

High-Performance, Militarized Mass Spectrometer System

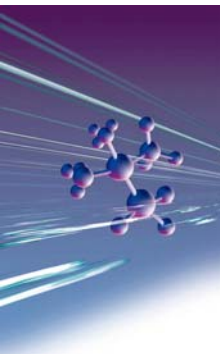
**HEMS 2009 Conference
September 22-24, 2009
Santa Barbara, CA**



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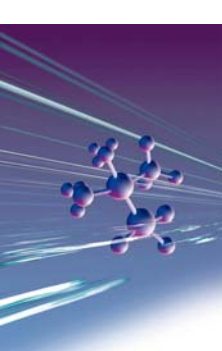
Content

- ◆ Portable QitTof™ (Quadrupole ion trap, time-of-flight) MS
 - *Dual EI/PI source*
 - *High speed MS/MS*

- ◆ Results and Applications
 - *Direct vapor sampling*
 - *Fast GC sampling*
 - *CW detection in air, soil, and water by PI/QitTof MS/MS*
 - *BW detection by Py/GC PI/QitTof MS*

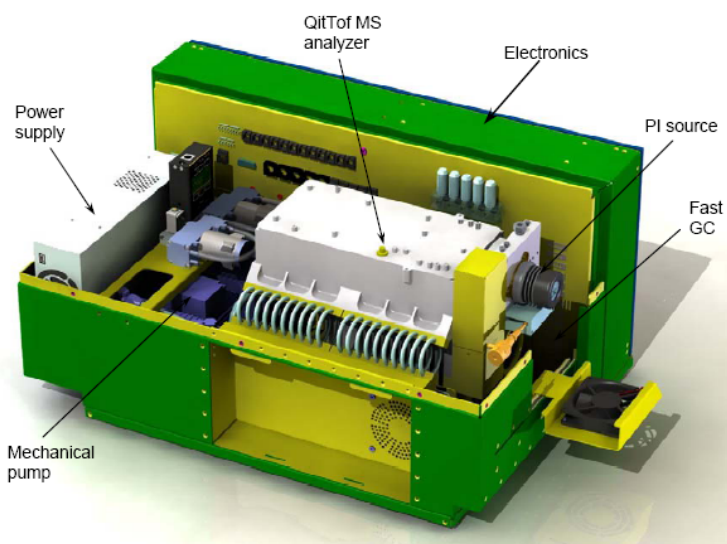
- ◆ HiPR (High-Performance Ruggedized) MS
 - *Partnership with Northrop Grumman*
 - *Technical specifications*
 - *CWA/TICs detection*





Latest Portable QitTof MS Systems

FieldMate™ Benchtop MS



22x16x14 in and 60 lb without aerosol collector

HiPR MS



- DoD mobile CWA/TIC capable
- Developed in partnership with Northrop Grumman
- 28x22x17 in and 150 lb

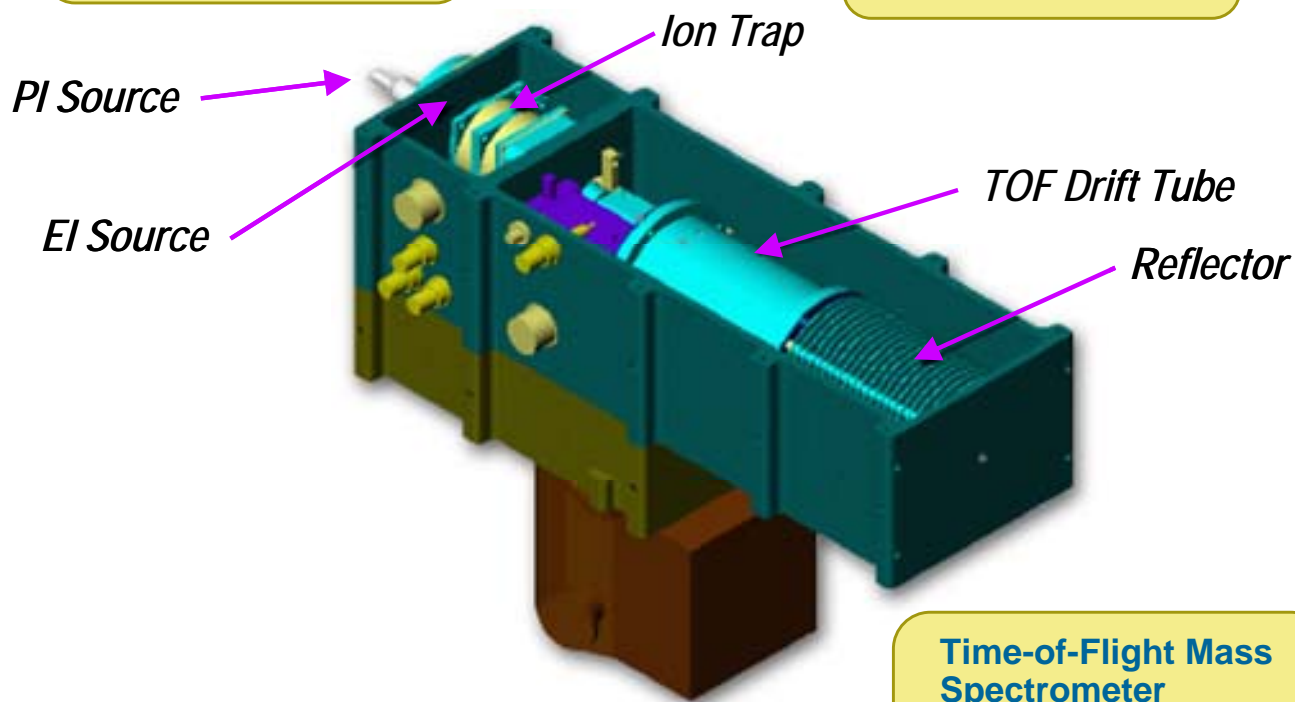
Compact EI/PI QitTof™ MS

Dual Photoionization / Electron Ionization

- Direct air sample
- Optional samplers, e.g. GC

Quadrupole Ion Trap

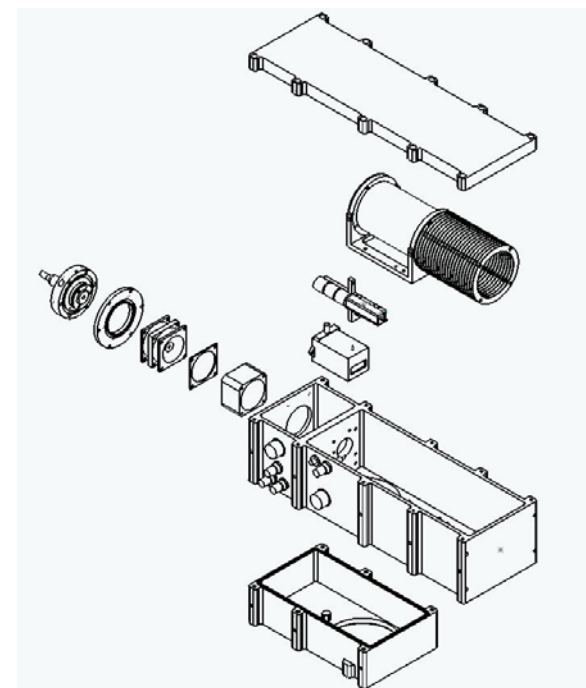
- Storage of ions
- MS / MS capable



Time-of-Flight Mass Spectrometer

- Full mass scans
- High-speed MS (60 Hz)
- Stable accurate masses

Novel differential pumping with split-flow TMP for high gas throughput

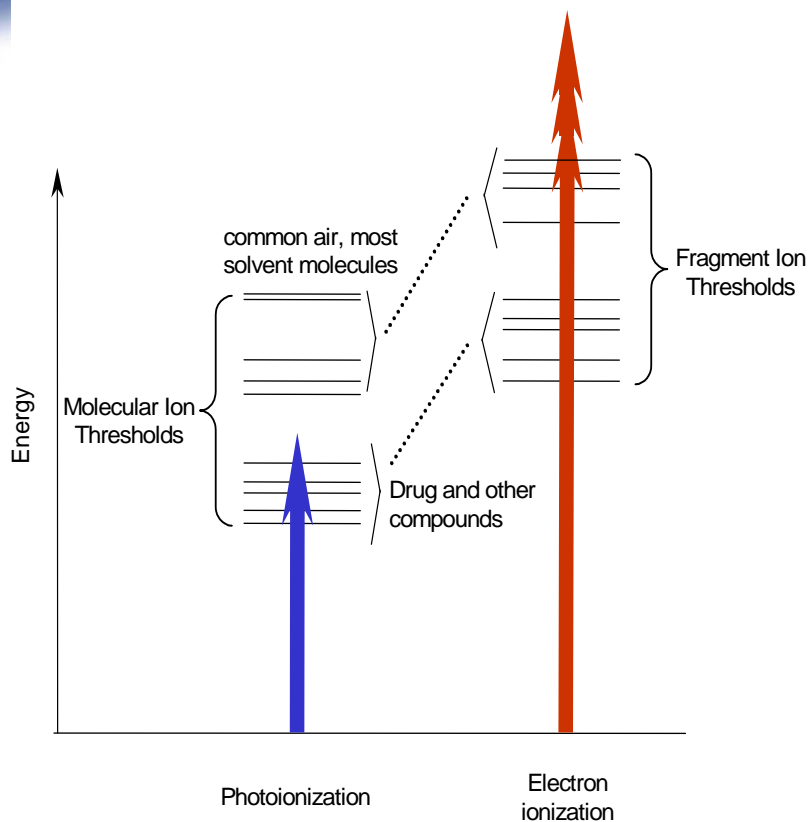


**Robust, economical design,
engineered for simplicity**

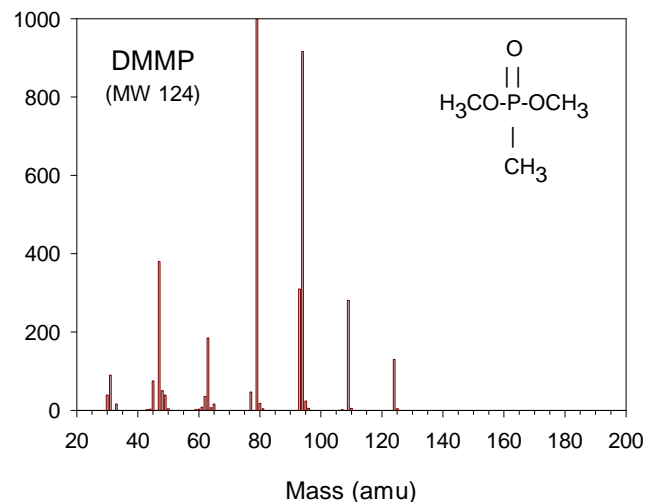


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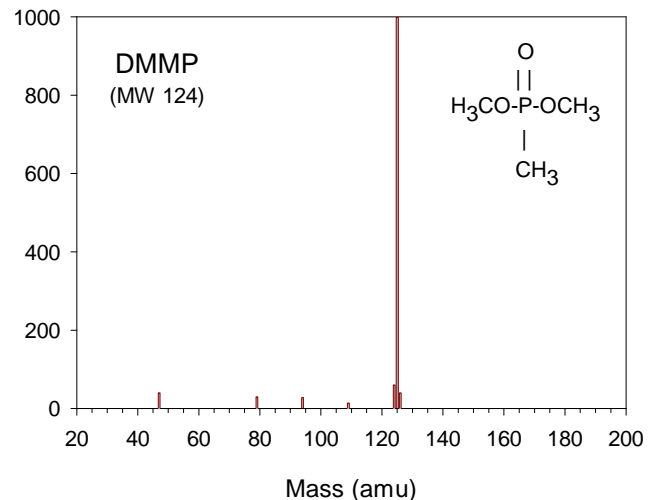
Photoionization vs. Electron Ionization



Electron ionization MS



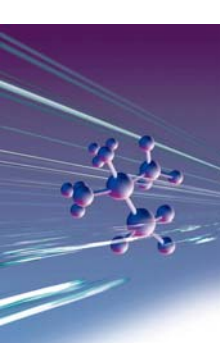
Photoionization MS



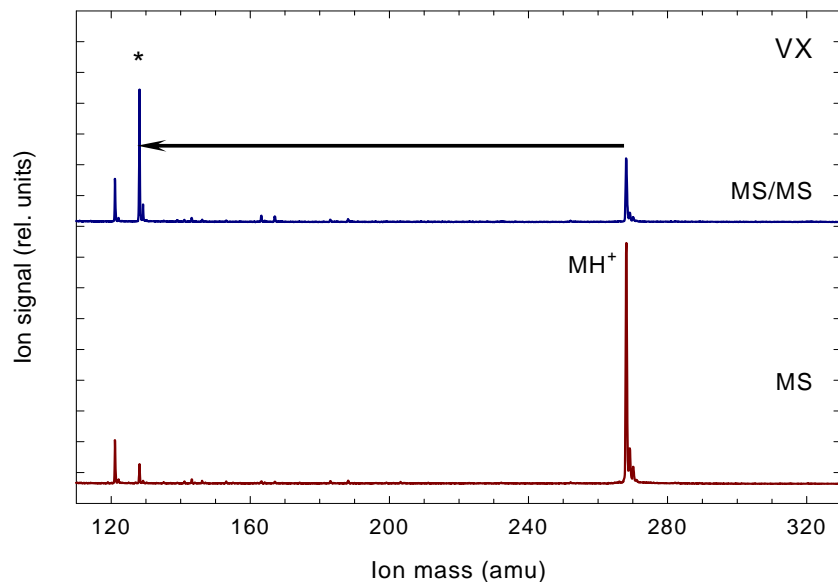
Benefits of photoionization source

- Near universal detection efficiency for many classes of compounds
- Parent ion signal with minimum fragmentation
- Minimum air and solvent signal
- Minimum ion suppression



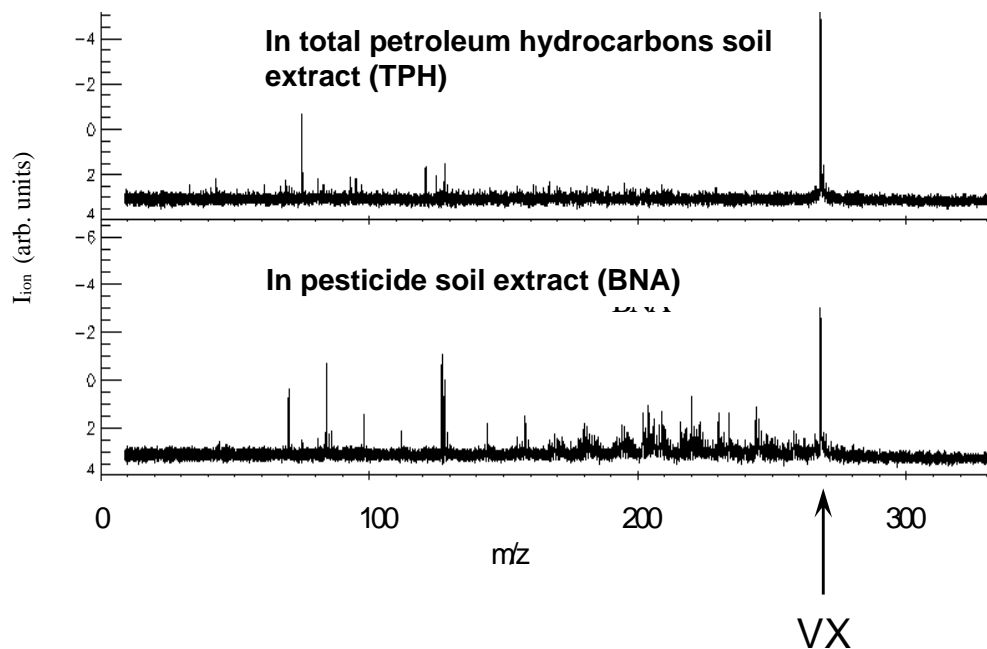


CW Detection by PI/QitTof MS/MS



PI MS of VX

- Distinct VX parent ion (bottom trace)
- Confirmatory MS/MS (top trace)



PI MS of VX in spiked soil extracts

0.012 mg/mL (0.83 ppm)

Agents detected by PI MS:

VX

GA, GB, GD, GF

HD, HN1, HN2

CR, CS, BZ



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CWs and Related Compounds Detected

Chemical Weapons Convention Treaty - Compliance Monitoring Compound List

Schedule-1 compounds

Toxic

VX
GA (Tabun)
GB (Sarin)
GD (Soman)
GF

HD (sulfur mustard)
HN-1 (Nitrogen mustard)
HN-3

CR
CS

Precursors (Binary)

QL
DF

Schedule-2 compounds

Toxic

BZ

Precursors

Diisopropyl methylphosphonate
Diethyl methylphosphonate
Dimethyl methylphosphonate
Diethyl ethylphosphonate
Diethyl methylphosphonothioate
Isopropyl methylphosphonic acid
Cyclohexyl methylphosphonic acid
Pinacolyl methylphosphonic acid
Methyl phosphonyl dichloride
3-quinuclidinol
Benzilic acid
Pinacolyl alcohol
Thiodiglycol
N,N-diethylethanolamine
1,4-dithiane
Thiodiglycol sulfoxide
Methylamine
Isopropylamine
Thioxane

Schedule-3 compounds

Precursors

Phosphorus oxychloride
Dimethyl phosphite
Trimethyl phosphite
Diethyl phosphite
Triethyl phosphite
Triethanolamine
N-ethyldiethanolamine
N-methyldiethanolamine

Decomposition Products

Methylphosphonic acid
Ethylmethylphosphonic acid
EMPTA
2-chlorodiethylsulfide

Other relevant compounds

VX disulfide
YL

Not detected: Phosgene, chloropicrin ; Detectable by EI





CW Detection in Water

◆ Specifications

- **Sensitivity:** 1-6 pg and 1-6 ng/mL (3σ MDL) for DMMP, DEMP, DEEP, DIMP
- **P_D , P_{FP} :** $P_D > 99\%$, $P_{FP} < 0.2\%$ for all four CW surrogates at 30 ng/mL (0.03 mg/L)
- **Dynamic range:** 5 decade, >3 decade linear
- **Speed:** 45 s per sample by autosampler including 2 washes

◆ Live Agent Testing

Chemical Warfare Agents in H₂O - ppb are in units of (mole analyte)/(mole H₂O)

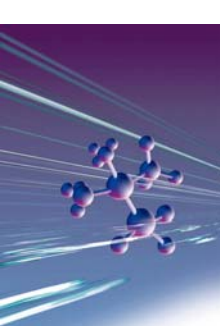
Compound	Name(s)	MW	Mass Obs	3σ LOD (ng)	3σ LOD (ppb)	Agent type
HN-1	Bis-(2-chloroethyl)ethylamine	170.08	170	0.131	14	Mustard
HN-3	Tris-(2-chloroethyl)amine	204.54	204	0.071	6	Mustard
GA	Tabun or Ethyl N,N-dimethylphosphoroamidocyanidate	162.13	163	0.354	39	Nerve
GB	Sarin or Isopropyl methylphosphonofluoridate	140.10	141 (99)	1.2 (.239)	154 (31)	Nerve
GD	Soman or Pinacolyl methyl phosphonofluoridate	182.18	99	0.678	67	Nerve
GF	o-Cyclohexyl-methylfluorophosphonate	180.20	99	0.491	49	Nerve
VX	o-Ethyl-3-(2-isopropylaminoethyl)methyl phosphonothiolate	267.38	268	0.166	11	Nerve

Measurements made at ECBC

◆ References

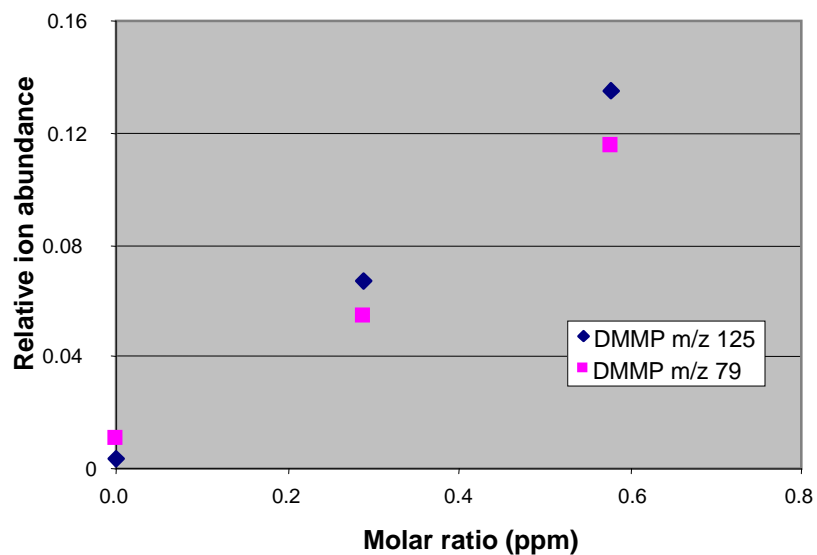
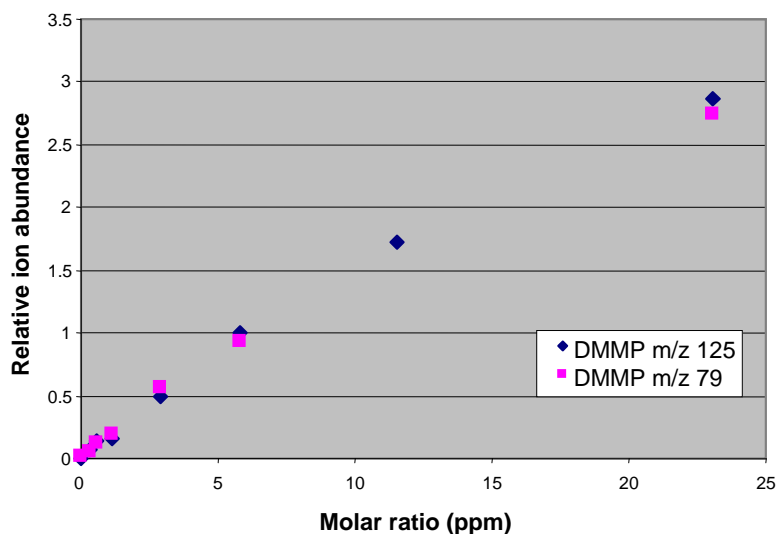
- J. A. Syage, S-S. Cai, J. Li, and M. D. Evans, "Direct Sampling of Chemical Weapons in Water by Photoionization Mass Spectrometry" *Anal. Chem.* **78**, 2967-76 (2006).
- J. A. Syage, "Guarding Drinking Water Against Chemical Weapons Attack," *Water & Wastes Digest* **45**(1), 22 (2005).
- J. Calles, R. Gottler, M. Evans, and J. Syage, "Early Warning Surveillance of Drinking Water by Photoionization Mass Spectrometry," *J. AWWA* **97**(1), 62-73 (2005).
- J. Wu, J. Gleenlee, and J. Syage, "Rapid Screening for Chemical Weapons Infiltration in Drinking Water," *J. AWWA* **96**(12), 44-47 (2004).





CW Real-Time Air Sampling

Field-Portable QitTof Linearity Measurements



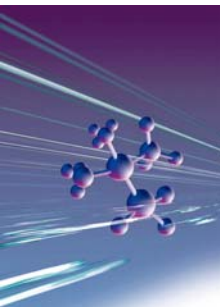
Real-time direct air sampling of DMMP

Mole fract.(ppm)	%RSD	LOD (ppb)	LOD (pg)
23.1	3.0%	13.7	33.7
11.5	0.9%	11.4	28.0
5.8	0.9%	9.9	24.3
2.9	2.2%	9.9	24.4
1.2	2.2%	11.9	29.3
0.6	4.7%	7.3	18.0
0.3	9.4%	7.3	18.0

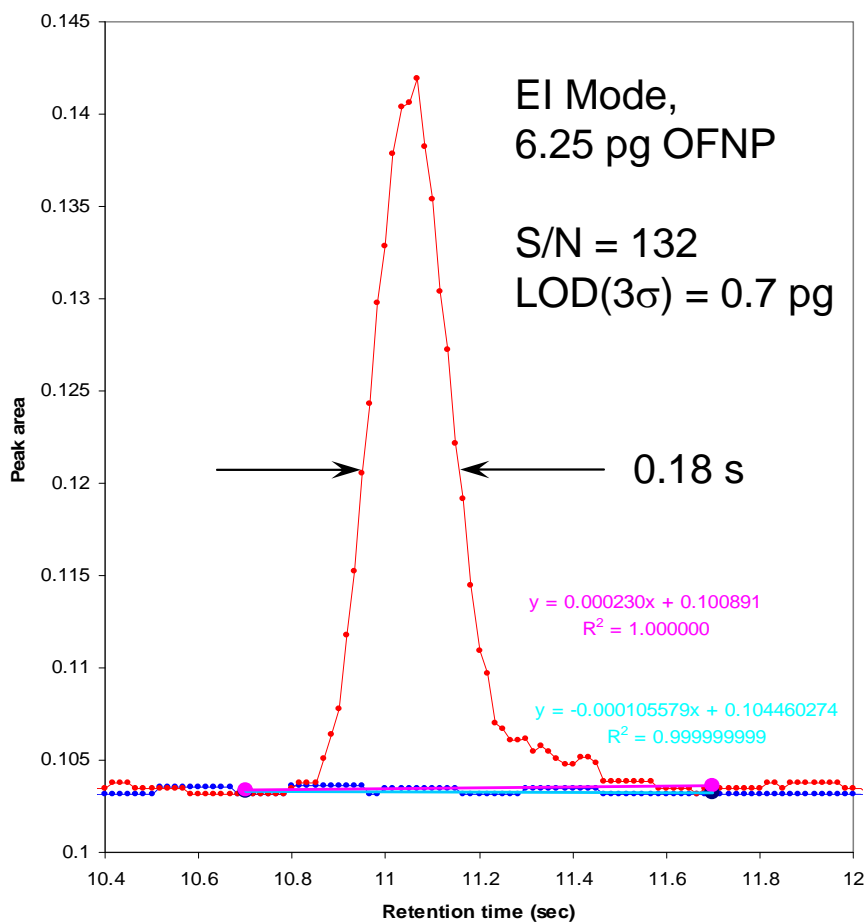
LOD: 10 ppb (DMMP) direct air sampling
Corresponds to about 20-30 pg

Dynamic Range: 10 ppb to 30 ppm (nearly linear)

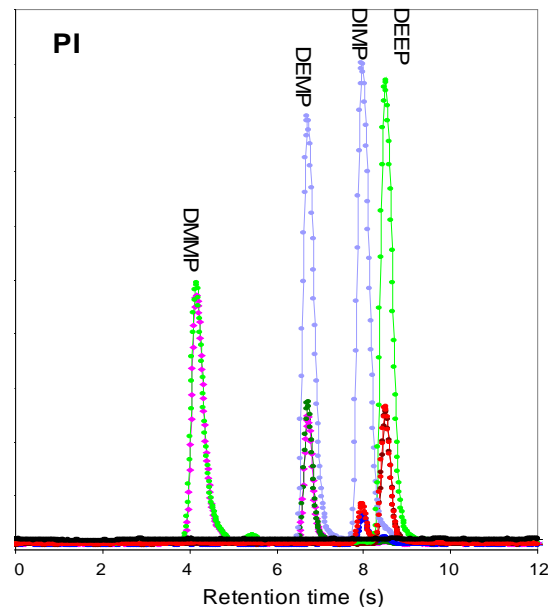
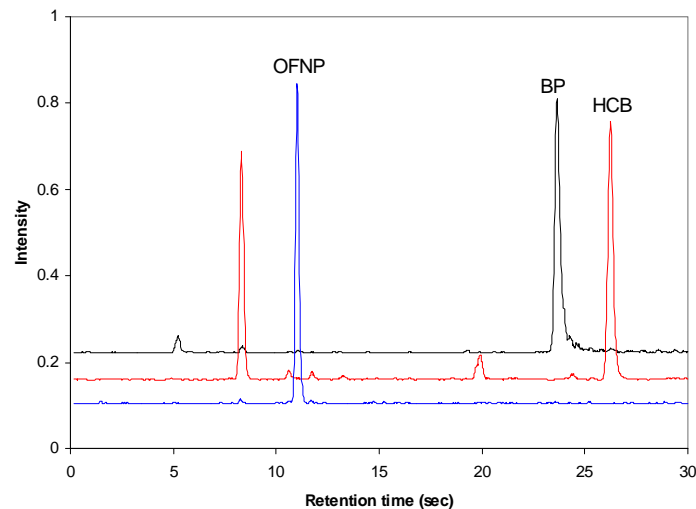




High-Speed, High-Sensitivity GC/QitToF MS

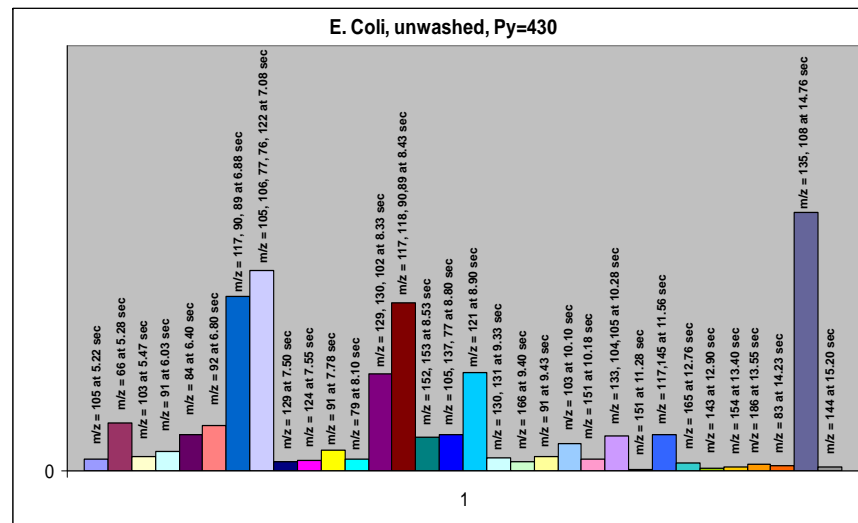
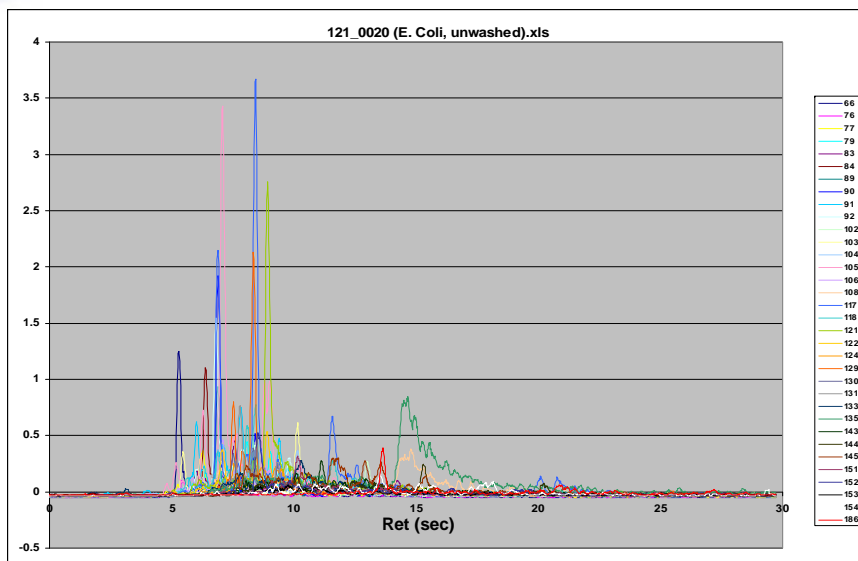


Comparable sensitivity to
Agilent 5973 GC/MS
(S/N = 20 for 1 pg OFNP)

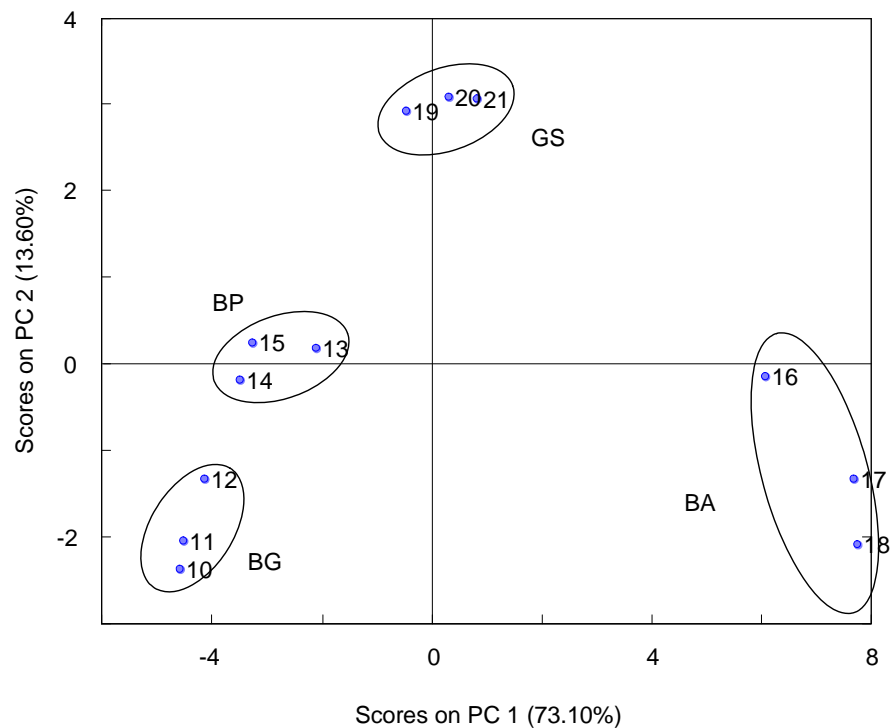


<10 pg full scan mode LODs
<10% RSD for 12 pg to 2.5 ng injections

BW Detection by Py/GC – PI/QitTof MS



Pyrolysis of 3 μ g of E. Coli: Histogram based on the integrated intensities for selected retention times and ion masses



PCA plot showing excellent discrimination for similar gram positive bacteria

Jack A. Syage, Brian J. Nies, and Matthew D. Evans, A. Peter Snyder, Waleed M. Maswadeh, and Ashish Tripathi, "Rapid CB Monitoring by Pyrolysis/GC Photoionization Mass Spectrometry," *Proc. of 2nd Joint Conf. Point Det. for CB Defense*, (2003).



High Performance Ruggedized (HiPR) MS

Broad spectrum threat detection on a single platform



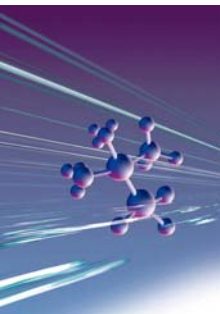
40"x22"x17", 180 lbs

- ◆ Modular hardware and software design
- ◆ Detection and identification of all chemical threats in seconds
- ◆ Reliable biological detection on the move
- ◆ Adaptable, easily reconfigured for changing threat environment
- ◆ High sensitivity and selectivity
- ◆ Low FAR and high P_D

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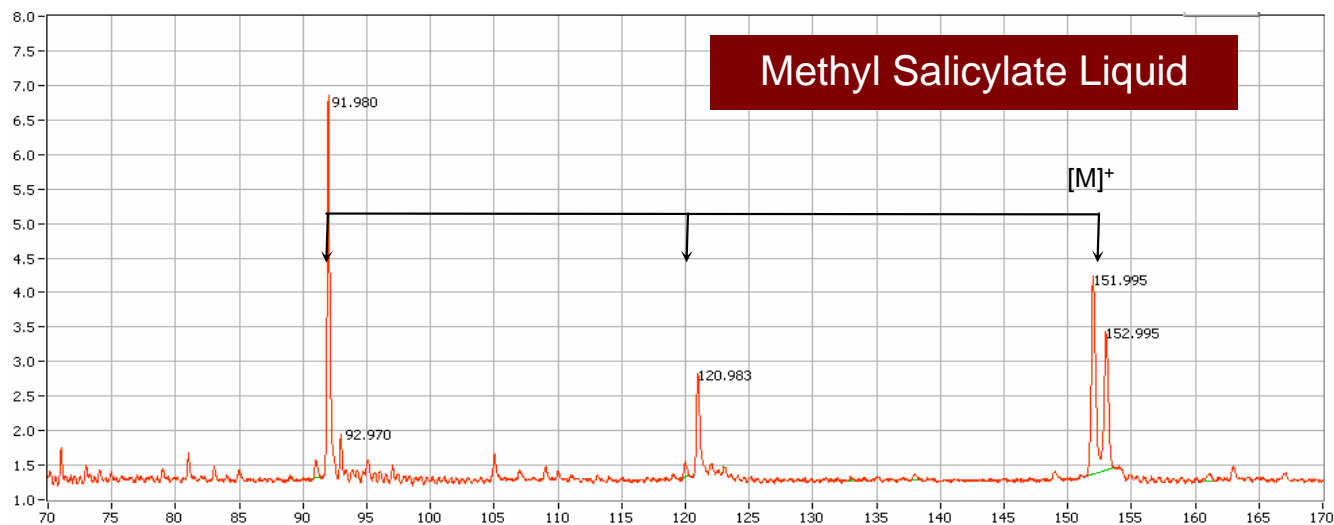
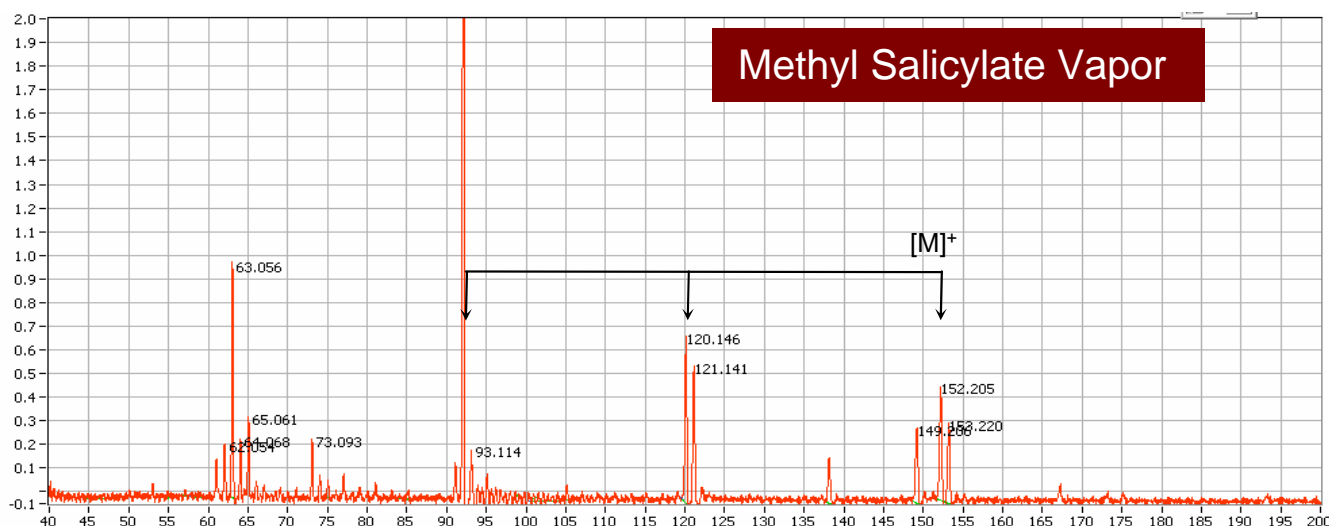


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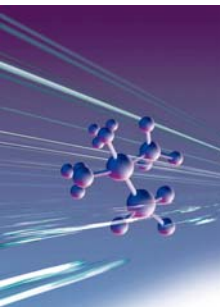
CWA Simulant Detection

Demonstrated detection of >17 CWAs and Simulants in solid, liquid, and vapor form at 1000x lower levels than required



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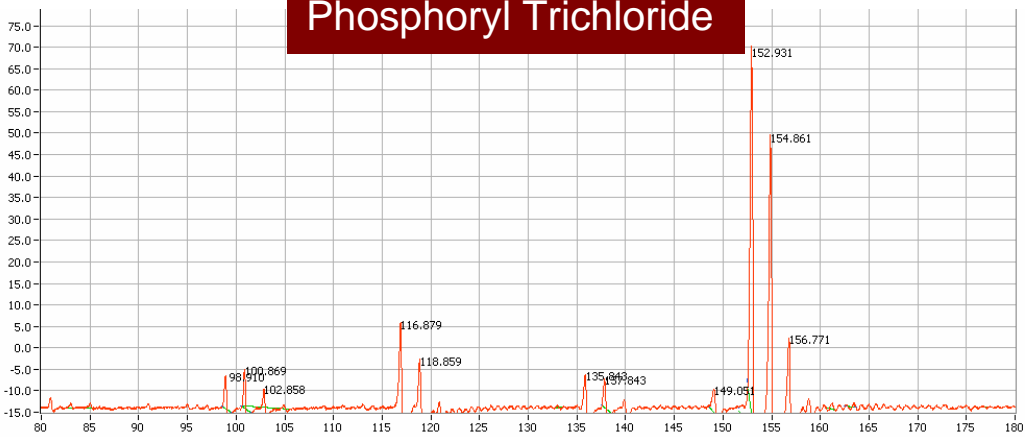




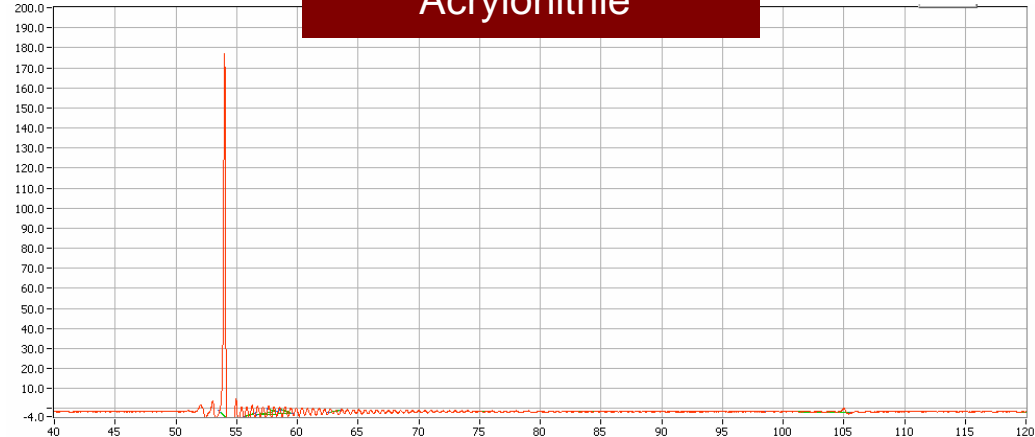
TICs Detection

Demonstrated detection of >25 TICs below Immediately Dangerous to Life and Health (IDLH) values

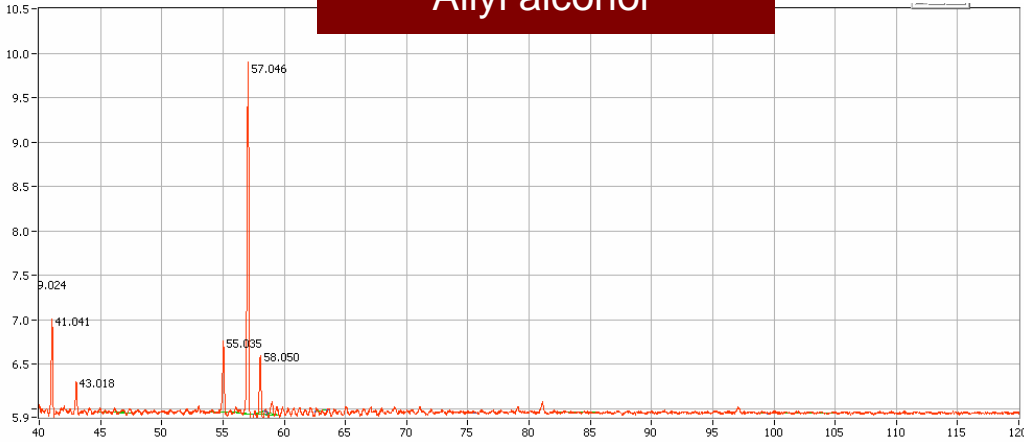
Phosphoryl Trichloride



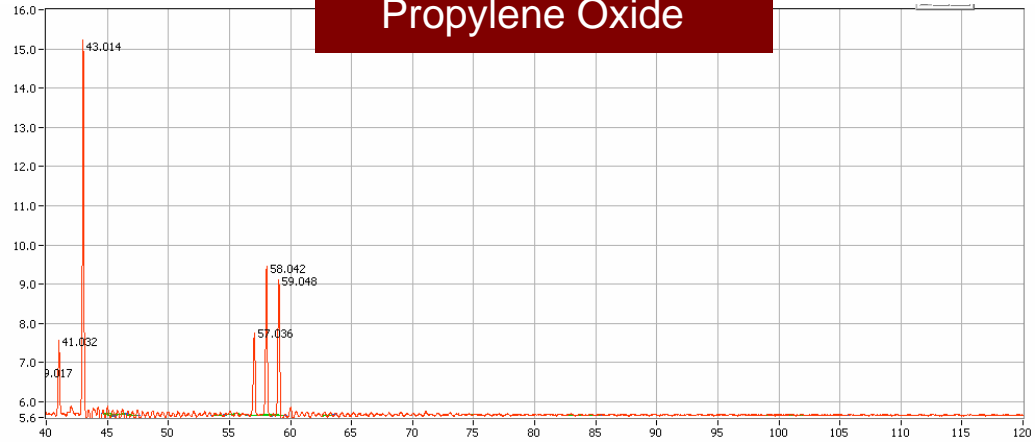
Acrylonitrile

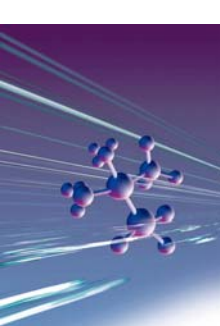


Allyl alcohol



Propylene Oxide

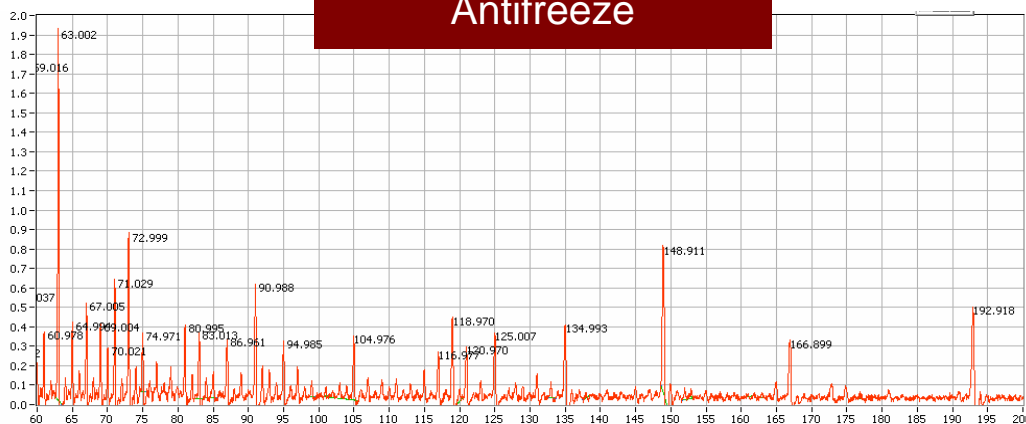




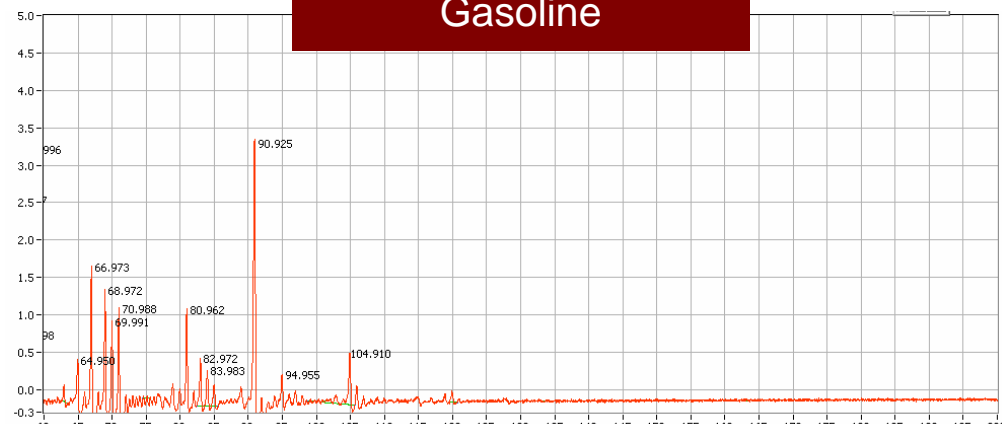
Background and Interferent Rejection

High resolution MS can detect agents in the presence of very complex and 100x more concentrated POLs

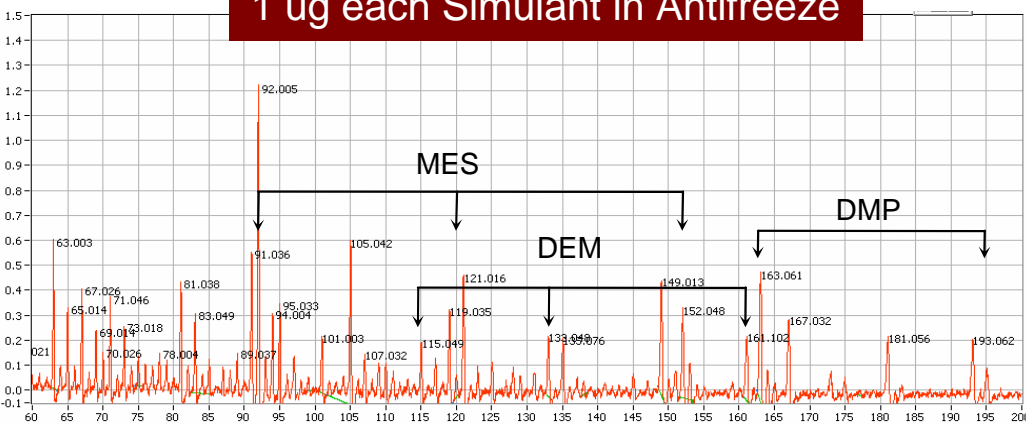
Antifreeze



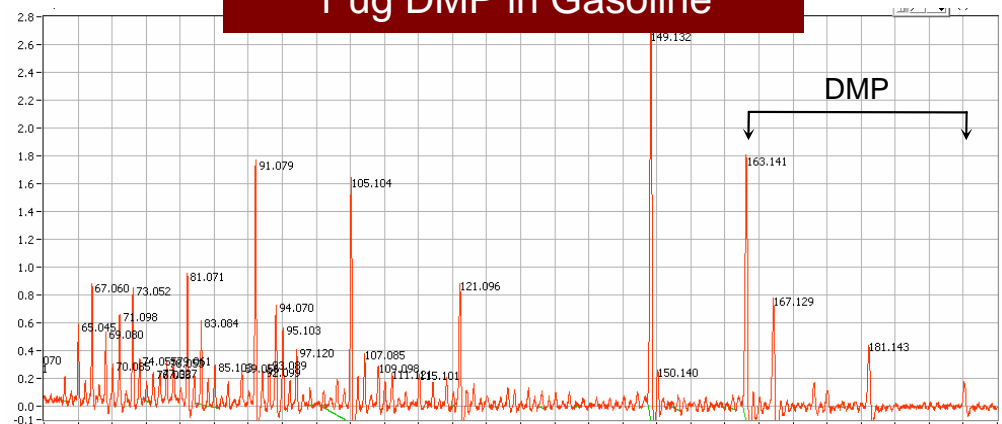
Gasoline

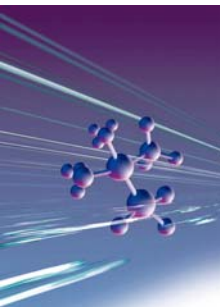


1 ug each Simulant in Antifreeze



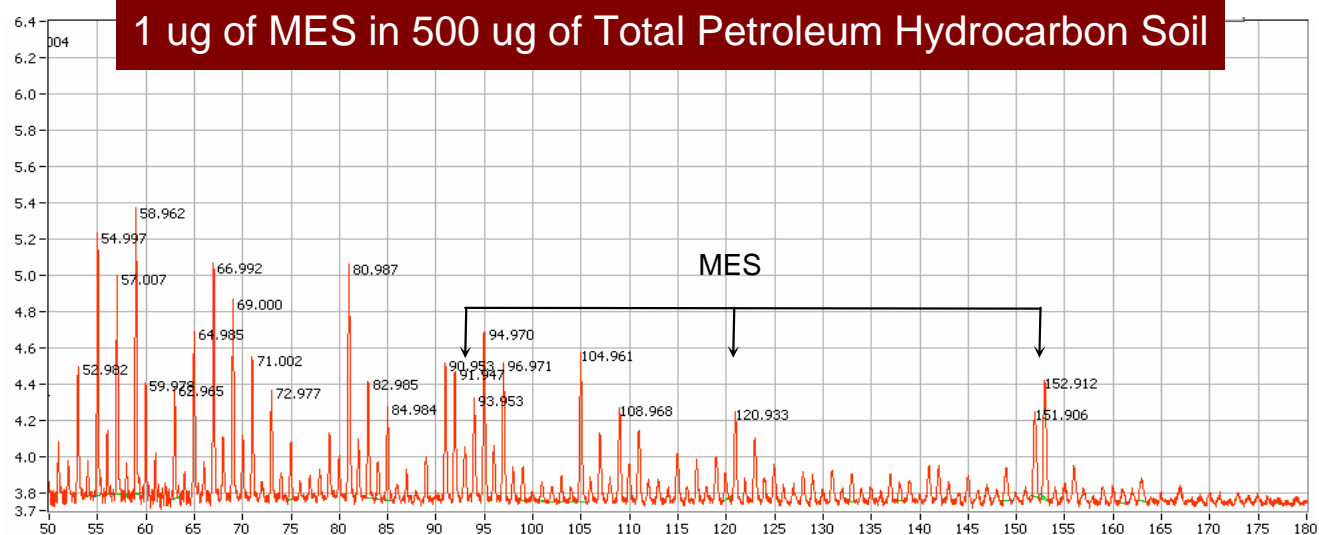
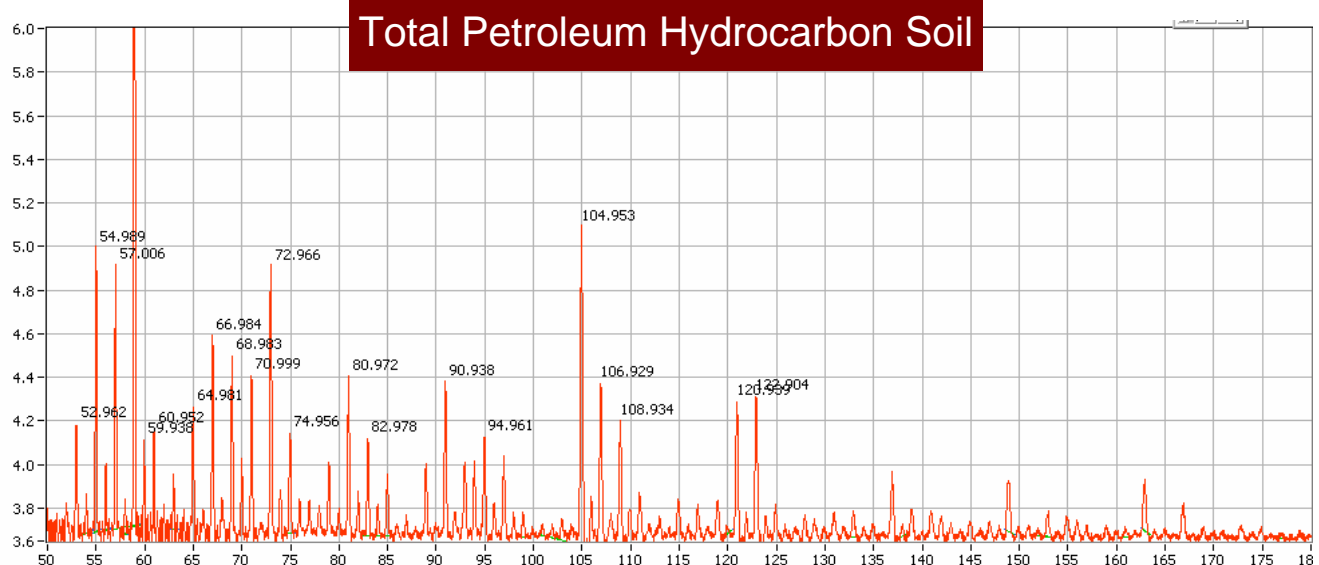
1 ug DMP in Gasoline





Background and Interferent Rejection

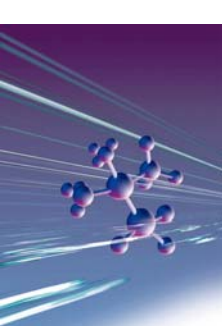
High resolution MS can detect agents in the presence of very complex and 500x more concentrated soil backgrounds



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Application





Summary

- ◆ Major innovations in MS transitioned to product
 - *QitTof MS is an exceptionally powerful analyzer*
 - *Dual EI/PI is a very flexible multimode source available for widespread screening applications*

- ◆ Demonstrated detection of wide range of threat compounds
 - *CWs, BWs, TICs, explosives, and narcotics*
 - *High performance detection in portable systems*
 - *60 Hz MS and 30 Hz MS/MS allows for high-throughput, high-speed screening*

- ◆ Acknowledgment
 - *We are grateful to Northrop Grumman for their support and for the leadership of Dr. Daniel Dickinson*
 - *This work would not have been possible without the talent and hardwork of the Syagen technical and engineering team*