

What's in the air we breathe?

Chemical fingerprinting of PM_{2.5} by TD-GC×GC-TOF MS



Who are SepSolve Analytical?

Experts in analytical chemistry

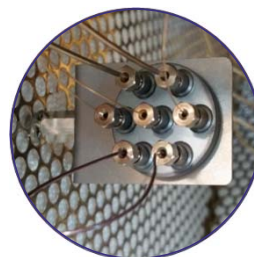


MARKES
international

 **SepSolve**
Analytical



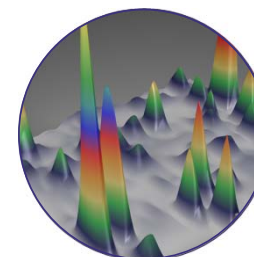
Sample preparation



Separation



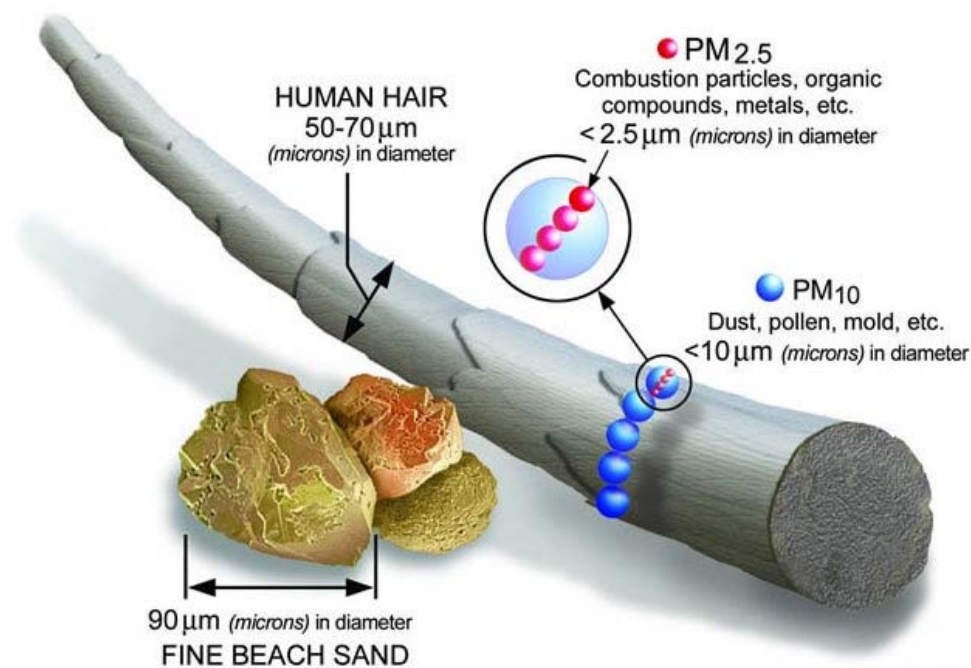
Identification



Data analysis

Particulate matter (PM) in air

- Airborne particulate matter is made up of a collection of solid and/or liquid materials of various sizes
 - PM_{2.5} (fine particles): $d \leq 2.5 \mu\text{m}$
 - PM₁₀ (coarse particles): $d \leq 10 \mu\text{m}$
- PM pollution consists of materials (including dust, smoke, and soot) either:
 - Directly emitted into the air
 - Result from the transformation of gaseous pollutants



Source: www.epa.gov/pm-pollution/particulate-matter-pm-basics

Sources of particulate matter



Industry
(power plants, factories...)



Vehicle emissions

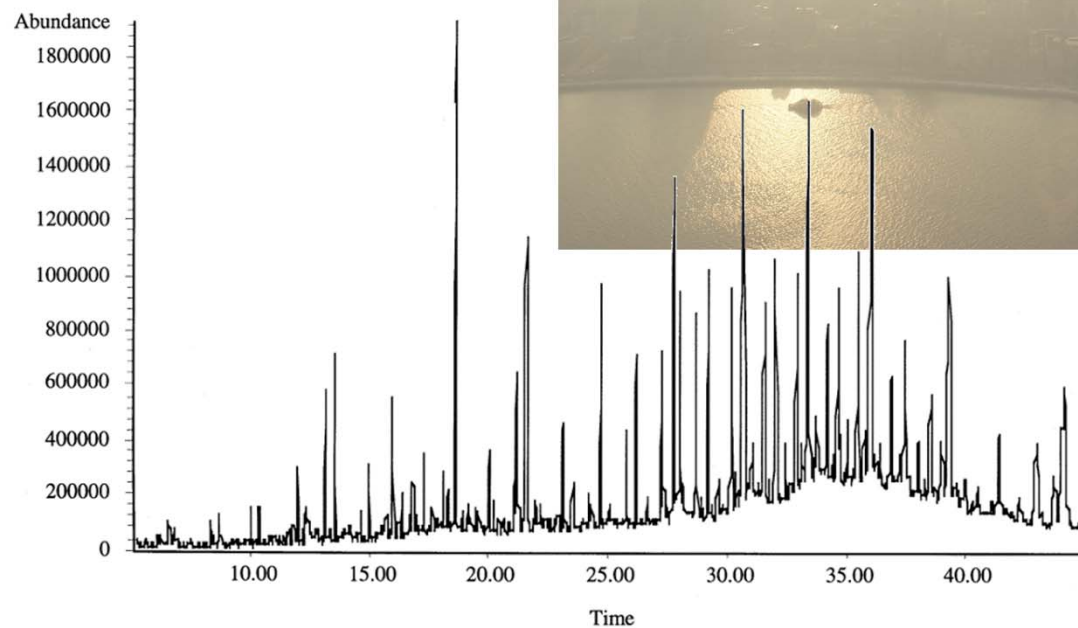


Natural Sources
(forest fires, volcanoes...)

Analysis of PM 2.5

The Challenges

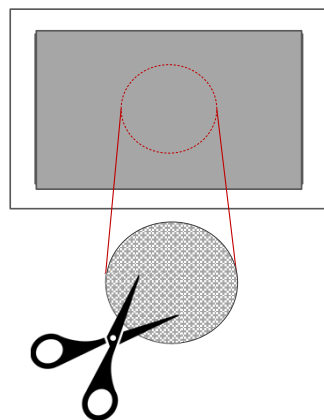
- Time-consuming sample preparation
- Wide range of chemical classes
- Complex chromatograms



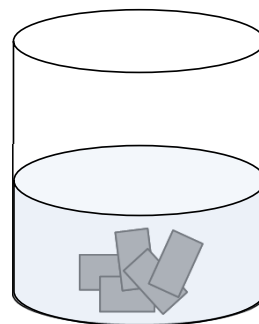
Previous approaches sample preparation



Sampling of PM_{2.5} on to quartz filter using in-situ sampler



PM_{2.5} filter cut or punched into sections



Solvent extraction with sonication

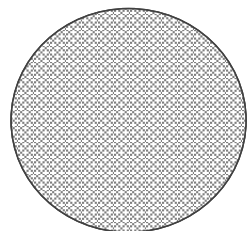


Evaporation – blow down with nitrogen

- Manual, time-consuming and costly
- Multiple handling steps can lead to error

New approach to PM2.5 analysis

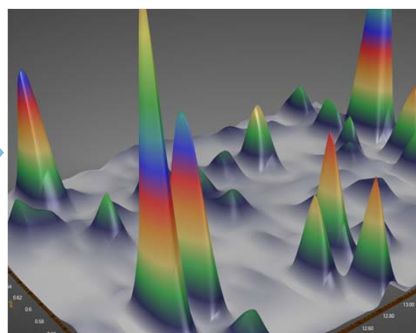
Direct desorption of filter for TD-GC×GC-TOF MS



Cut/rolled sections of
a PM2.5 filter



Place inside empty TD
tube for direct desorption



Enhanced separation by
INSIGHT-GC×GC

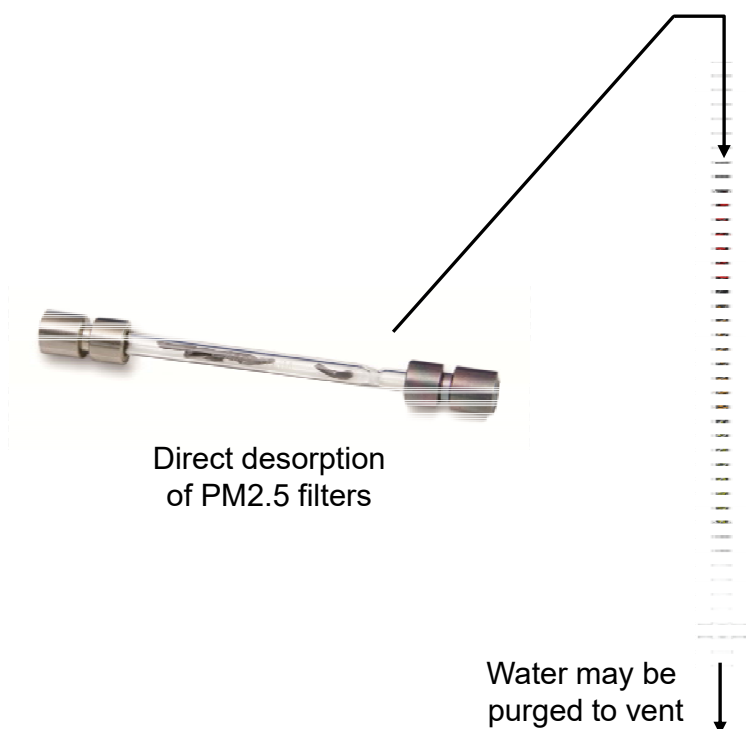


Confident identification
by BenchTOF

- Minimal sample preparation
- No solvents required

Direct desorption

Simplified sample preparation for PM2.5

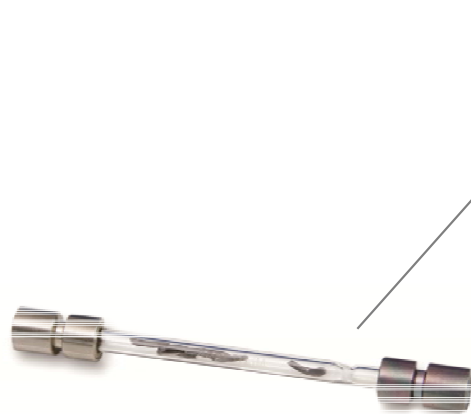


TD100-xr
Automated thermal desorber

- PM2.5 filter is placed within an empty TD tube and heated to desorb analytes on to the focusing trap
- Electrically-cooled focusing trap concentrates VOCs and SVOCs

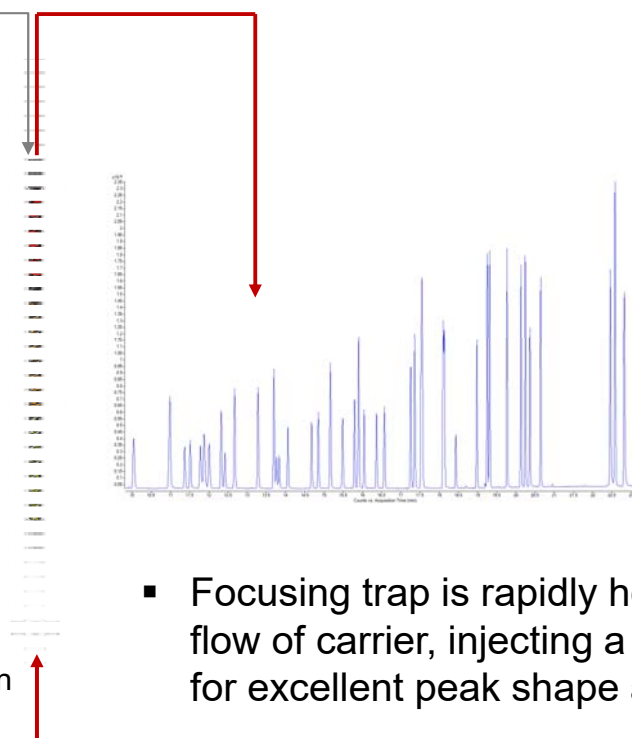
Direct desorption

Simplified sample preparation for PM2.5



Direct desorption
of PM2.5 filters

'Backflush' operation
for trap desorption



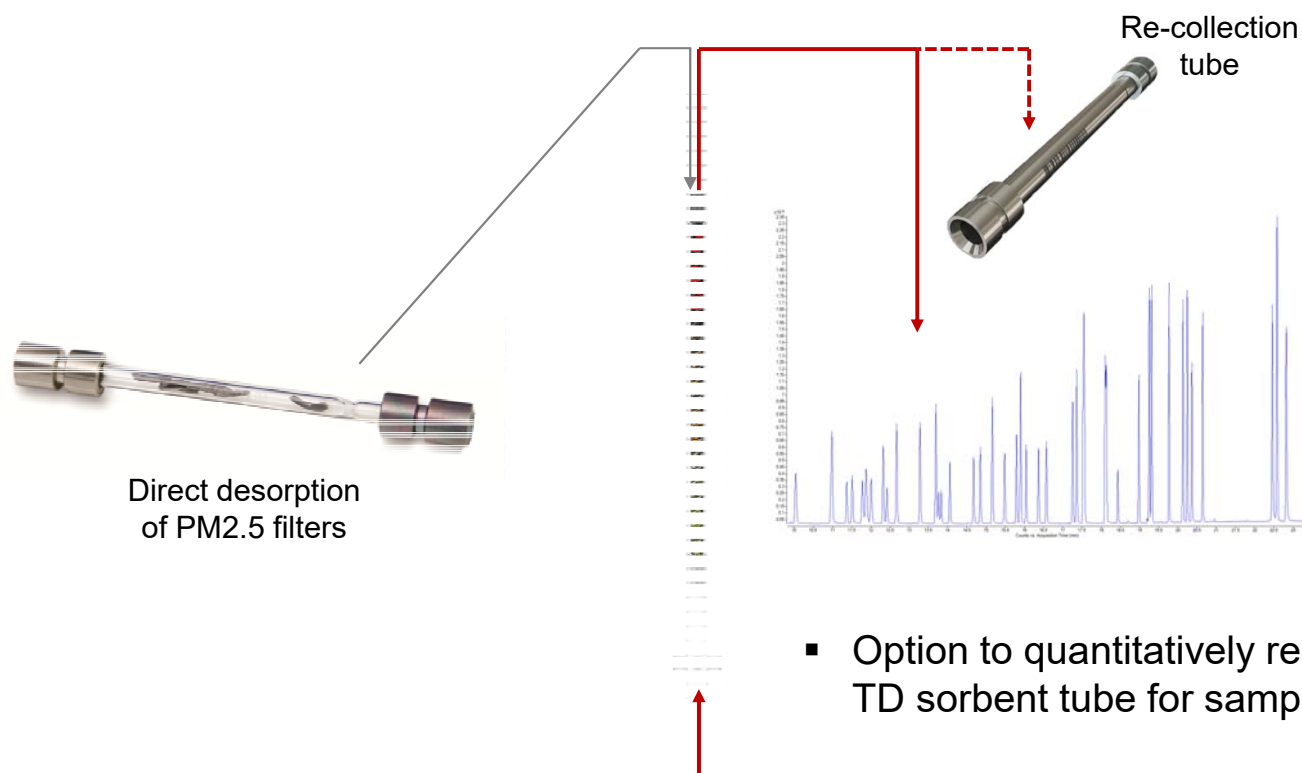
- Focusing trap is rapidly heated (up to 100 °C/s) in a reverse flow of carrier, injecting a narrow band of vapour into the GC for excellent peak shape and high sensitivity



TD100-xr
Automated thermal desorber

Direct desorption

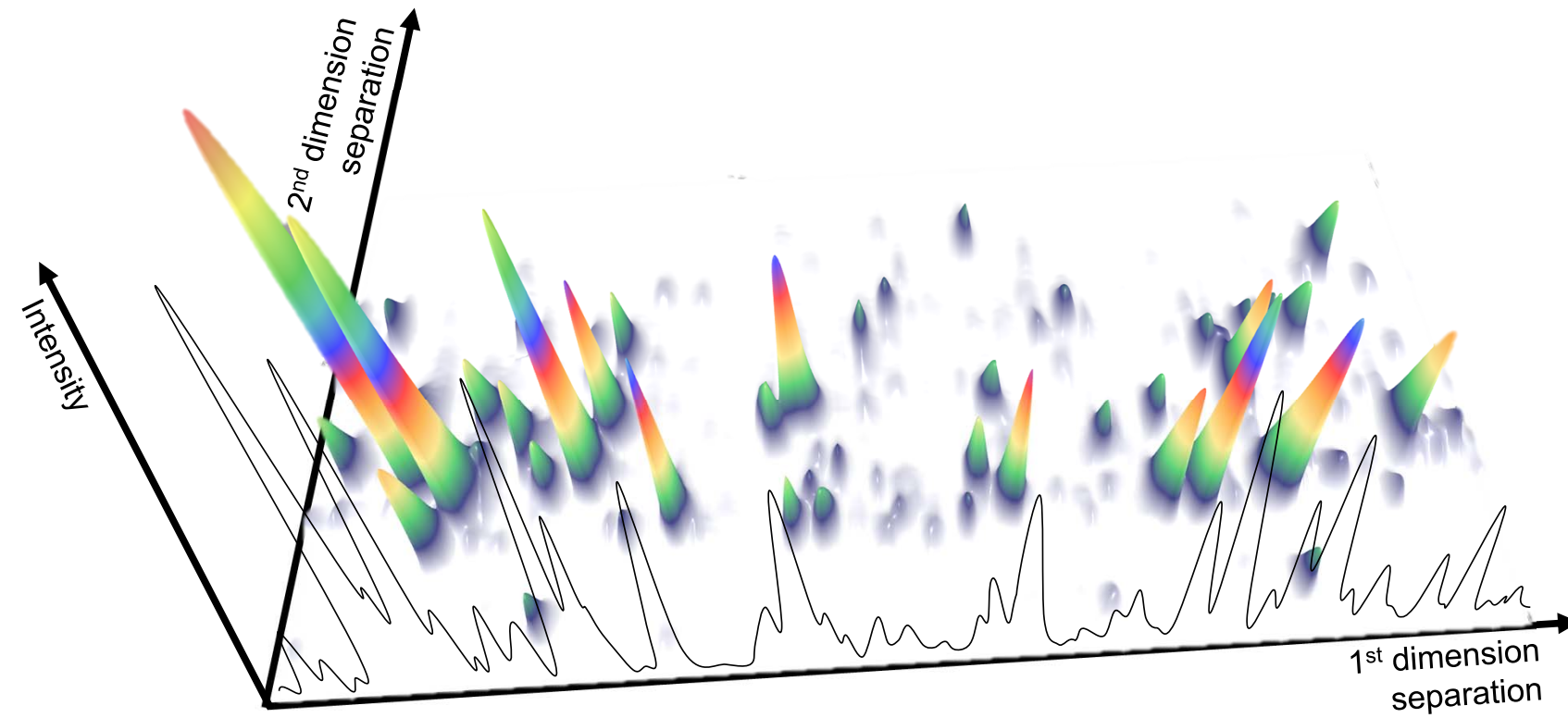
Simplified sample preparation for PM2.5



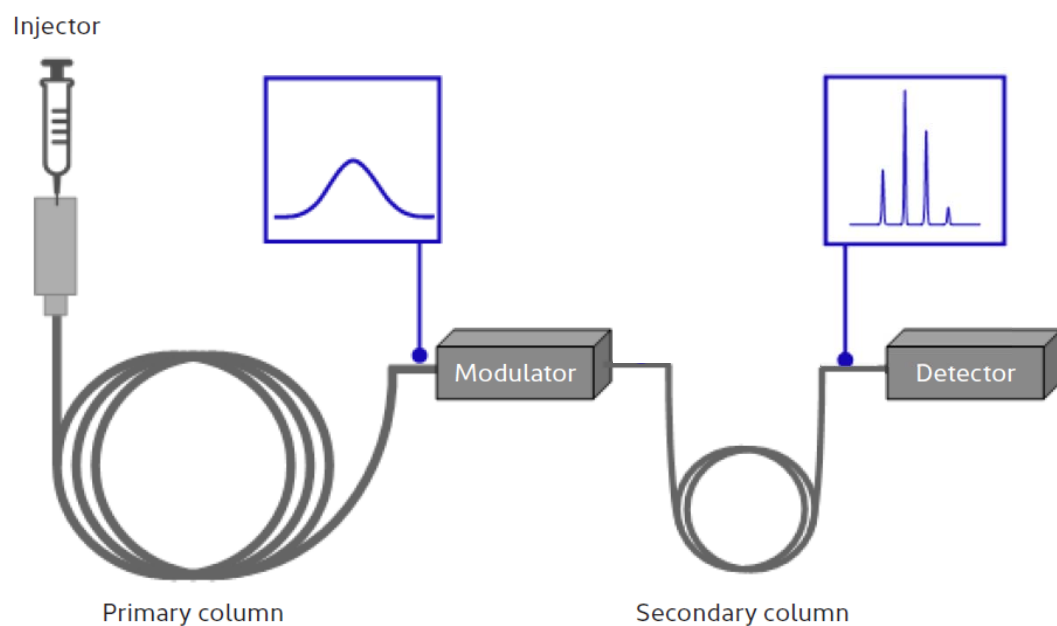
TD100-xr
Automated thermal desorber

- Option to quantitatively re-collect the split flow on to a clean TD sorbent tube for sample archiving and repeat analysis

What is GC×GC?



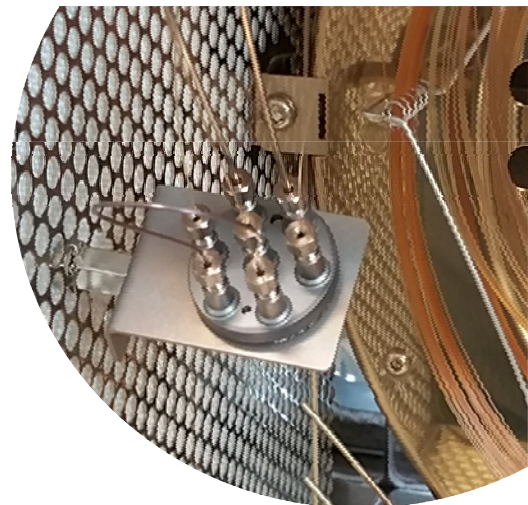
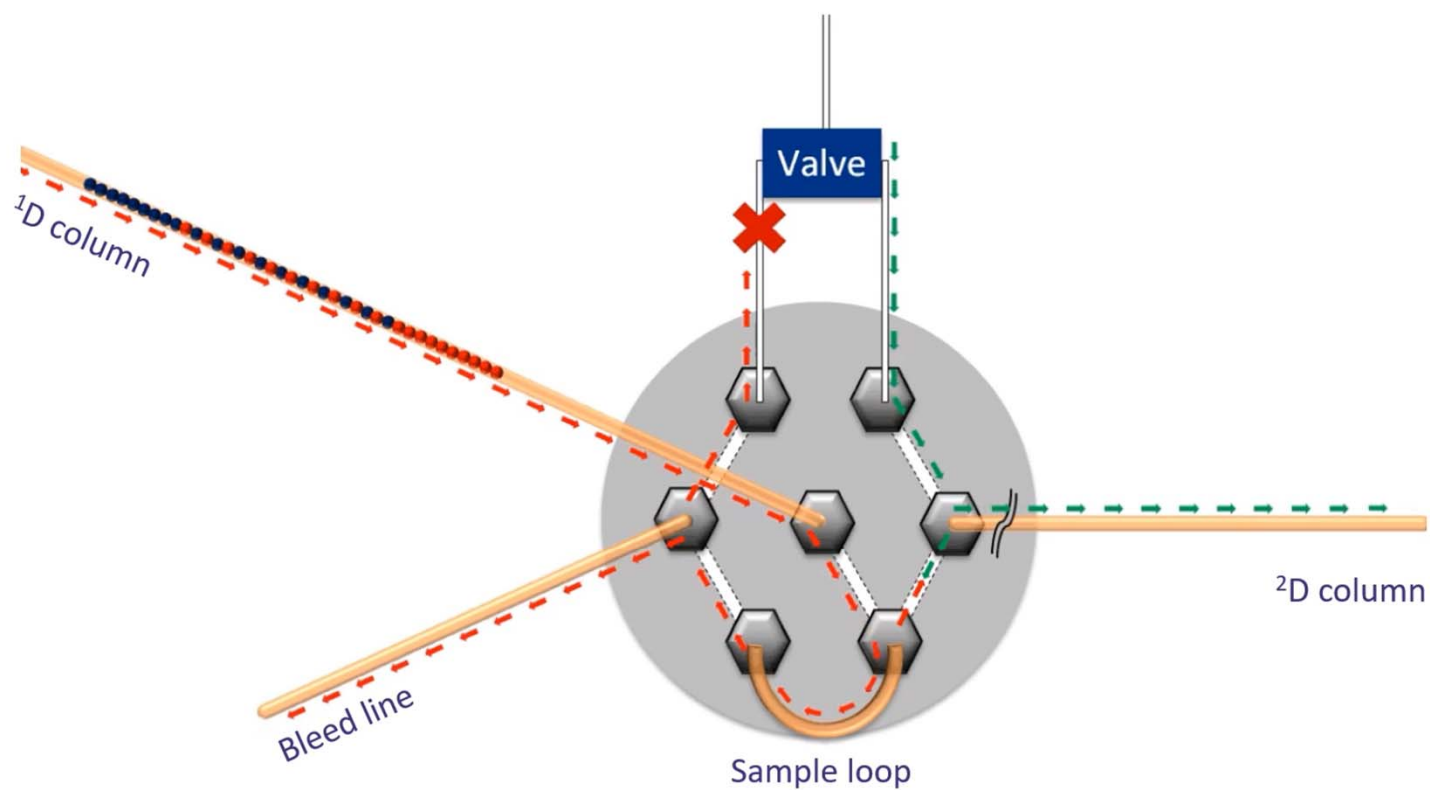
What is GC×GC?



- The modulator is the 'beating heart' of a GC×GC system
- Advances in flow modulation have made GC×GC more suitable for routine analysis

Reverse fill/flush flow modulator

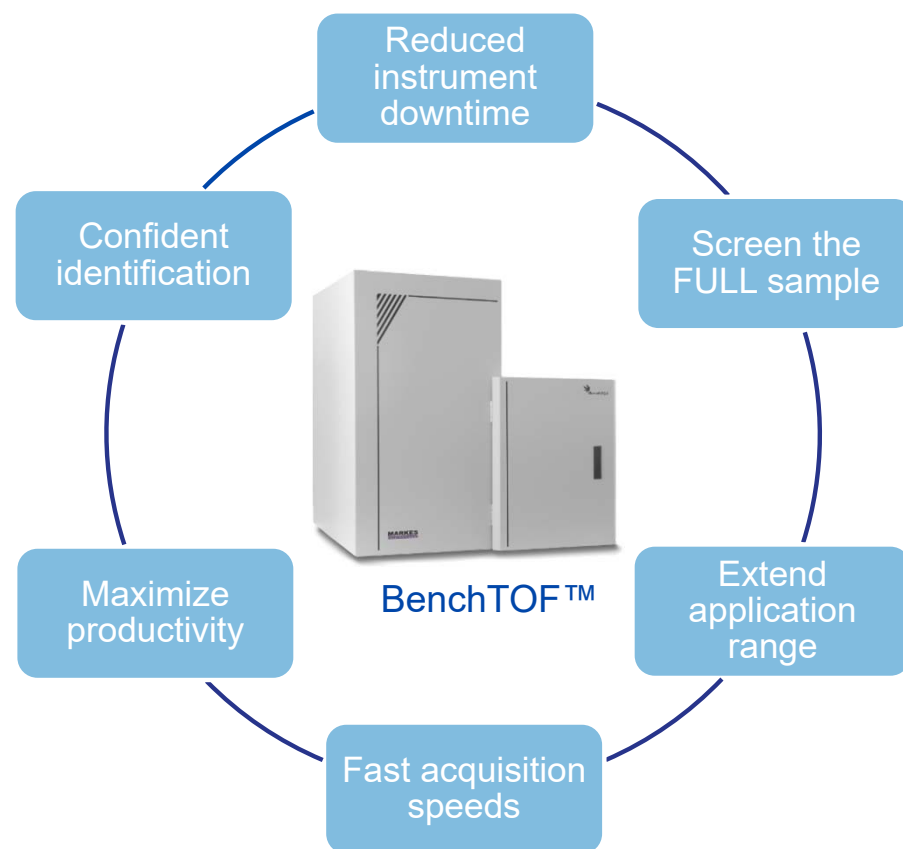
How does it work?



Why choose TOF mass spectrometry?

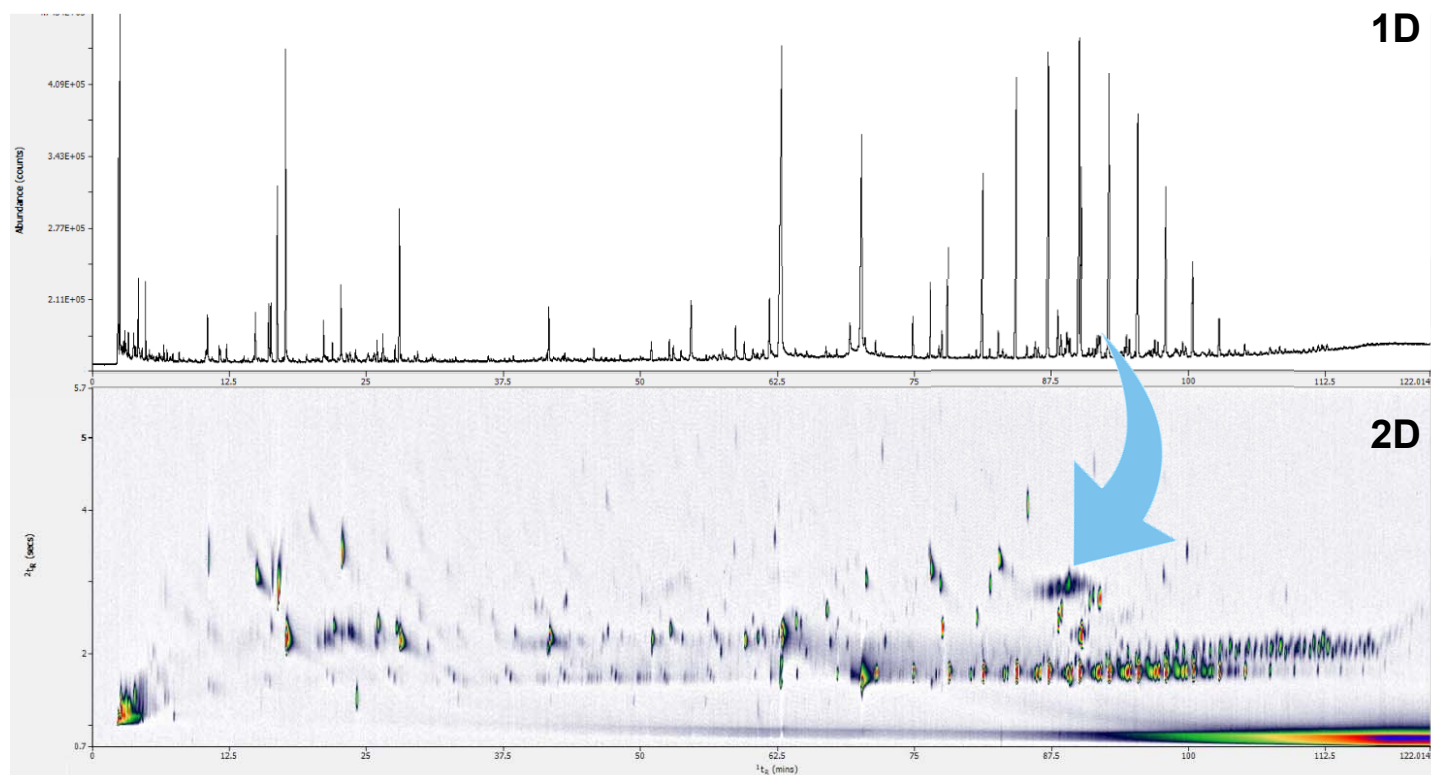
BenchTOF™

- Highly sensitive, confident identification of targets and non-targets
- Reduced instrument downtime through long-term stability and minimal maintenance requirements
- Acquisition speeds are ideal for GC×GC



PM 2.5 analysis

Gaining an additional level of detail...

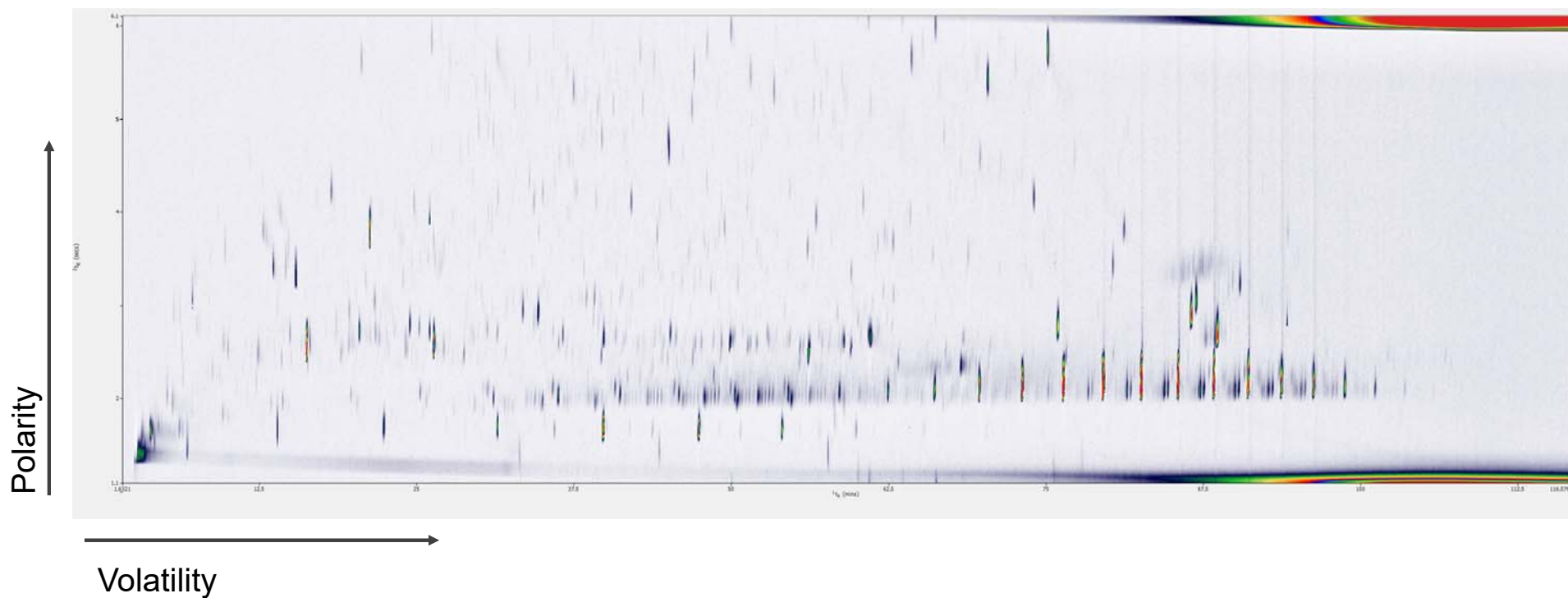


1D TD-GC-FID

2D TD-GC×GC-TOF MS

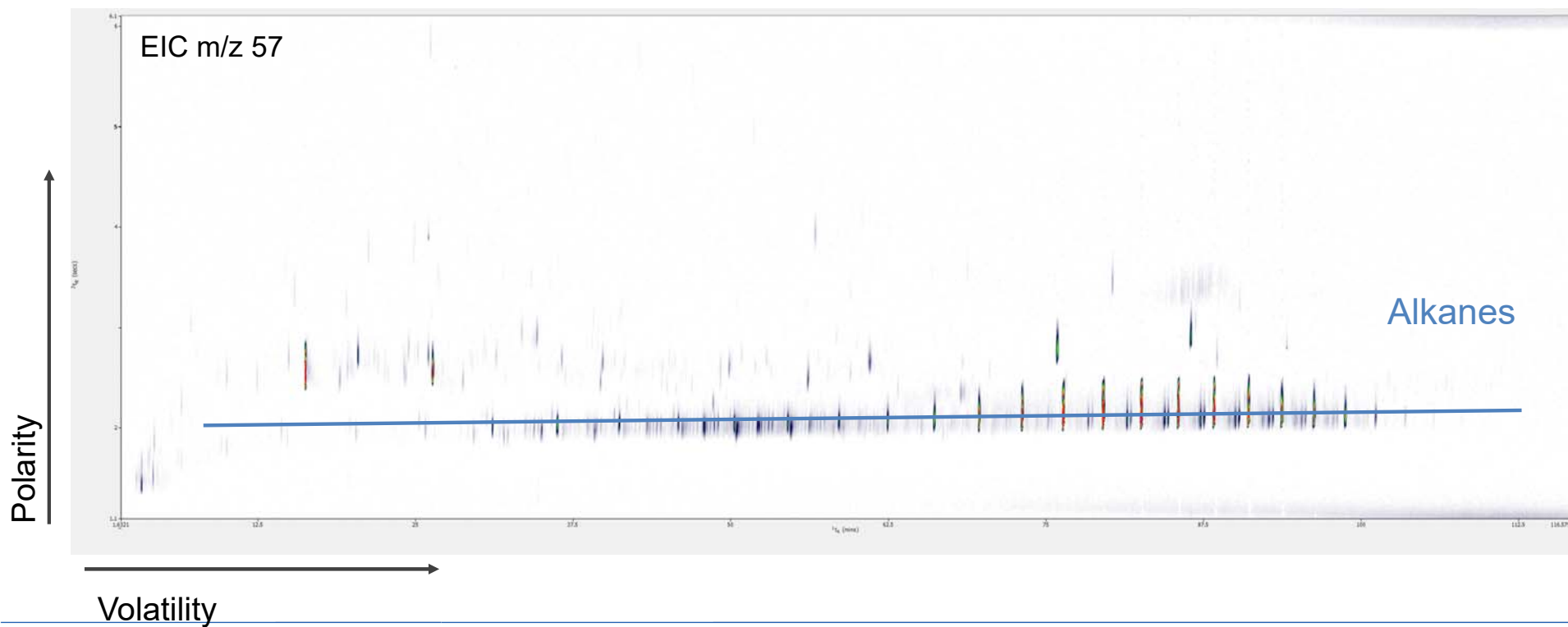
Enhanced separation of PM2.5

Wide-ranging chemical classes in a single run



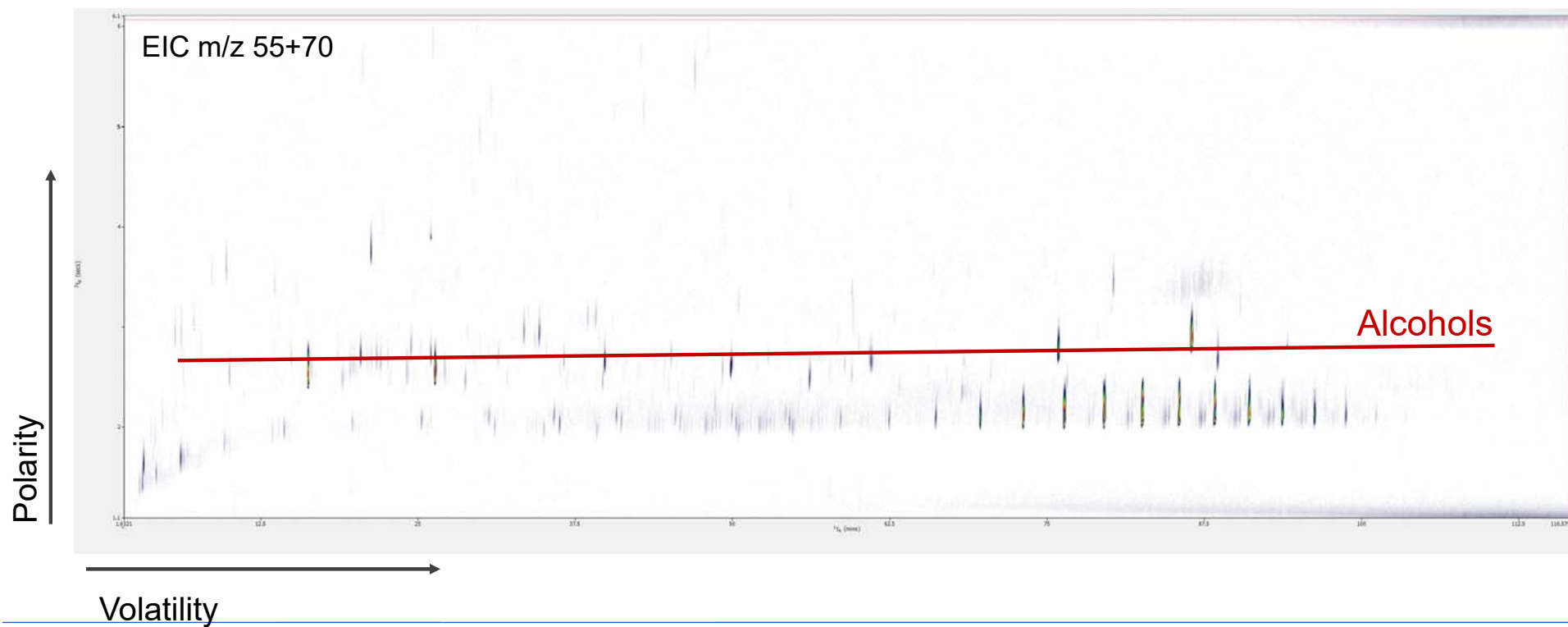
Enhanced separation of PM2.5

Wide-ranging chemical classes in a single run



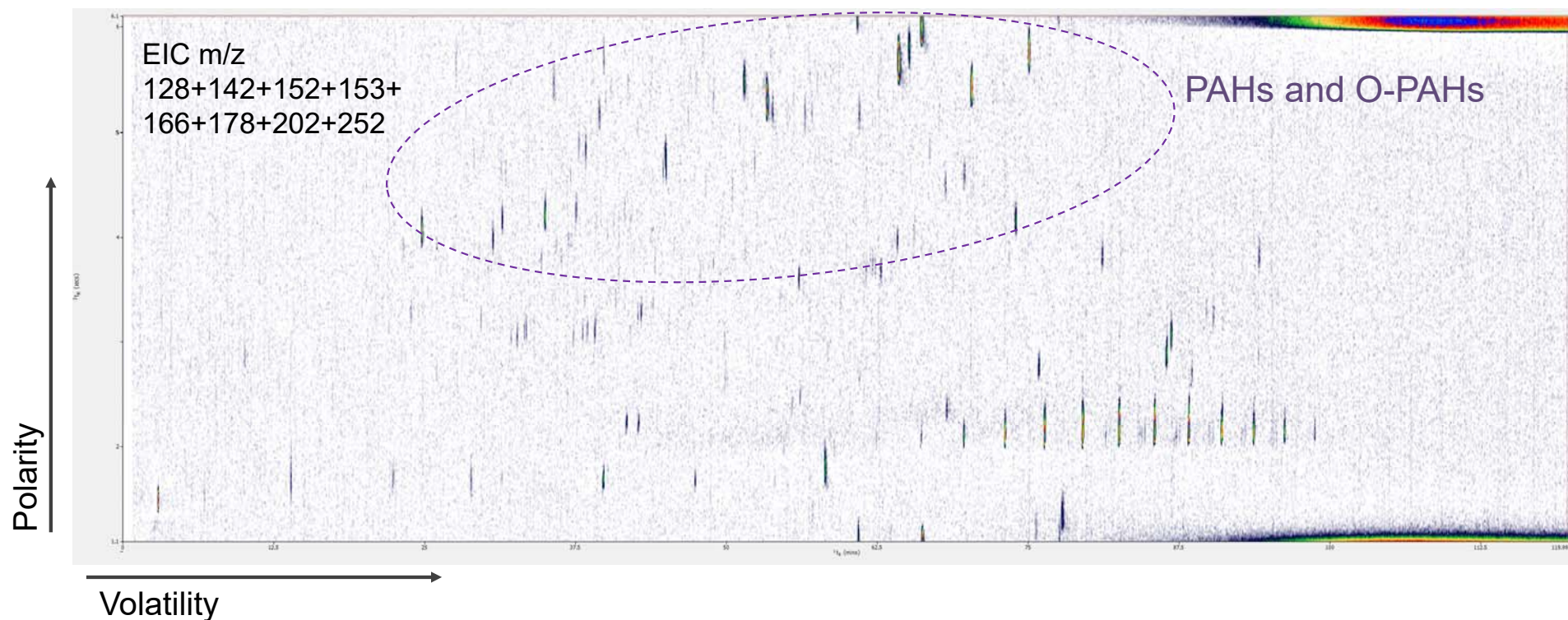
Enhanced separation of PM2.5

Wide-ranging chemical classes in a single run

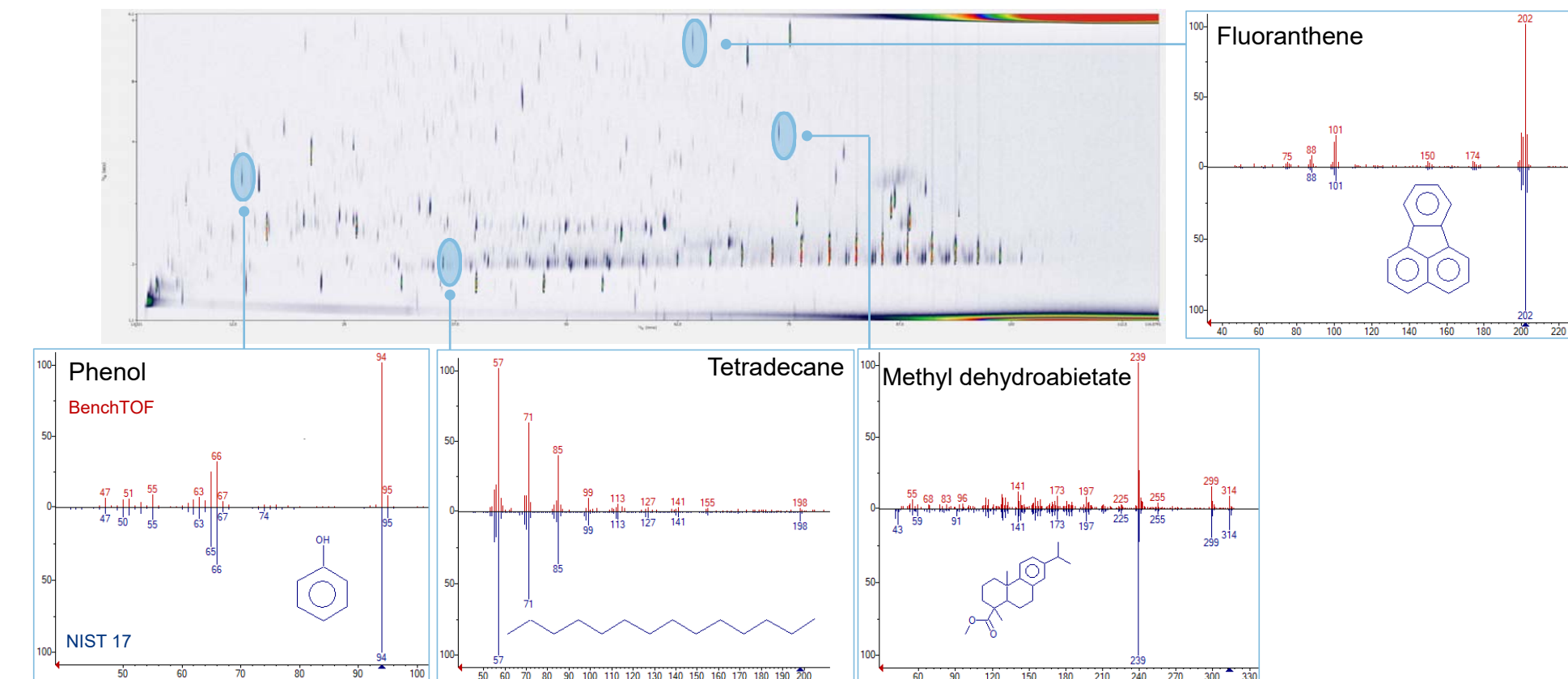


Enhanced separation of PM2.5

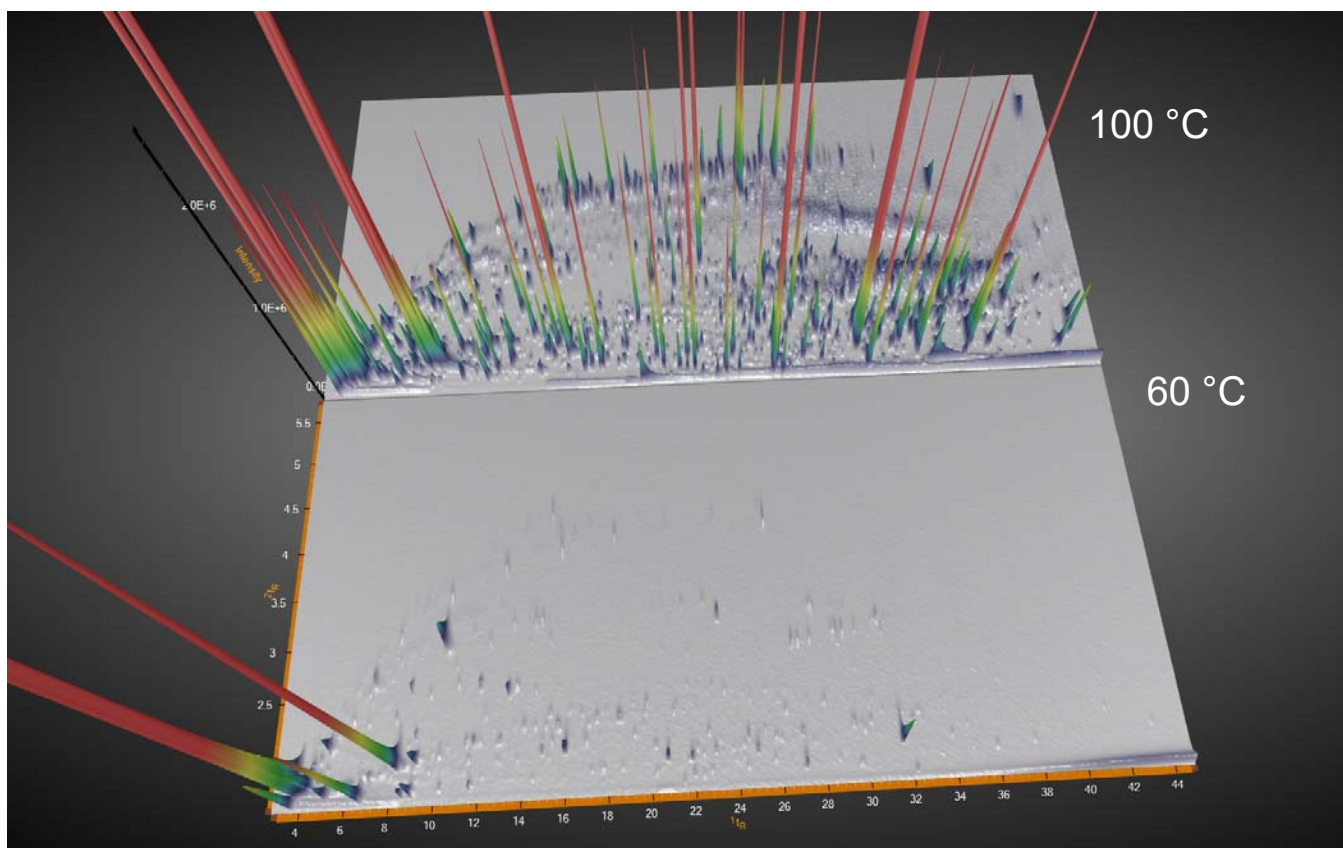
Wide-ranging chemical classes in a single run



Confident identification by BenchTOF



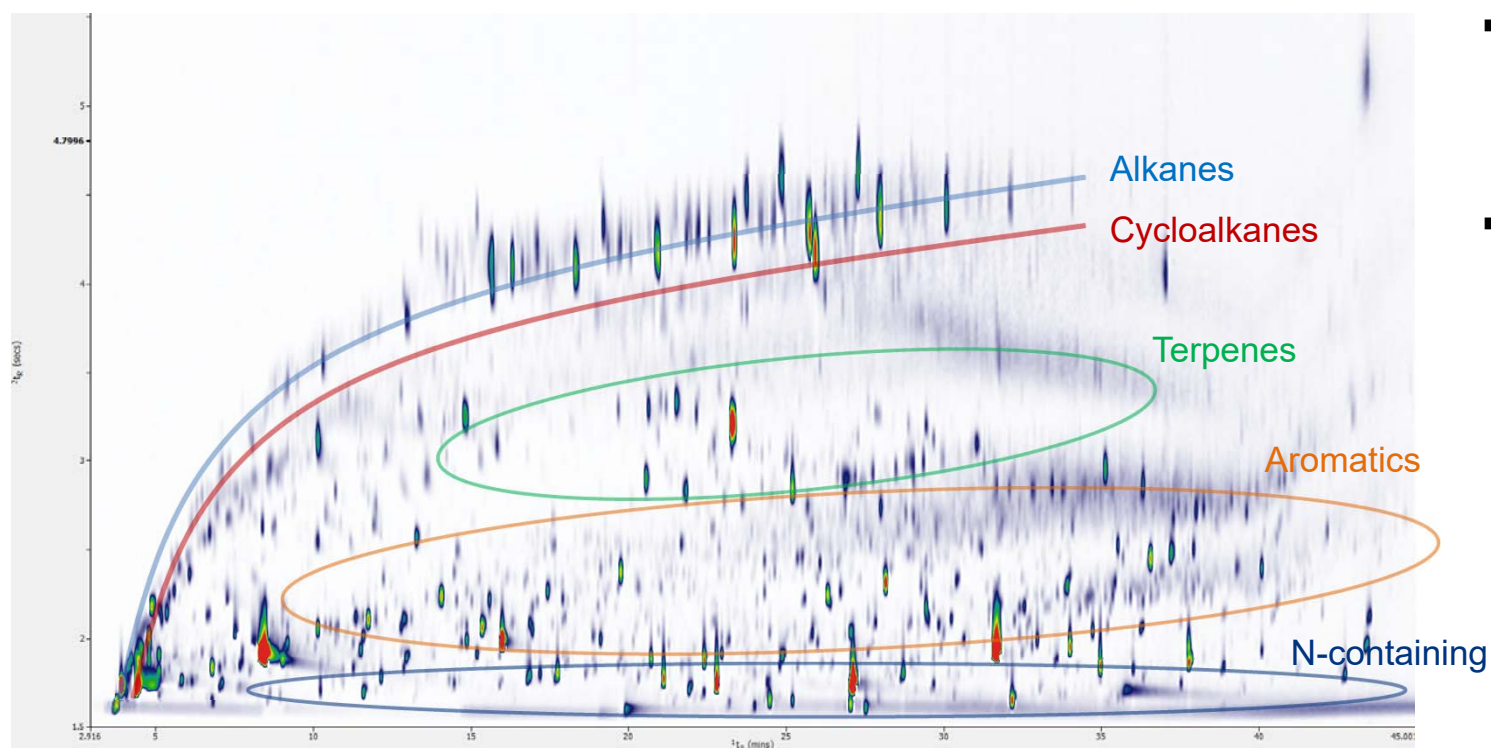
Tyre emissions as contributors to particulate matter



- Analysis of worn tyre by Micro-Chamber/Thermal Extractor™ and TD-GC×GC-TOF MS
- 10-fold increase in the number of peaks detected at 100 °C compared to 60 °C

Enhanced separation of chemical classes

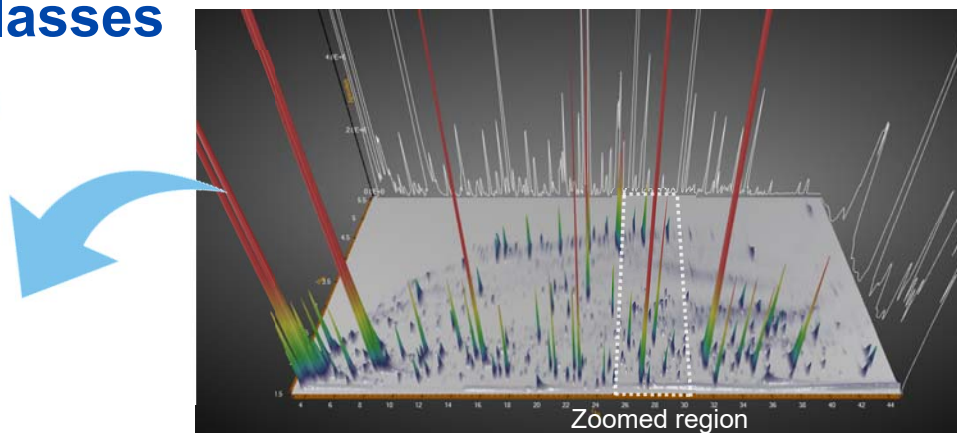
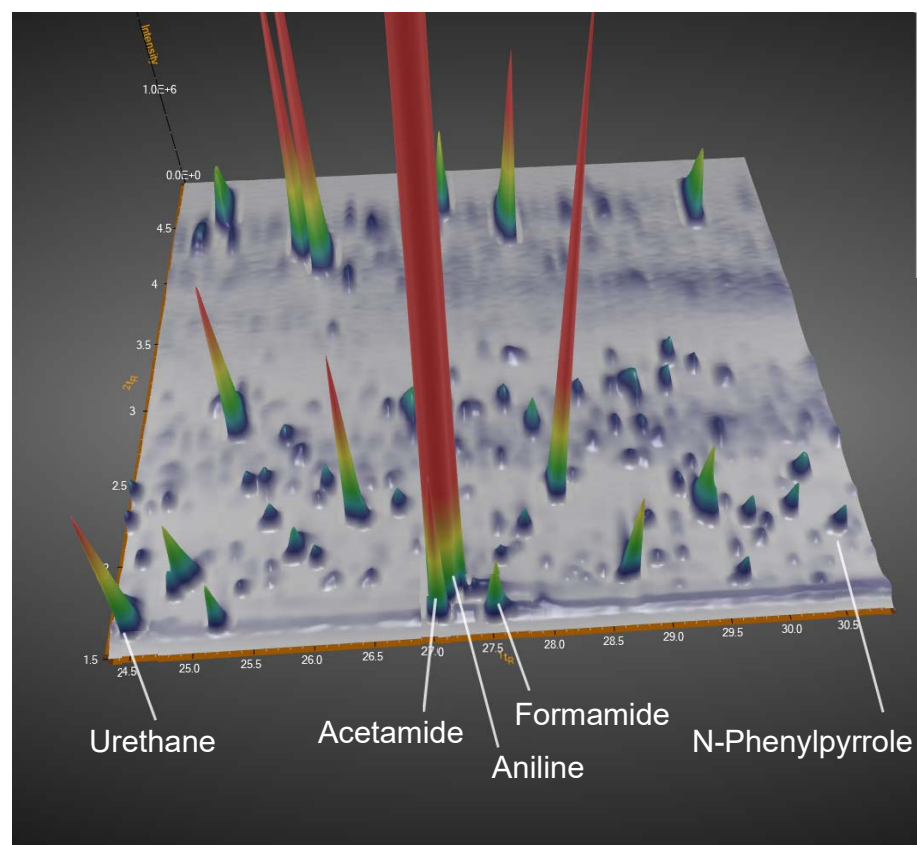
Tyre emissions at 100 °C



- Wide-ranging analytes identified
- Many of which are potentially harmful to health

Enhanced separation of chemical classes

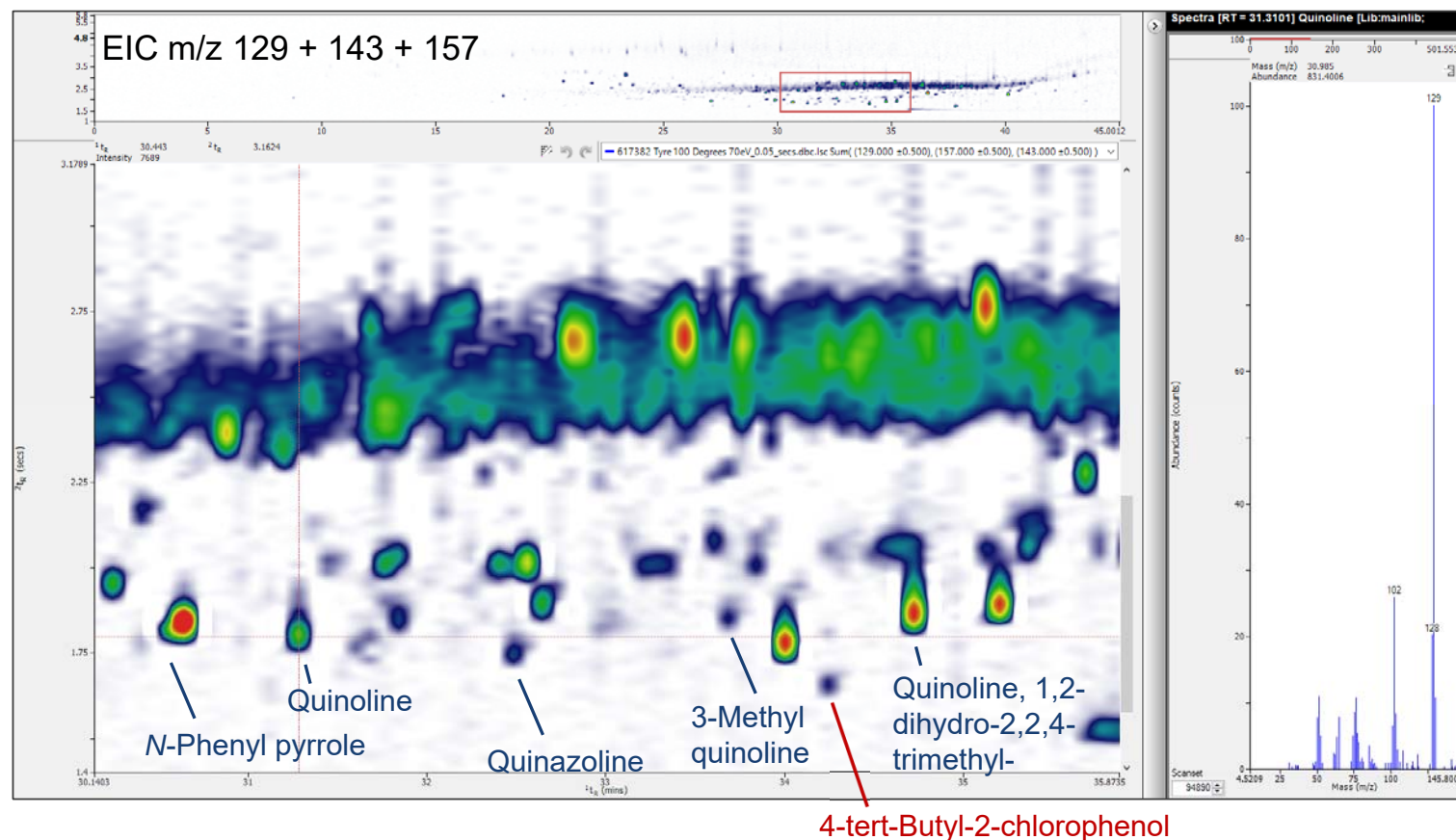
Nitrogen-containing compounds in tyre emissions



- **>70 N-containing compounds** identified by screening against NIST database
- Multiple coelutions would have occurred in a 1DGC separation

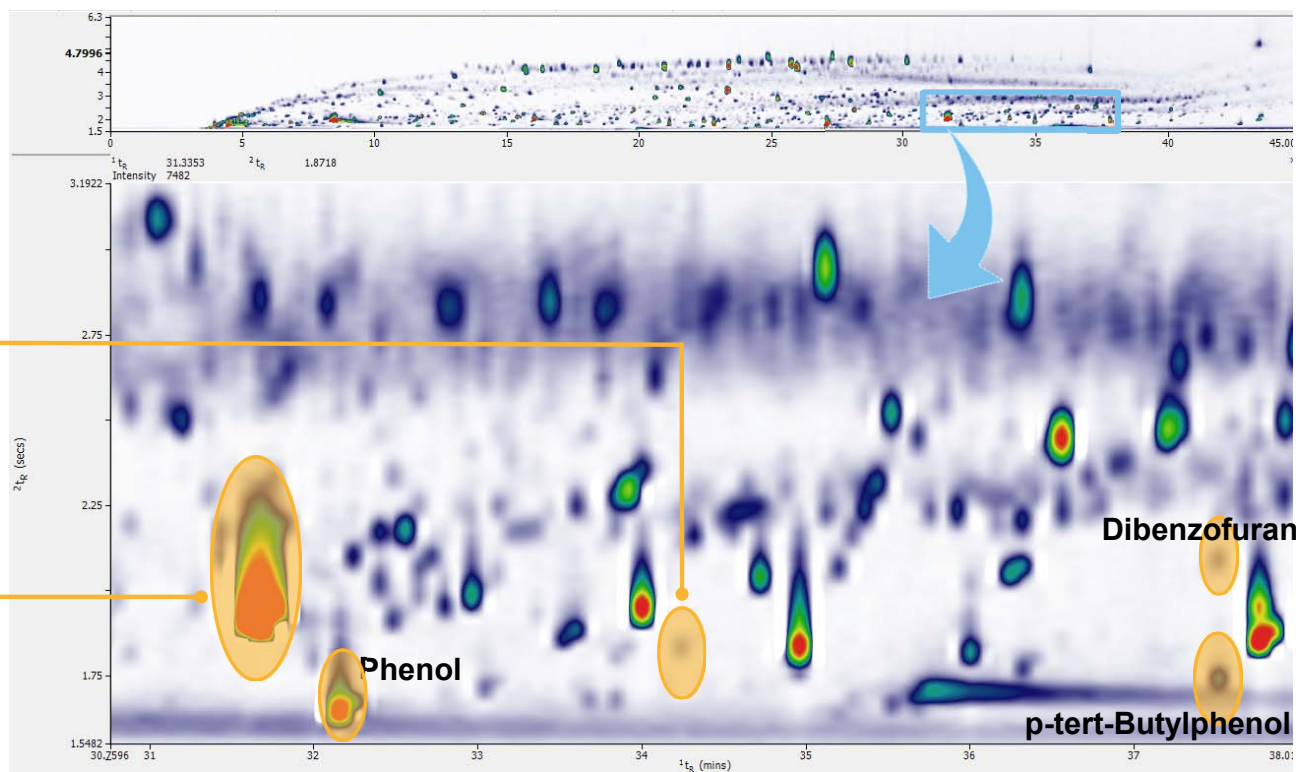
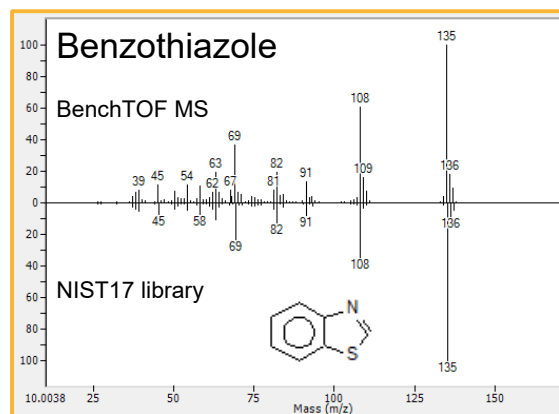
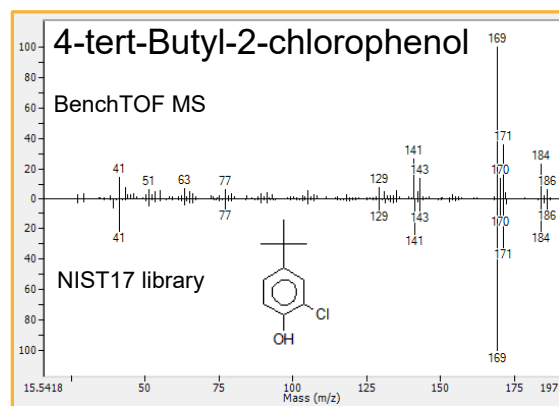
Tyre emissions at 100 °C

Nitrogen-containing compounds



- **>70 N-containing compounds** identified by screening against NIST database

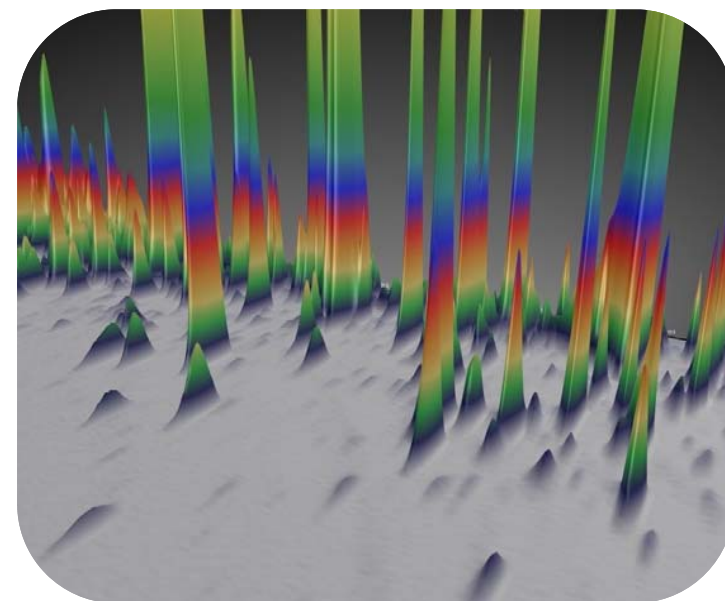
Confident identification of compounds of concern



Summary

Discover more – Deliver more

- There is a wealth of information available in chemical fingerprinting of PM2.5
- Thermal desorption can simplify sample preparation for analysis of PM2.5 and provide re-collection capabilities for repeat analysis
- GC×GC allows you to discover more about sample composition, for enhanced separation of a wide range of analytes
- BenchTOF mass spectrometers provide confident identification of targets and non-targets, for robust screening of potentially harmful compounds





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