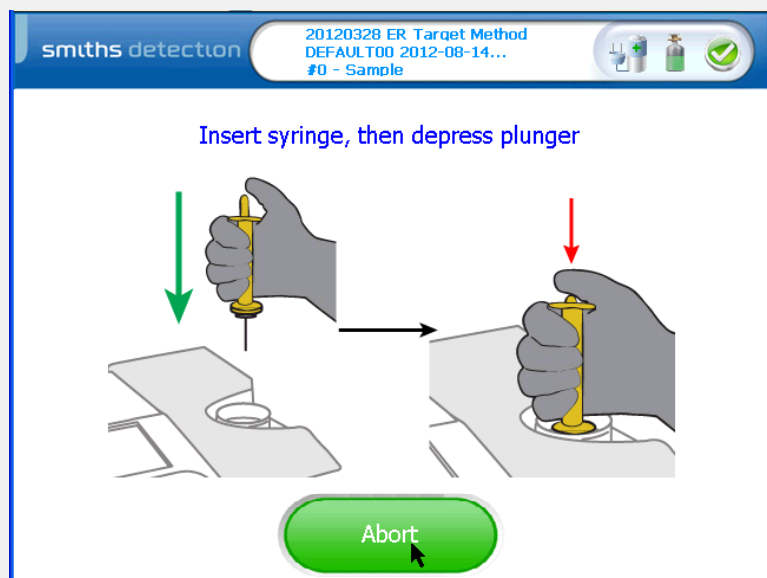
# Environmental/Ruggedness

- Sealed Enclosure
  - DECON capable
  - Dust, Sand
- Shock tested
  - Bumpers, chassis
  - Drop tested at 1.5' (all sides)
- Shake/Vibration Tests
  - 10.5, 60, and 152.5 Hz
  - 30 min (all sides)
- Efficient heat transfer
  - Stand alone operation at 38°C ambient conditions
  - Operation at 45°C ambient conditions with the use of cold pack
  - GC column be cooled to ~ 50°C;  $T_{\text{turbo}}$  must be < 60°C

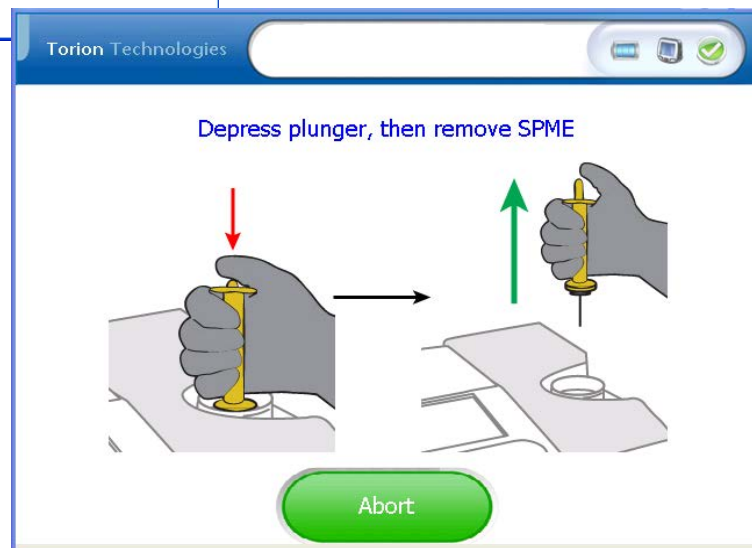


# Software Designed for Ease of Use

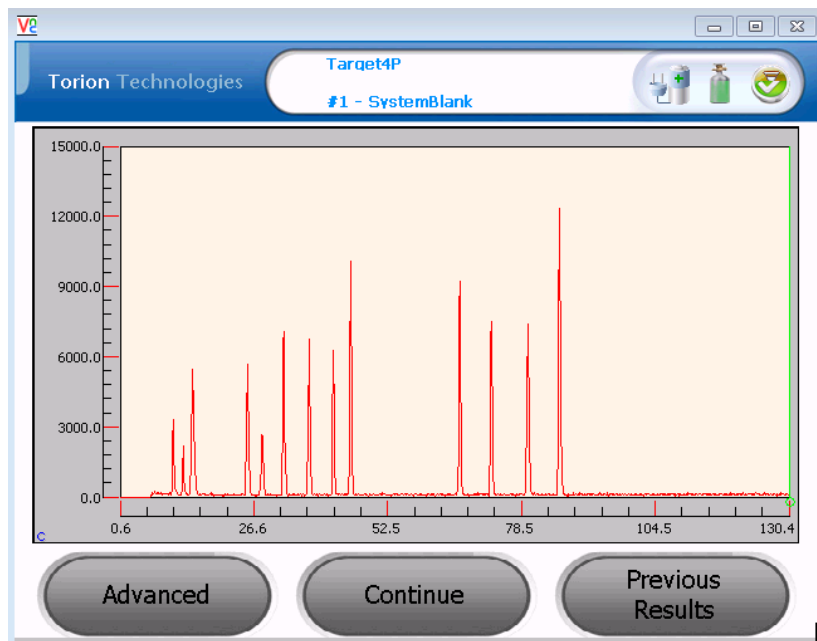
- All instrument operation software is resident on the GC/MS system (external notebook connection available but not required)
- Windows CE Operating System
- Self-diagnosing and easy to setup. Autocalibration and validation.
- Touch screen and simple keypad navigation and operation in PPE
- Results presented in a clear, concise way for non-expert users



# Non-expert User Software

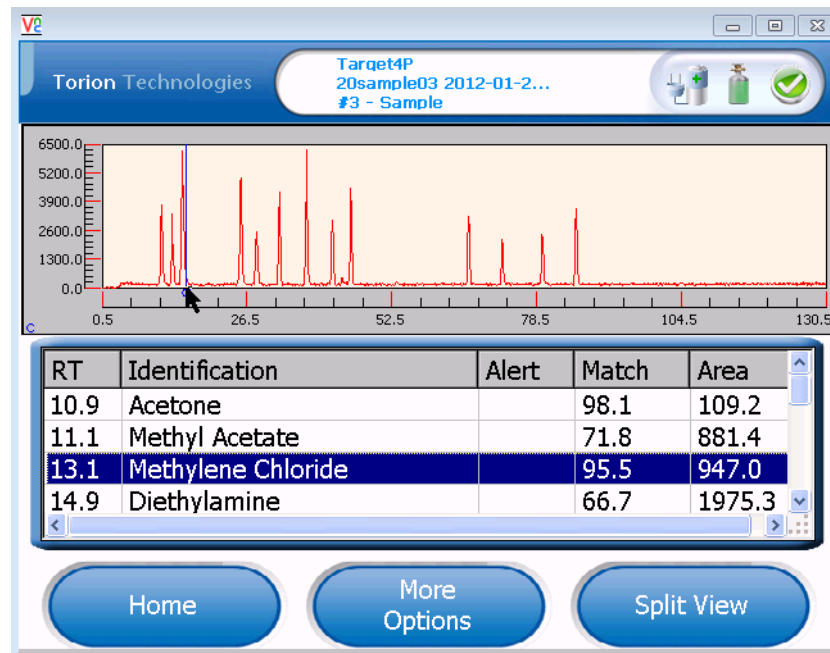


# Active Real-time Display



During Run

## Post-run Showing Target Library Hits and Unknown Identifications

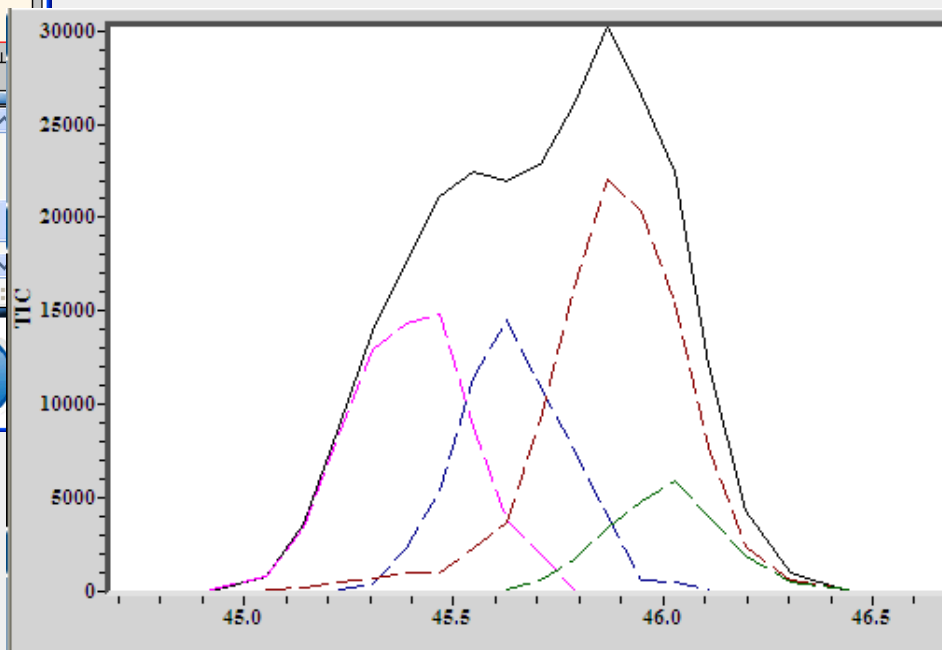
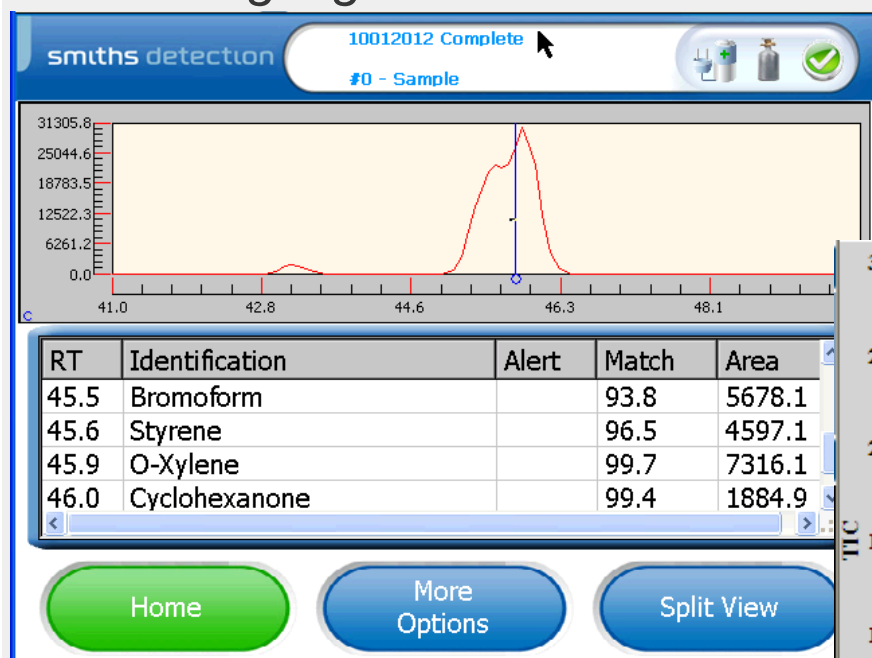


- CHROMION™ Peak Deconvolution/Extraction and Unknown Identification using On-board Libraries (customizable libraries supported)
- Quantitation Parameters Stored in Libraries, Executed Automatically.
  - Removable Data Media, Remote Data Transfer

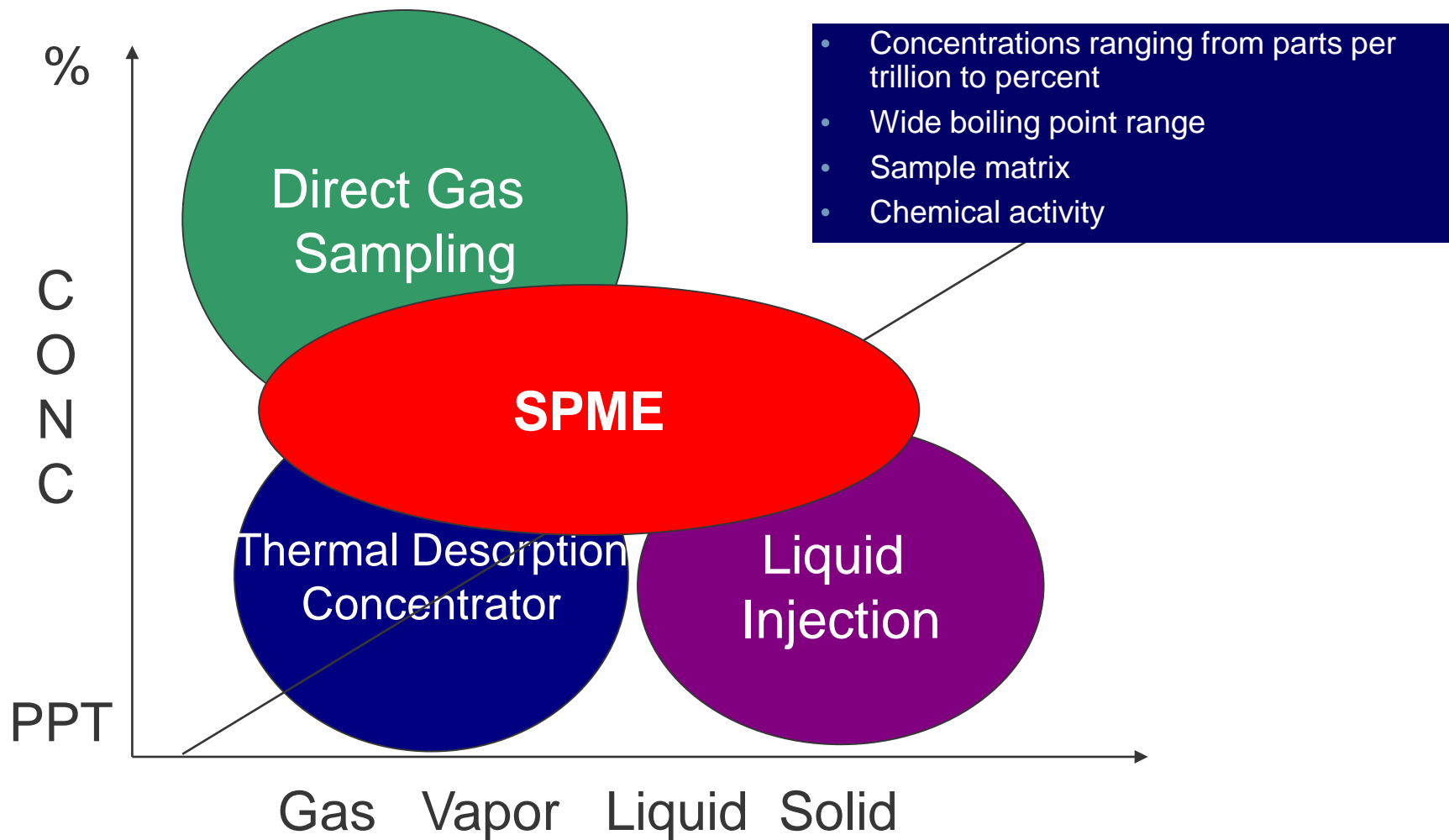


# Ease-of Use: Automatic On-board Deconvolution

- Four overlapping peaks identified using proprietary deconvolution and searching algorithms in both on-board and PC-based software



# The Challenge of a Universal Sampler



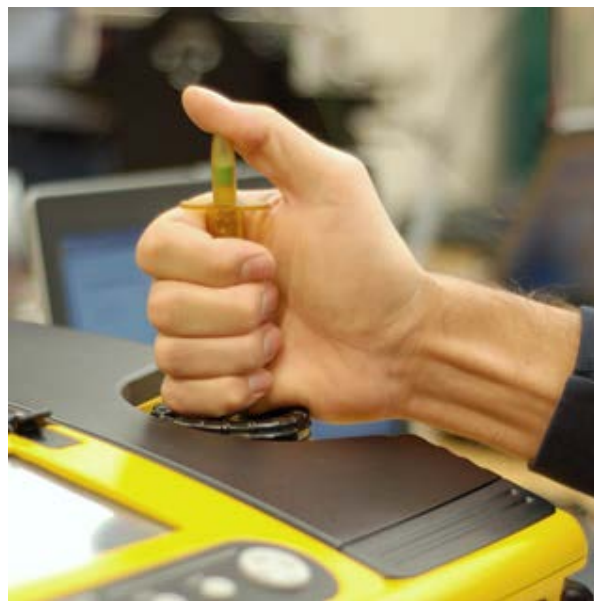
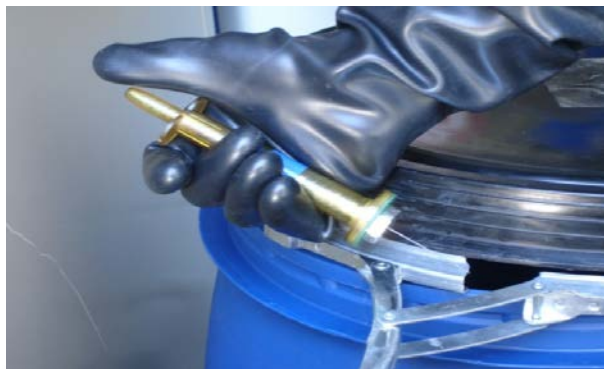
# SPS™-3 Field Portable Sample Preparation Station



- Portable:
  - Weight 10.05 lbs
  - Size: 12.5" x 10.8" x 7.8"
  - On-Board Helium Gas Supply
  - Battery Power: 15 runs
  - Key Pad Operation
  - LCD
- Multiple Functions
  - Internal Standard (IS)
  - Sample Desorption (SD)
  - Heated Headspace (HS)
  - Purge & Trap (PT)

# Sample Introduction Methods

Solid Phase  
Micro  
Extraction  
(SPME)

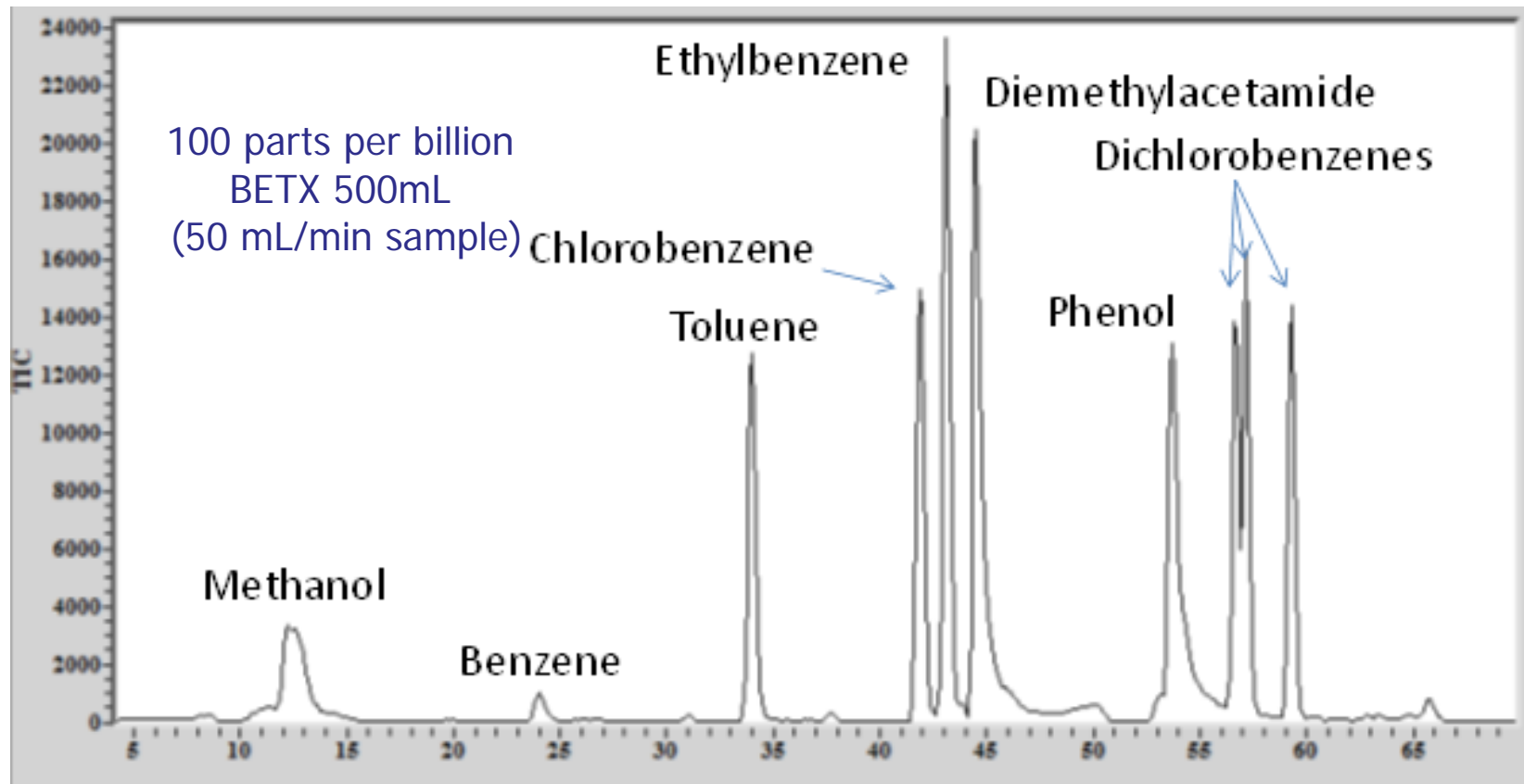


CUSTODION®

Needle Trap



# Air Sampling Using Needle Trap





“Lab data is not as good as you think and field data is better than you think.”

*John Fitzgerald, Massachusetts DEP*



# Applications: Chemical Warfare Agent Detection

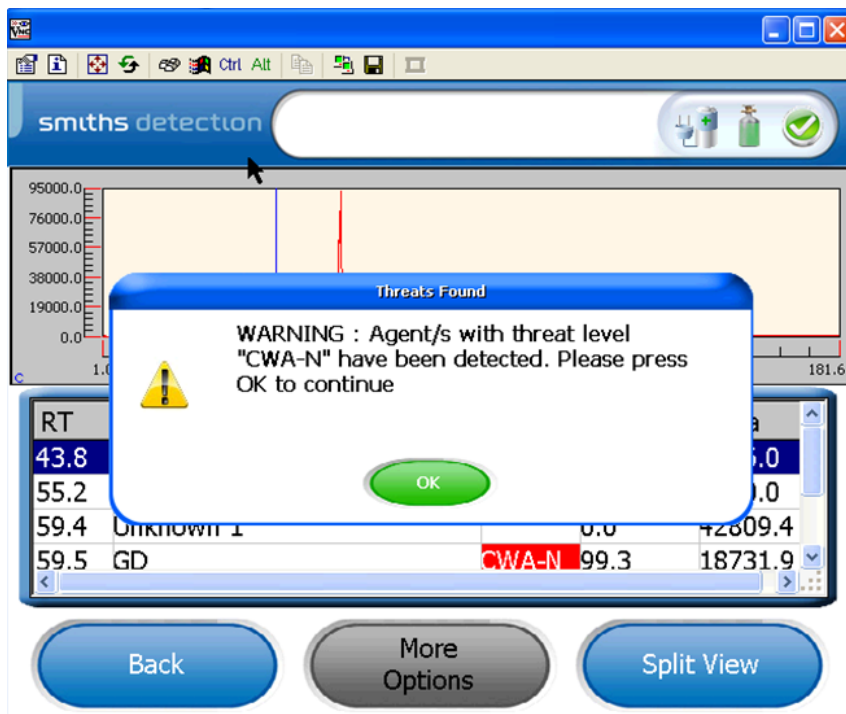


Table 1. CWA analysis detail

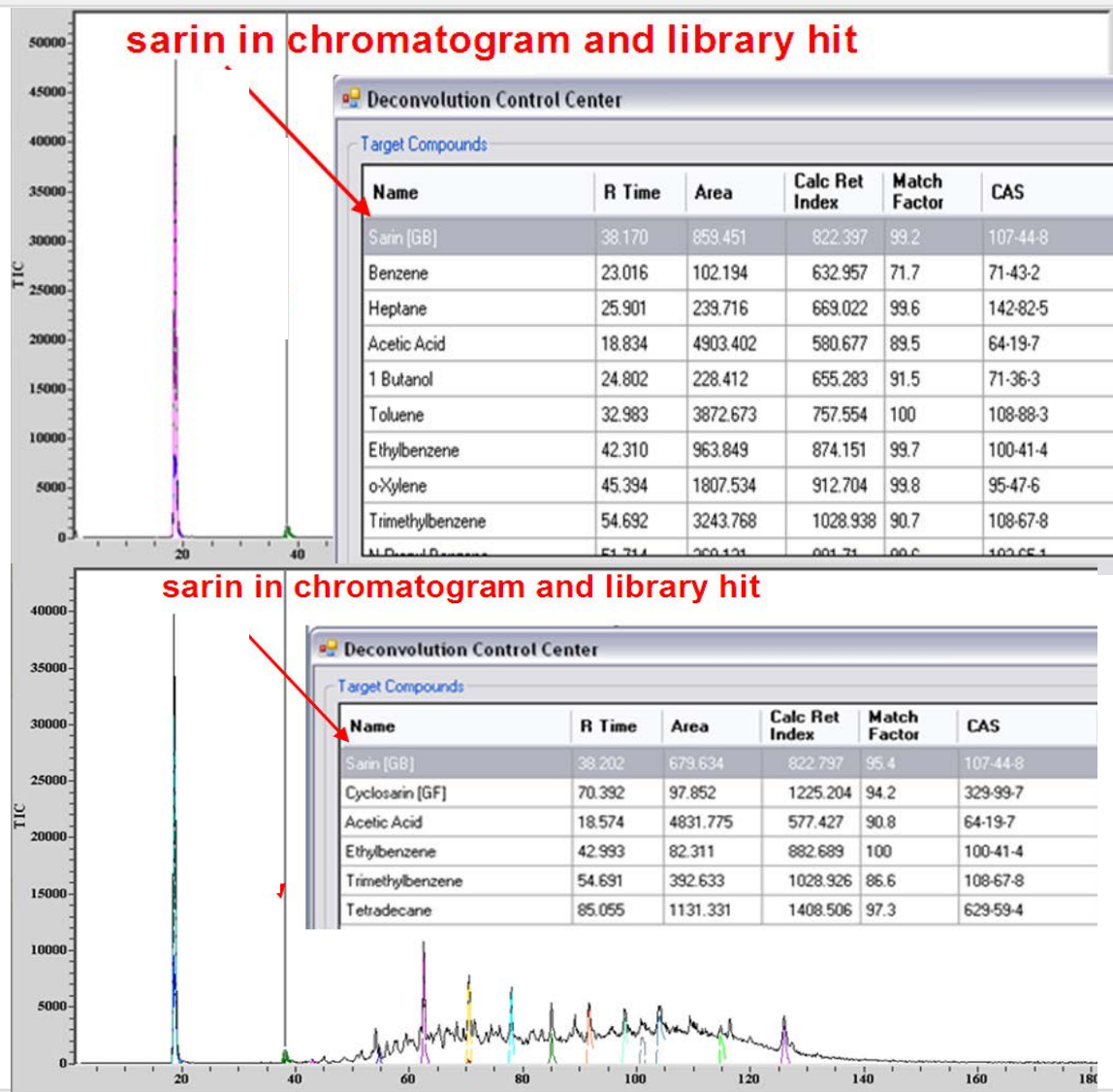
CWA	Agent Class	Molecular Structure
GB (Sarin)	Nerve	
GD (Soman)	Nerve	
GF (Cyclosarin)	Nerve	
GA (Tabun)	Nerve	
VX	Nerve	
VR (Russian VX)	Nerve	
HN3 (Nitrogen Mustard)	Vesicant	
L (Lewisite)	Vesicant	
HD (Sulfur Mustard)	Vesicant	
BZ	Incapacitating	

# Applications: CWA in Complex Samples



Sarin standard

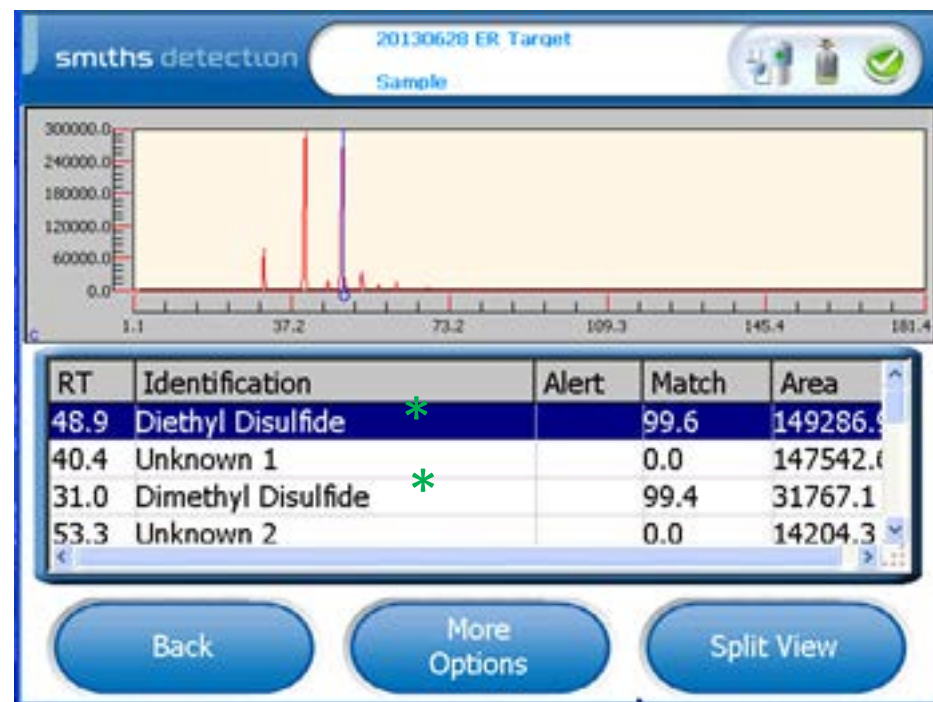
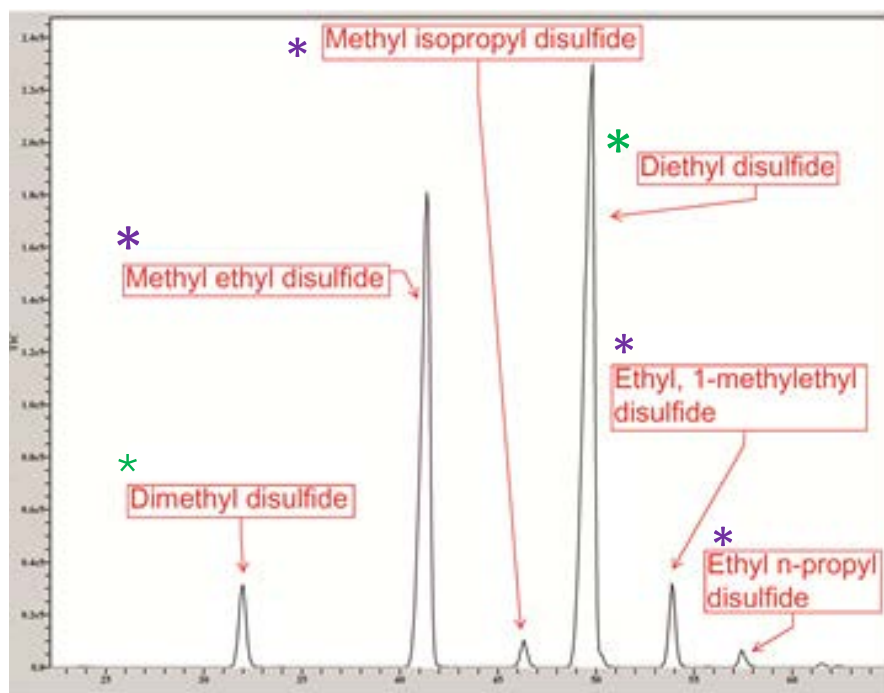
Sarin in Diesel Fuel



# Application: HAZMAT Responders - Onsite Analysis of Contents of a Leaking Cargo Tanker



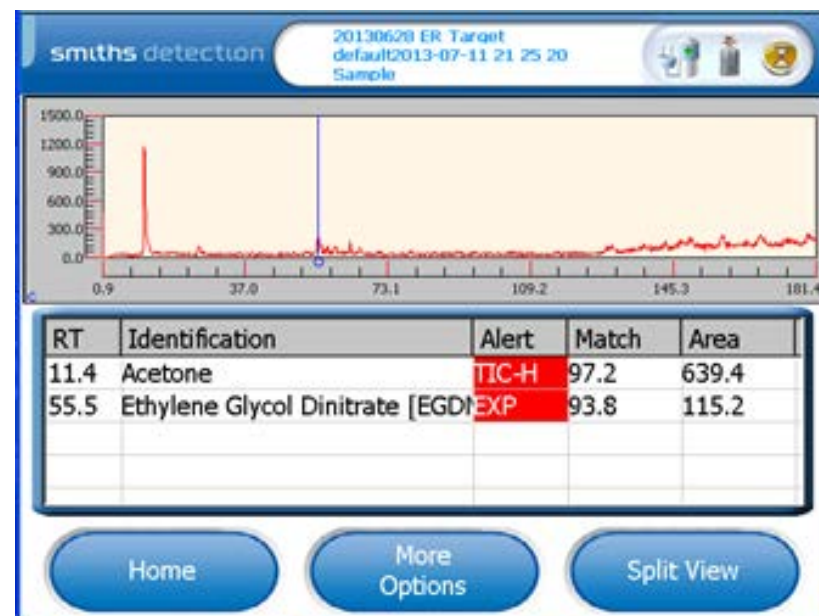
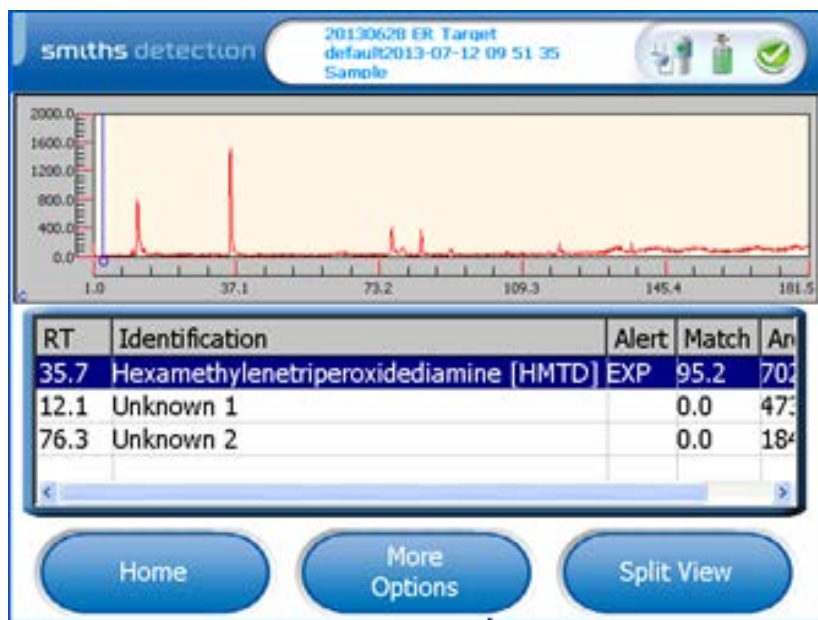
- Shipping manifest papers indicated only sodium sulfide and sodium hydroxide
- Onboard library identified 2 compounds (\*). Subsequent NIST library search identified remaining 4 (\*)



# Application: HAZMAT Responders Onsite Analysis of Explosives

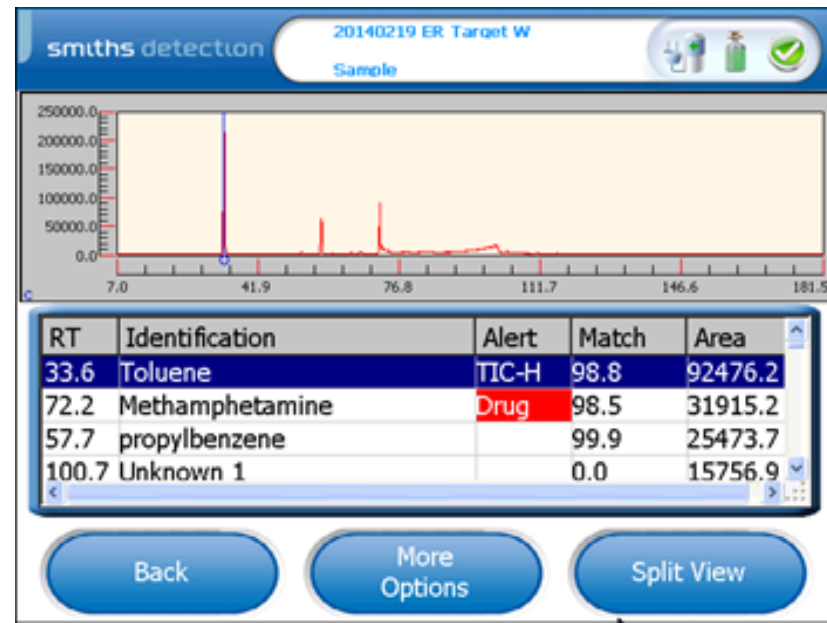
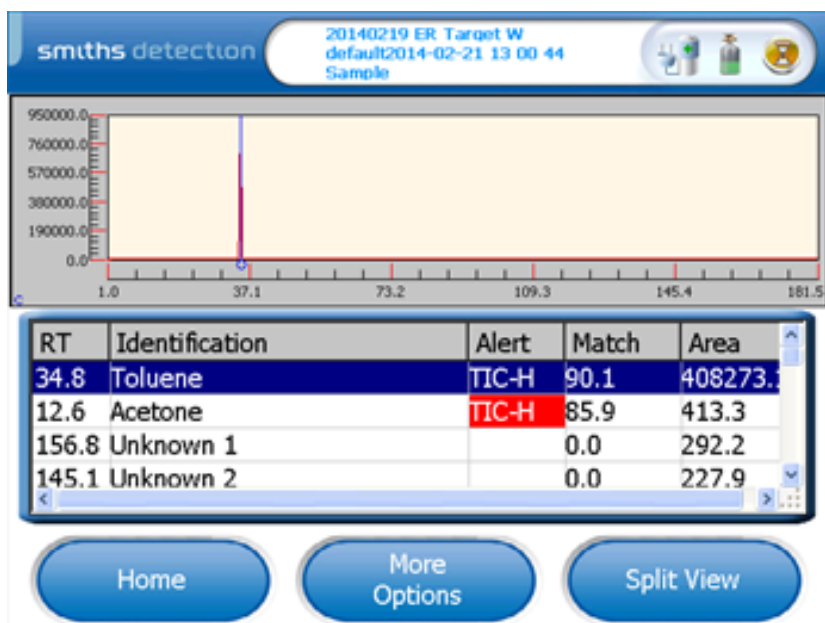


Headspace and acetone-rinse of residual explosives on improvised glassware





# Applicaton: Onsite Analysis of MethLab Chemicals



# Sample to Information: When and Where it's Needed

Smaller- Lighter-Faster



**ANYTIME  
ANYPLACE  
ANYWHERE**



The TRIDION™-9 is the world's fastest and most portable GC-TMS



# QUESTIONS?



**Bill Hahn**

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**732.648.6479 (mobile)**

**<http://torion.com/products/torion.html>**

**Special acknowledgement:**

**Warren Mino, Ph.D.**

**Smiths Detection**

**&**

**Steve Lammert**

**Perkin Elmer**