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Fast GC-TOFMS for High-throughput Screening of Environmental Contaminants

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Outline

- Challenges in monitoring water quality
- GC-TOF MS for water analysis
  - Potential limitations?
- Three potential solutions:
  - Deconvolution
  - Separation capacity of GCxGC
  - Soft electron ionisation

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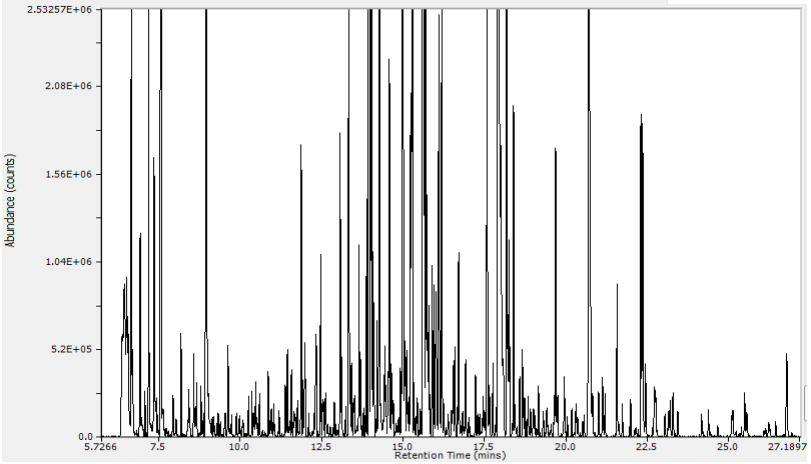
Monitoring water quality

- Focus is generally on “priority” substances, but what about those of emerging concern?
- Always need lower detection limits
- New monitoring methods and analytical techniques are now necessary

Issues with current methodology

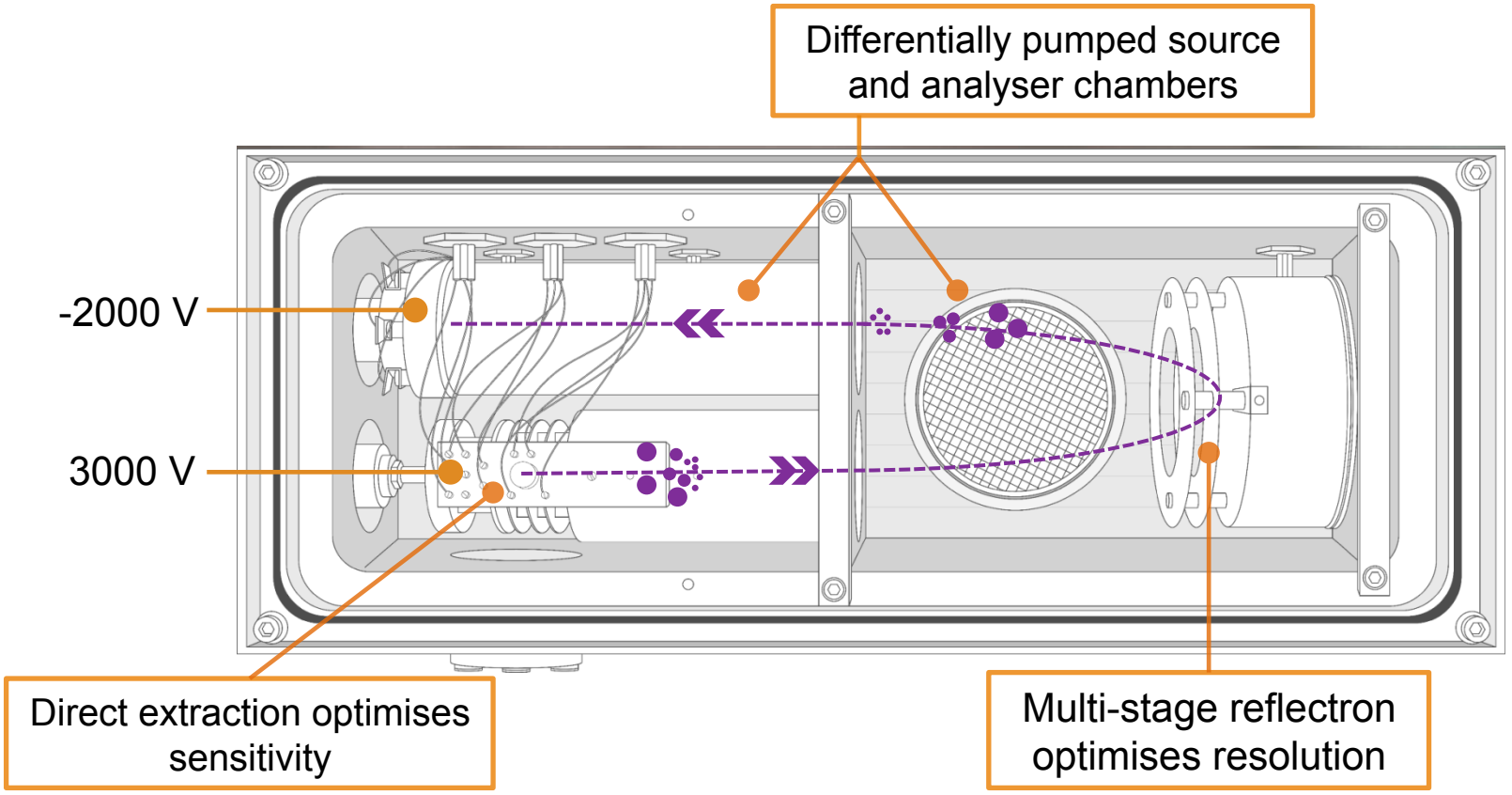
- 1D GC-MS is not able to resolve all components



- Grab sampling is limited

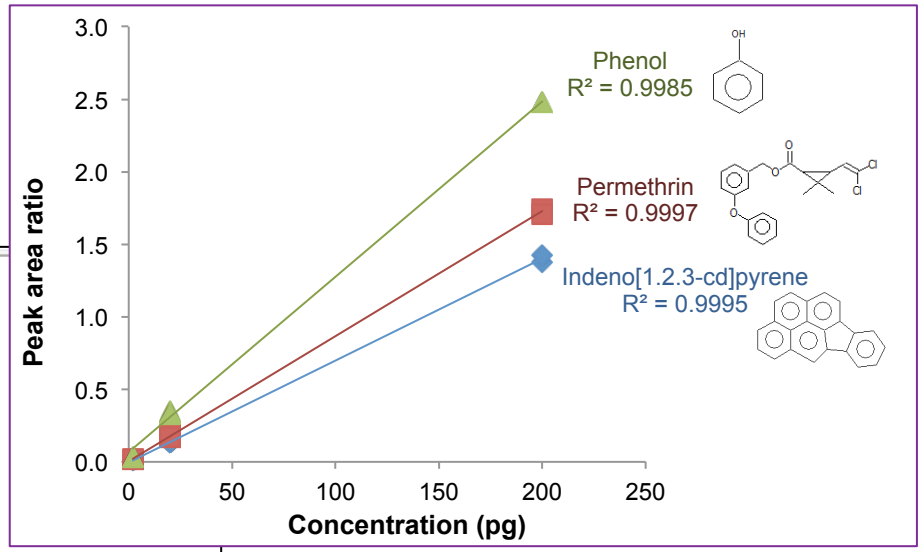
BenchTOF technology

Proprietary design

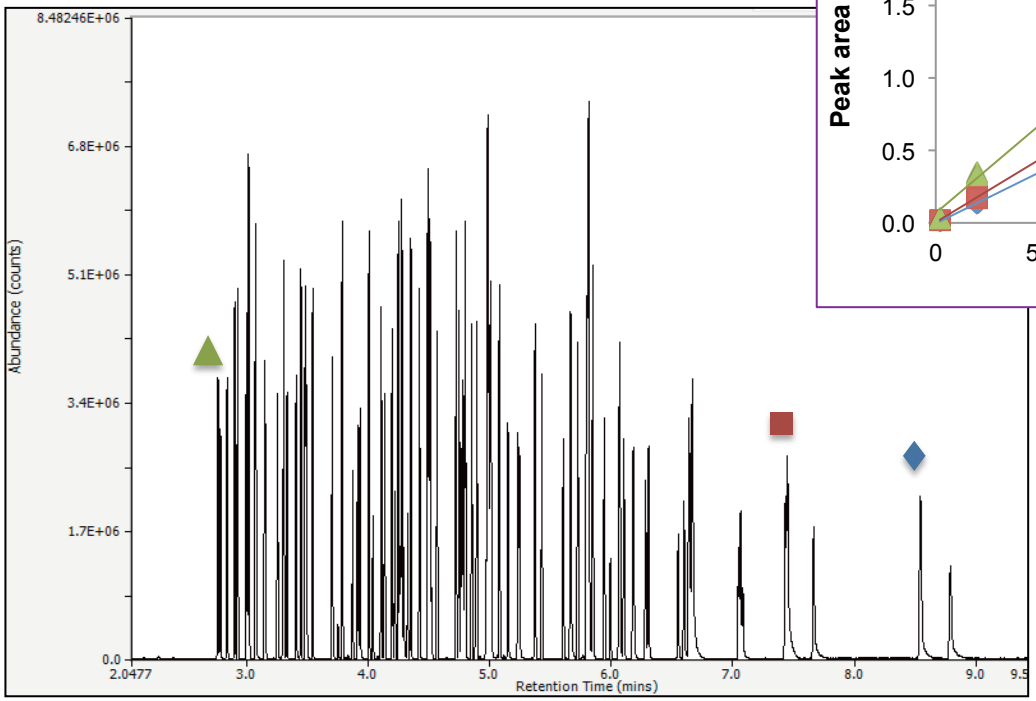


Benefits of GC-BenchTOF MS

Fast trace-level analysis

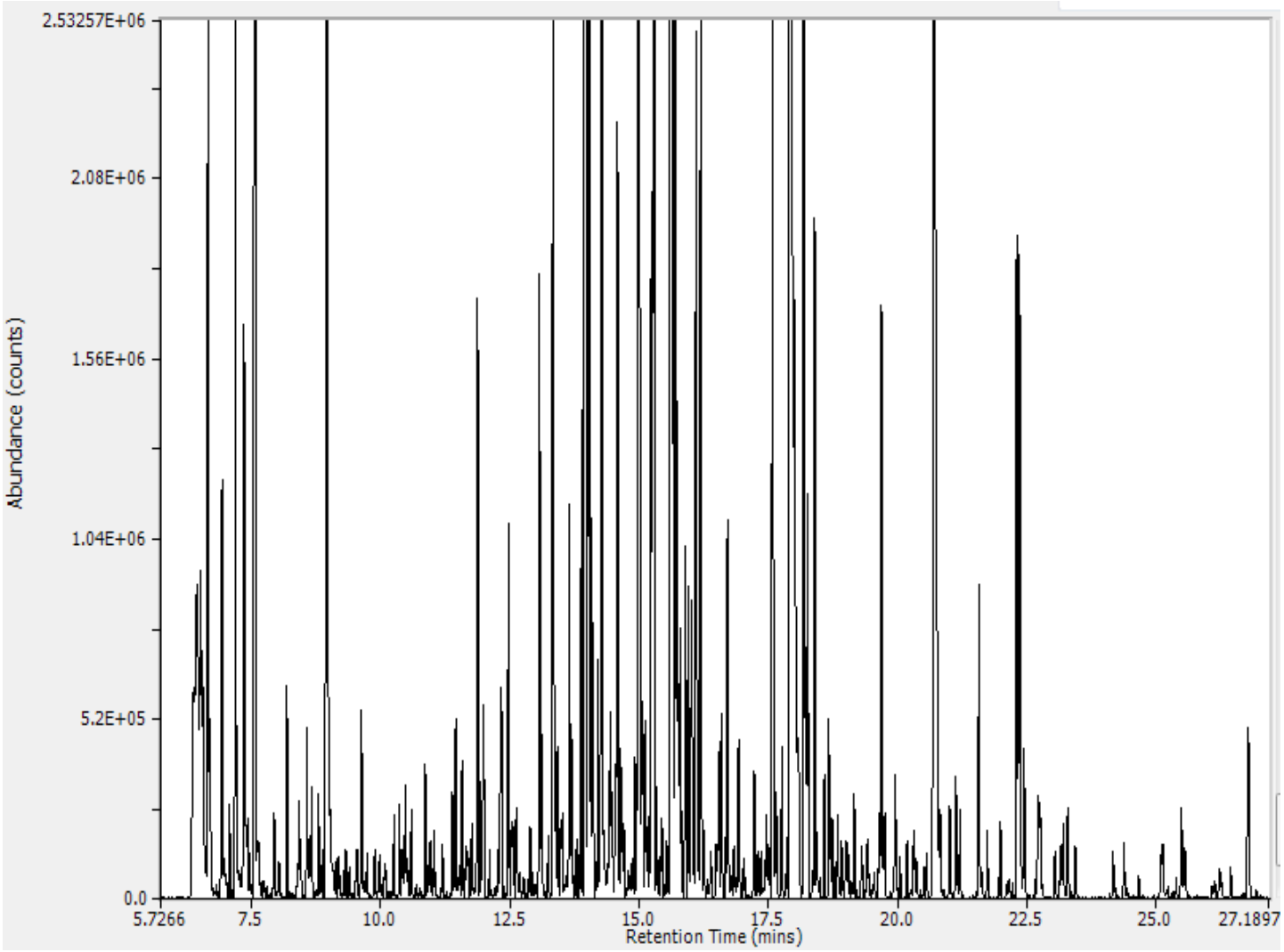


2 – 200 pg on column



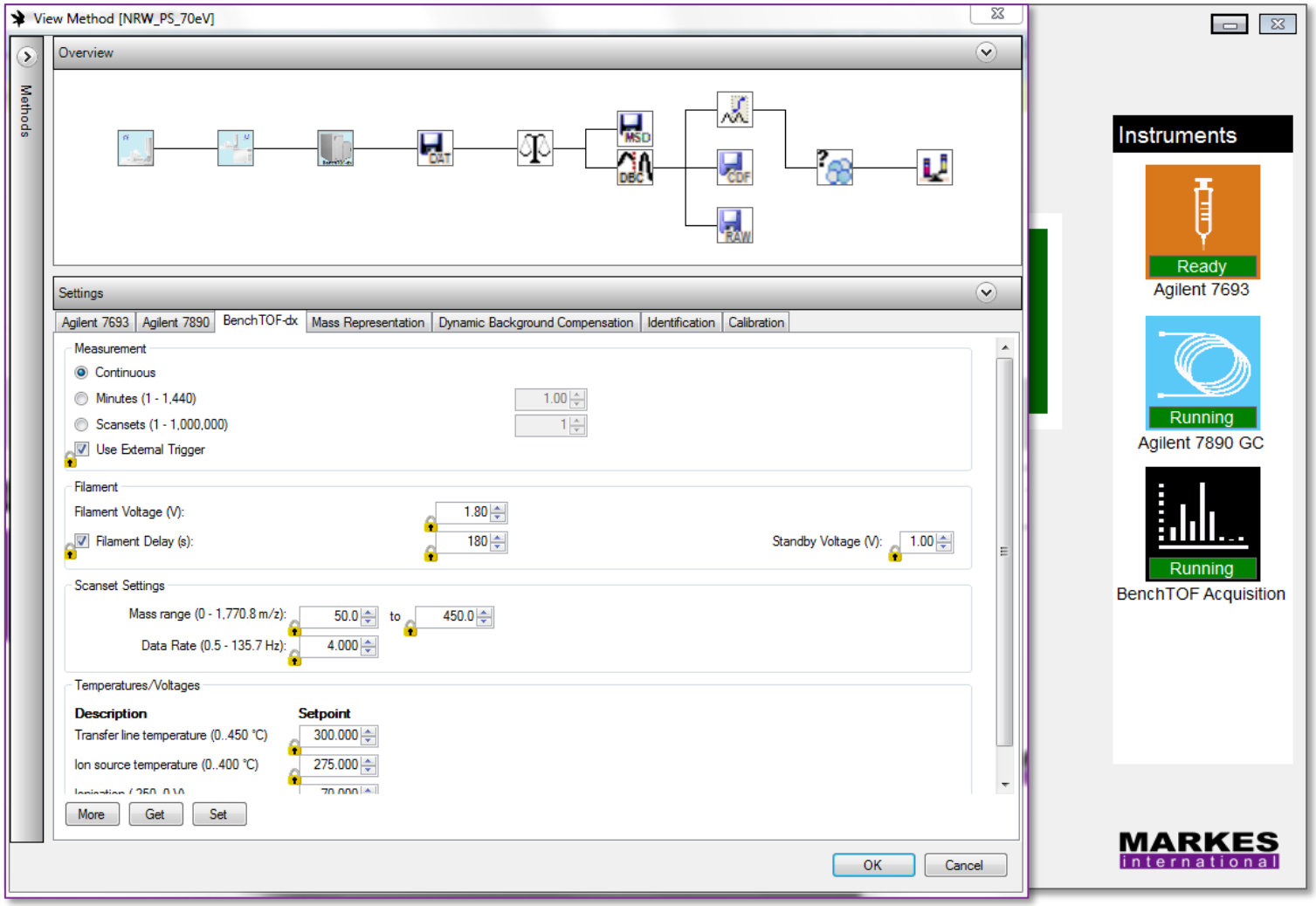
95 pollutants in less than 10 minutes

Problem #1: Is there enough separation capacity?



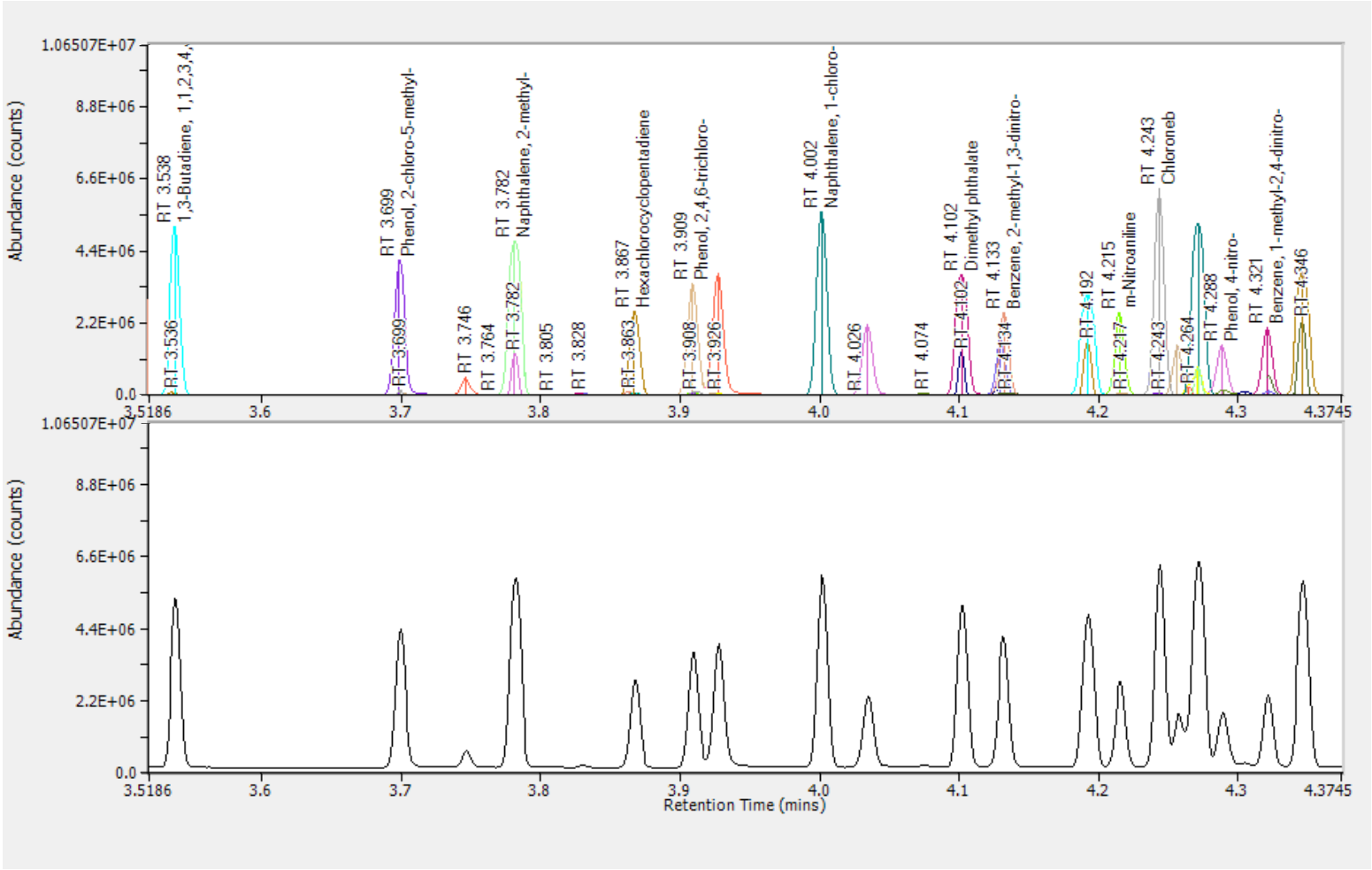
Potential solution?

Deconvolution



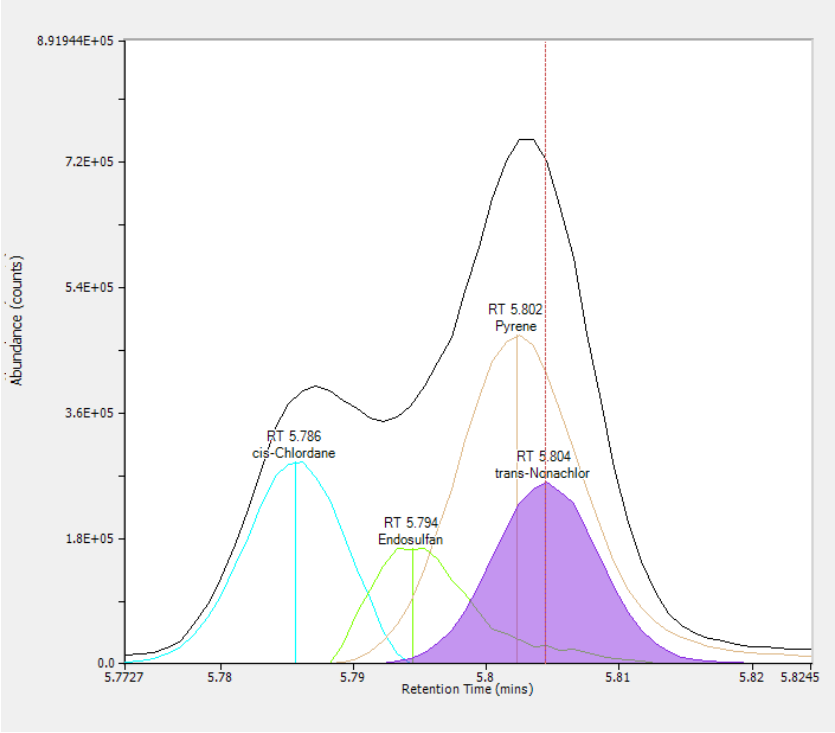
Real-time analysis

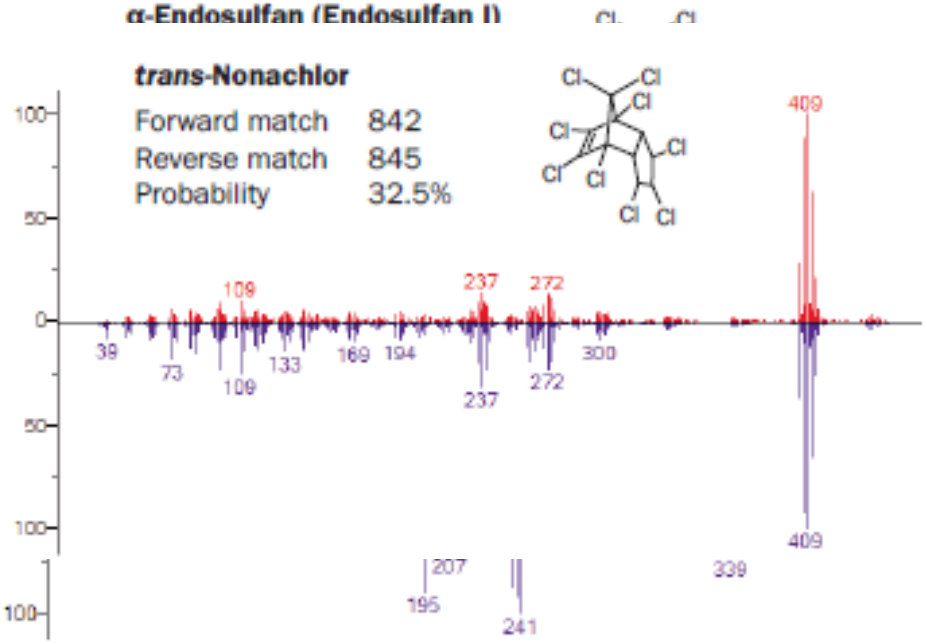
Results available on-the-fly



Confident identification of co-eluting peaks

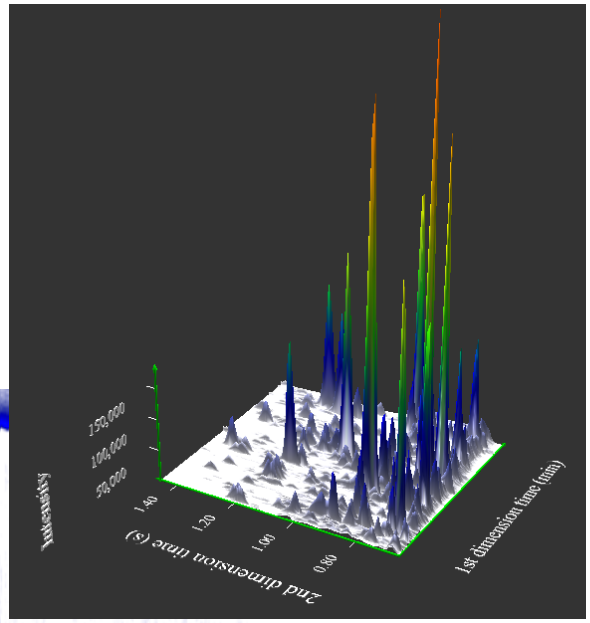
Deconvolution of four pollutants



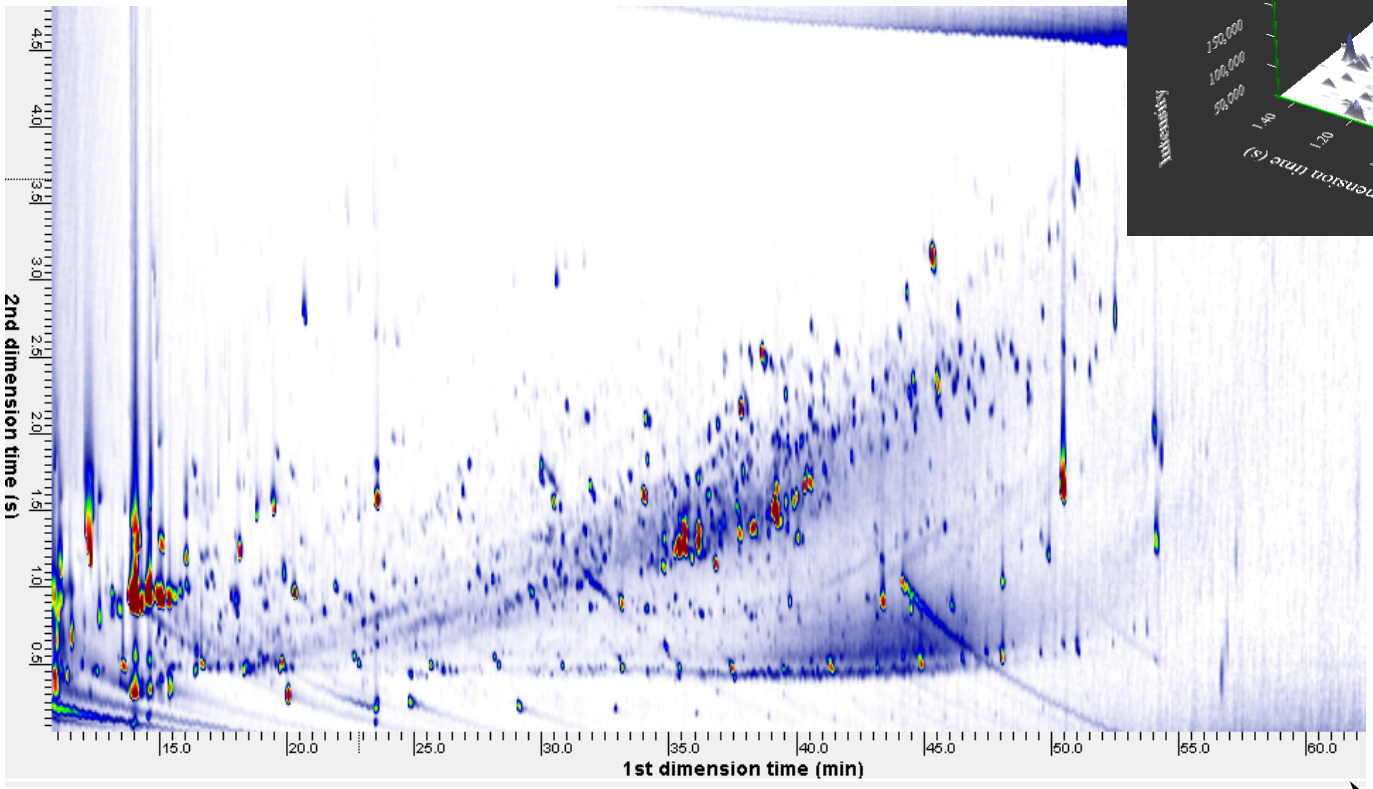


Another potential solution?

GCxGC TOF-MS



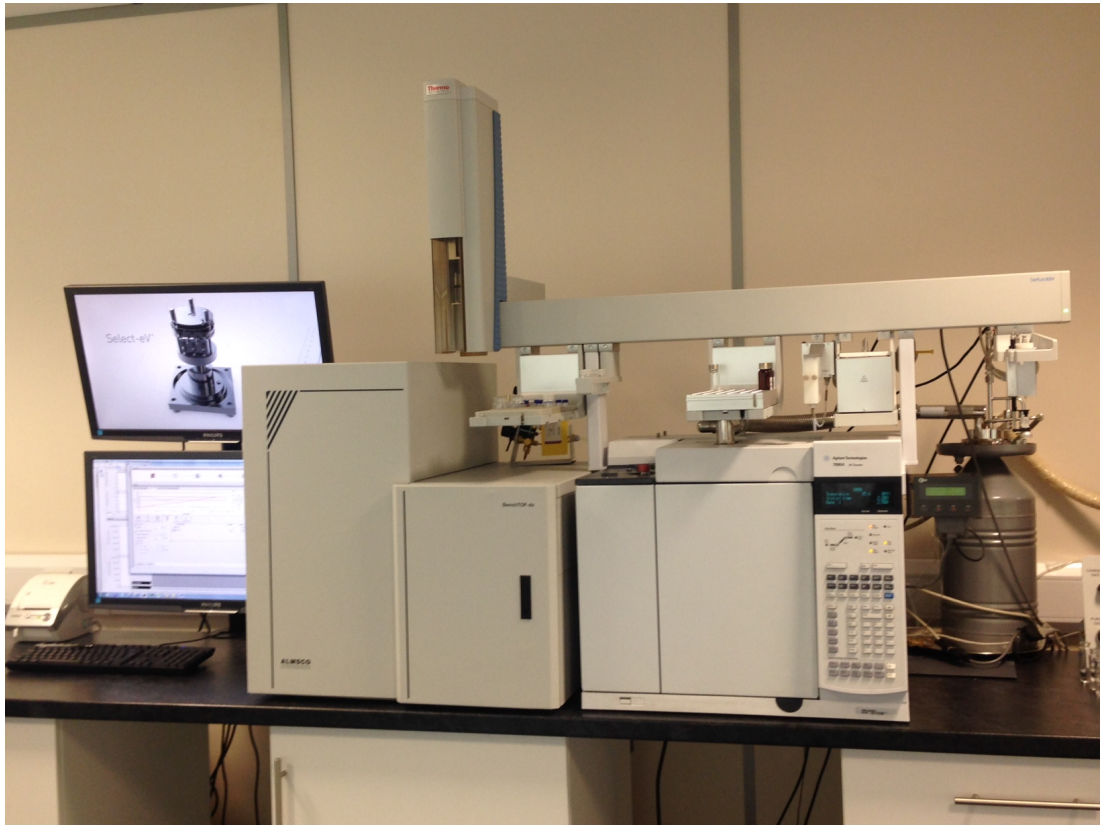
Polar column



Non-polar column

Analytical system

GCxGC-TOF MS

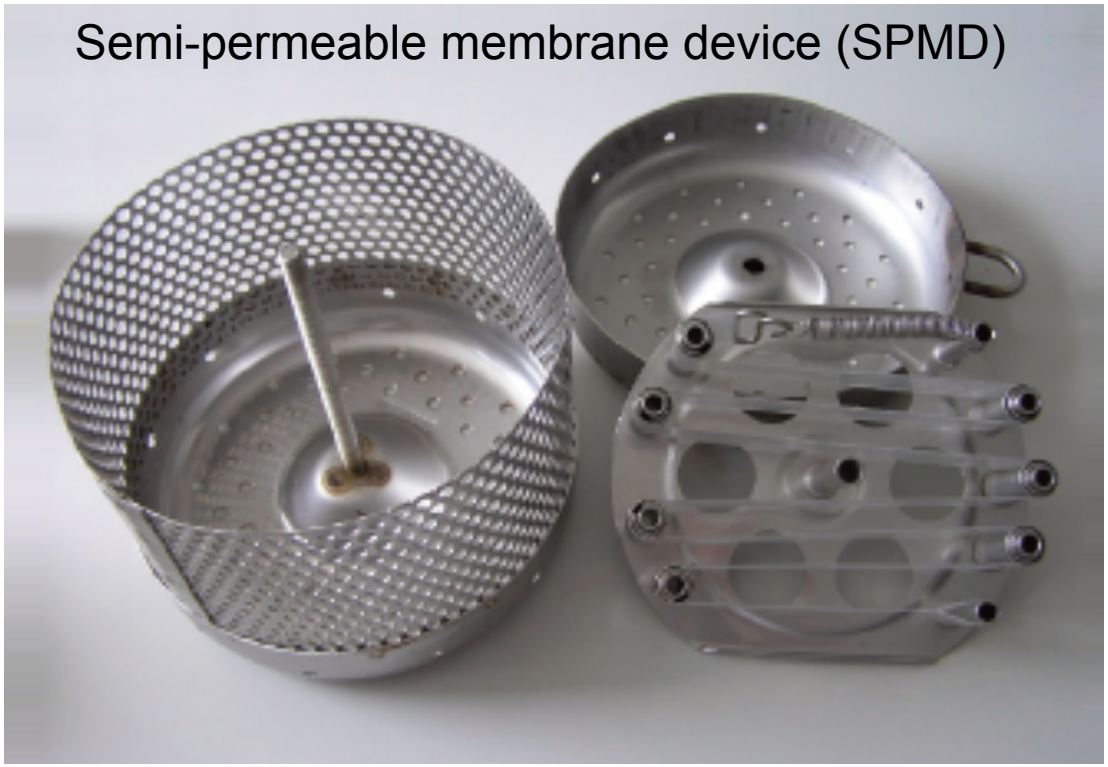


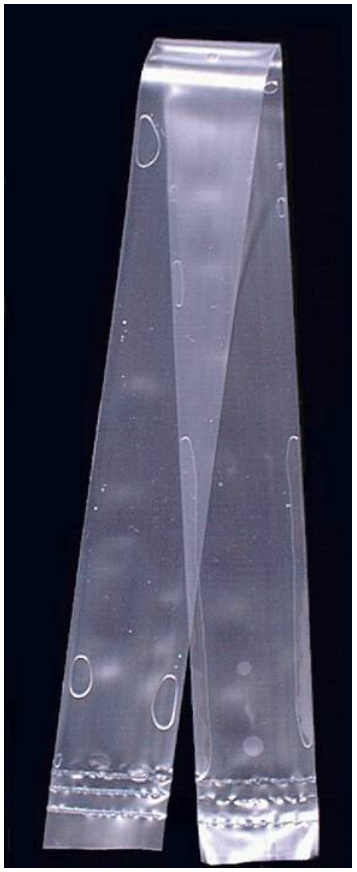
Column set:
1st dimension: SGE BPX5,
30 m × 0.25 mm × 0.25µm;

2nd dimension: SGE BPX50,
2 m × 0.1 mm × 0.1 µm;

Modulator:
Zoex ZX1 loop modulator
1 m as for second dimension
Modulation period = 5 s

Screening by passive sampling and GCxGC-TOF MS

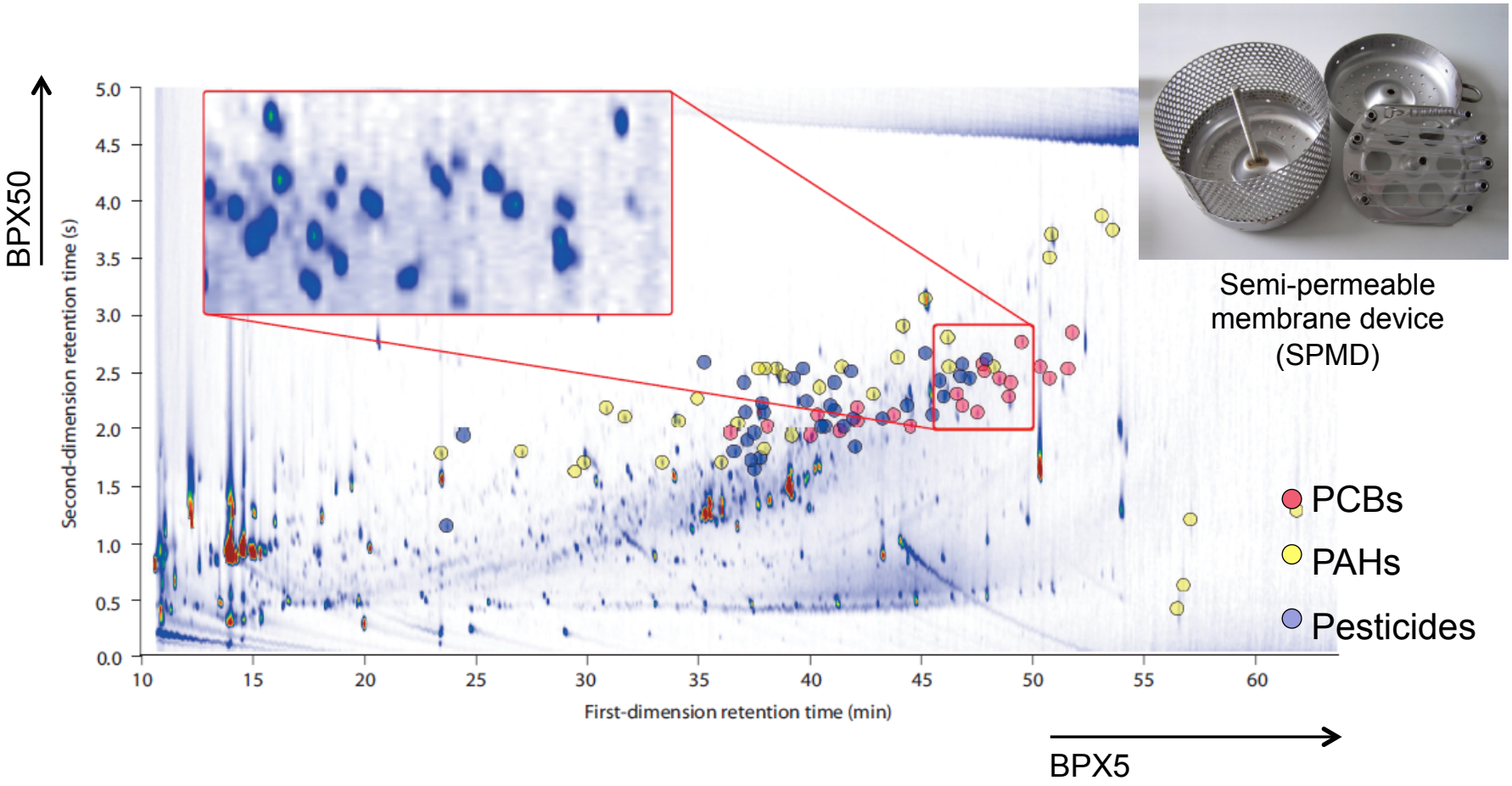




- Overcomes the limitations of grab sampling
- Designed to concentrate hydrophobic chemicals (with log Kow > 4)

Passive sampling of river water

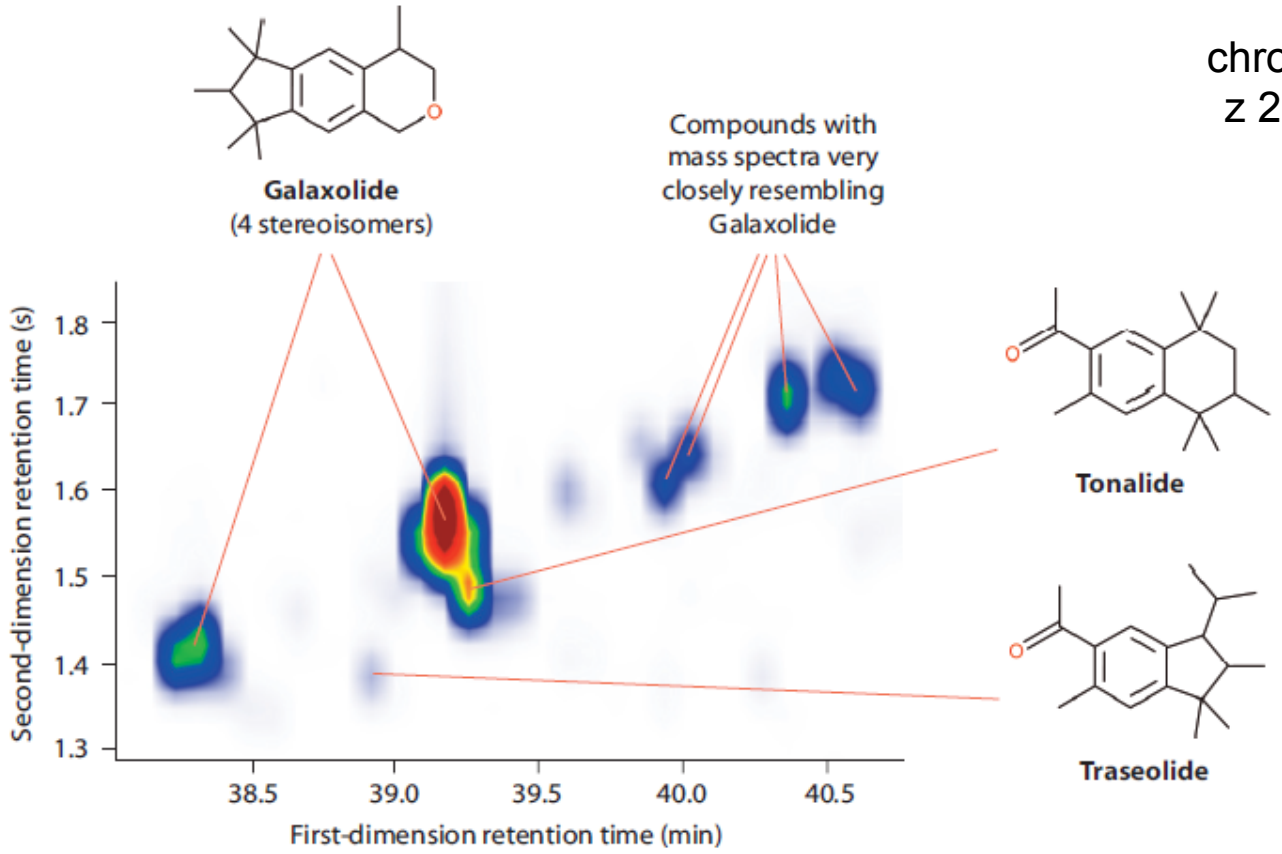
Over a 4-week period



Semi-permeable membrane device (SPMD)

Identification of emerging contaminants

Polycyclic musks



2D extracted-ion chromatogram (EIC) for m/z 215, 229, 243 and 258.

- Not restricted to priority pollutants – those of emerging concern are also monitored.

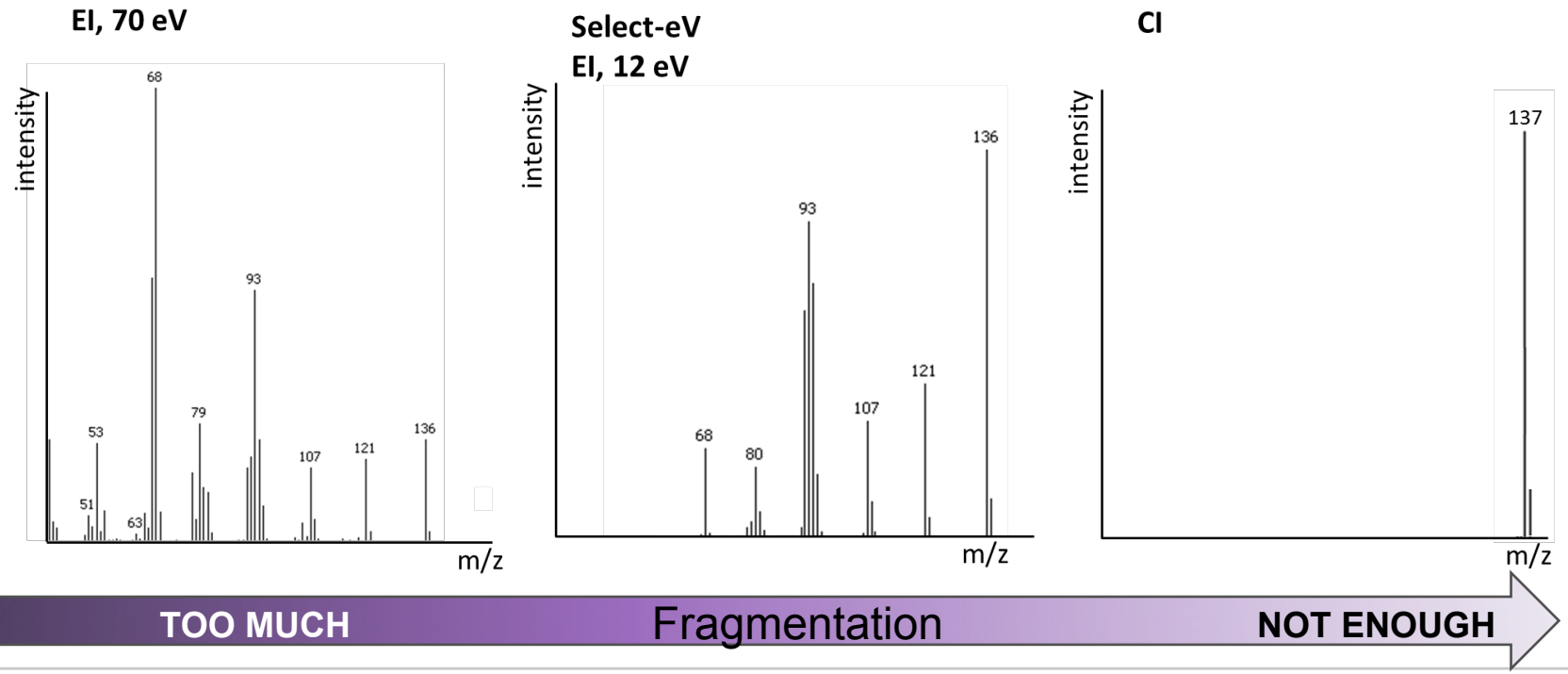
Increased confidence in identification

Compound	Class	NIST library match		
		GCxGC	1D GC (no deconvolution)	1D GC (with deconvolution)
Acenaphthylene	PAH	932	619	722
Fluoranthene	PAH	944	927	936
1,1'-Biphenyl, 2,2',3,4-tetrachloro-	PCB	870	800	819
2,3,3',5,5',6-Hexachloro-1,1'-biphenyl	PCB	844	776	795
DDT	Pesticide	835	790	801
Atrazine	Pesticide	842	603	620
Chlorpyrifos	Pesticide	824	684	701
Endrin	Pesticide	842	Not found	Not found
Galaxolide	Polycyclic Musk	879	835	835

Problem #2: Weak molecular ions &/or similar spectra

Challenges in soft ionisation

- Source-switching
- Optimise additional parameters
- Sensitivity loss
- Poor isomer speciation

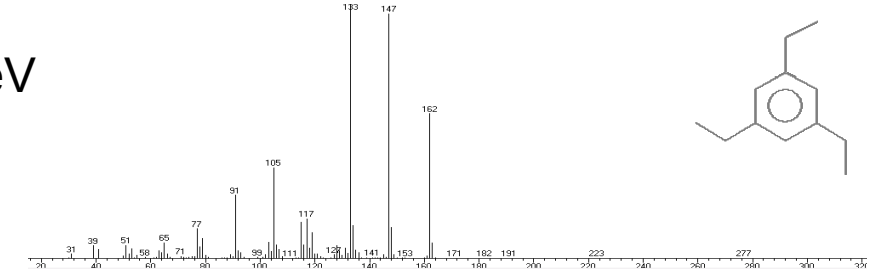


Soft electron ionisation

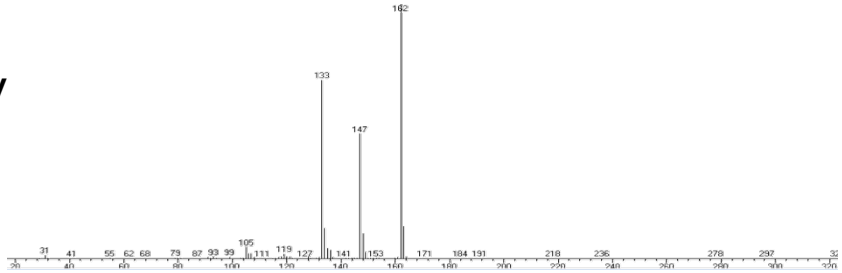
With no inherent loss in sensitivity

Select-eV

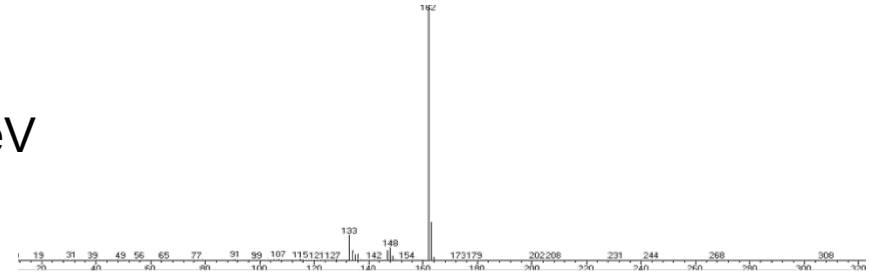
70 eV



16 eV

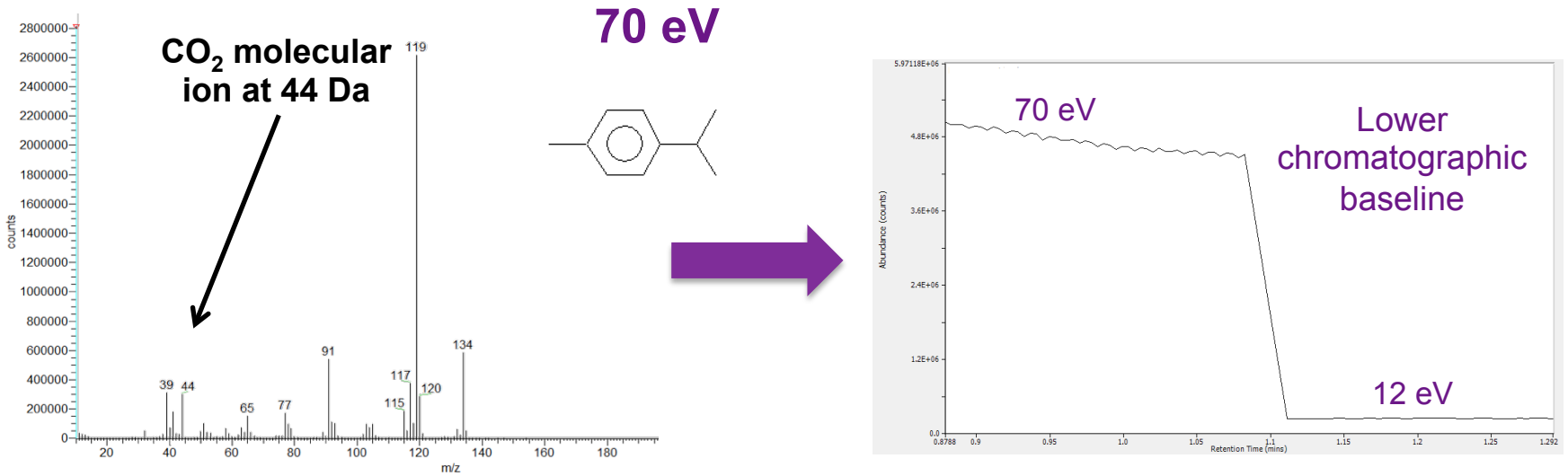


12 eV



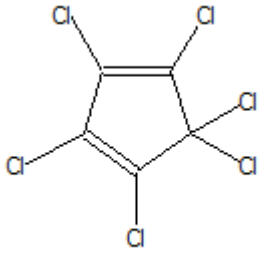
Selectivity enhancement at low eV

Reduced ionisation of common background/carrier gases

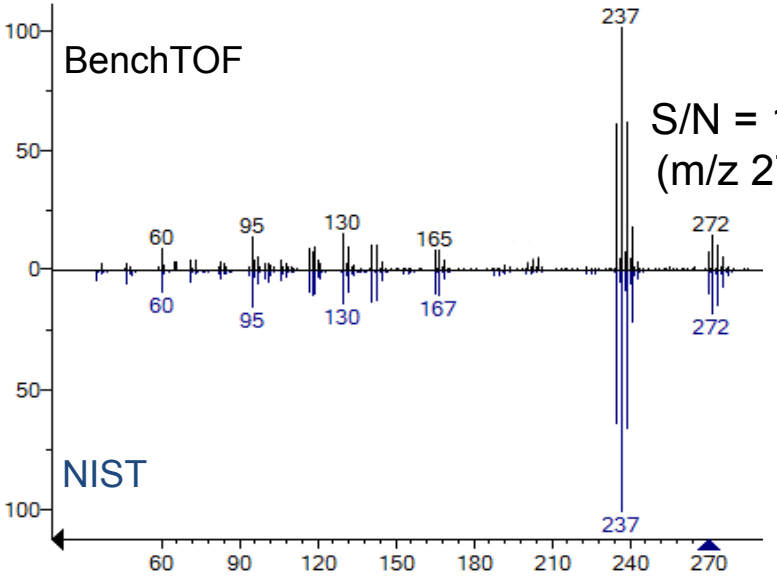


- Ionisation potential of common gases in GC–MS
  - CO_2: 13.8 eV
  - N_2: 15.6 eV
  - H_2: 15.4 eV
  - **He: 24.6 eV**

Hexachlorocyclopentadiene

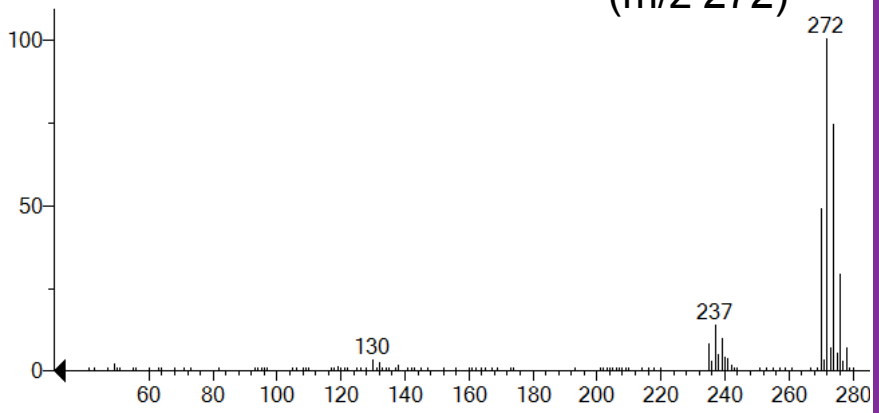


70 eV



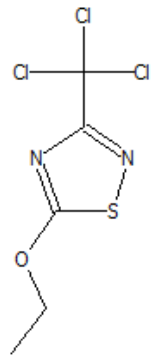
NIST MF = 845

11 eV

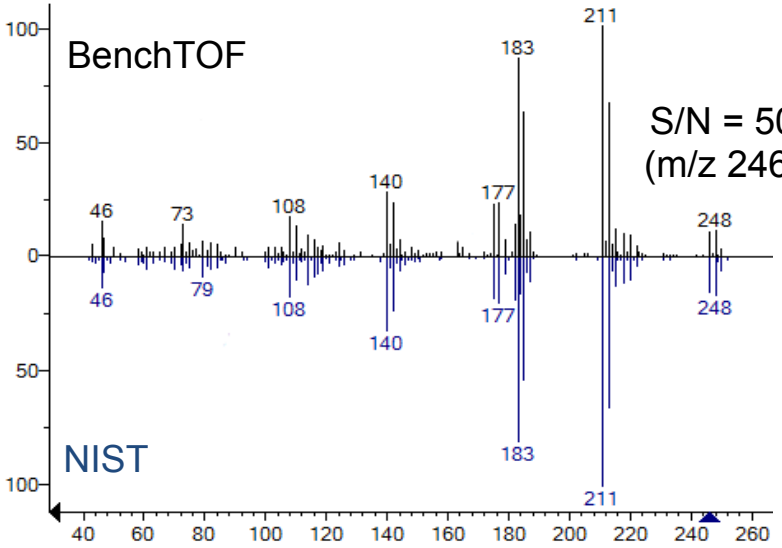


- Greater than 15x increase in signal-to-noise for m/z 272

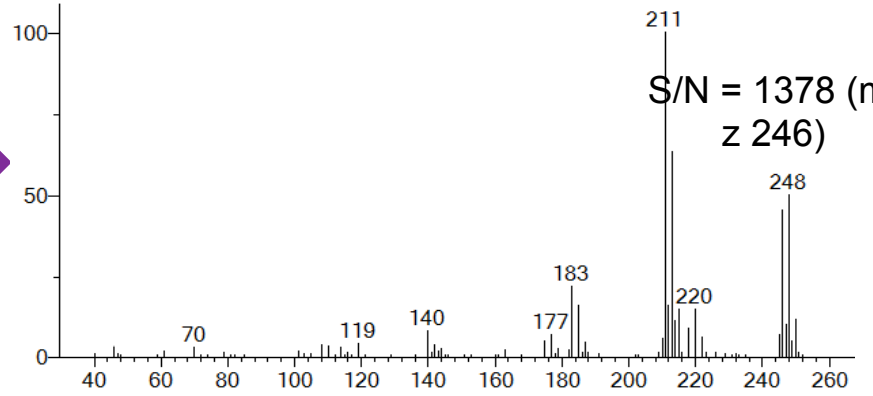
Etridiazole



70 eV



11 eV

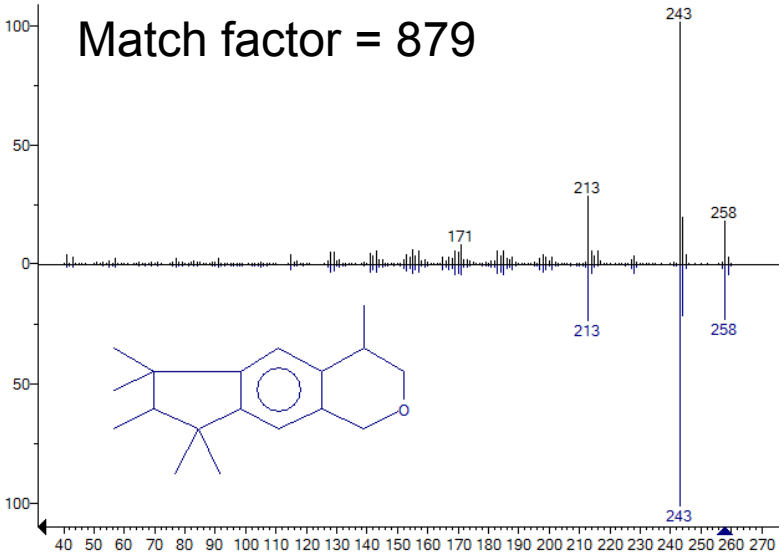


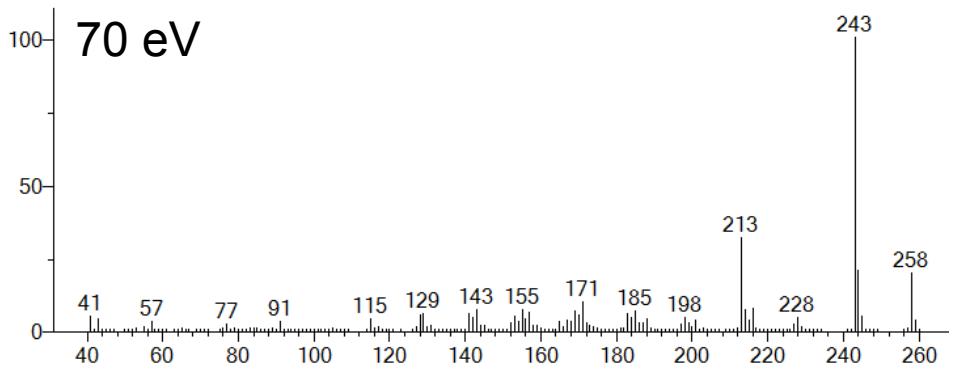
NIST MF = 819

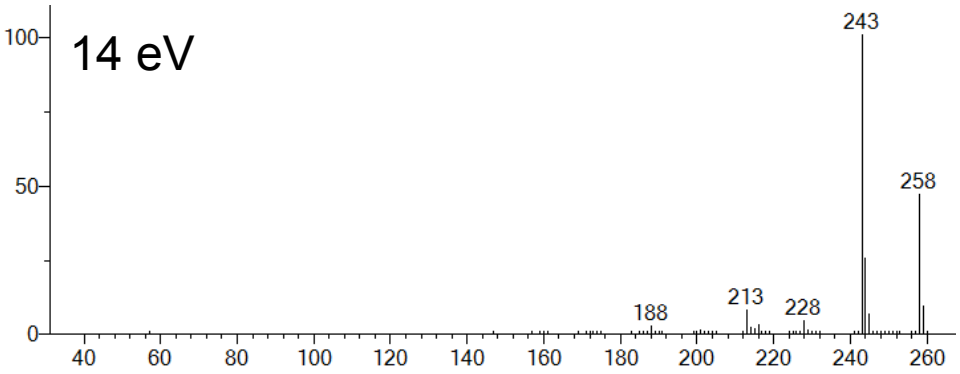
- Simplified spectrum at 11 eV
- Greater than 25x increase in signal-to-noise for m/z 246

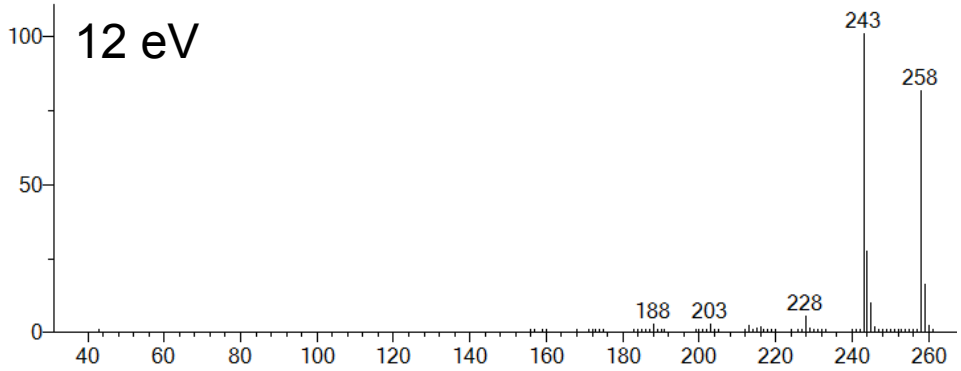
Polycyclic Musks

Galaxolide (HHCB)



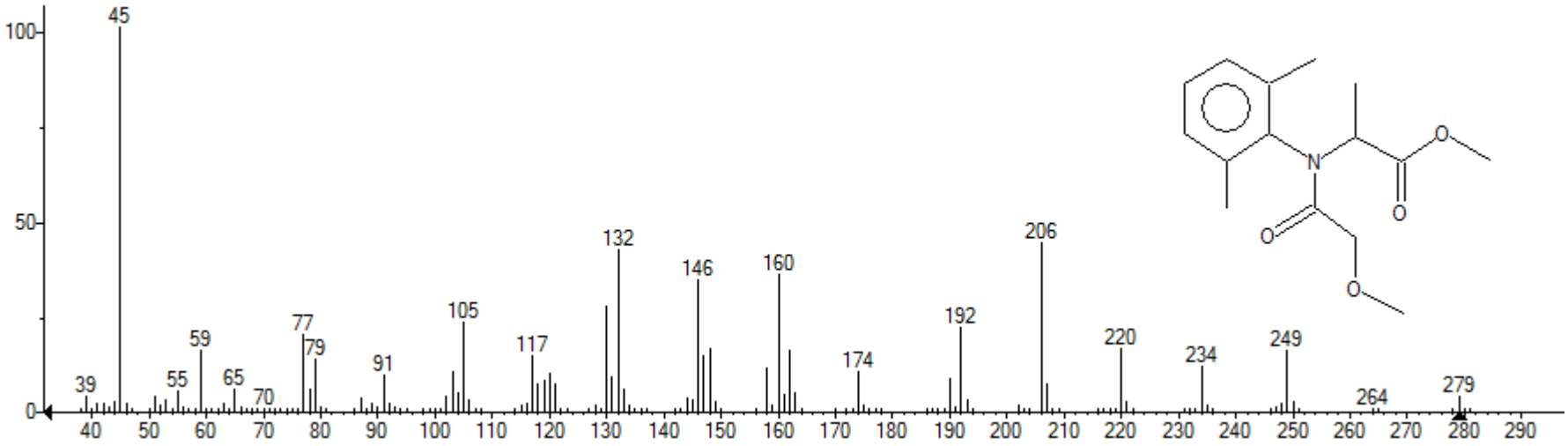




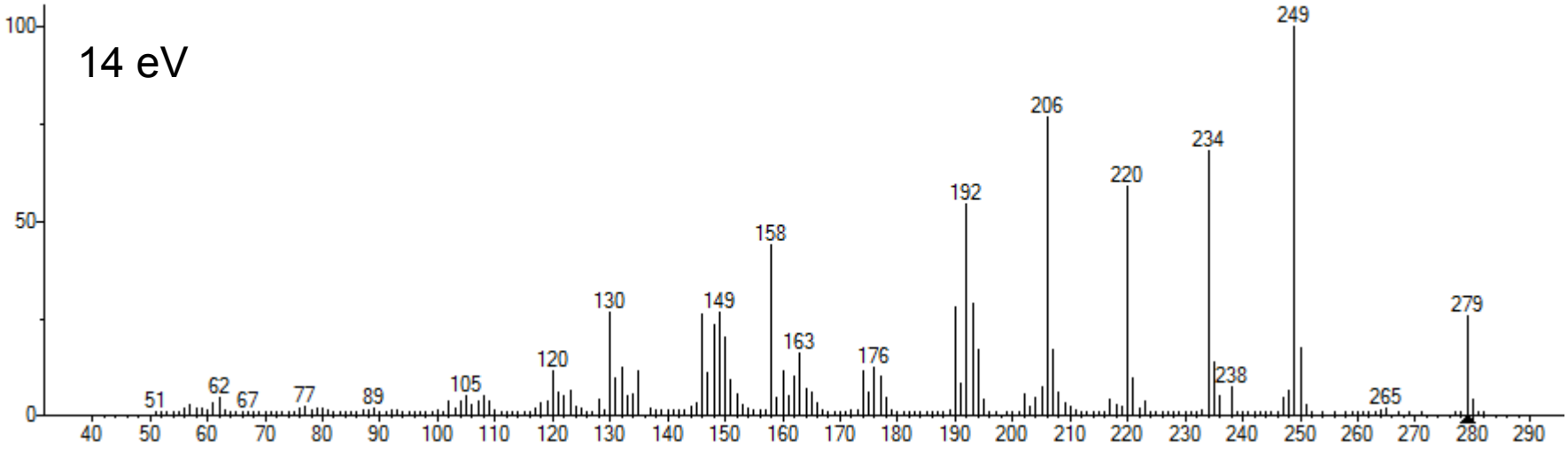


Metalaxyl

70 eV



14 eV



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Summary

- GC-TOF MS enables fast & simple, ultra trace-level detection of targets and unknowns in environmental samples.

- GCxGC-TOF MS gives enhanced separation and confident identification when screening complex matrices.

- Select-eV provides:
  - Simplified spectra for higher peak capacity
  - Improved sensitivity and selectivity
  - Complementary spectra for confident identification capacity

Thank you for listening!

Any Questions?

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