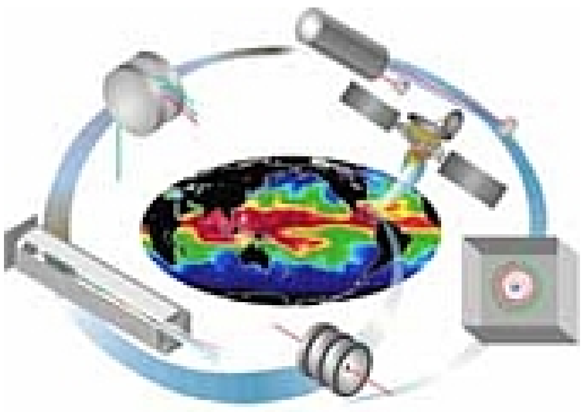
The GUARDION®-7 Hand-Portable GC-TMS: R*ecent Enhancements and New Applications*



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September 23rd, 2009

Presentation Outline

- Next Generation GC-TMS
  - Toroidal ion Trap Mass Spectrometer
  - Low Thermal Mass Capillary GC
  - SPME Sampling and Injection
  - Deconvolution Software
- Recent TMS Enhancements
- GC-TMS Applications

The Next Generation Hand-Portable GC-MS

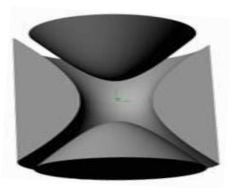
Next Generation MS: Smaller-Lighter-Faster

- Significant improvement from current instruments:
  - Size Reduction
  - Weight Reduction
  - Speed of Analysis
  - Ease of Use
- Operates reliably in harsh environments
- Lower sustainment costs
  - Consumables
  - Training
- Broader Analytical capabilities
  - Volatile and Semivolatile Compounds

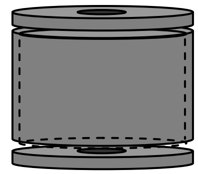
Advantages of Ion Traps for HEMS

- Simple, rugged design (no critical alignment of ion optics)
- Less stringent vacuum requirements (requires 1 mtorr operating pressure)
- High duty cycle ⇨ High sensitivity
- Low power (especially with small ion trap mass analyzers)
- High sensitivity and selectivity
- MS-MS capabilities

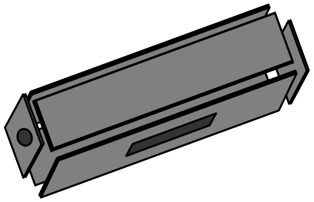
Different Ion Trap Configurations



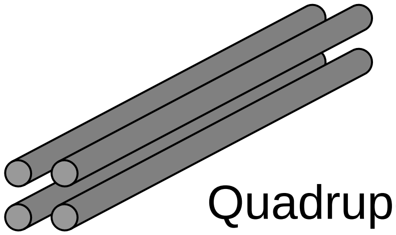
Quadrupole ion trap or Paul trap



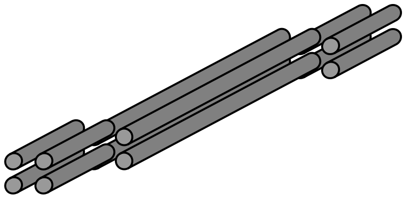
Cylindrical ion trap



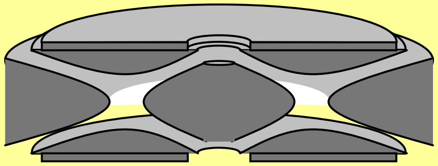
Rectilinear ion trap



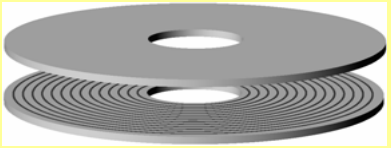
Quadrupole mass filter



Linear ion trap



Toroidal ion trap

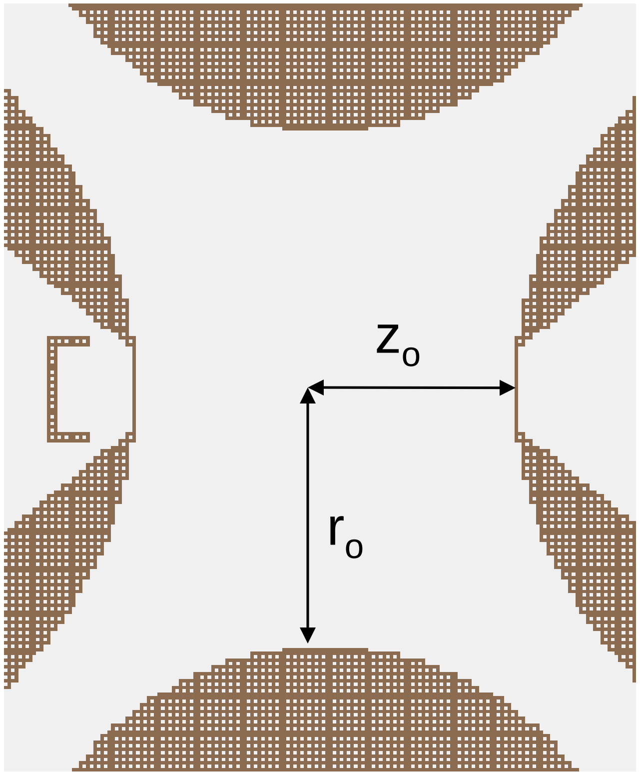


Halo ion trap

Mitigating Factors of Ion Traps

- 3-D ion trap is an “ion bottle” with somewhat fixed relative dimensions (r_o vs. z_o)
- Ion-ion repulsion (space charge)
- Commercial traps optimized at
  r_o = 1 cm, ~16 kV_{p-p}
- Further increase in r_o not practical due to arcing of RF high voltage
- Decrease of r_o yields lower RF power, but will lead to earlier onset of space charge

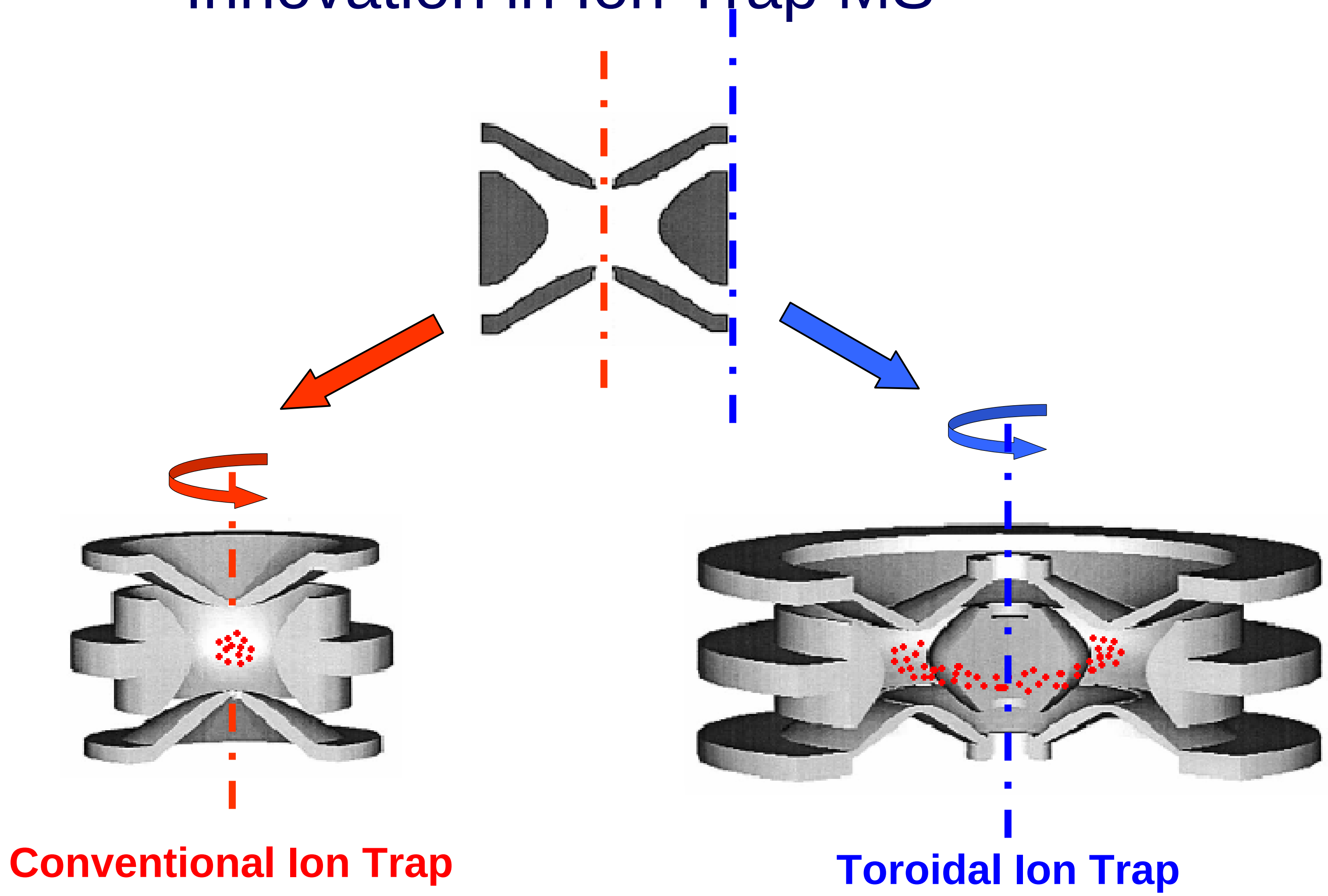
$$q = \frac{-8eV}{m(r_0^2 + 2z_0^2)\Omega^2}$$



Why Toroidal Ion Trap Mass Spectrometry?

- 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)
- Homogenous field (compared to linear ion traps)
  - No end effects. All spatial positions within mass analyzer are equivalent

Innovation in Ion Trap MS



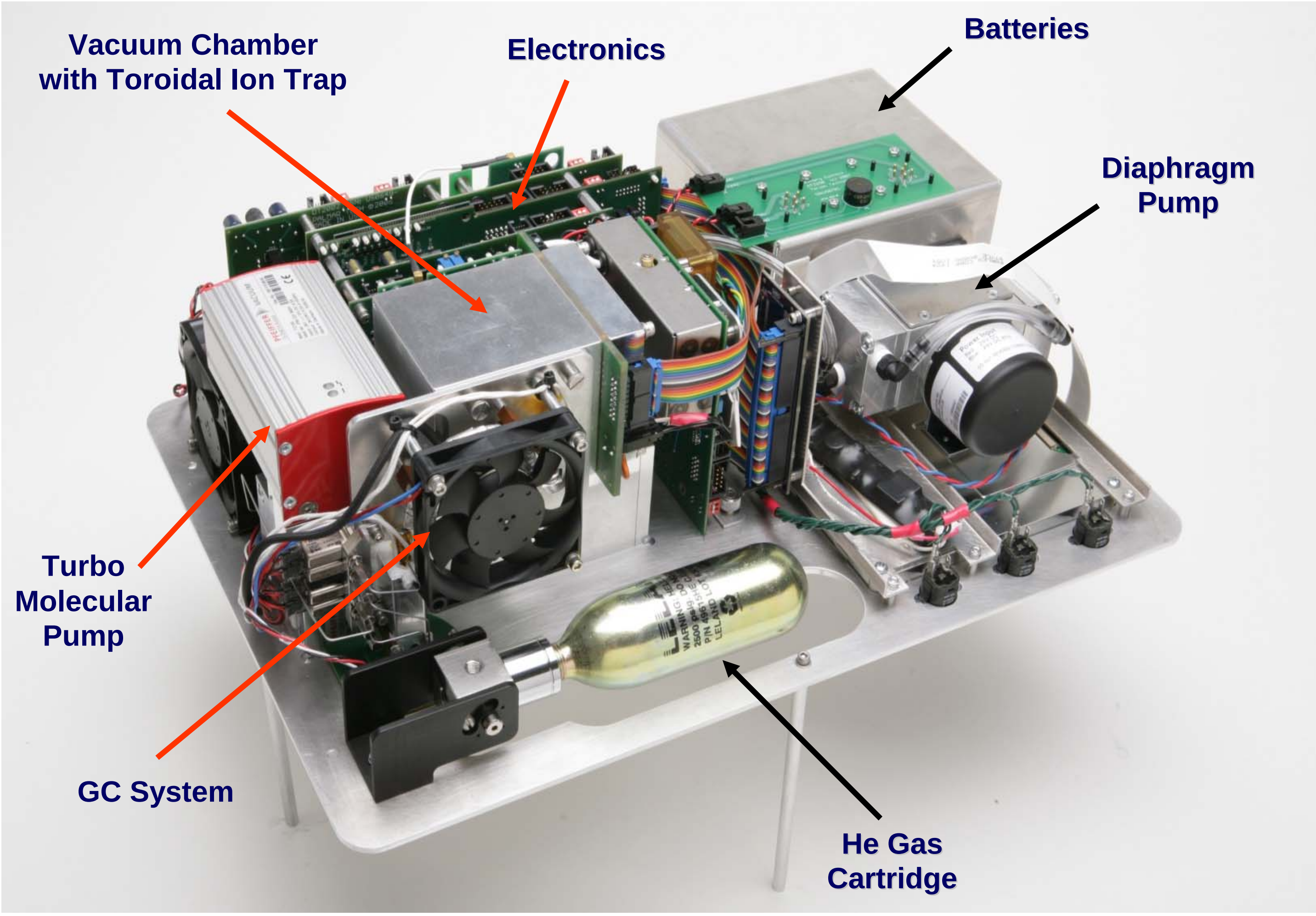
GUARDION®-7 GC-TMS Specifications

Specifications

- **Dimensions:** 47 cm x 36 cm x 18 cm
- **Weight: <13 kg or 28 lbs** (including batteries)
- **Peak Power**: ~ 80 W
- **Sample Introduction**: SPME
- **GC**: MXT-5, 5 m x 0.1 mm x 0.4 µm
- **TMS:** Toroidal Ion Trap
- **Mass Range**: 45 to 500 Daltons
- **Resolution**: 0.55 at m/z 91 (toluene)

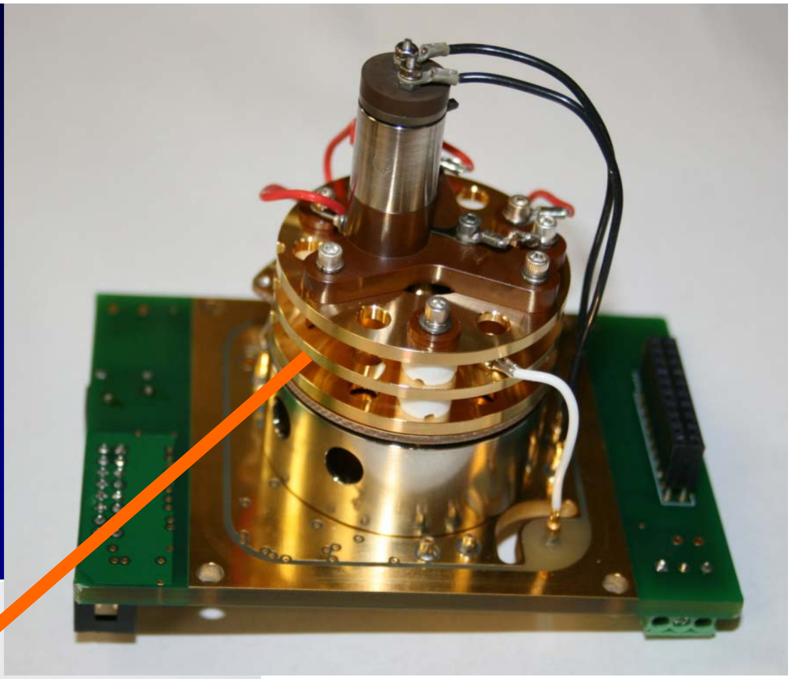
  0.80 at m/z 223 (diethylphthalate)
- **Vacuum**: turbo molecular/diaphragm pump
- **Helium Cartridges:** ~300 x 5 minute runs
- **Batteries:** ~50-75 x 5 minute runs

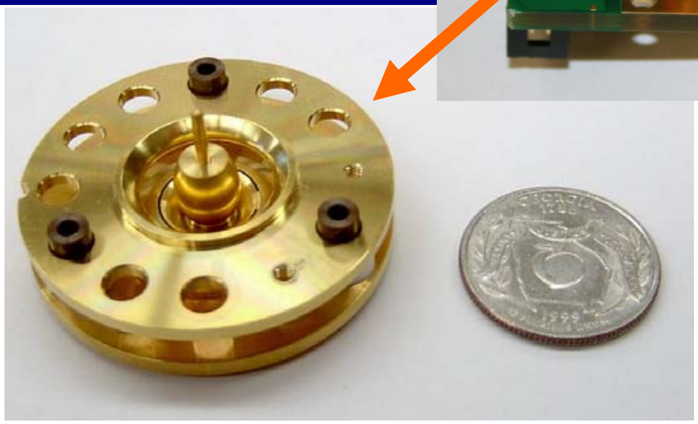
Torion GUARDION®-7 GC-TMS Components



Miniaturized Toroidal Ion Trap Mass Spectrometer

- RF Trapping Field:
  - 4 MHz
  - 1200 (max) $V_{p\text{-}p}$
- Resonance Ejection:
  - 1.8 MHz - 110 KHz
  - 5 V amplitude
- Pressures:
  - He buffer gas: 10^{-3} to 10^{-4} mbar
- r° = 2 mm





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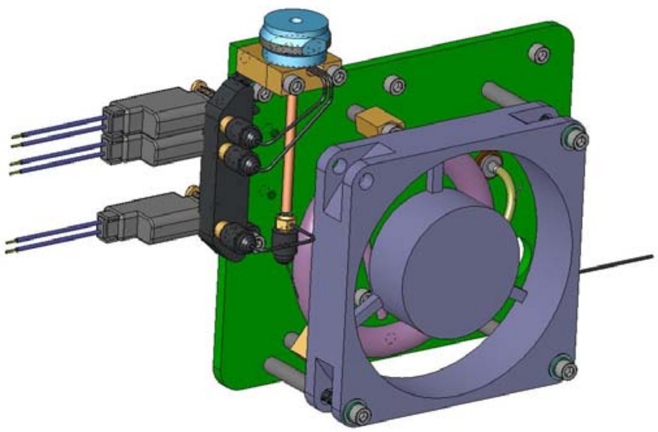
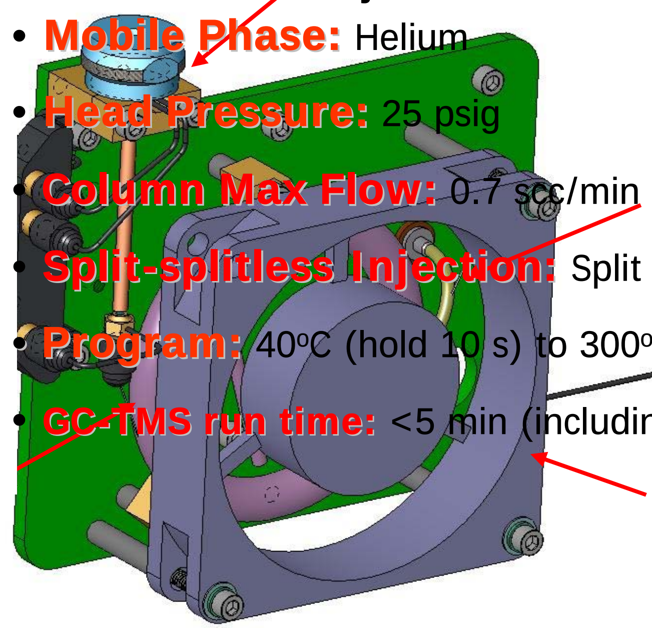
LTM Capillary Gas Chromatograph

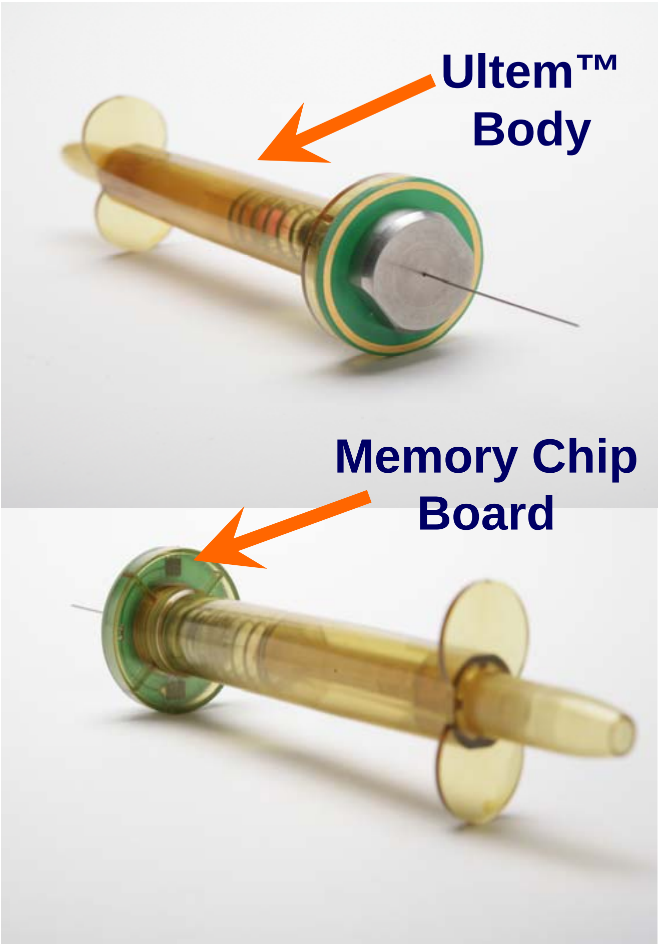
- **Column:** MXT-5 (5 m x 0.1 mm x 0.4 μm)
- **Mobile Phase:** Helium
- **Head Pressure:** 25 psig
- **Column Max Flow:** 0.7 scc/min @ 20ºC
- **Split-splitless Injection:** Split ratio 20
- **Program:** 40ºC (hold 10 s) to 300ºC (hold 10 s) @ 120ºC/min
- **GC-TMS run time:** <5 min (including cooling & data analysis)





Advantages of SPME Sample Collection and Injection

- Solvent-free
- Reusable
- Finite sampling capacity
- Simple to use
- Faster than other extraction techniques
- Low cost per sample
- Applicable to air, liquid, and solid samples
- Different phases available for selective sampling



Easy to Use Software

- On-board and Computer-based Software
- Three button instrument operation
- Simple GUI interface - results are clear and concise
- Automated target compound identification

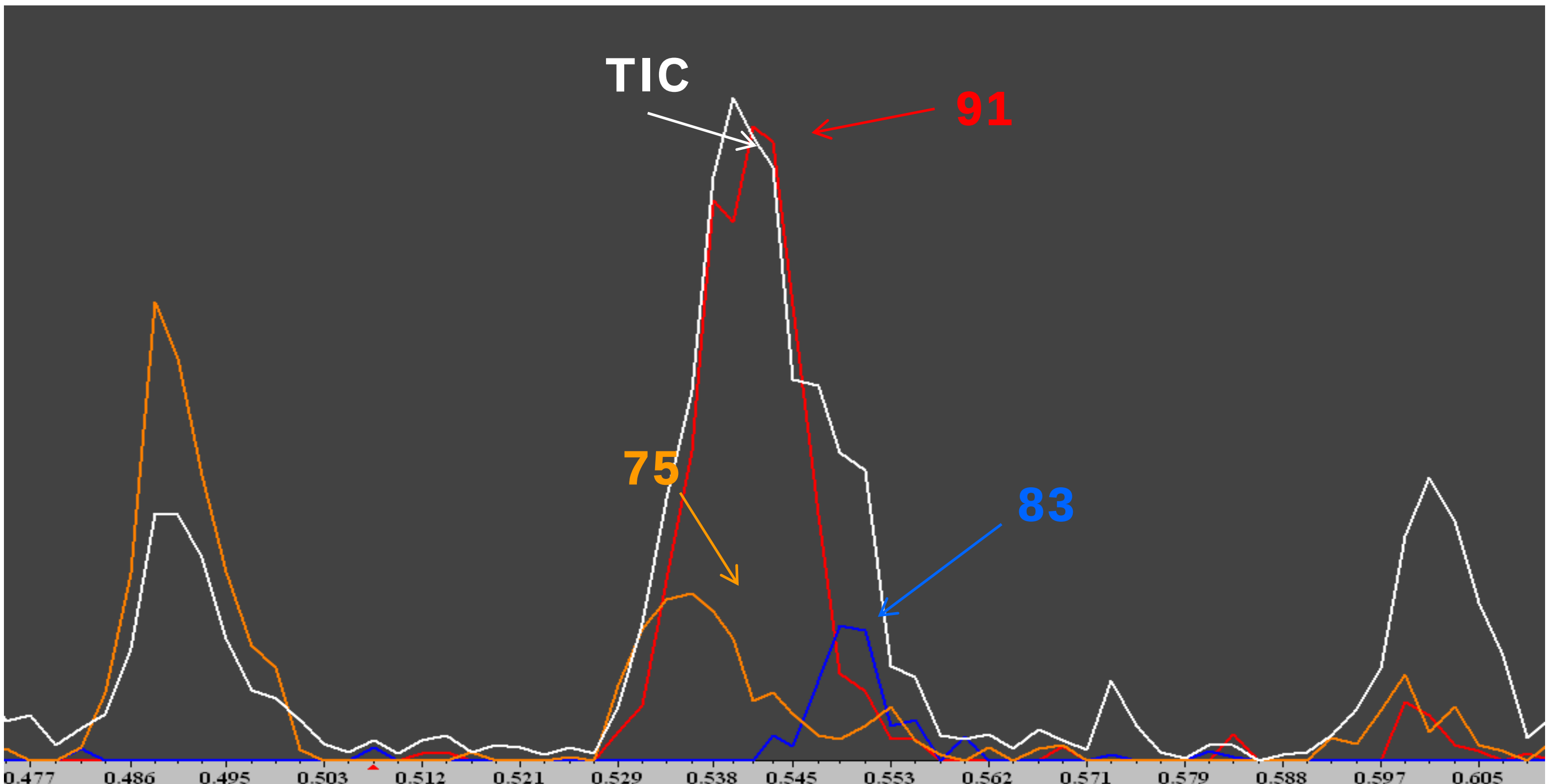
Found 12 of 12 compounds in C03003C0

Chemical	HL	RT	A%	Conf
Benzene	TIC-M	30	0.698	96
Toluene	TIC-M	44	1.184	97
Tetrachloroethylene	TIC-M	48	0.102	88
1,2-dibromoethane	TIC-M	49	0.040	85
Tribromomethane	TIC-M	57	0.470	94
p-Bromofluorobenze	TIC-M	61	0.033	65
Butyl benzene	TIC-M	75	0.224	95
Di-n-butyl sulfide	TIC-M	78	1.287	94
Nitrobenzene	TIC-M	81	0.093	91

Up | Done | Down

On Board Peak Deconvolution

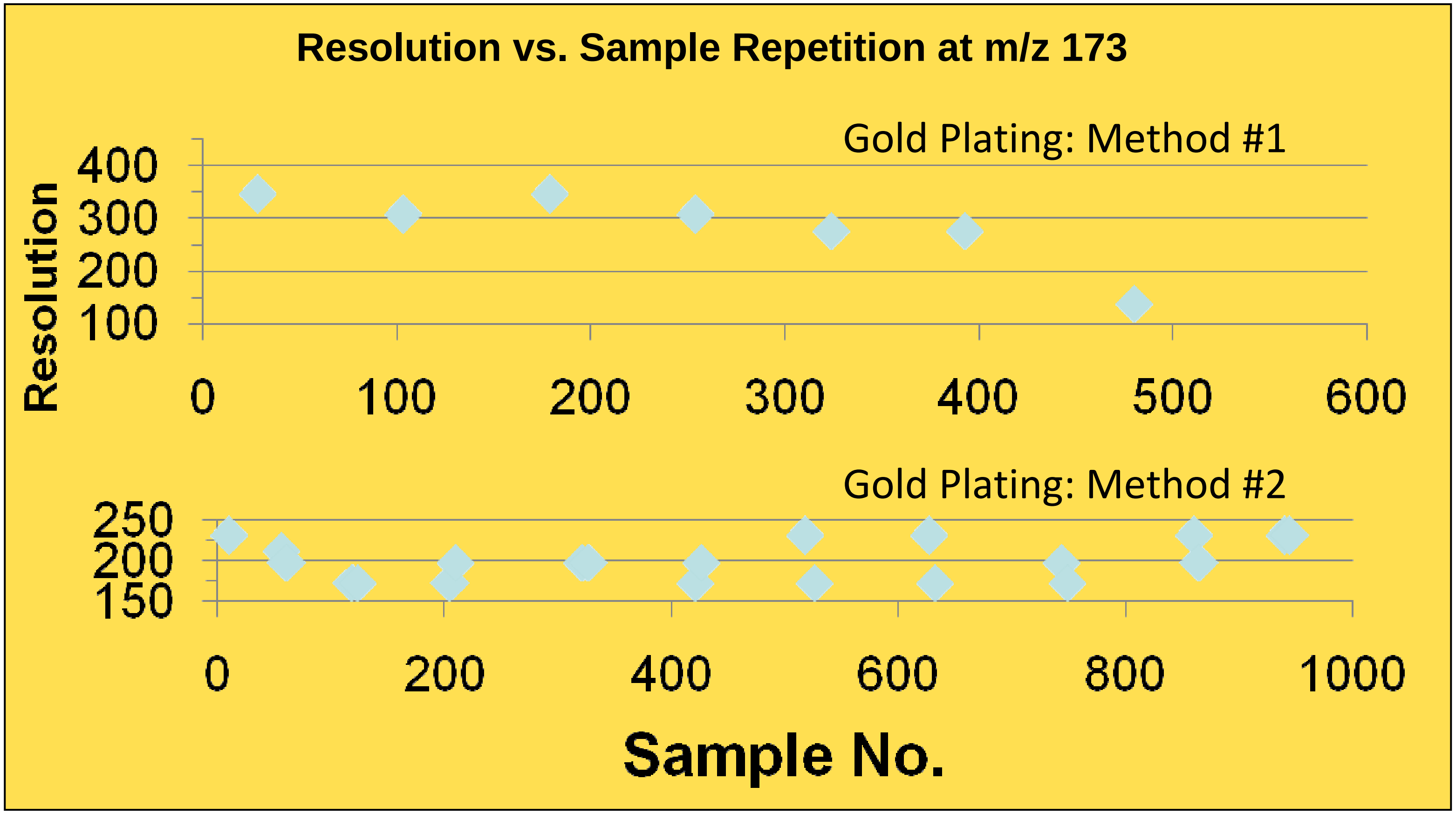
- Original mass spectral data effectively resolved into components
- Extract accurate individual mass spectra for each analyte
- Accurately distribute the signal from masses shared by several components



Recent TMS Enhancements

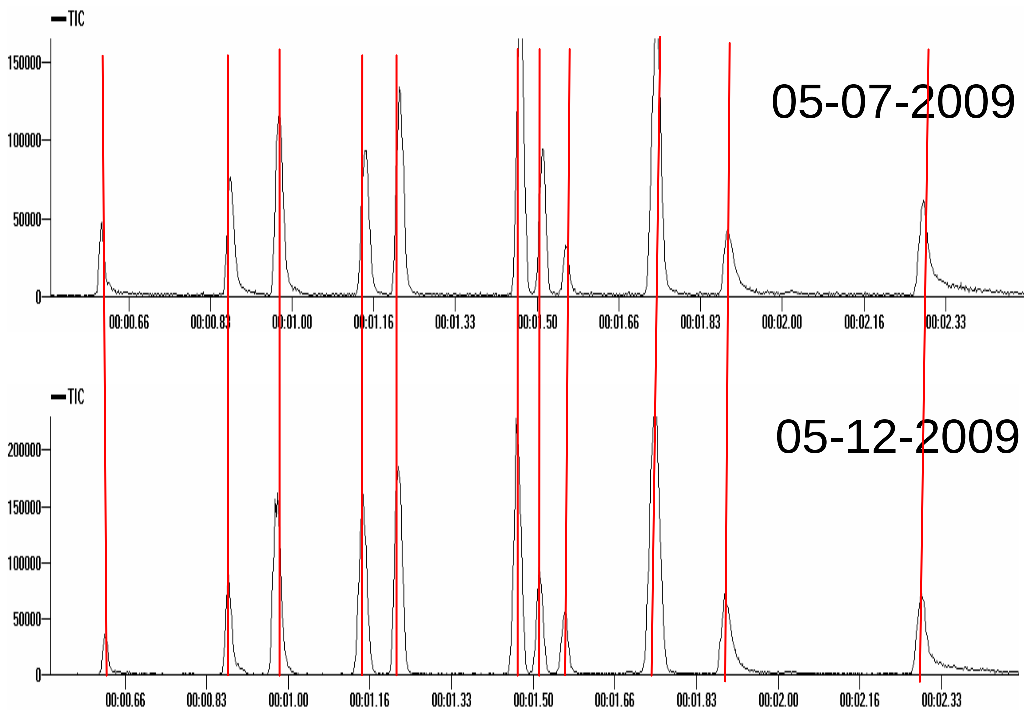
- Surface Finish
- Electronic Pressure Control
- Better Modeling
- Improved Slit Design

Effects of Surface Finish on TMS Performance



Electronic Pressure Control

- Increase chromatographic performance and reproducibility for more accurate target compound identification
- Improves MS reproducibility due to constant helium levels in trap



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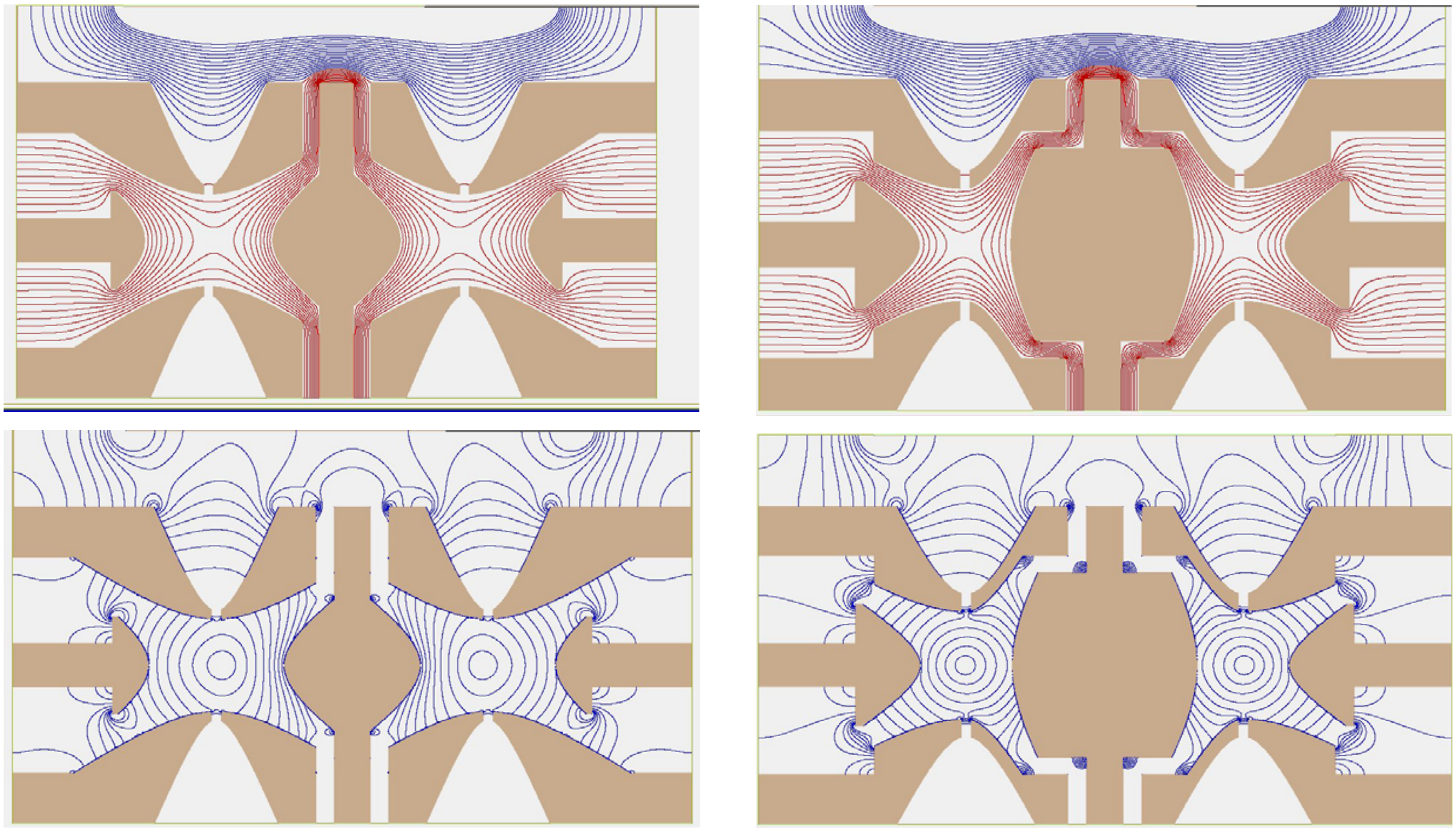
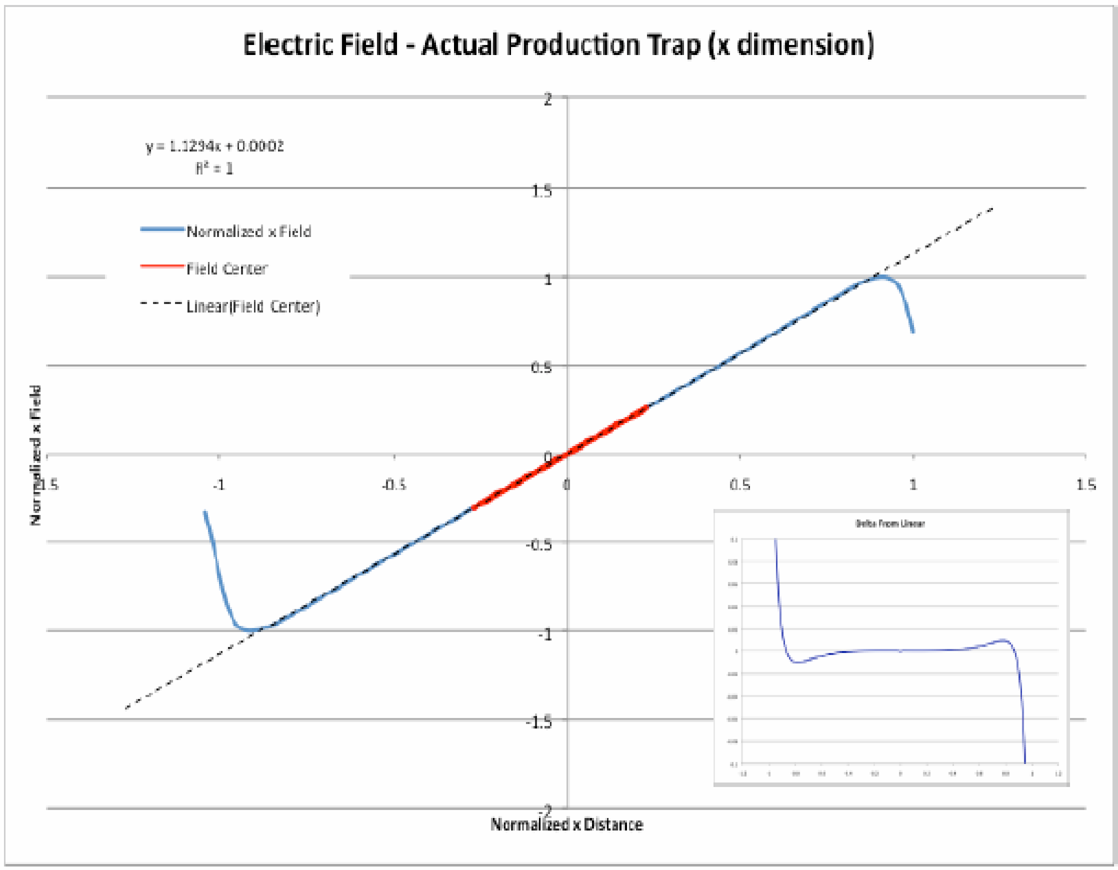
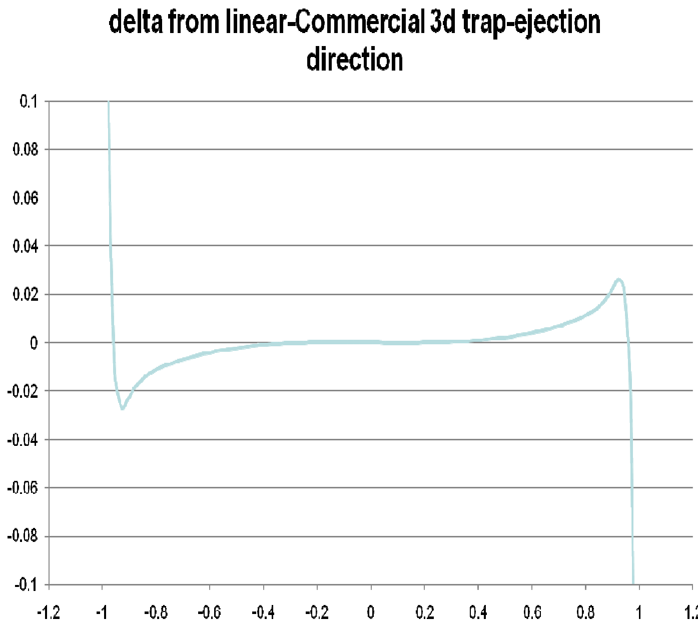
Simion Equipotential and Potential Gradient Plots

Symmetric Toroidal Trap | Asymmetric Toroidal Trap



Electric Field Gradient Plots for TMS and CIT





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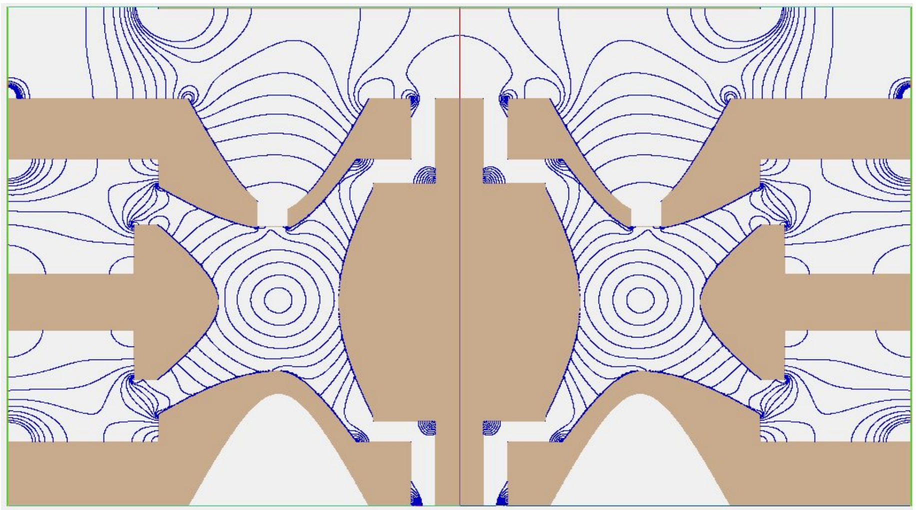
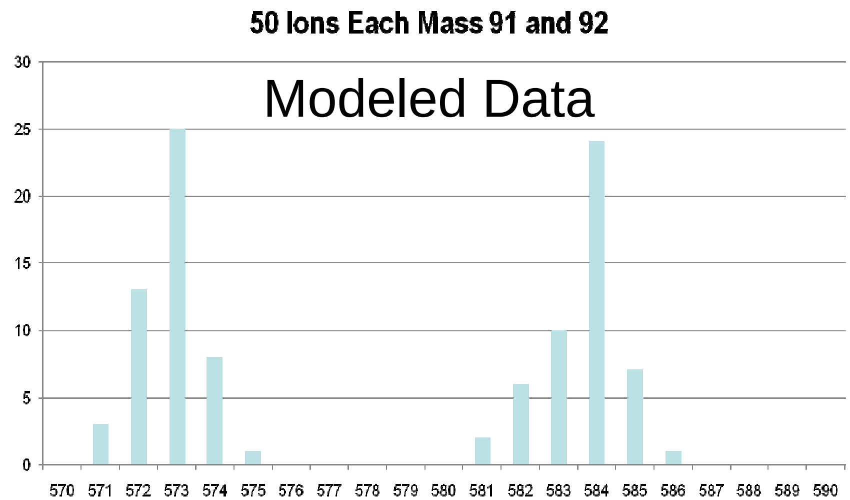
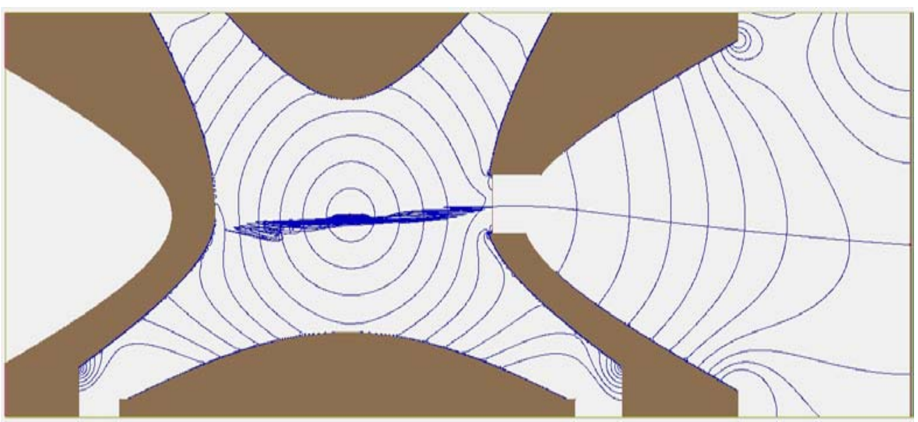
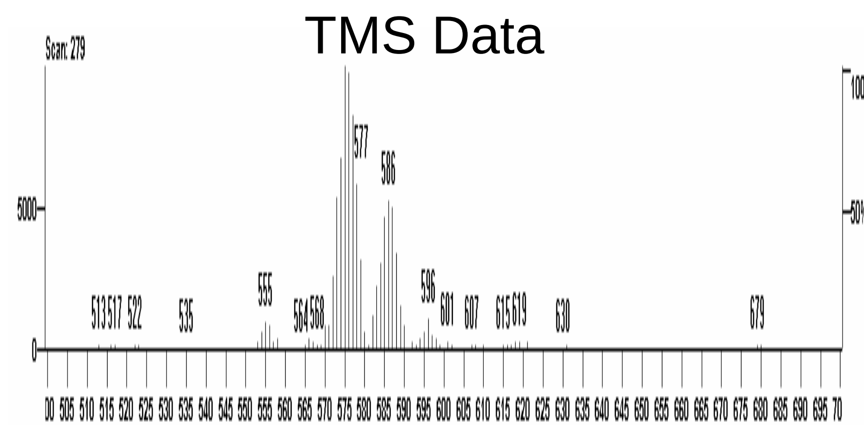
Simion Potential Gradient Plot and Ion Flight Modeling

Asymmetric Toroidal Trap with Screened Slit Modification

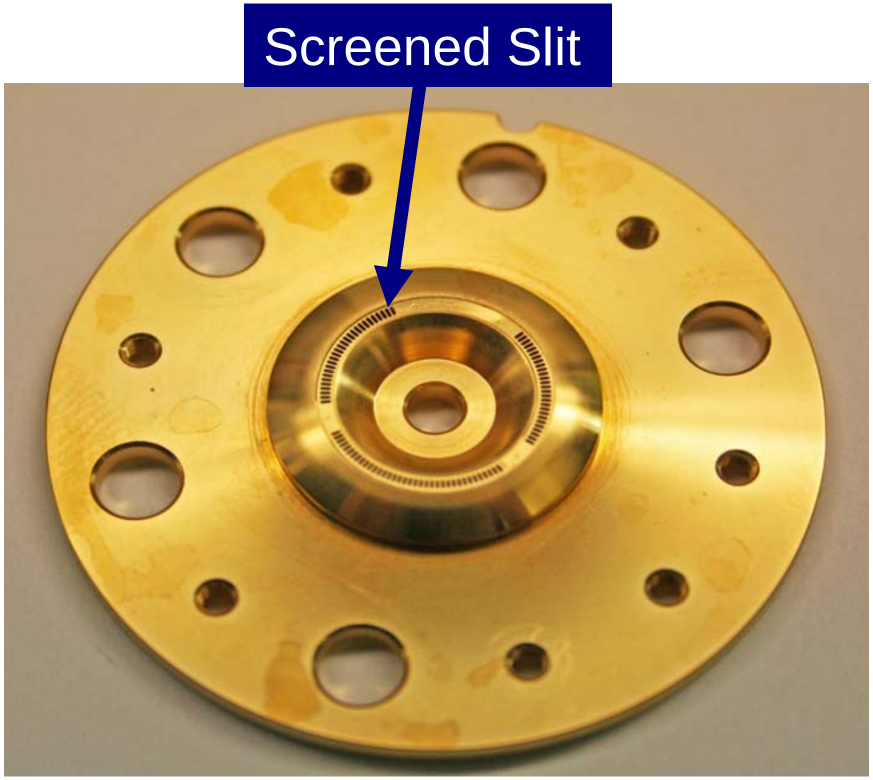






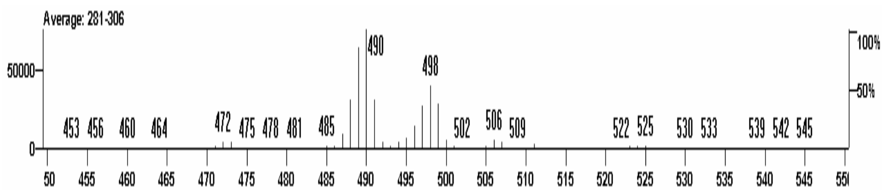


EDM and Screened Slits: Detector-side End Cap

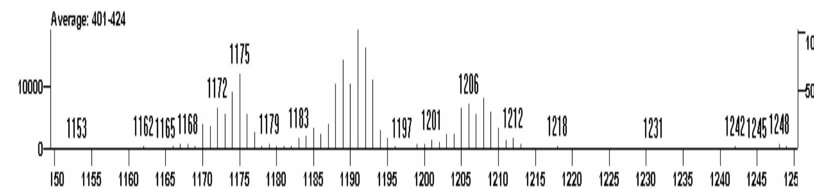


Raw Data From EDM and Screened Slits

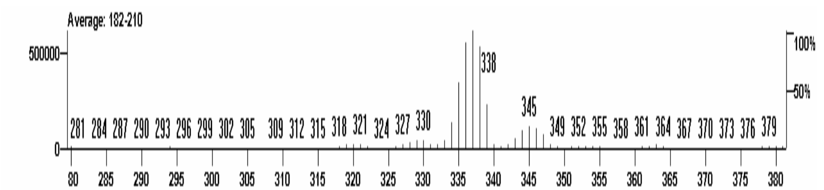
Toluene Mass 91 and 92 EDM Slits



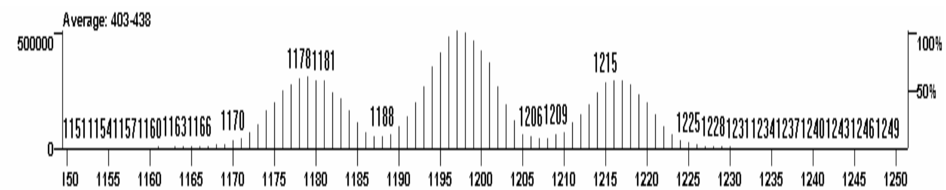
Bromoform Mass 171, 173 and 175 EDM Slits



Toluene Mass 91 and 92 Screened Slits



Bromoform Mass 171,173 and 175 Screened Slits



Average of All Scans Across Chromatographic Peak

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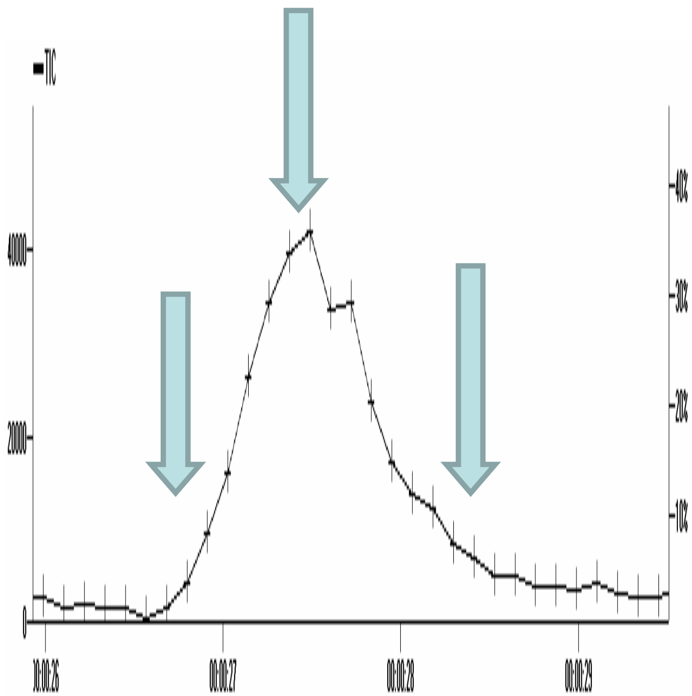
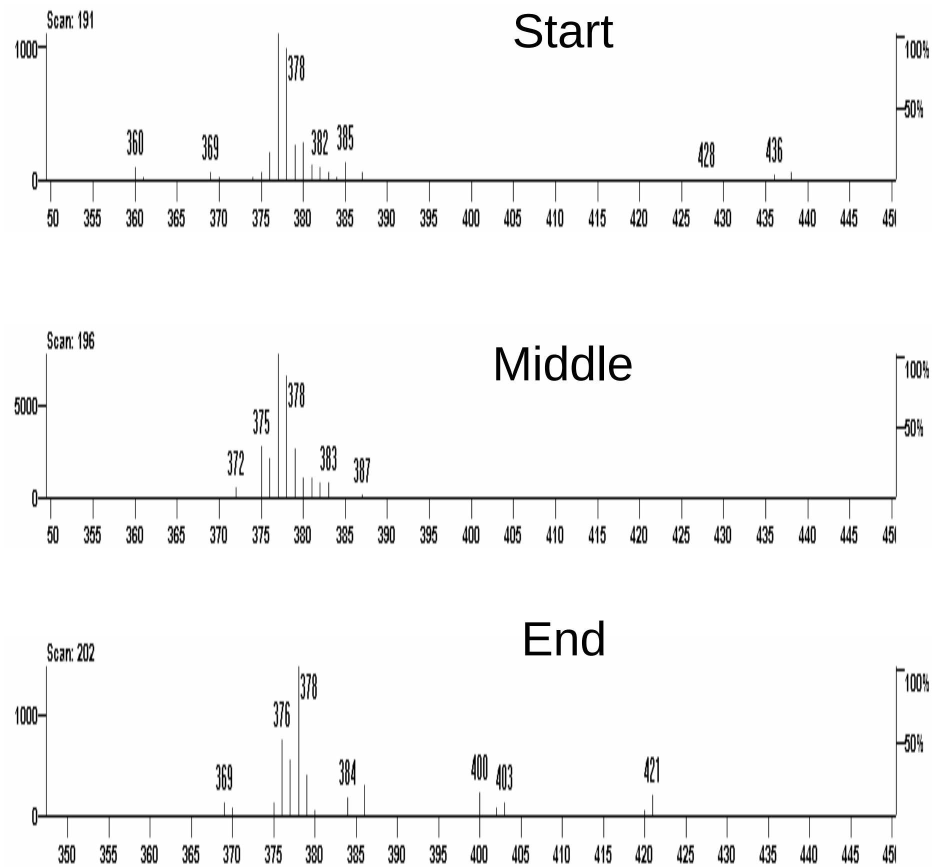
Scan-to-Scan Reproducibility with EDM Slit Trap

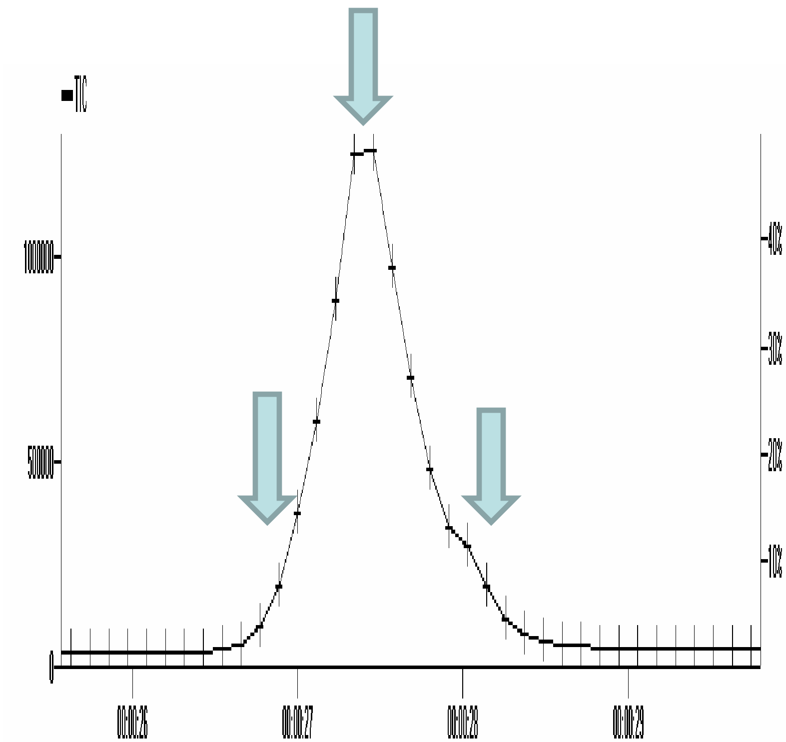
Toluene

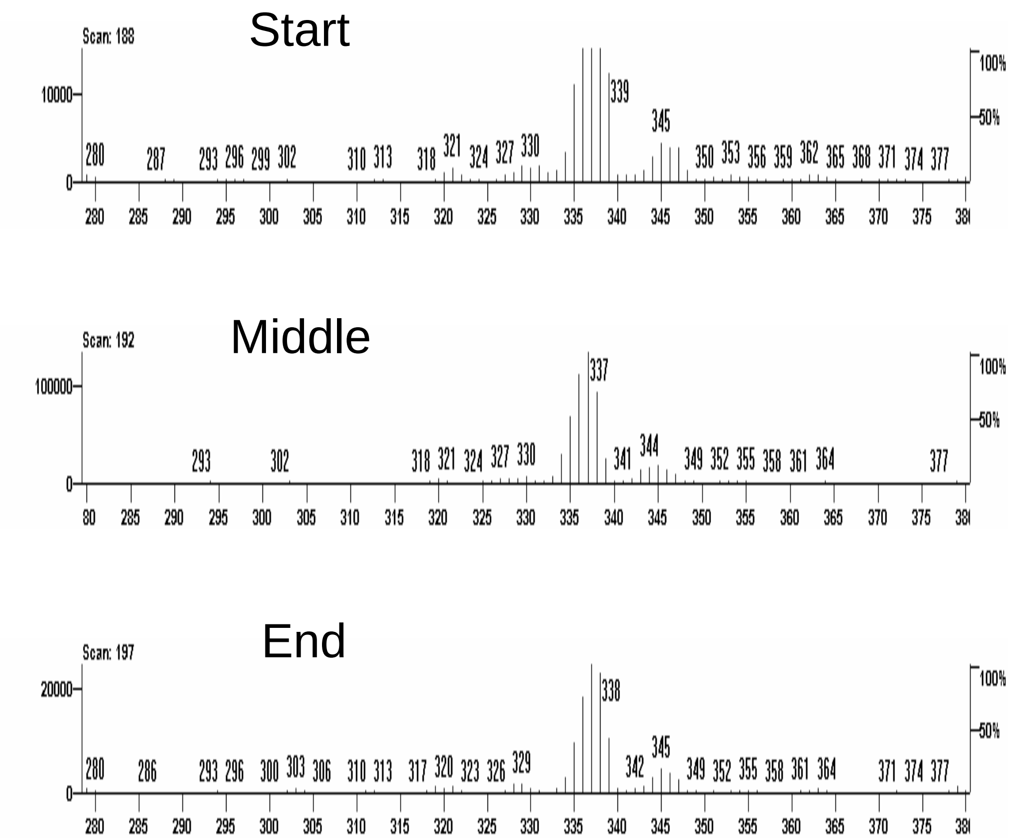




Scan-to-Scan Reproducibility with Screened Slits

Toluene





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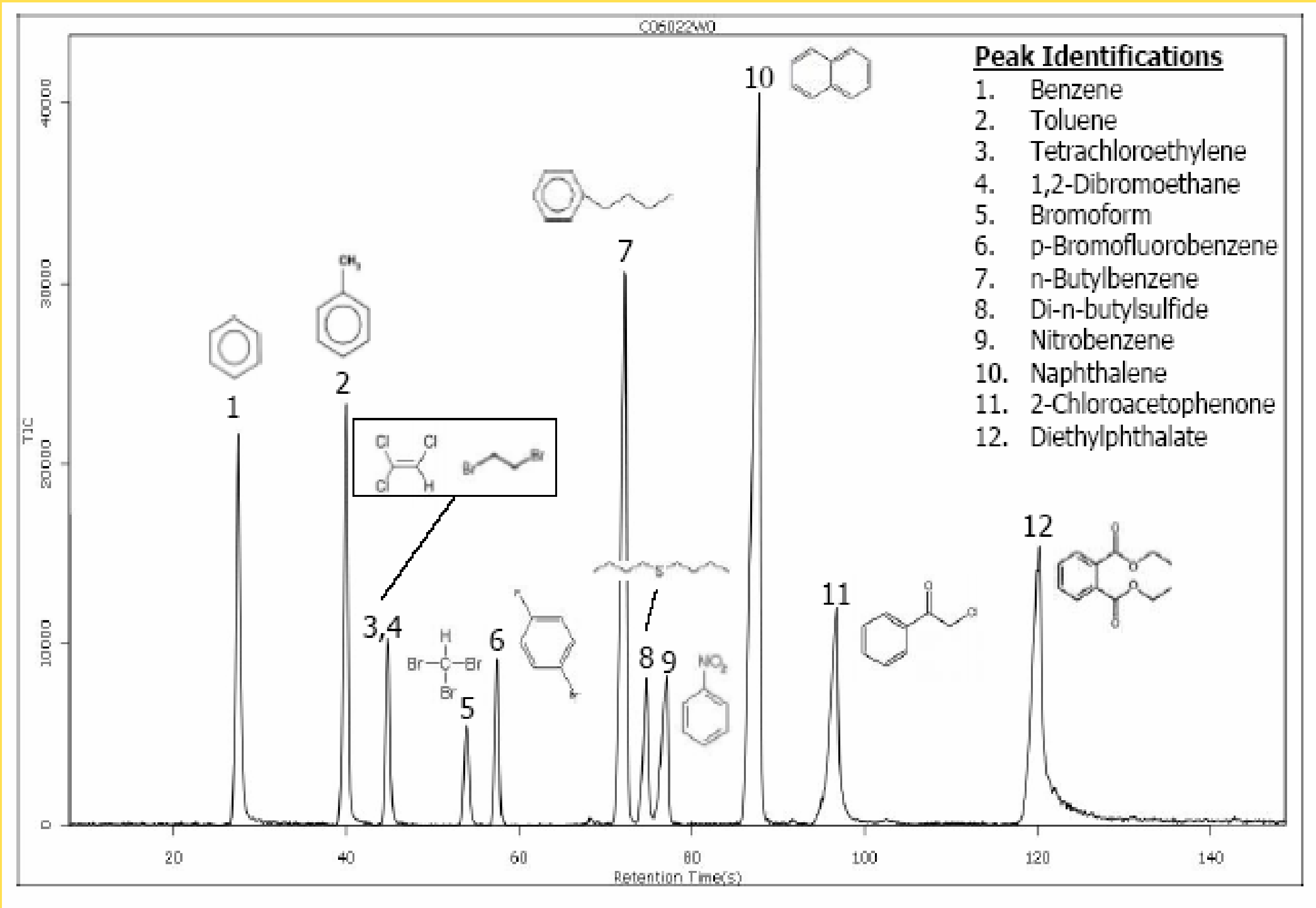
Recent GC-TMS Applications

GC-TMS Analysis of Hazardous Compounds



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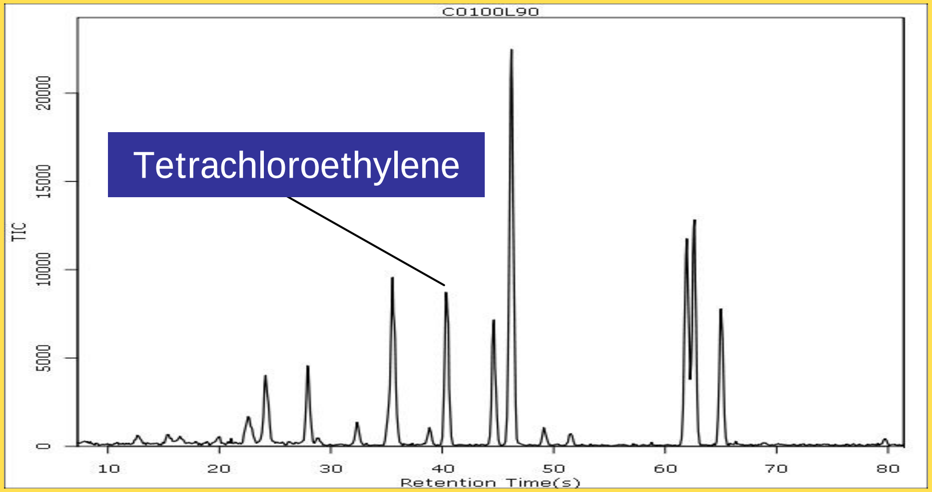
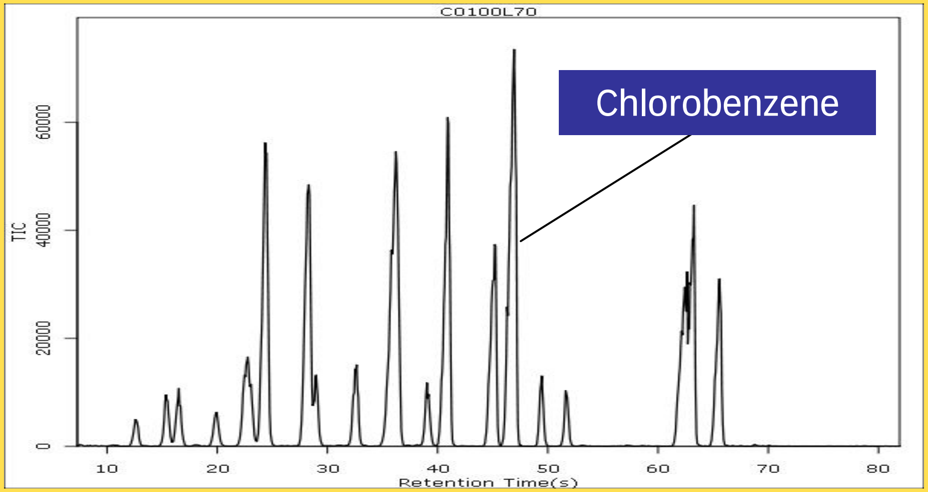
Volatiles (VOCs) in Water

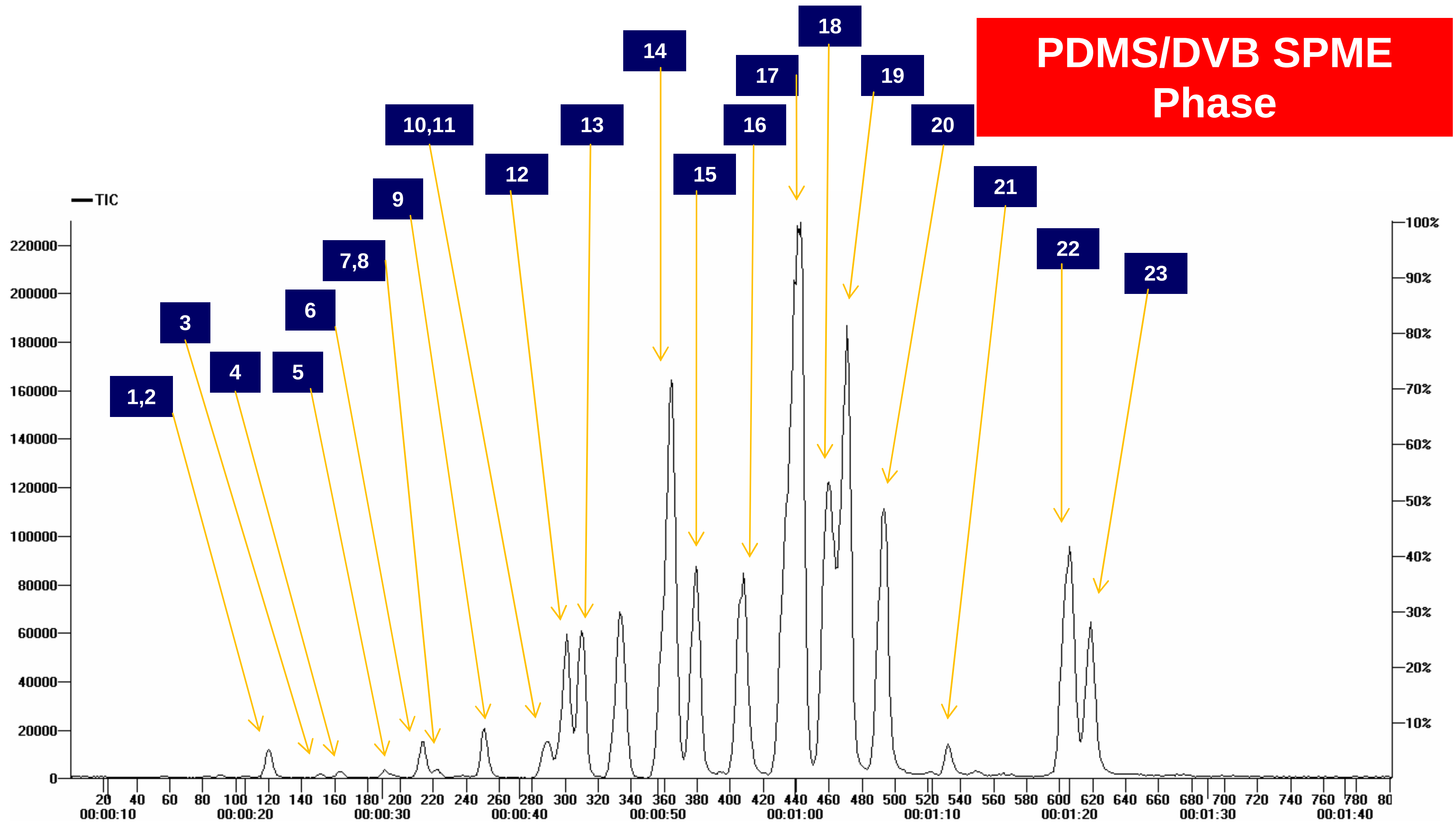


Headspace
75 ppb in water



Direct sampling
20 ppm in water

Volatiles (VOCs) in Soil



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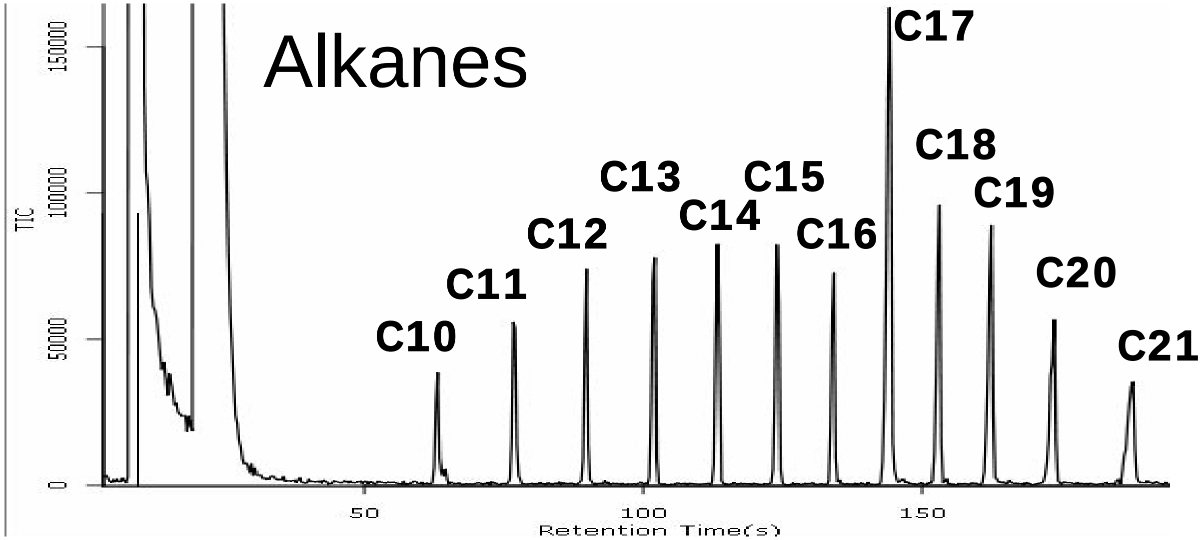
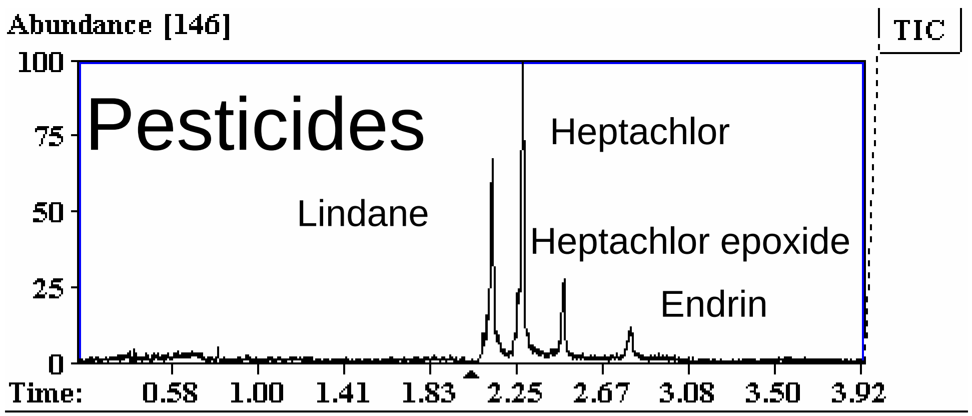
Analysis of Semivolatile Compounds



C-20 BP = 342.7ºC



Melting point of Endrin = 200ºC

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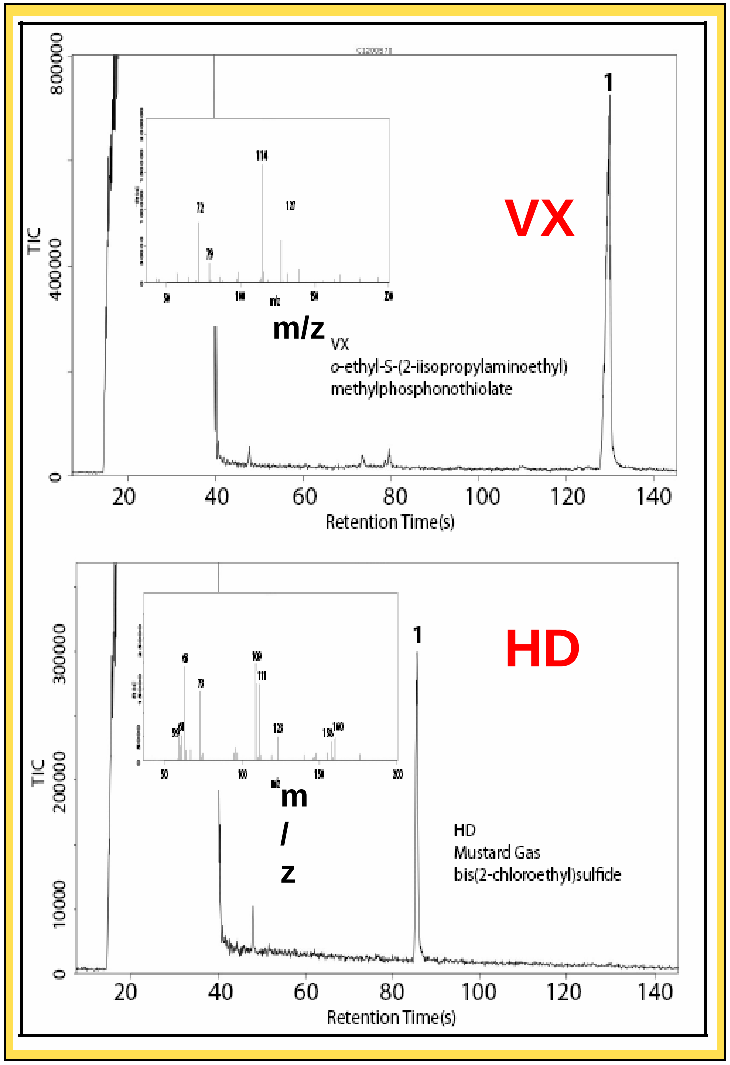
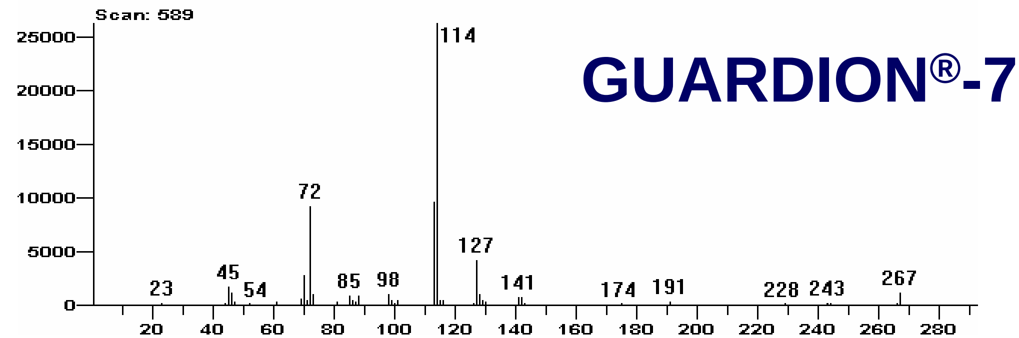
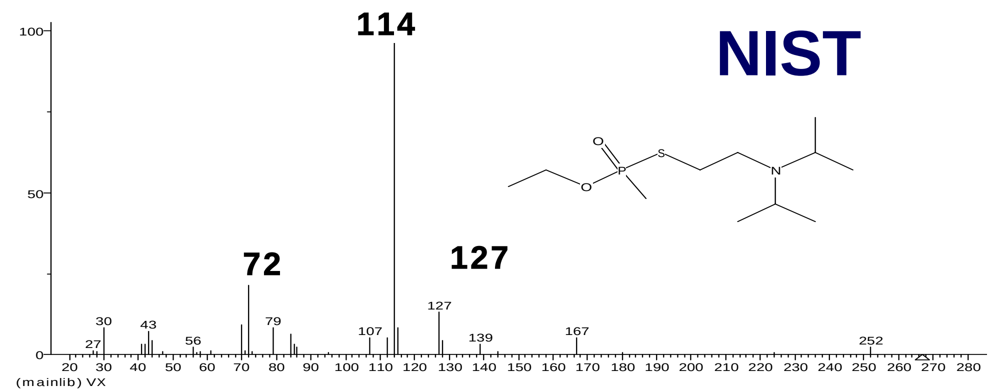
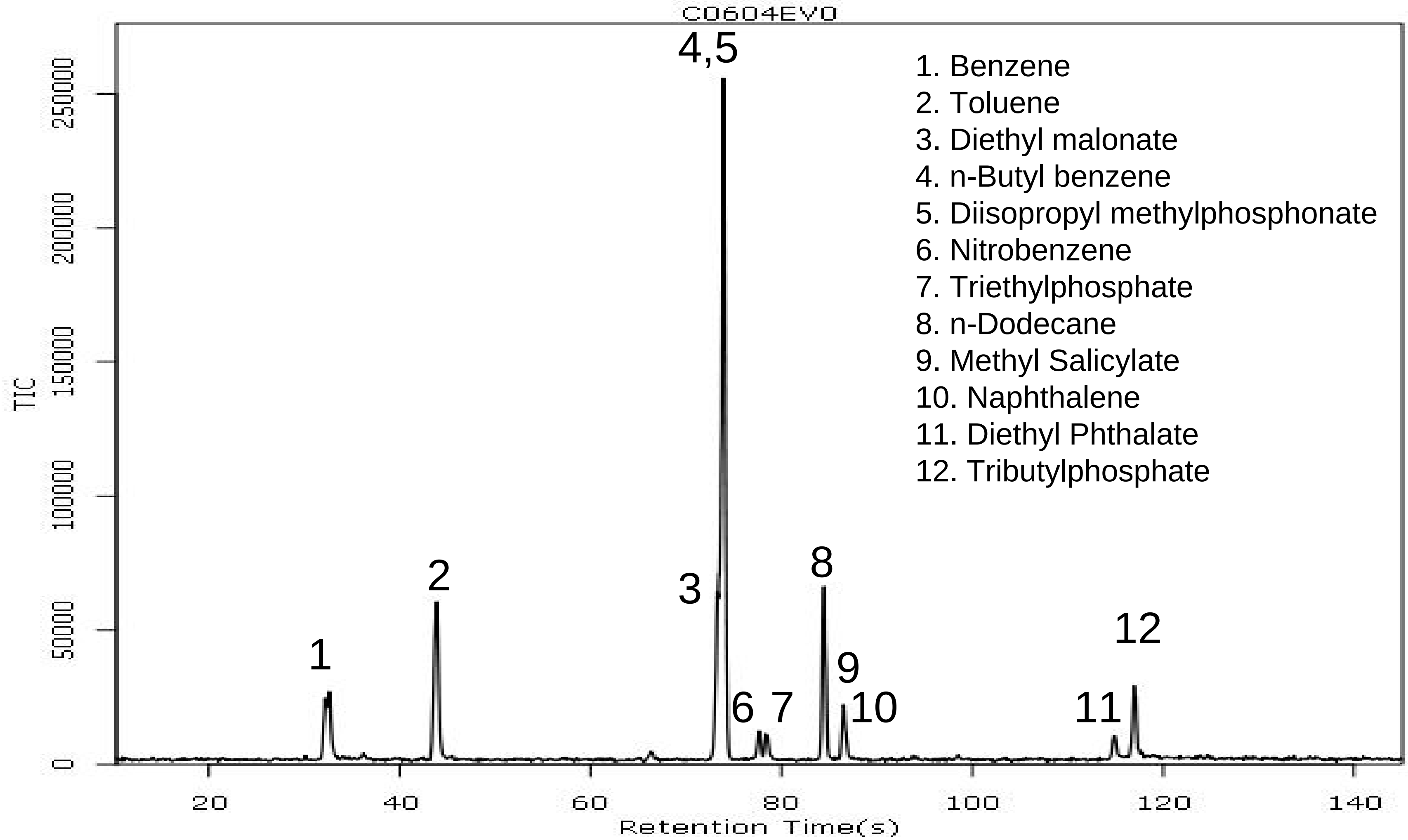
Analysis of Chemical Warfare Agents



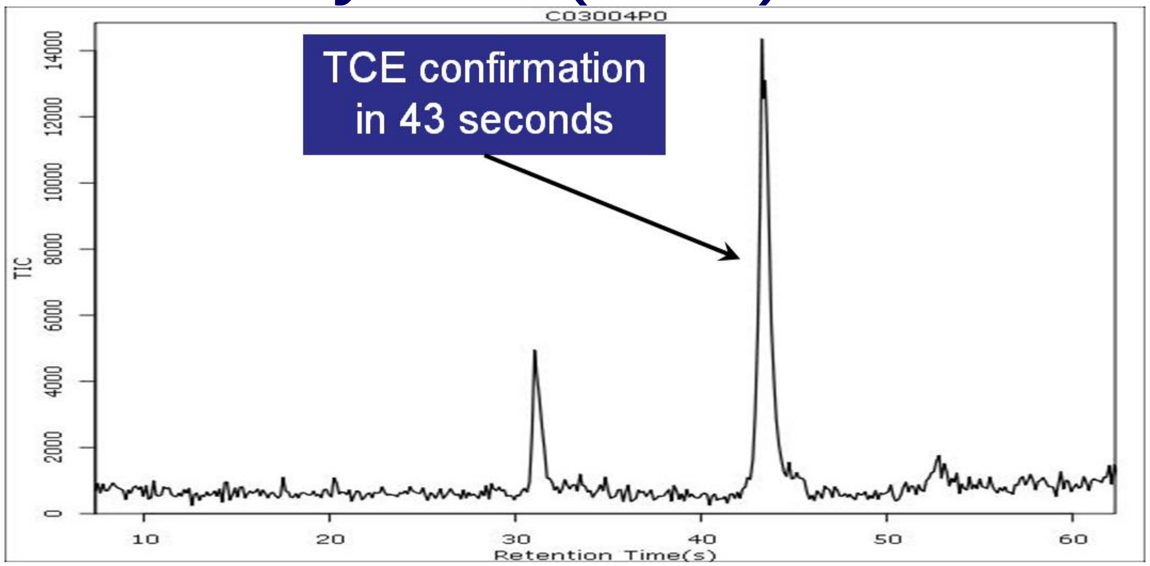


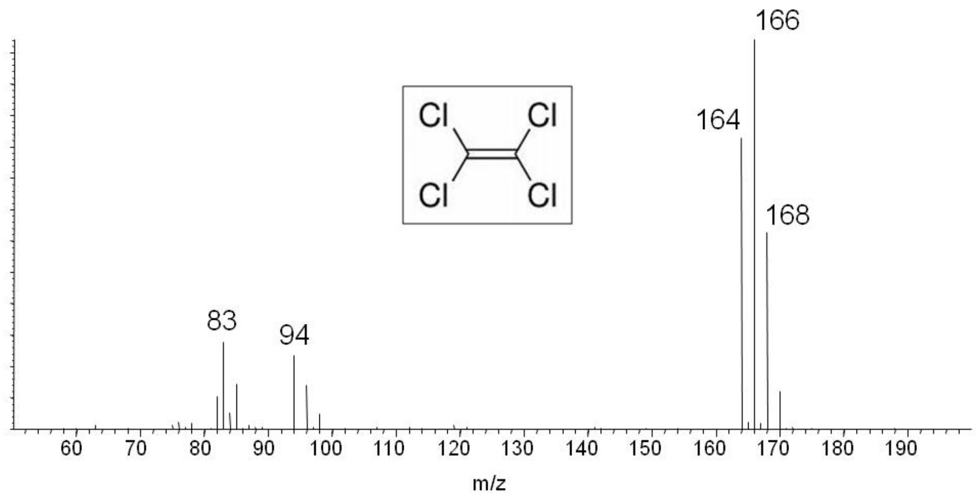


CWA Simulants and TICs

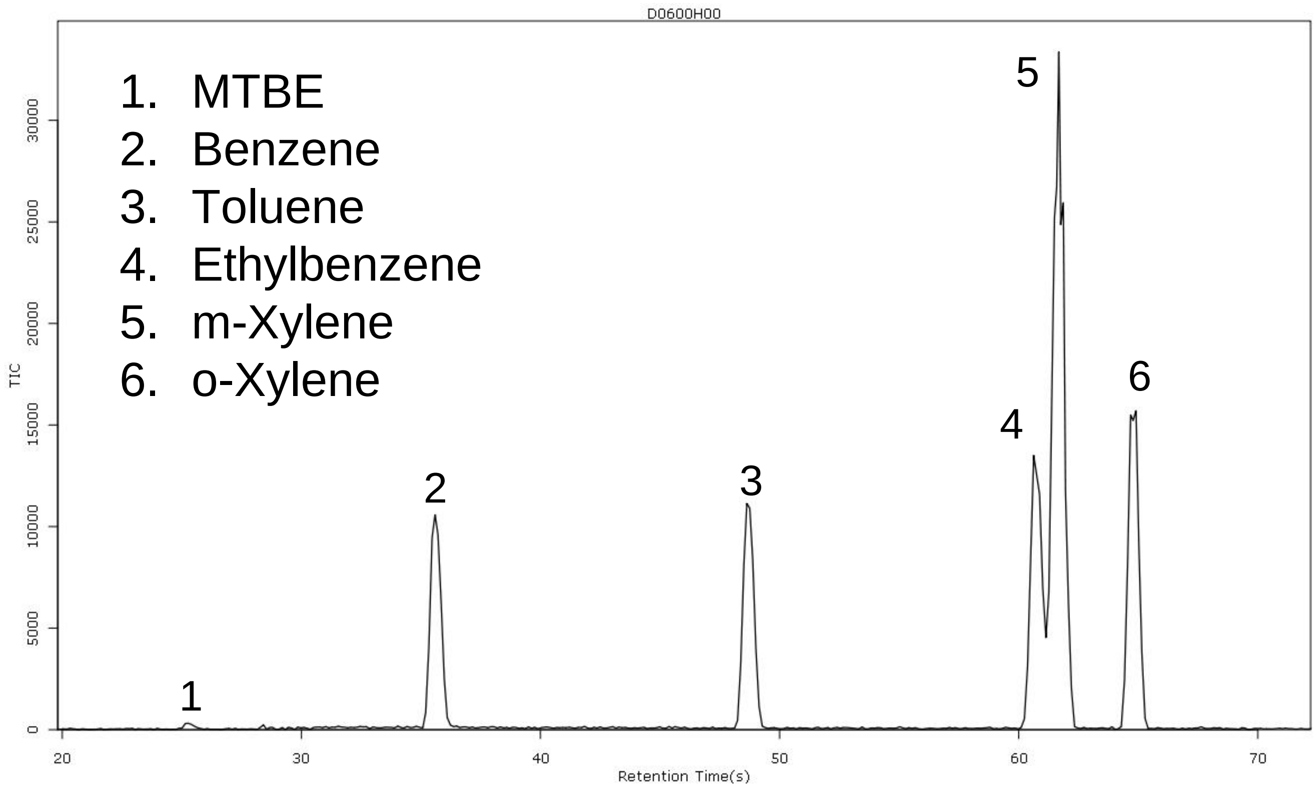


Tetrachloroethylene (TCE) Contamination





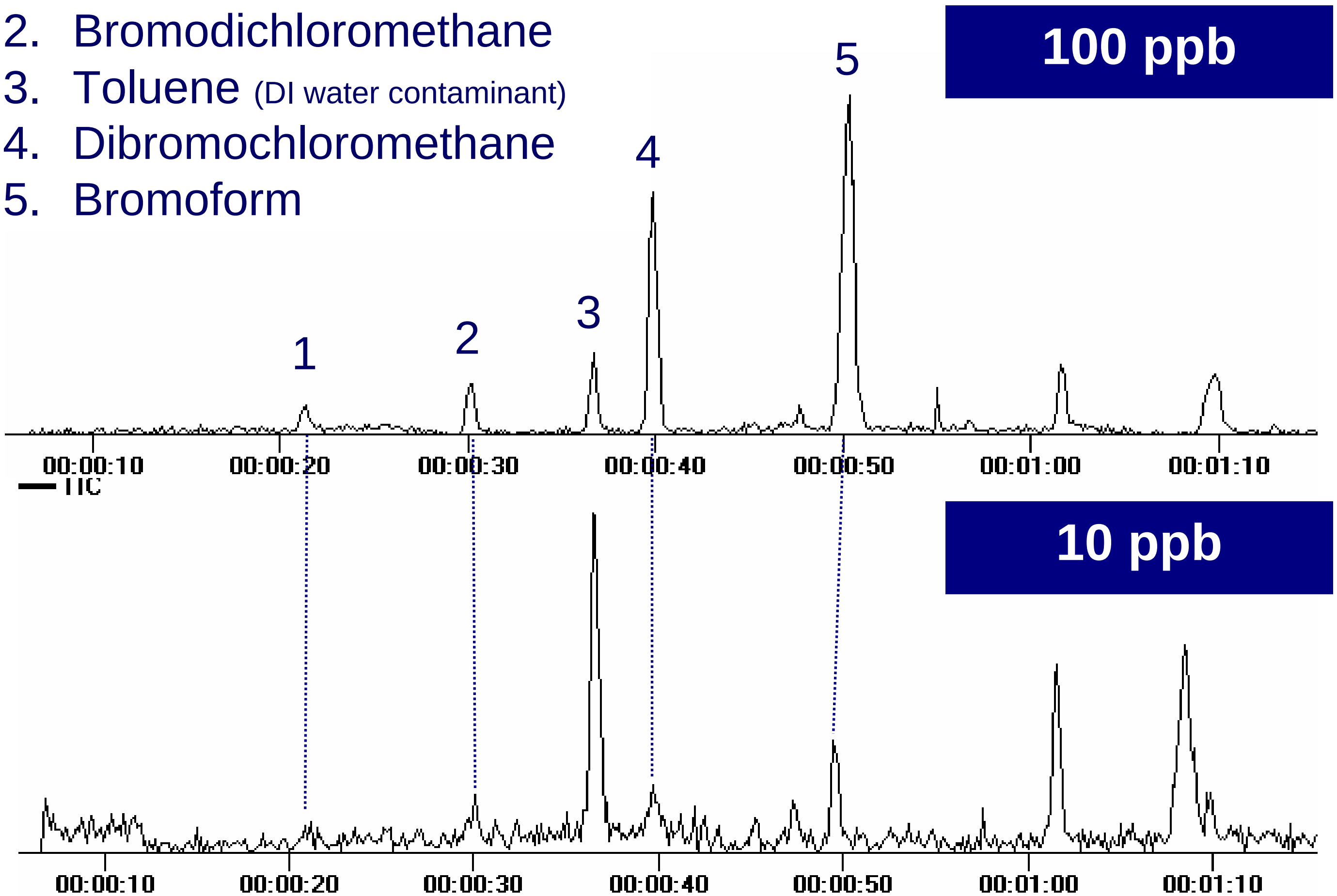
BTEX & MTBE in Ground Water



15 s headspace sample, 10 ppm

SPME Analysis of Trihalomethanes in Water

1. Chloroform
2. Bromodichloromethane
3. Toluene (DI water contaminant)
4. Dibromochloromethane
5. Bromoform



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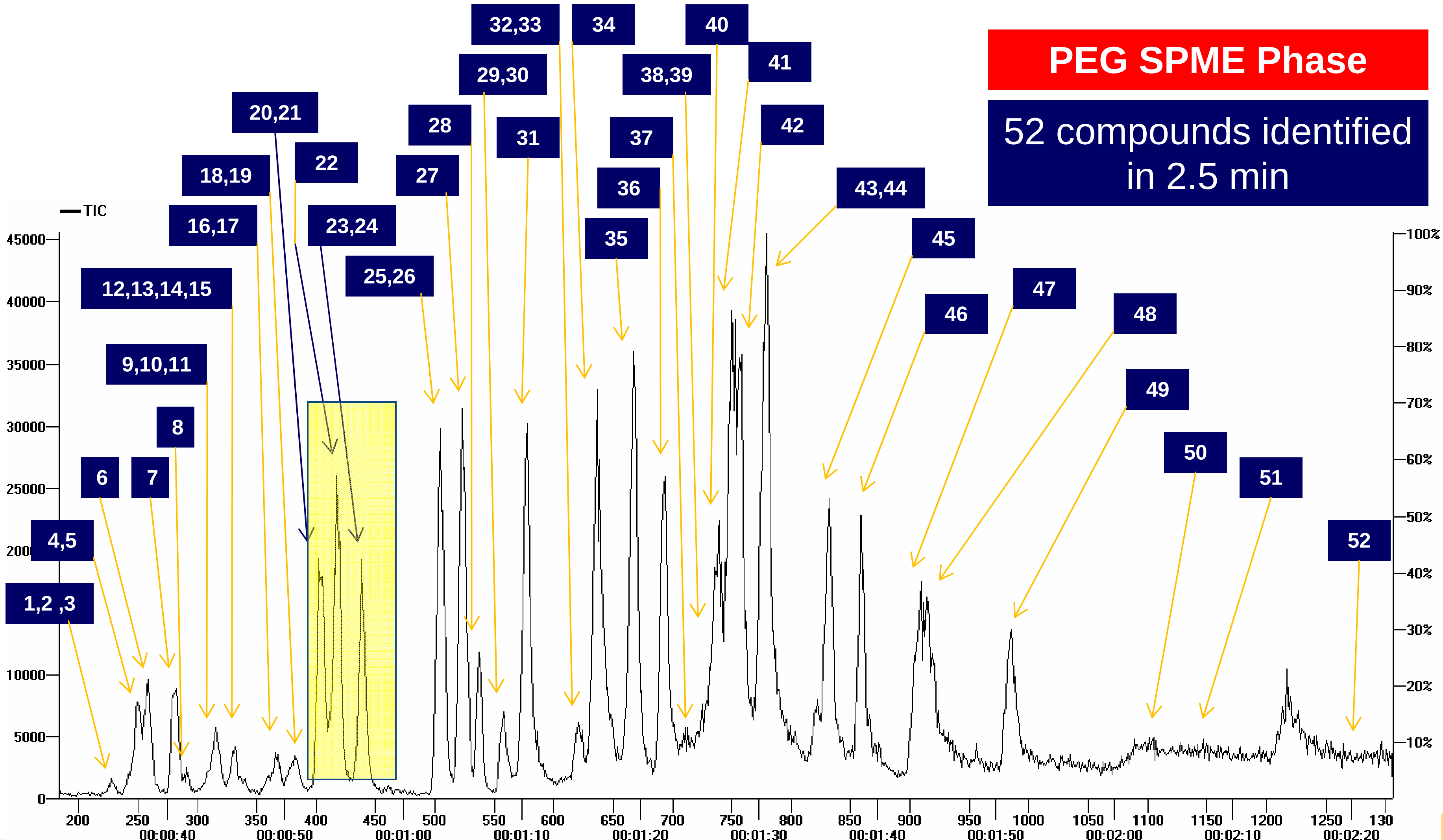
Semivolatiles (SVOCs) in Water

PEG SPME Phase

52 compounds identified in 2.5 min



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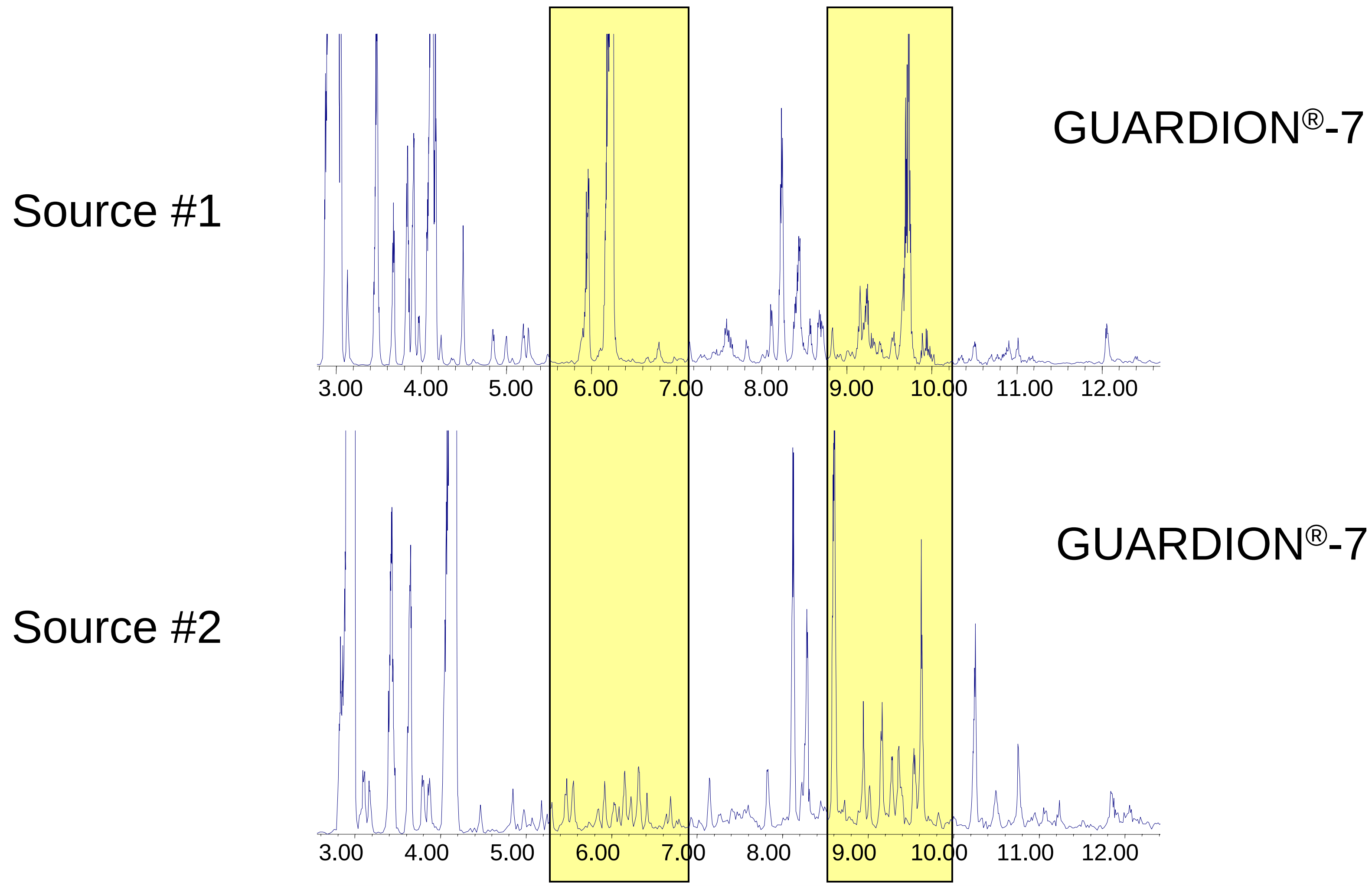
Spiked into Tap Water: 1-10 ppm each

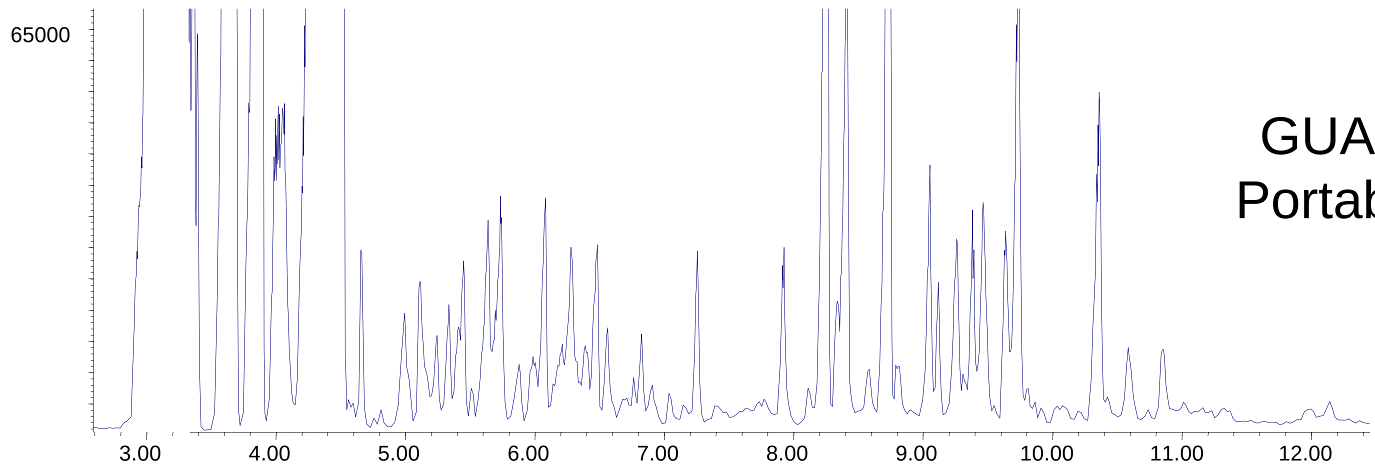
Semivolatiles (SVOCs) in Water

1	Aniline	19	2,4-Dimethylphenol	37	2,4-Dinitrotoluene
2	Phenol	20	2,4-Dichlorophenol	38	2,3,4,6-Tetrachlorophenol
3	Bis(2-chloroethyl)ether	21	1,2,4-Trichlorobenzene	39	2,3,5,6-Tetrachlorophenol
4	2-Chlorophenol	22	Naphthalene	40	Diethylphthalate
5	1,3-Dichlorobenzene	23	4-Chloroaniline	41	4-Chlorophenyl phenyl ether
6	1,4-Dichlorobenzene	24	Hexachlorobutadiene	42	Fluorene
7	1,2-Dichlorobenzene	25	4-Chloro-3-methylphenol	43	Diphenylamine
8	Bis(2-chloroisopropyl)ether	26	2-Methylnaphthalene	44	Azobenzene
9	Benzyl alcohol	27	1-Methylnaphthalene	45	4-Bromophenyl phenyl ether
10	N-Nitroso-di-n-propylamine	28	Hexachlorocyclopentadiene	46	Hexachlorobenzene
11	Hexachloroethane	29	2,4,6-Trichlorophenol	47	Phenanthrene
12	2-Methylphenol	30	2,4,5-Trichlorophenol	48	Anthracene
13	4-Methylphenol	31	2-Chloronaphthalene	49	Di-n-butylphthalate
14	3-Methylphenol	32	2-Nitroaniline	50	Fluoranthene
15	Nitrobenzene	33	Dimethylphthalate	51	Pyrene
16	Isophorone	34	Acenaphthylene	52	Benzyl butyl phthalate
17	2-Nitrophenol	35	Acenaphthene		
18	Bis(2-chloroethoxy)methane	36	Dibenzofuran		

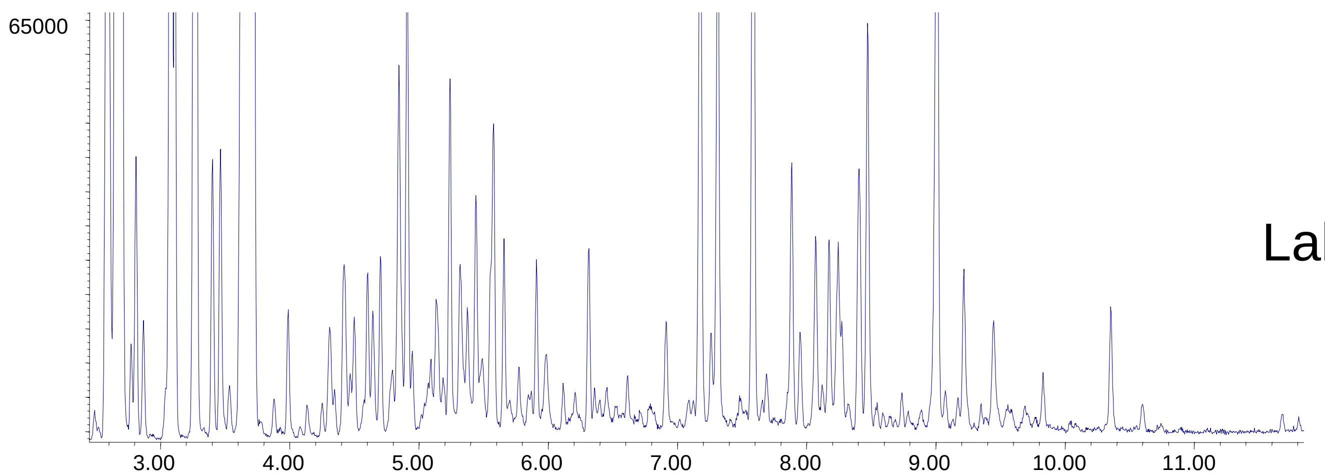
Frankincense (spice)



Frankincense (Source #2)



GUARDION®-7
Portable GC-TMS



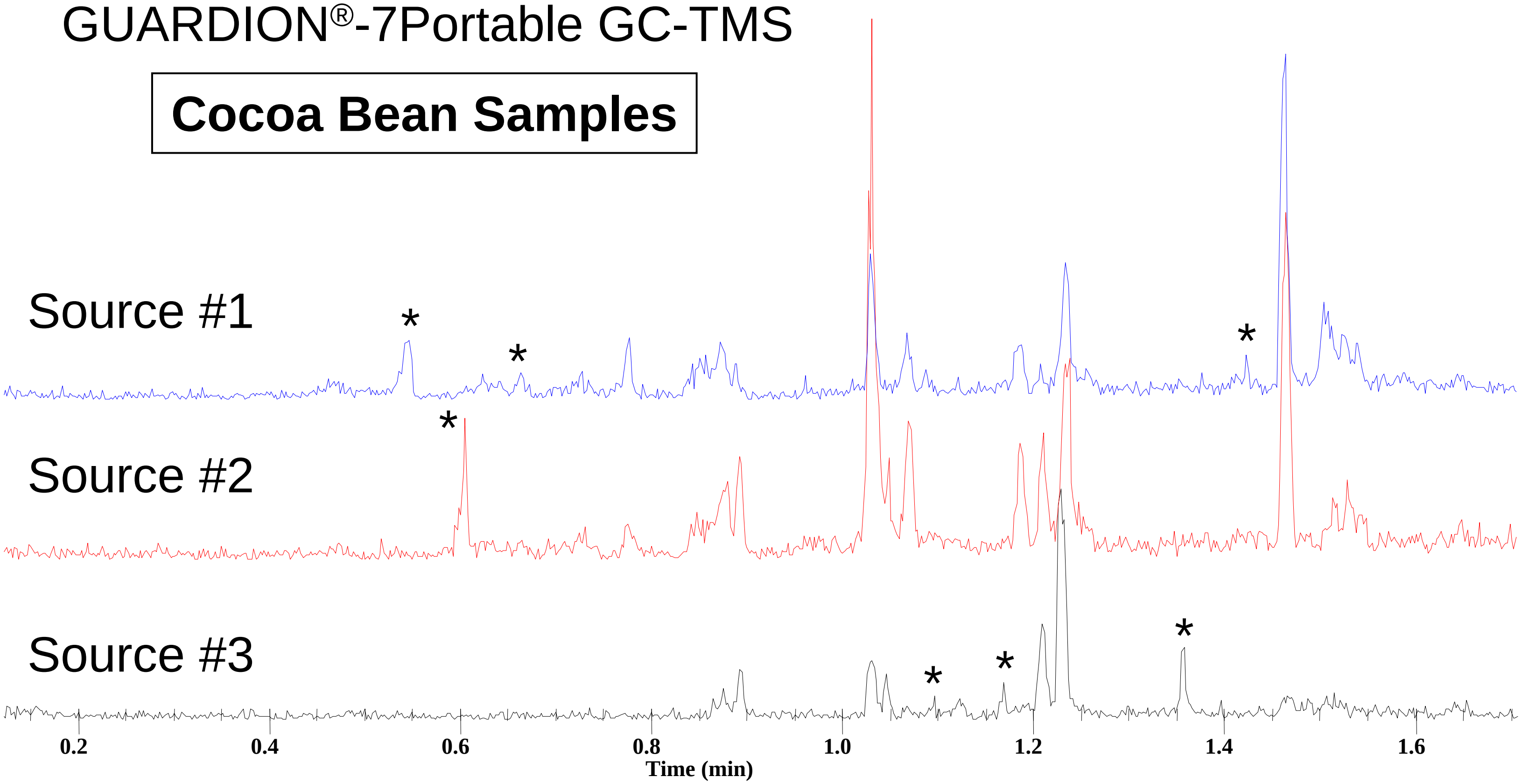
Agilent
Laboratory GC-MS

TORION®

Raw Materials Food Quality Monitoring

GUARDION®-7Portable GC-TMS

Cocoa Bean Samples



PDMS/DVB SPME fiber, 20 min headspace exposure, 65°C

* Potential food quality biomarkers

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Questions-Discussion