What's in the air we breathe?
Chemical fingerprinting of PM2.5 by TD-GC×GC-TOF MS

Who are SepSolve Analytical?

Experts in analytical chemistry
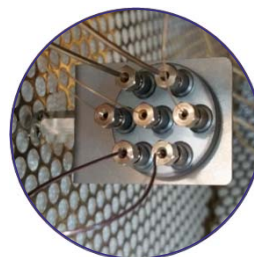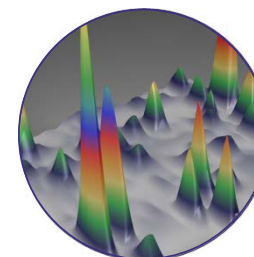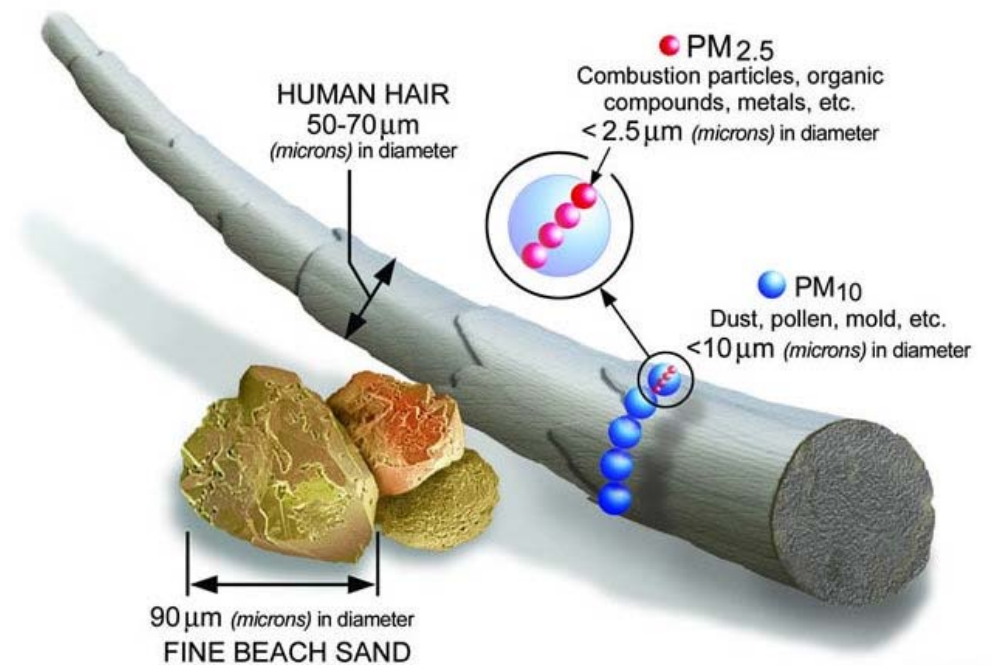

Sample preparation

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
  - PM2.5 (fine particles): d ≤ 2.5 µm
  - PM10 (coarse particles): d ≤ 10 µm

- PM pollution consists of materials (including dust, smoke, and soot) either:
  - Directly emitted into the air
  - Result from the transformation of gaseous pollutants

HUMAN HAIR
50-70 µm
(microns) in diameter

PM2.5
Combustion particles, organic compounds, metals, etc.
<2.5 µm *(microns)* in diameter

PM10
Dust, pollen, mold, etc.
<10 µm *(microns)* in diameter

90 µm *(microns)* in diameter
FINE BEACH SAND

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

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Sources of particulate matter

Industry
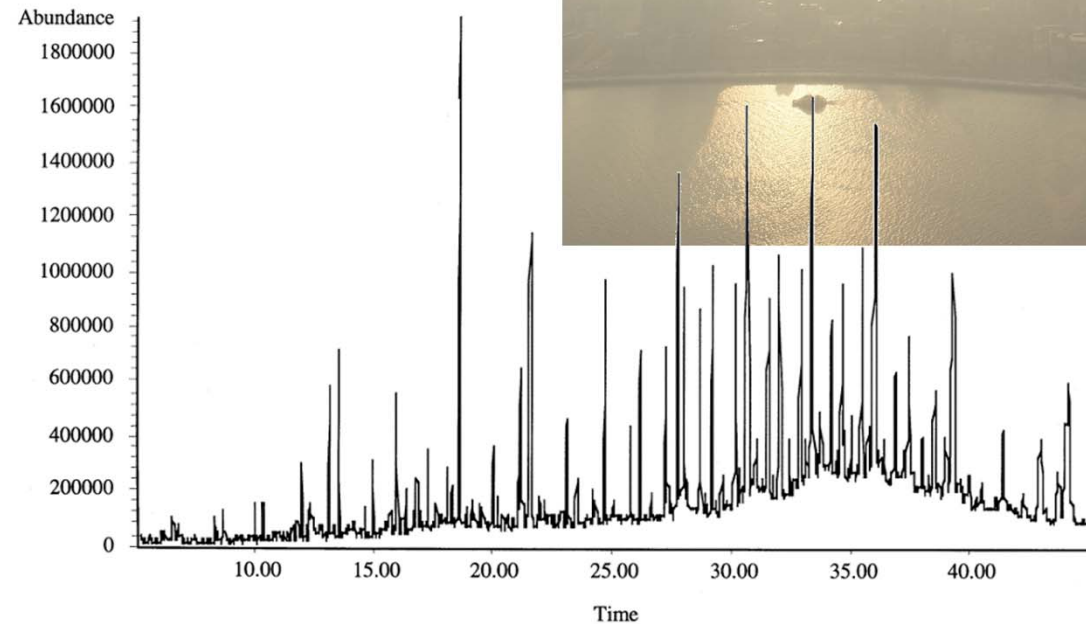(power plants, factories…)

Vehicle emissions

Natural Sources
(forest fires, volcanoes…)
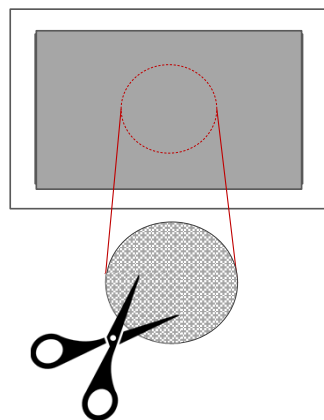
Analysis of PM 2.5

The Challenges

- Time-consuming sample preparation

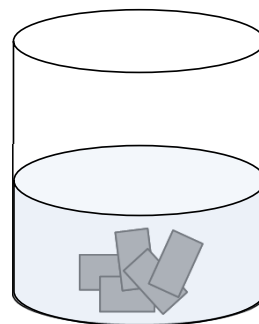- Wide range of chemical classes

- Complex chromatograms

Previous approaches sample preparation

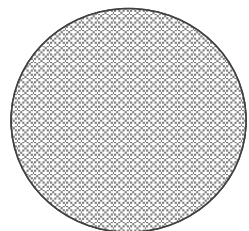| Sampling of PM2.5 on to quartz filter using in-situ sampler | PM2.5 filter cut or punched into sections | Solvent extraction with sonication | Evaporation – blow down with nitrogen |

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

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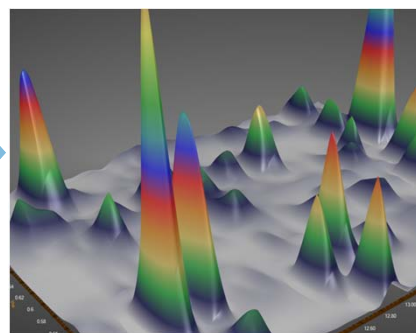Analytical

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

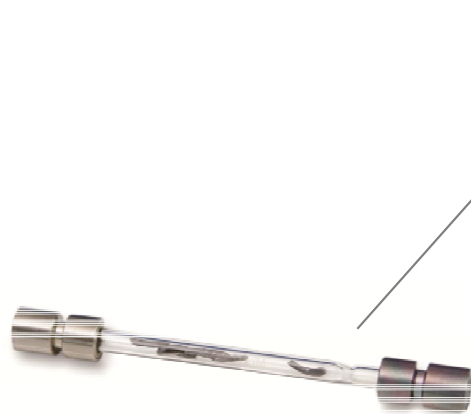# Direct desorption

Simplified sample preparation for PM2.5

TD100-xr
Automated thermal desorber

Direct desorption
of PM2.5 filters

Water may be
purged to vent
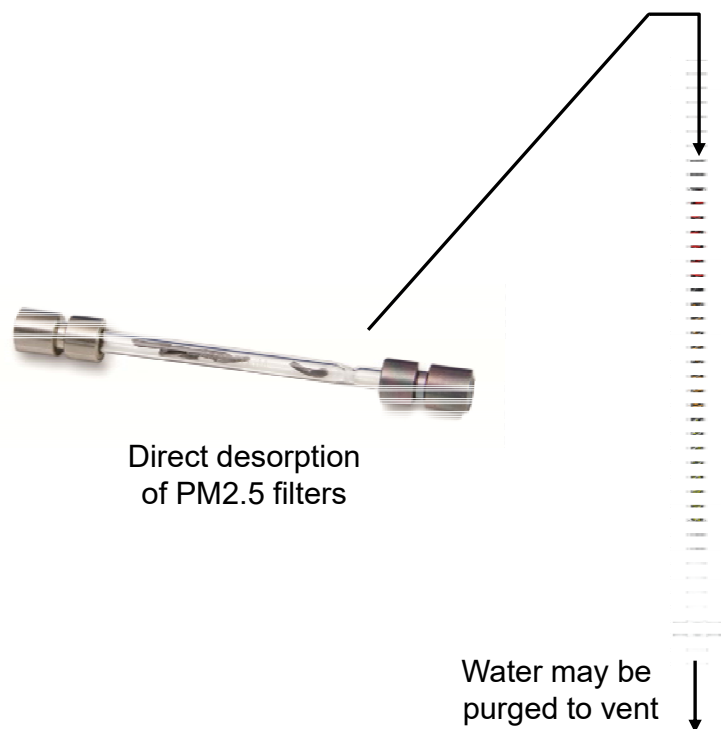
- PM2.5 filter is placed within an empty TD tube and heated to desorb analytes on to the focusing trap

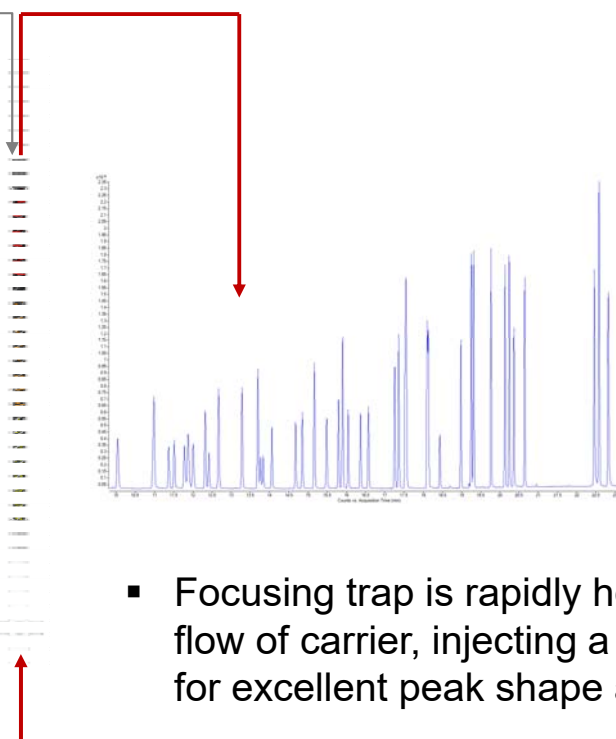- Electrically-cooled focusing trap concentrates VOCs and SVOCs

Direct desorption

Simplified sample preparation for PM2.5

TD100-xr
Automated thermal desorber

Direct desorption
of PM2.5 filters

'Backflush' operation
for trap desorption

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

Direct desorption

Simplified sample preparation for PM2.5

Re-collection tube

TD100-xr
Automated thermal desorber

Direct desorption
of PM2.5 filters
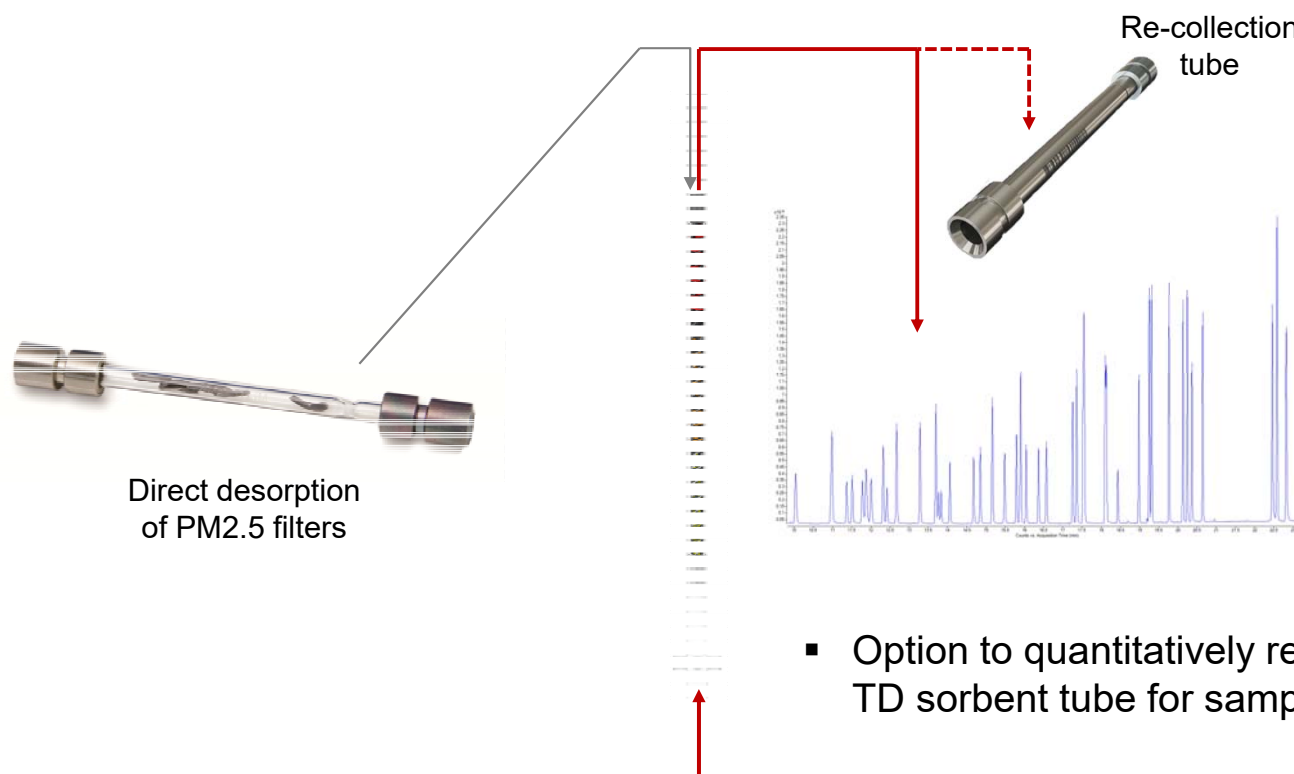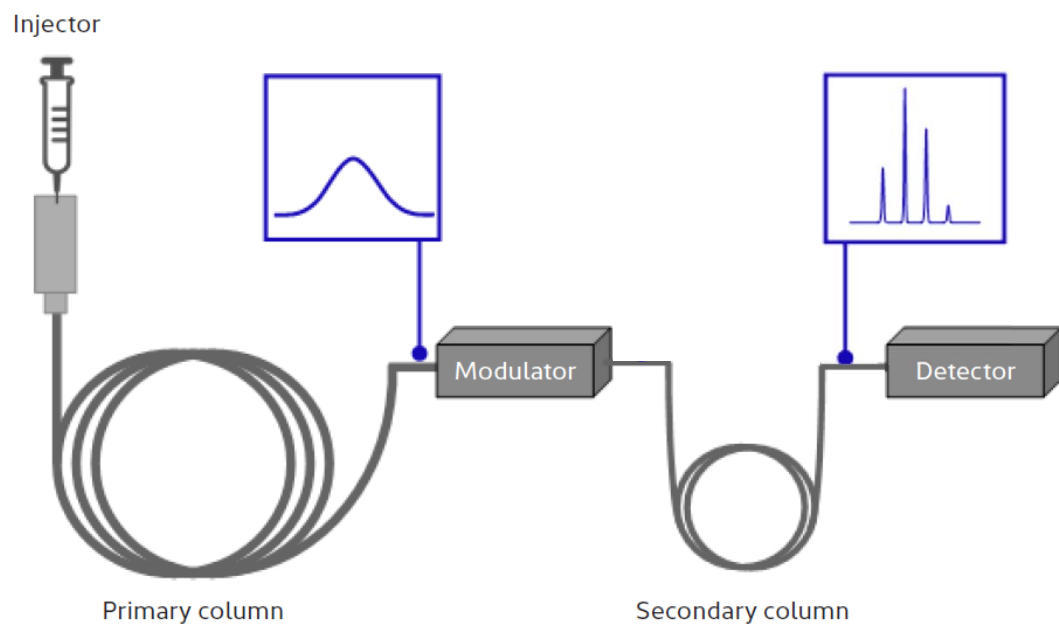
- Option to quantitatively re-collect the split flow on to a clean TD sorbent tube for sample archiving and repeat analysis

What is GC×GC?

2nd dimension separation

Intensity

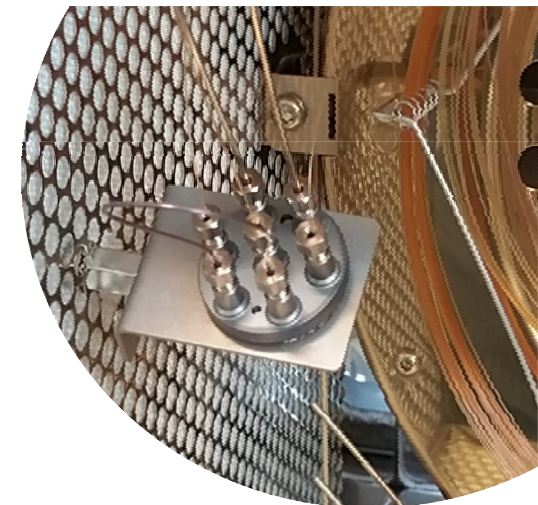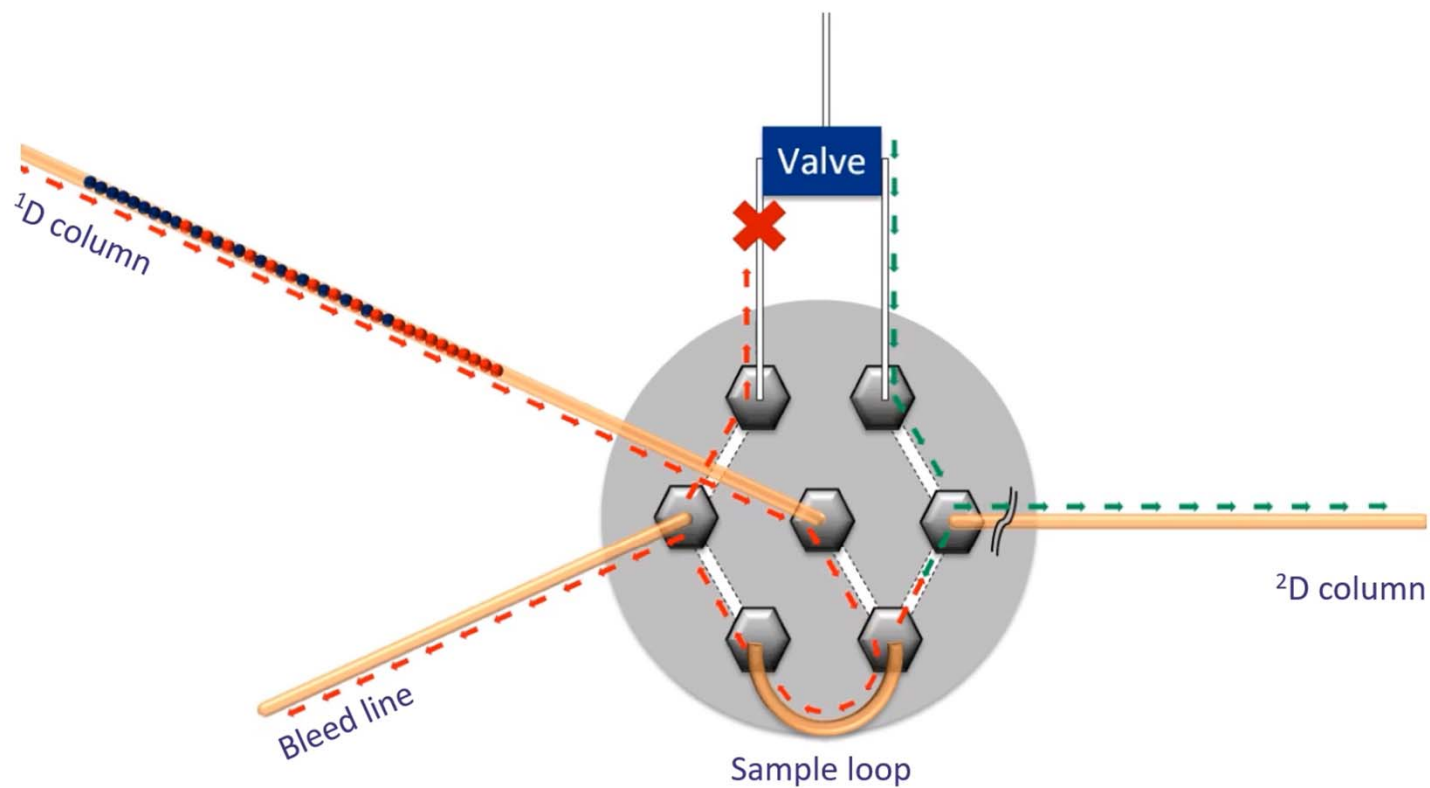1st dimension separation

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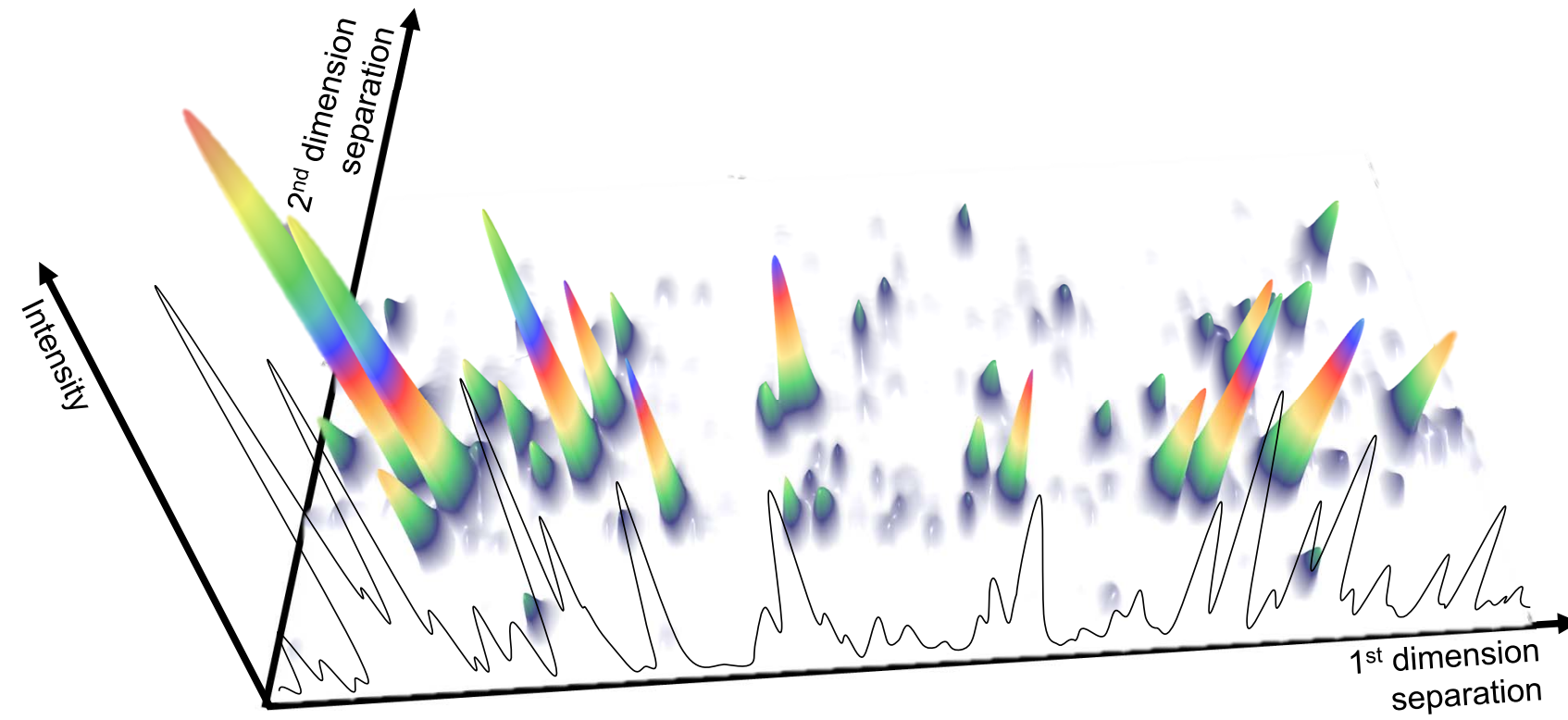
What is GC×GC?

- The modulator is the 'beating heart' of a GC×GC system

- Advances in flow modulation have made GC×GC more suitable for routine analysis

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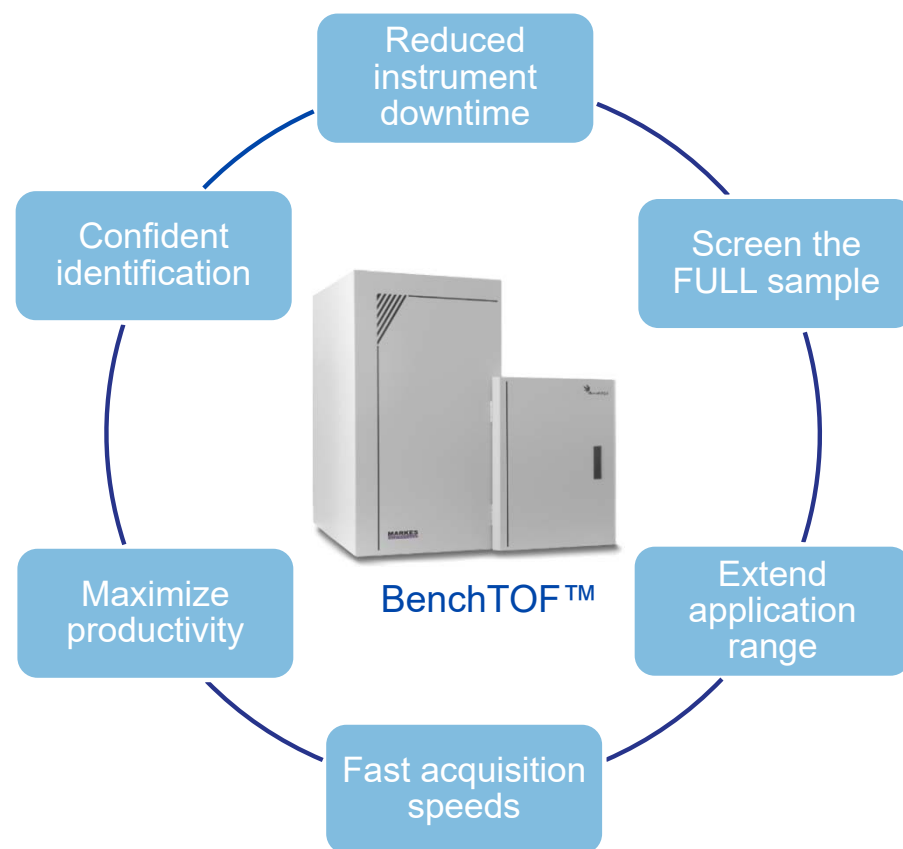# Reverse fill/flush flow modulator

How does it work?
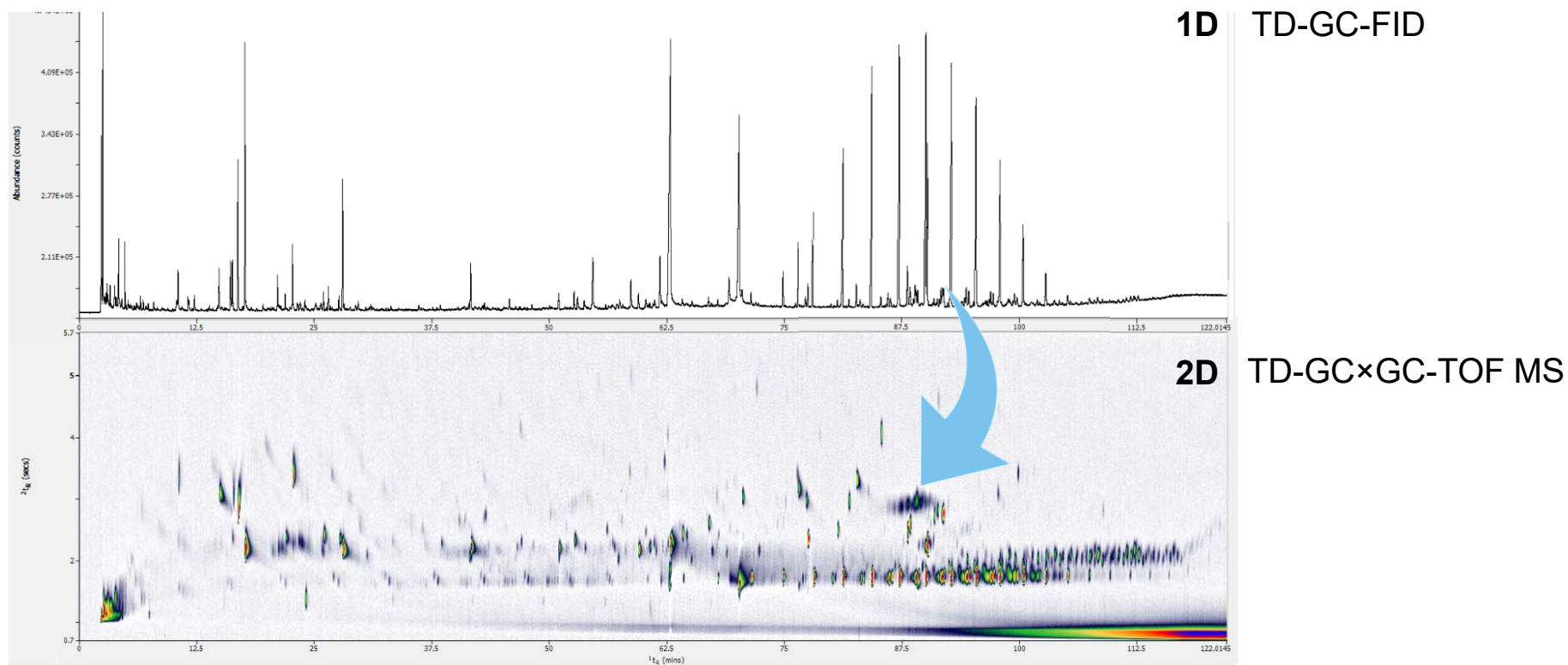
Why choose TOF mass spectrometry?

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

Reduced instrument downtime

Screen the FULL sample

Confident identification

BenchTOF™

Maximize productivity

Extend application range

Fast acquisition speeds

PM 2.5 analysis

Gaining an additional level of detail…

1D TD-GC-FID

2D TD-GC×GC-TOF MS

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Enhanced separation of PM2.5

Wide-ranging chemical classes in a single run

Polarity

Volatility

Enhanced separation of PM2.5

Wide-ranging chemical classes in a single run

EIC m/z 57

Alkanes

Polarity

Volatility
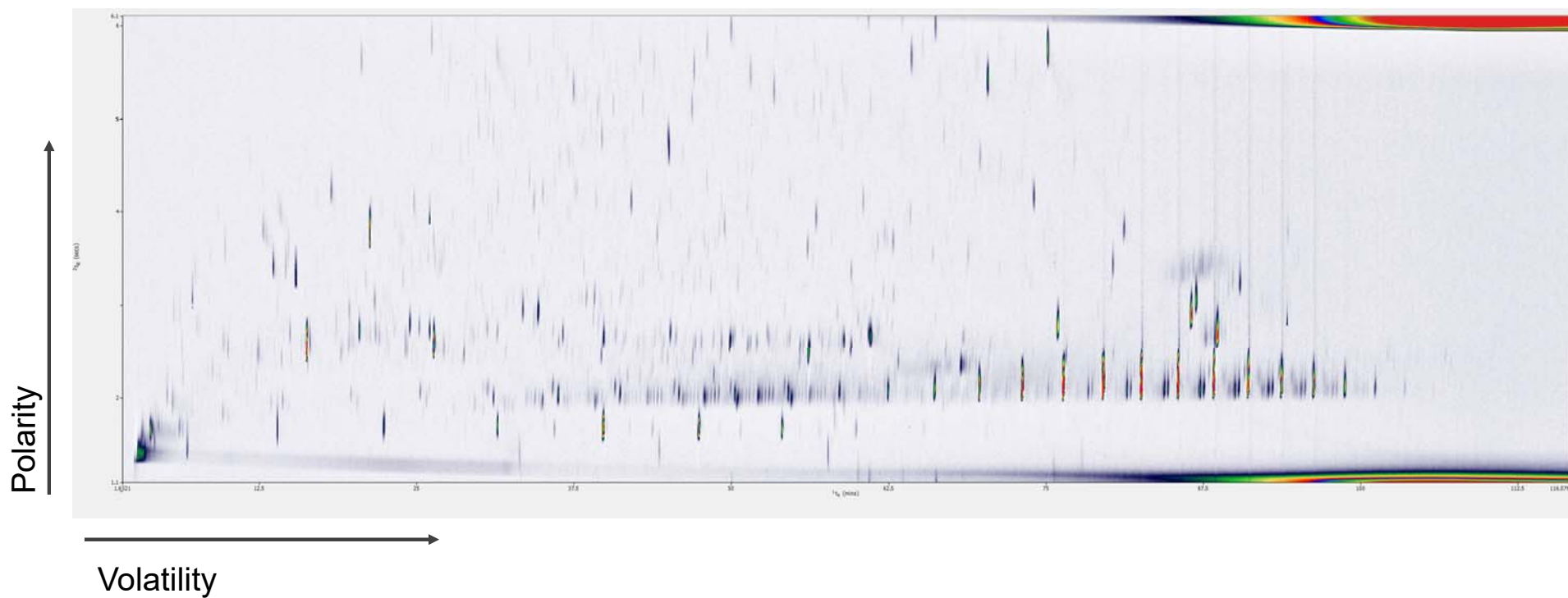
Enhanced separation of PM2.5

Wide-ranging chemical classes in a single run

Enhanced separation of PM2.5
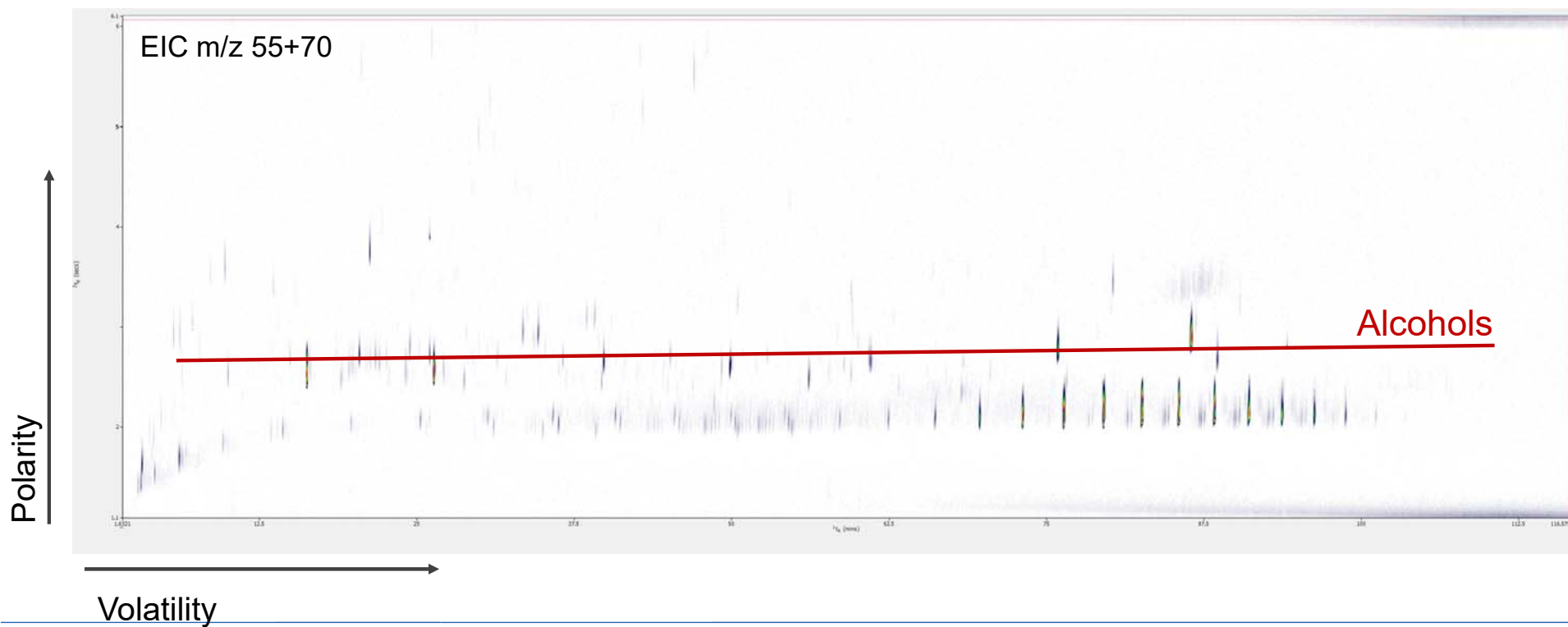
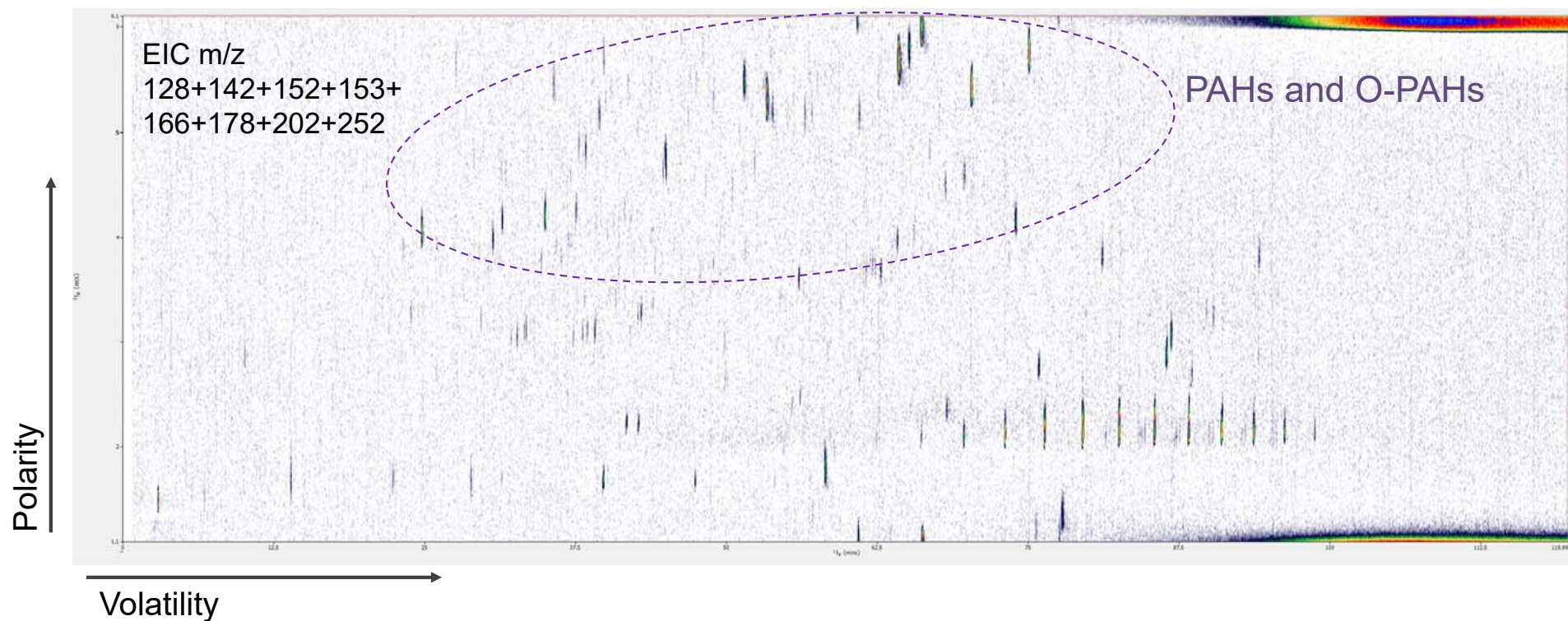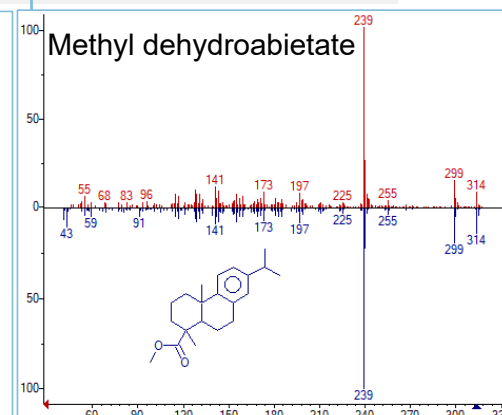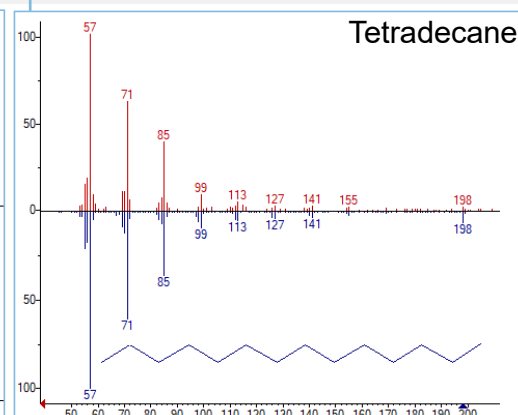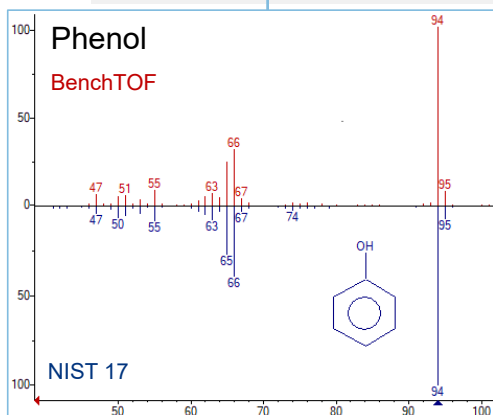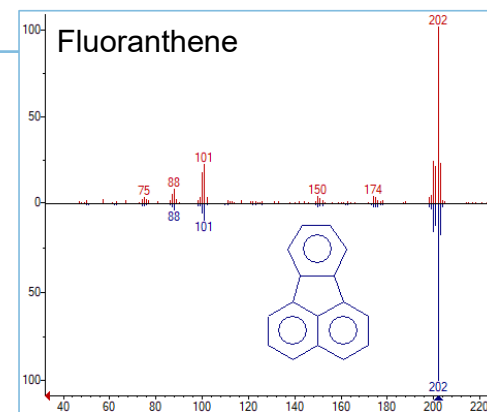Wide-ranging chemical classes in a single run

EIC m/z
128+142+152+153+
166+178+202+252

PAHs and O-PAHs

Polarity

Volatility

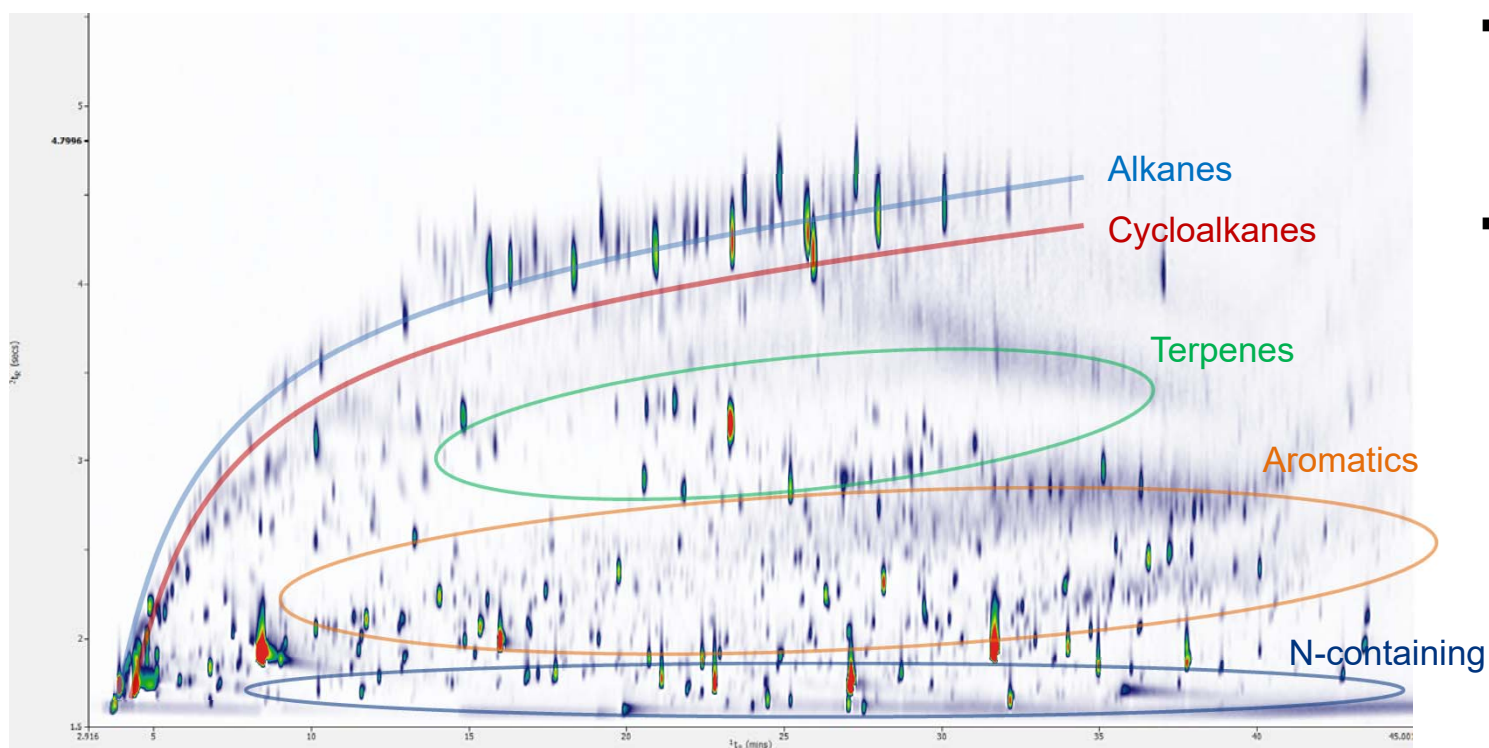# Confident identification by BenchTOF
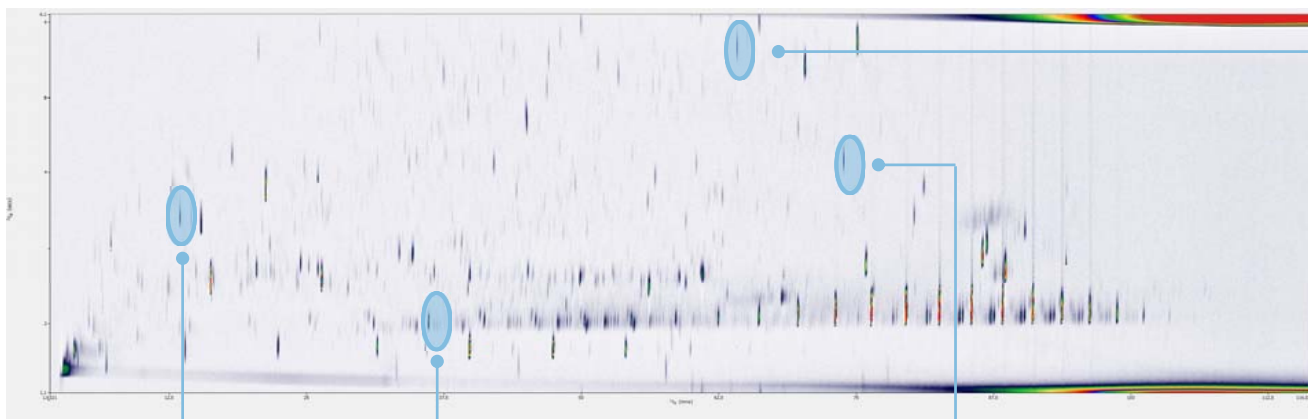
Tyre emissions as contributors to particulate matter

100 °C

60 °C
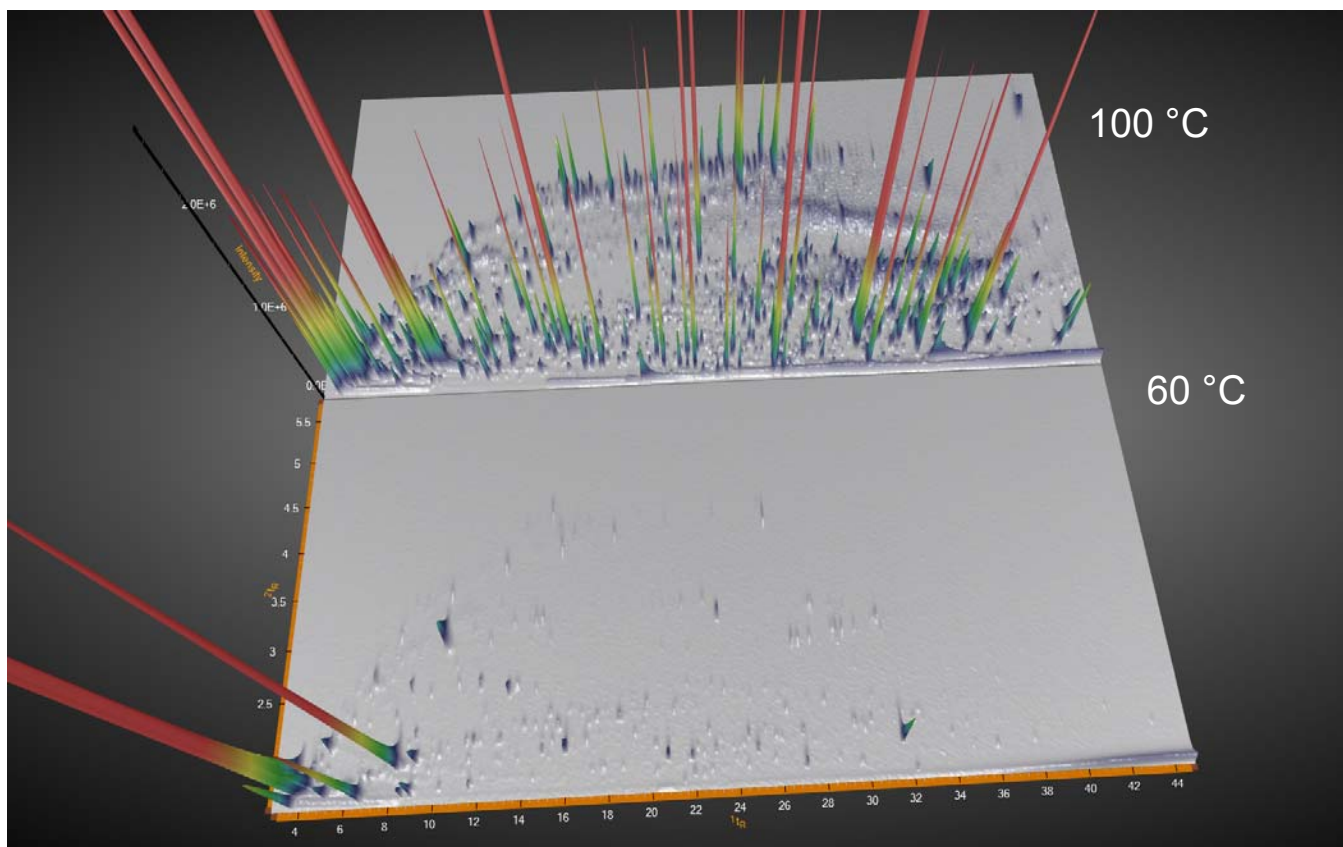
- Analysis of worn tyre by Micro-Chamber/Thermal Extractor™ and TD-GC×GC-TOF MS

- 10-fold increase in the number of peaks detected at 100 °C compared to 60 °C

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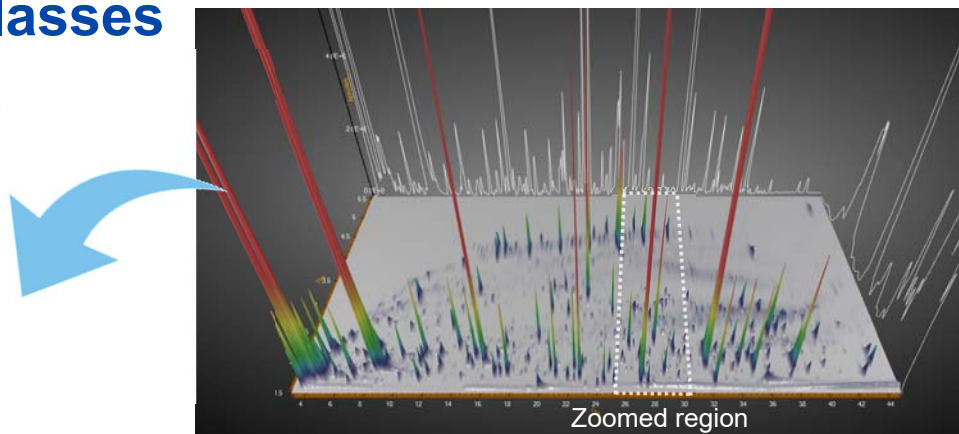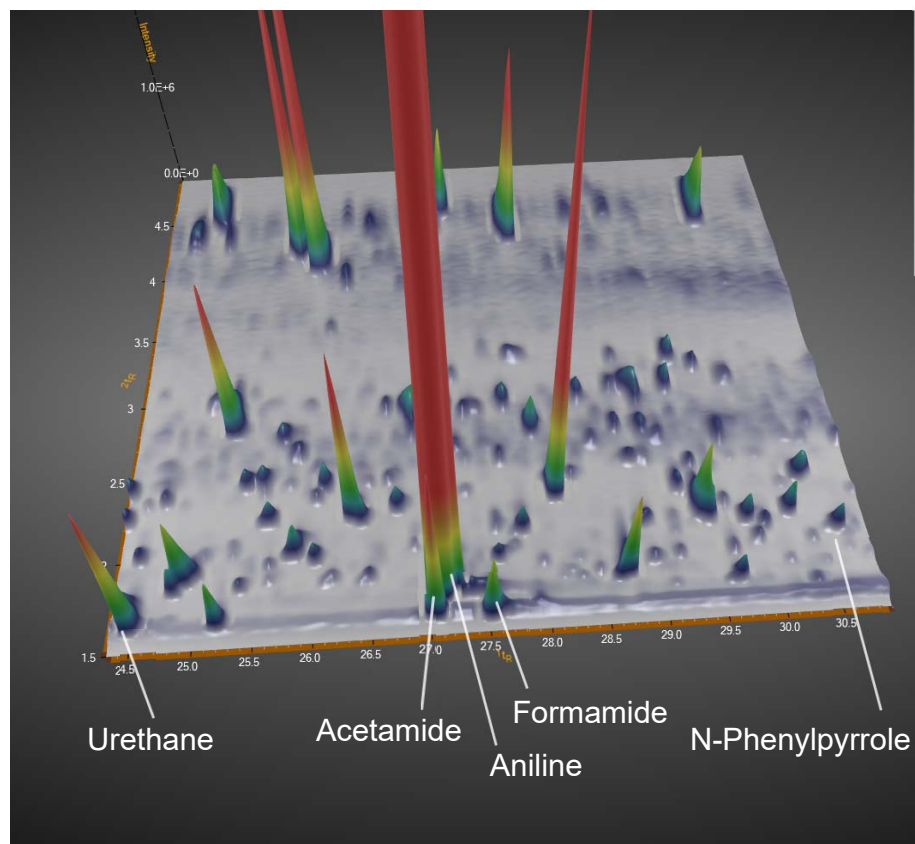
Enhanced separation of chemical classes

Tyre emissions at 100 °C

- Wide-ranging analytes identified

- Many of which are potentially harmful to heath

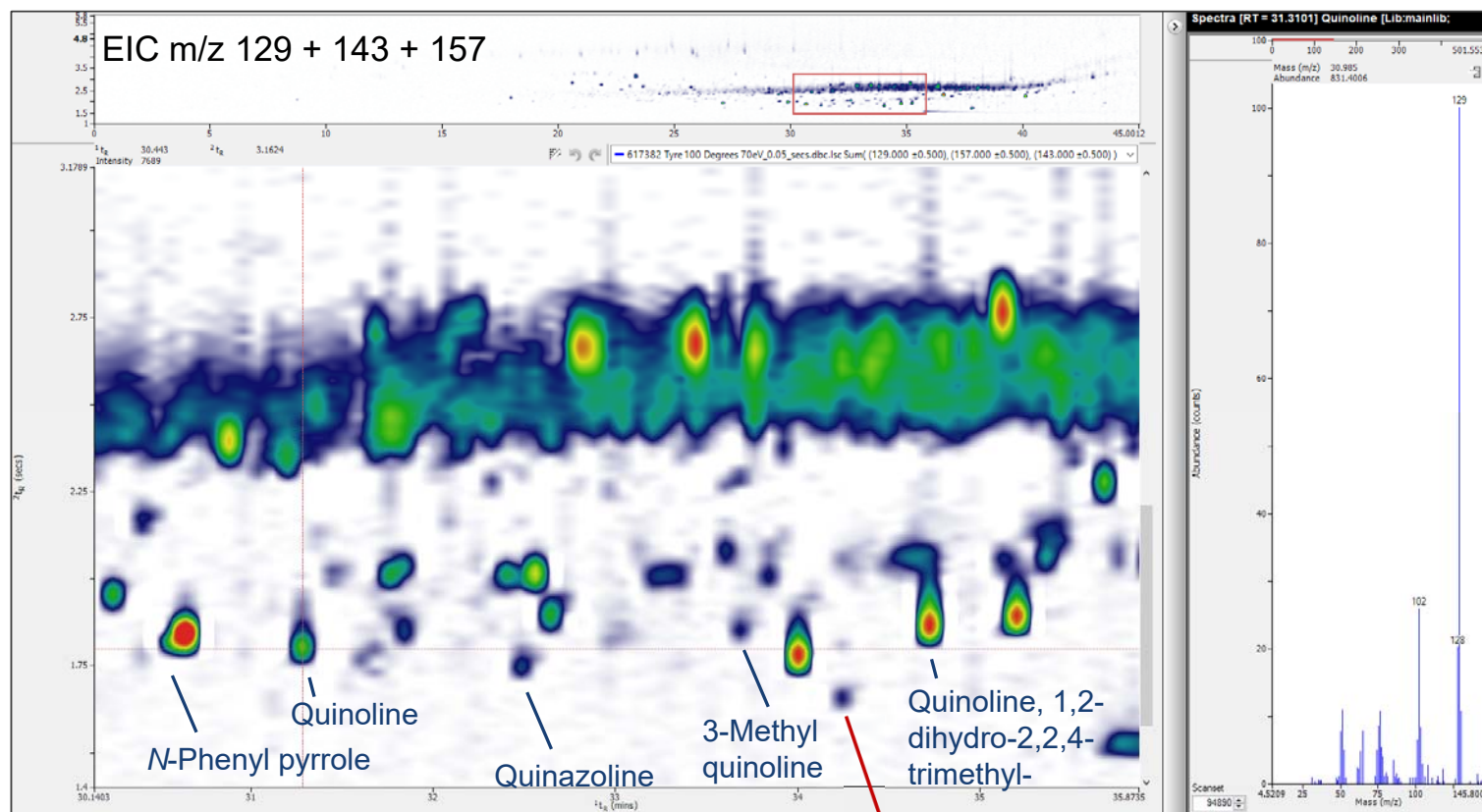# Enhanced separation of chemical classes

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

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Tyre emissions at 100 °C

Nitrogen-containing compounds

EIC m/z 129 + 143 + 157

N-Phenyl pyrrole

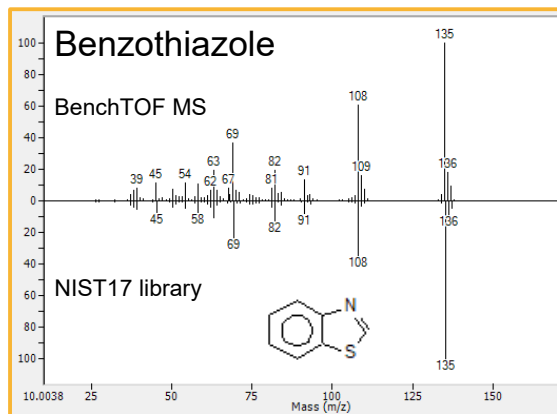Quinoline

Quinazoline

3-Methyl quinoline

Quinoline, 1,2-dihydro-2,2,4-trimethyl-
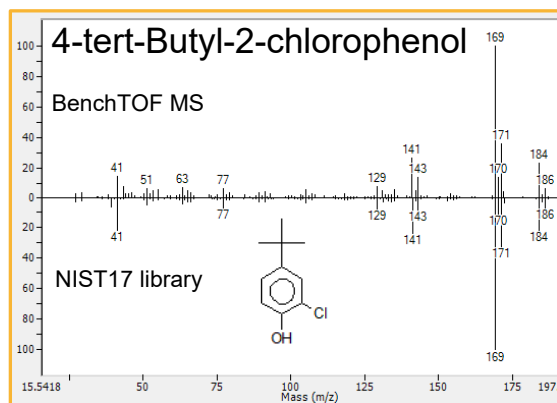
4-tert-Butyl-2-chlorophenol

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

Confident identification of compounds of concern
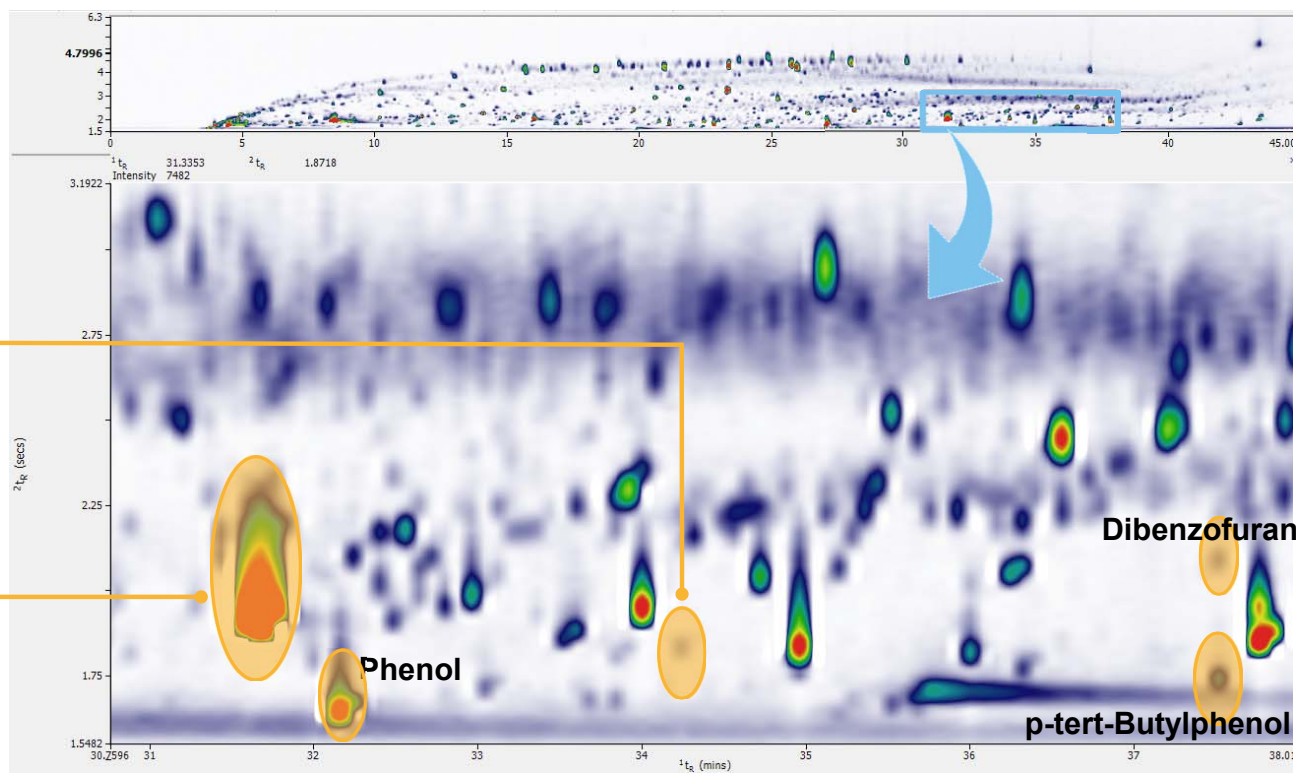
Summary

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
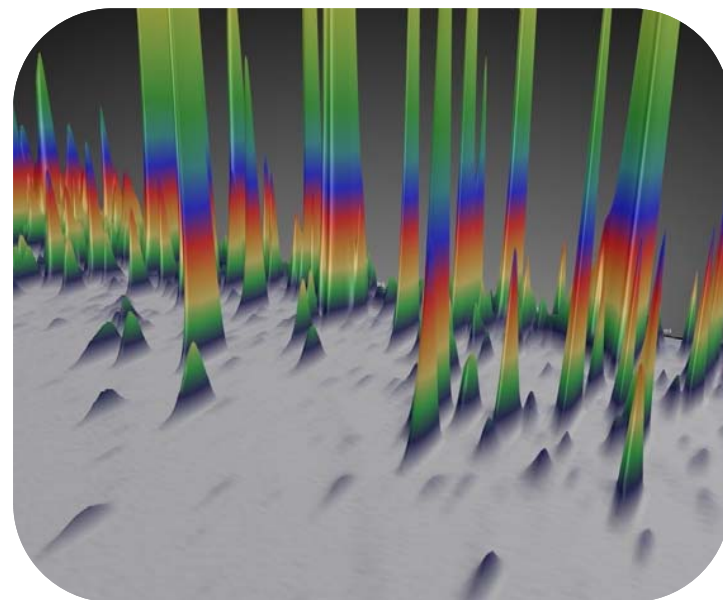
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