SepSolve Analytical

GC×GC–TOF MS for petrochemical fingerprinting

Wide-ranging petrochemical applications

CRUDE OIL FINGERPRINTING

OIL SPILL ANALYSIS

MATERIALS CHARACTERISATION

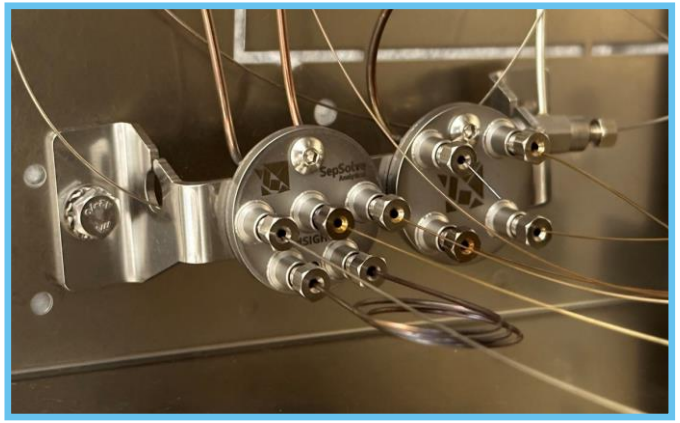
PYROLYSIS OILS & NOVEL FUELS

AVIATION FUELS

ODOURS FROM PLASTICS

GC×GC–TOF MS for petrochemical fingerprinting

INSIGHT-Flow

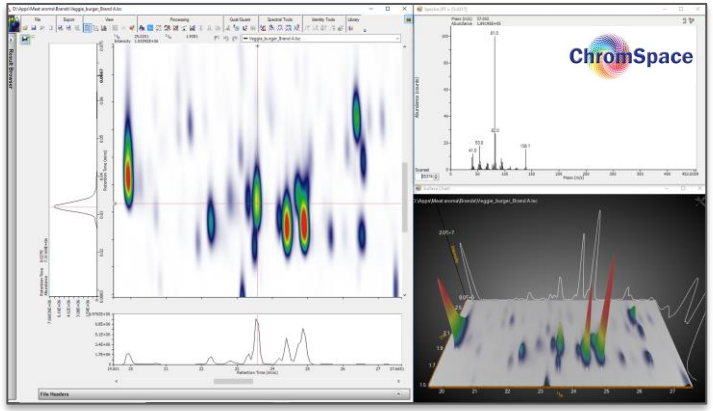


INSIGHT-Thermal

BenchTOF2™ time-of-flight MS

- ✓ Excellent sensitivity with full range spectra
- ✓ Reference-quality spectra
- ✓ Mass accuracy (<50ppm)
- ✓ Tandem Ionisation for unique soft ionisation
- ✓ Fast acquisition speeds (up to 400 Hz)

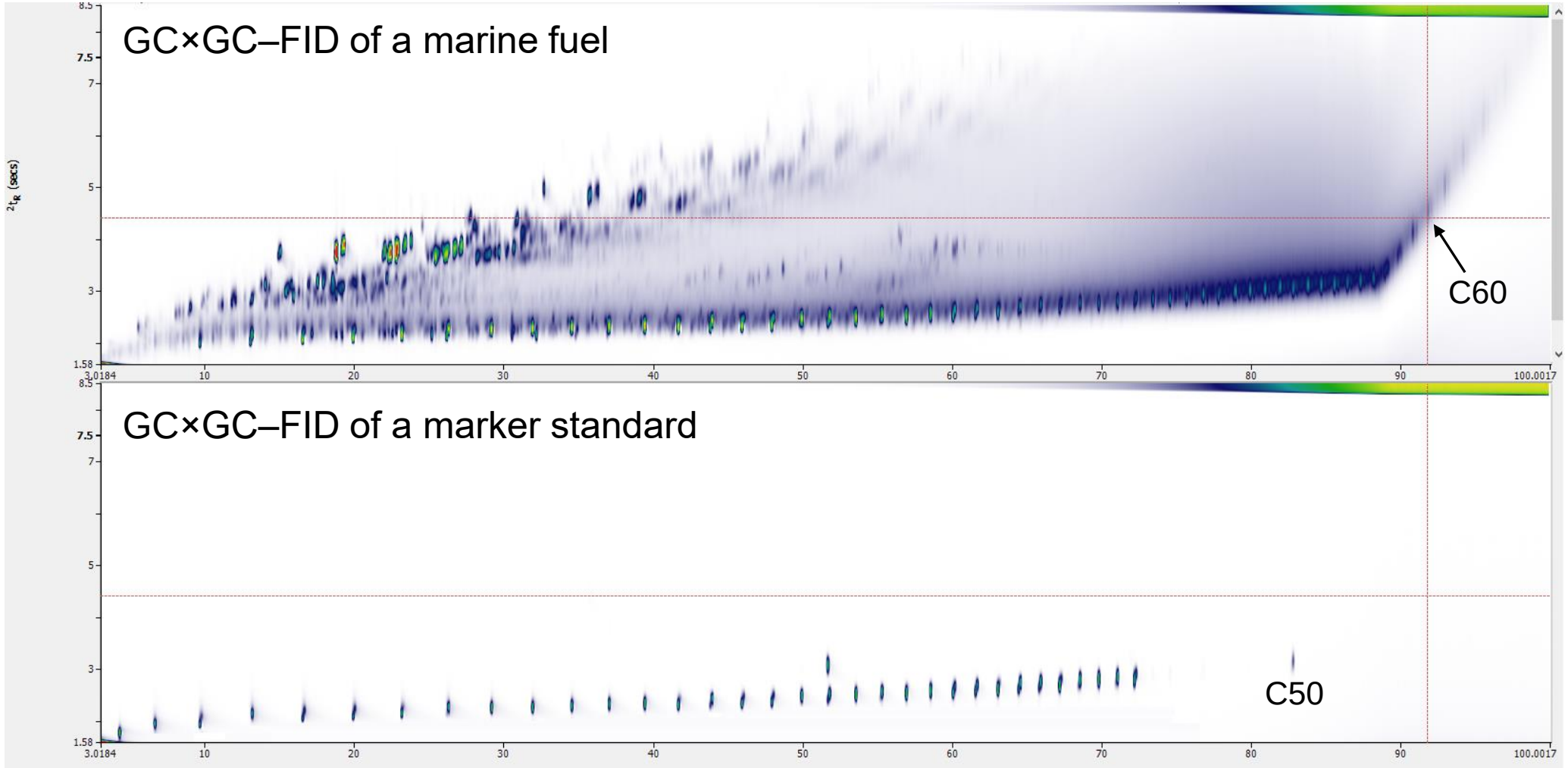
ChromSpace software



Wide analyte range

Flow modulation

Thermal modulation

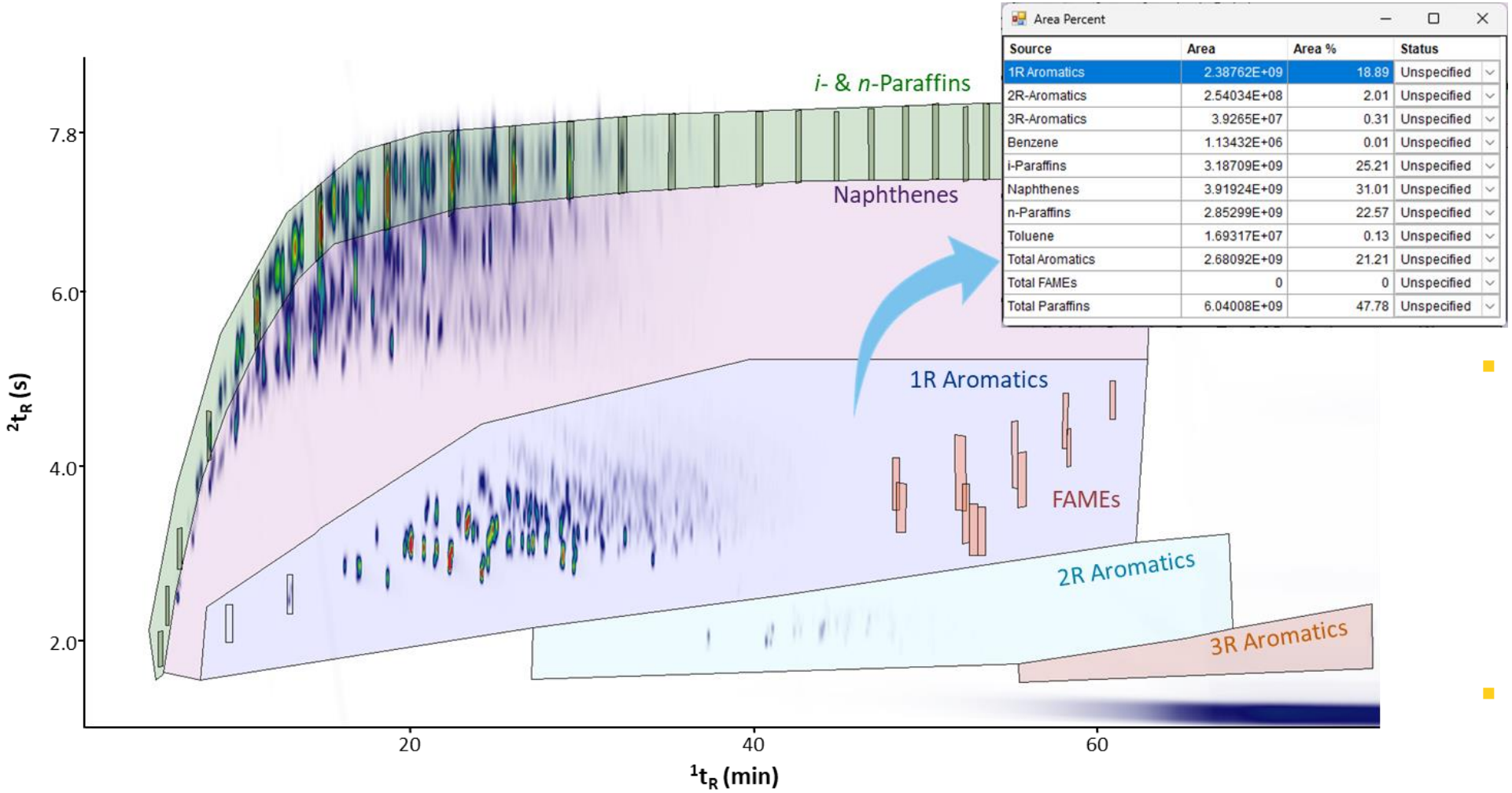


Example application: Analysis of aviation fuel

Flow modulation

Thermal modulation

Following ASTM Method D8396



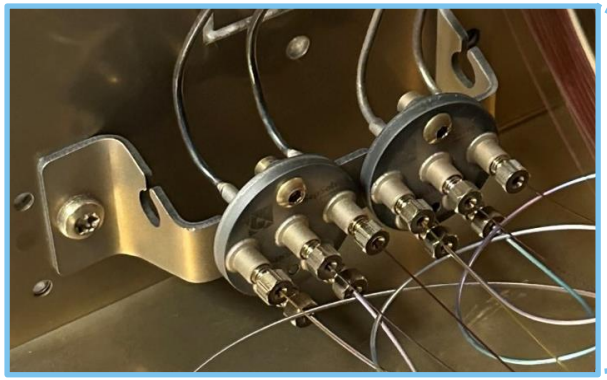
Area Percent

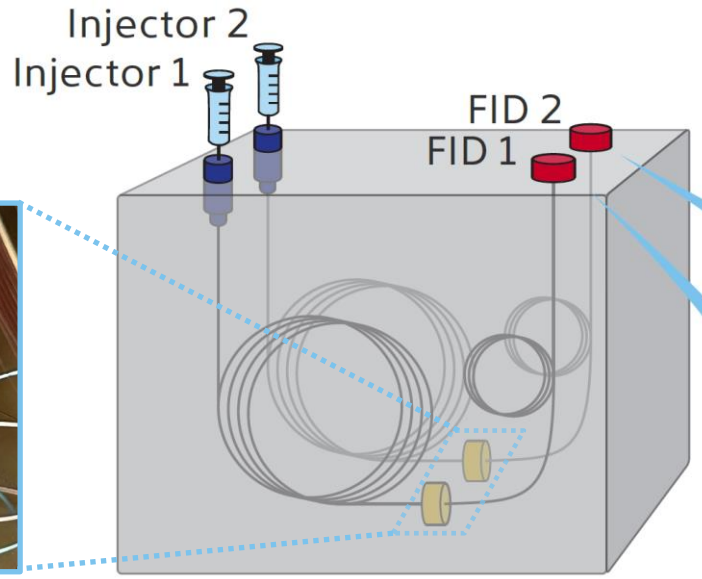
Source	Area	Area %	Status
1R Aromatics	2.38762E+09	18.89	Unspecified
2R-Aromatics	2.54034E+08	2.01	Unspecified
3R-Aromatics	3.9265E+07	0.31	Unspecified
Benzene	1.13432E+06	0.01	Unspecified
i-Paraffins	3.18709E+09	25.21	Unspecified
Naphthenes	3.91924E+09	31.01	Unspecified
n-Paraffins	2.85299E+09	22.57	Unspecified
Toluene	1.69317E+07	0.13	Unspecified
Total Aromatics	2.68092E+09	21.21	Unspecified
Total FAMEs	0	0	Unspecified
Total Paraffins	6.04008E+09	47.78	Unspecified

- Speciating hydrocarbons in middle distillates by ASTM Method D8396
- Easy reporting in ChromSpace®

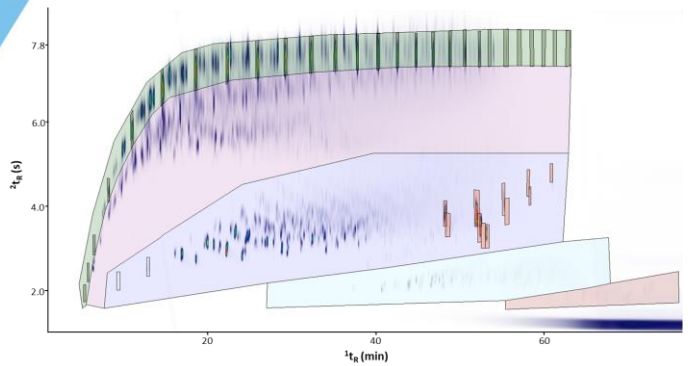
Enhanced productivity…

…through dual-channel GC×GC–FID

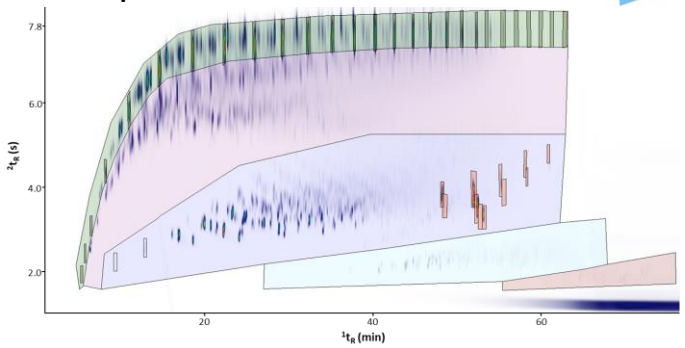




Sample 1



Sample 2



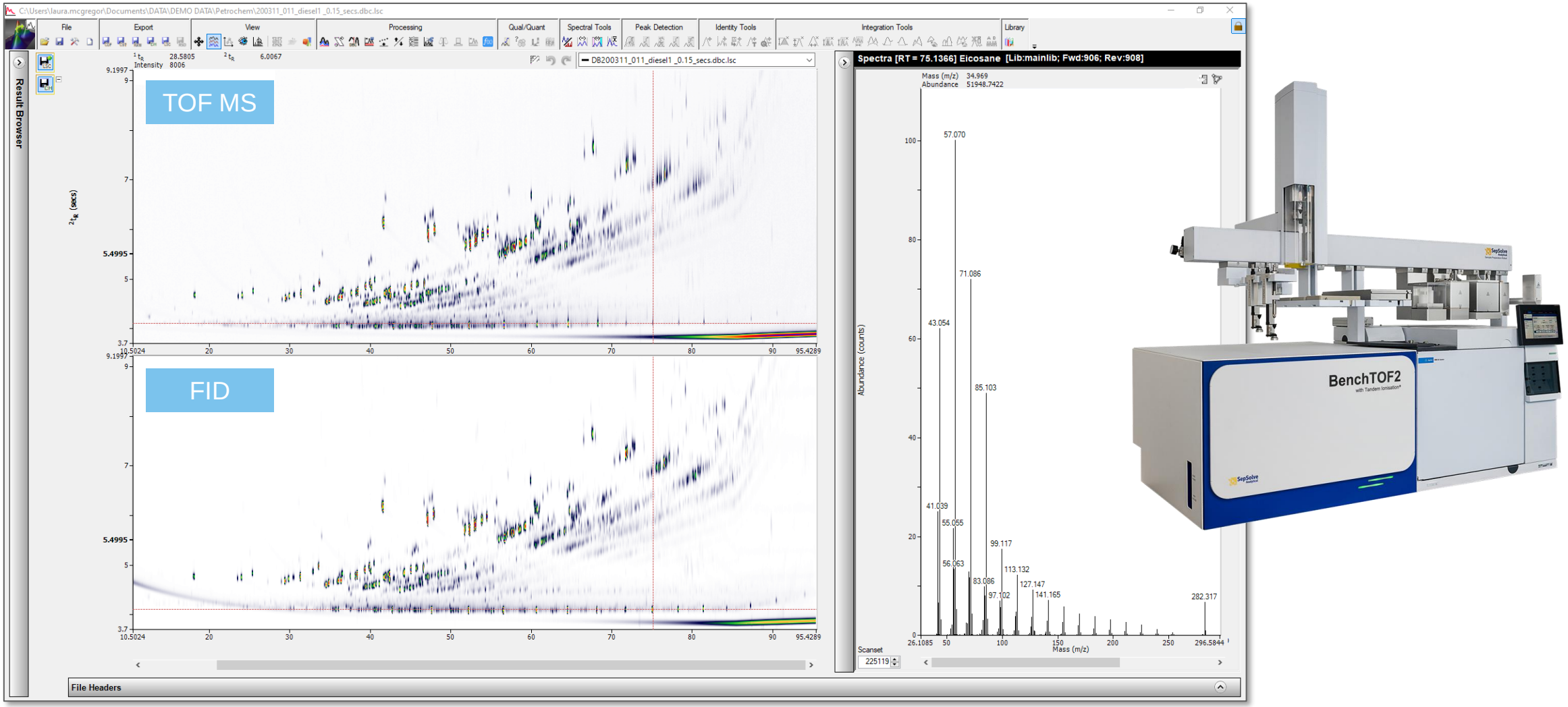
- Run two samples simultaneously with dual-channel GC×GC–FID to double the productivity of a single GC oven

Advantage of adding BenchTOF2

Flow modulation

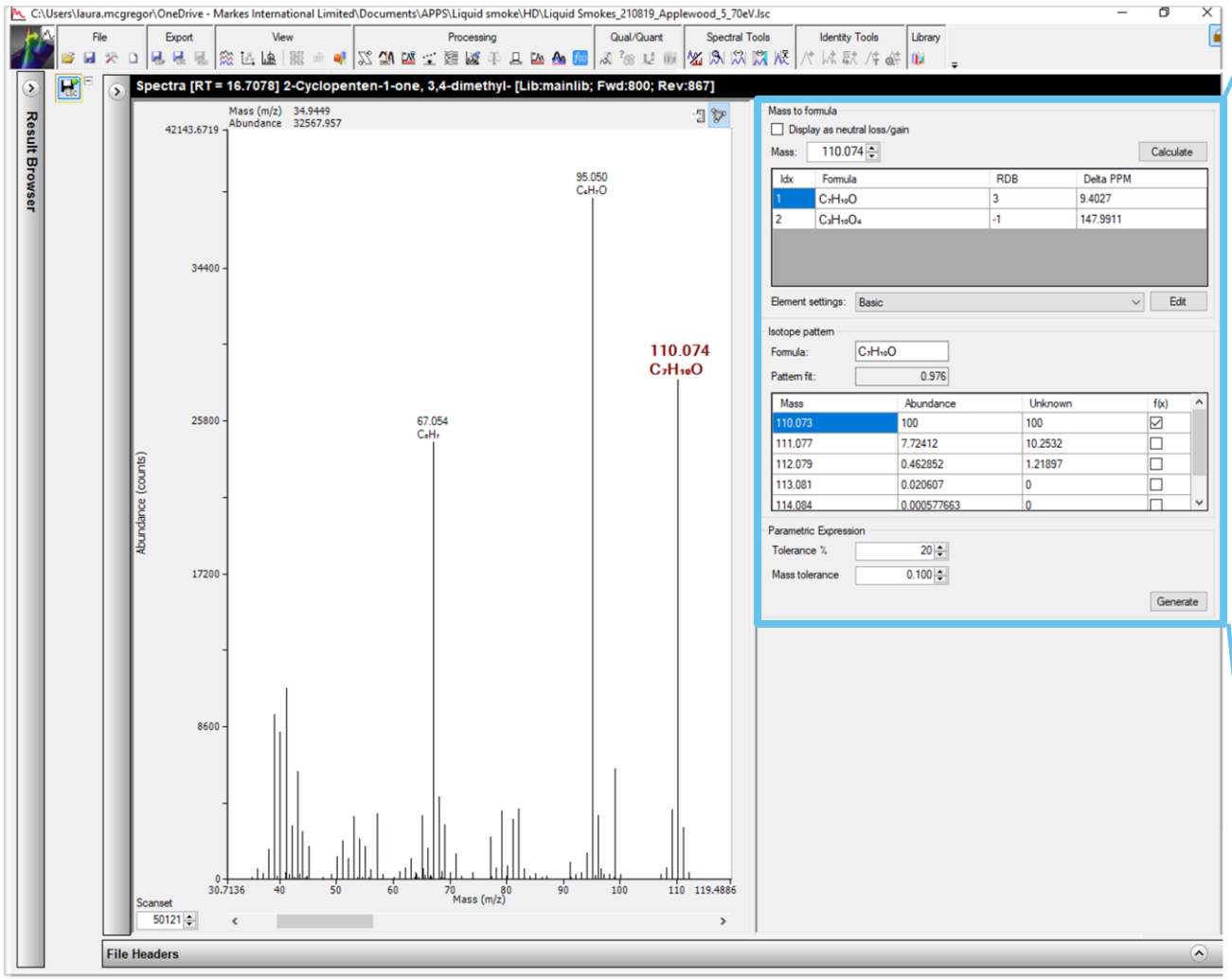
Thermal modulation

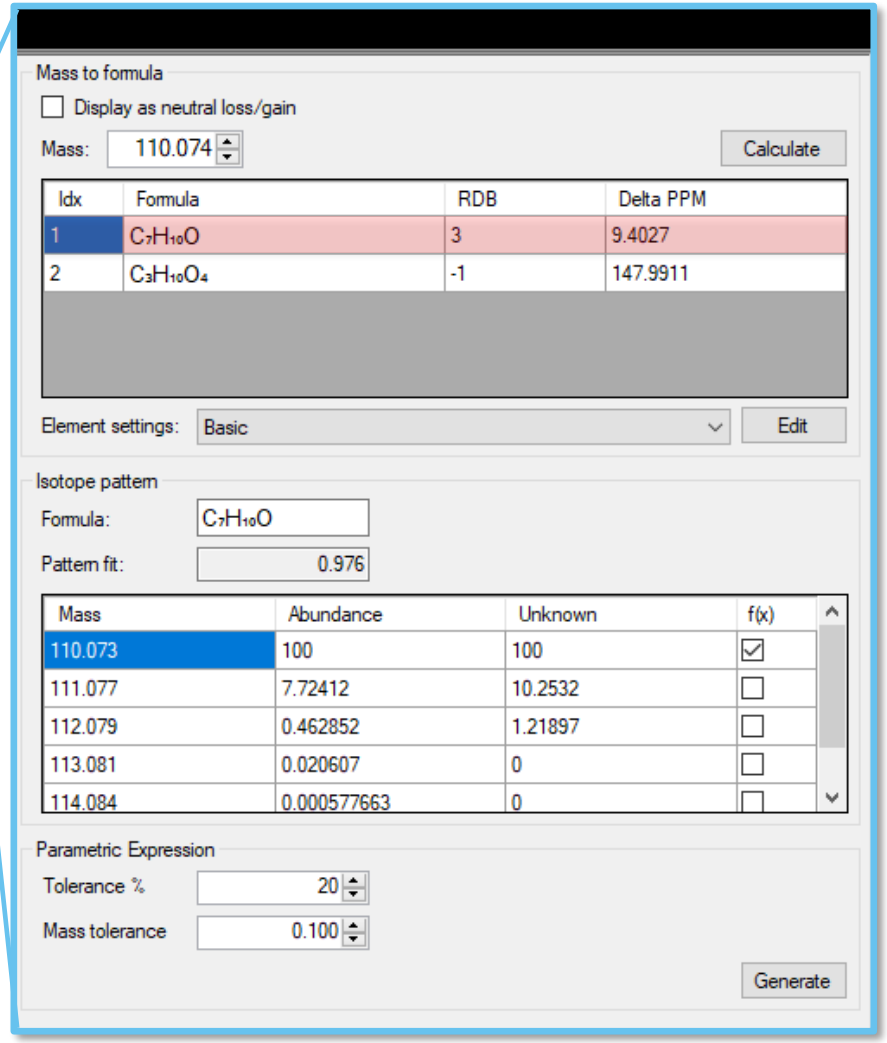
Analysis of diesel by GC×GC–TOF MS/FID



The importance of mass accuracy

Be sure you're identifying the correct compound





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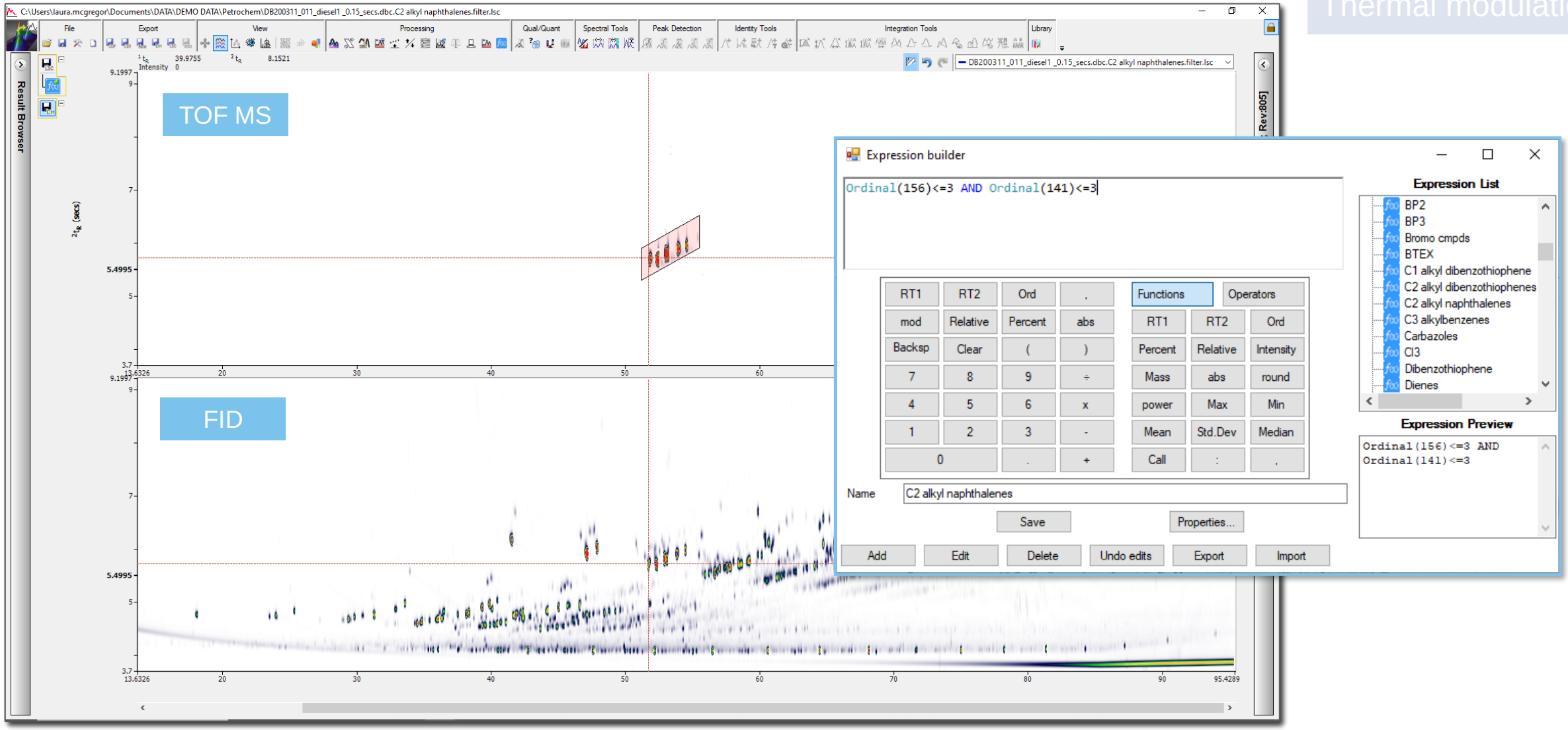
Making the most of mass spectral data

Flow modulation

Thermal modulation



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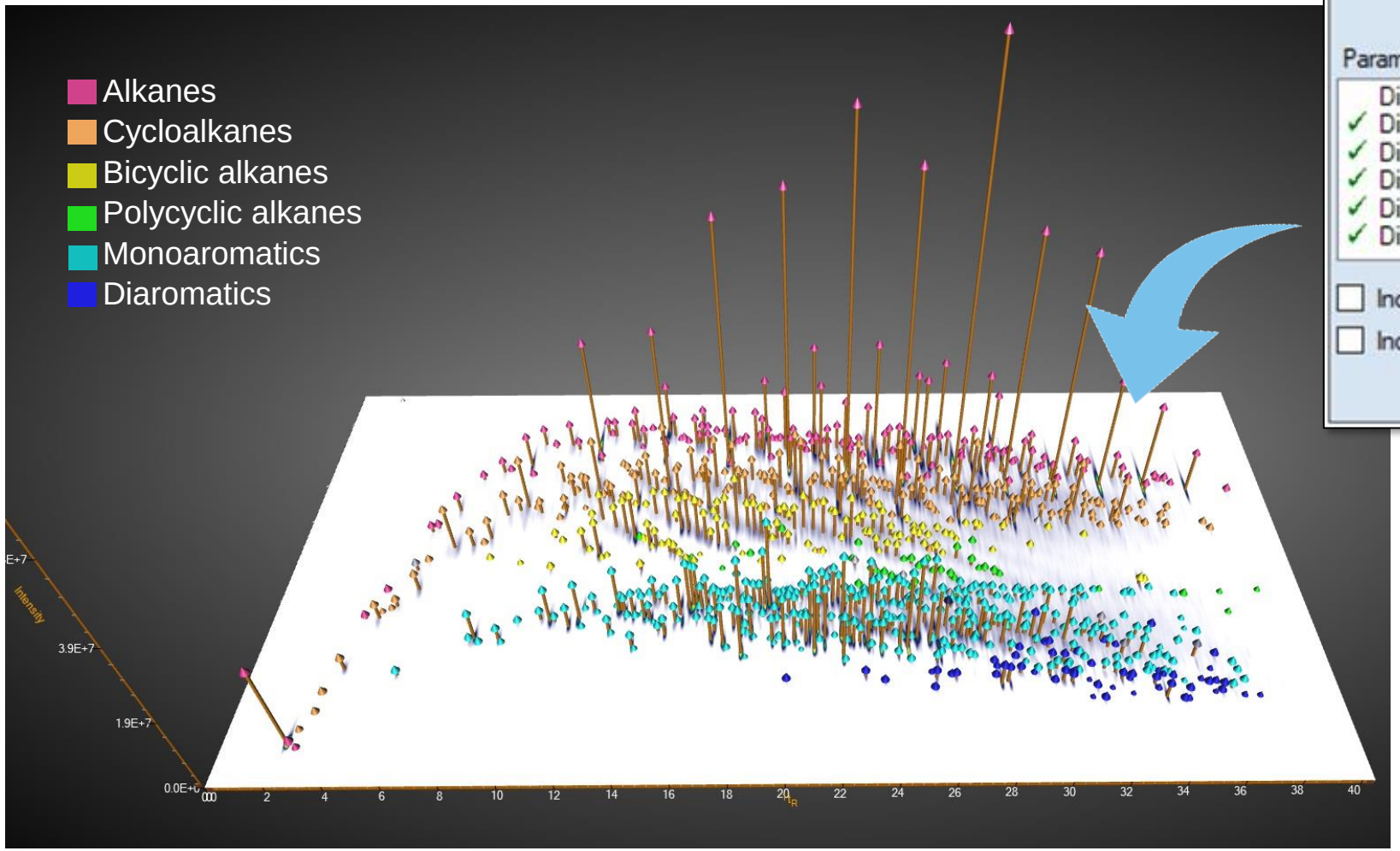
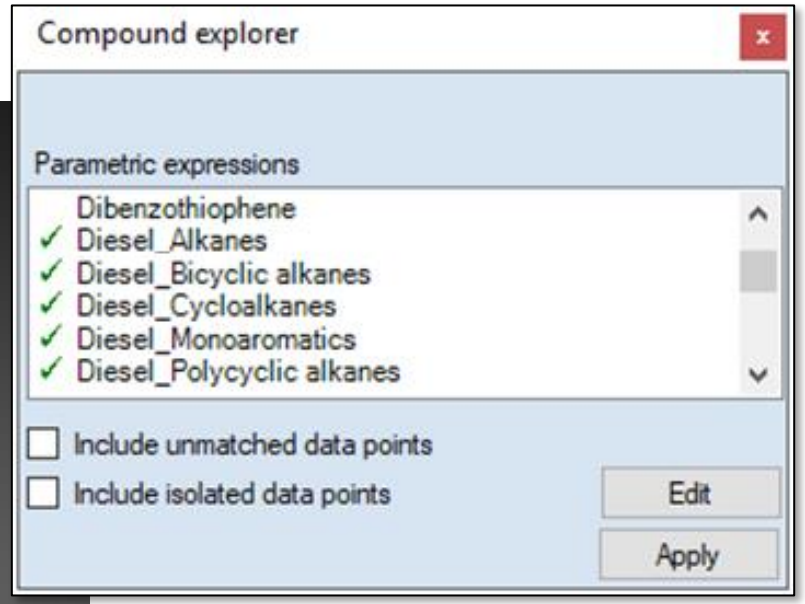
Making the most of mass spectral data

Classification of diesel by GC×GC–TOF MS





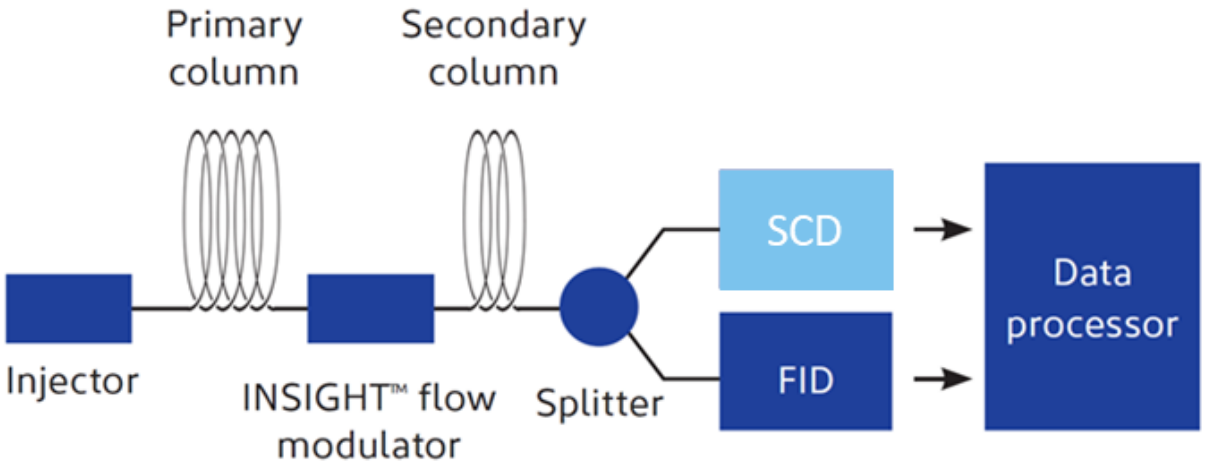
- Apply multiple expressions during integration to quickly classify the entire sample

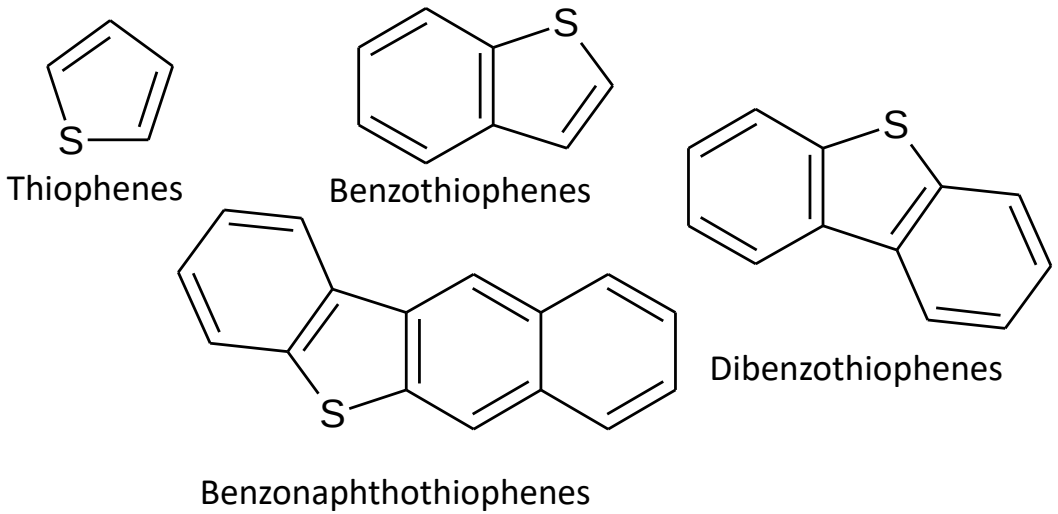
Simple set-up of parallel detection

Flow modulation

Thermal modulation

Classification of sulfur species using GC×GC–SCD/FID



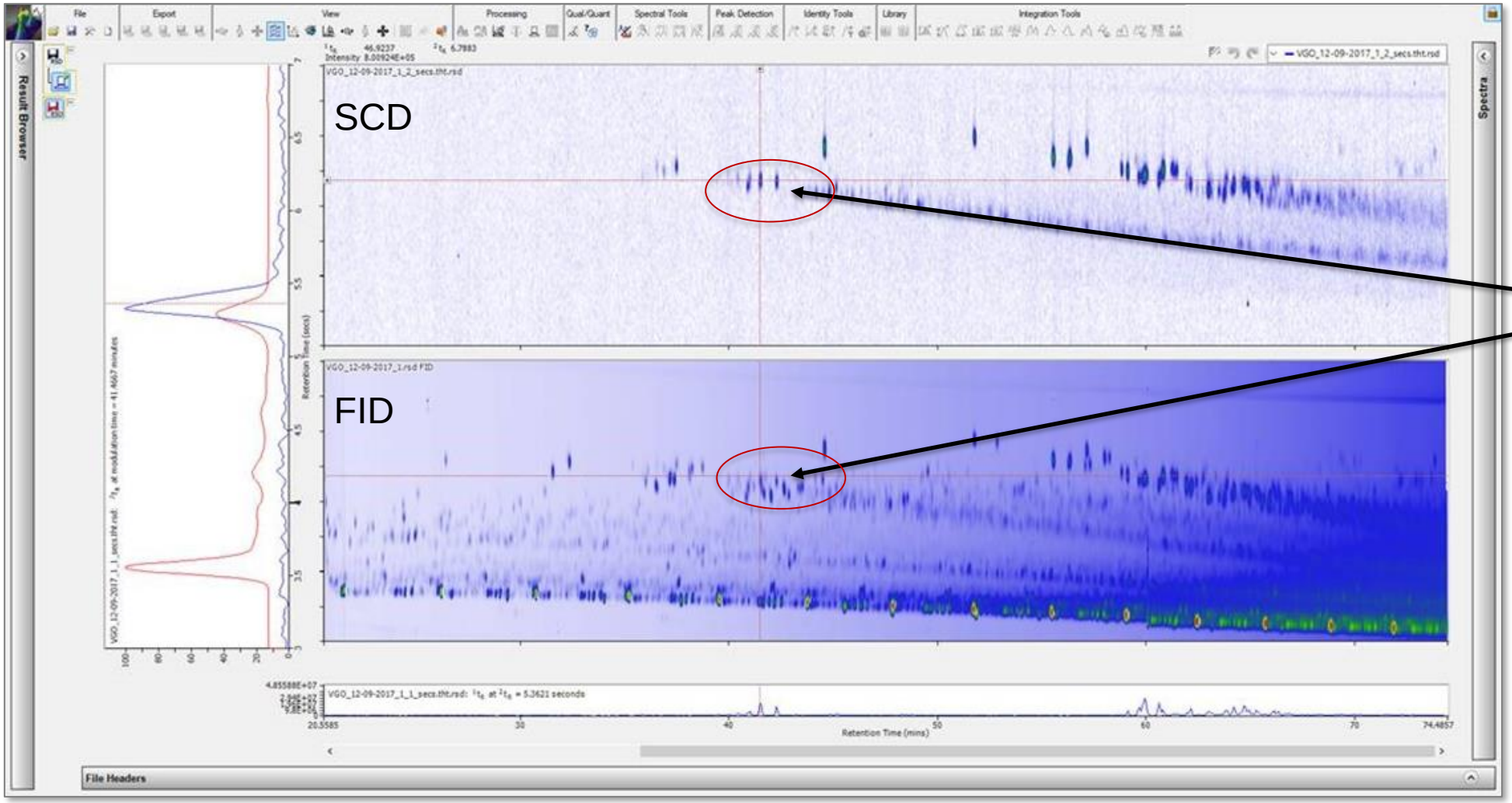


- Sulfur species often elute in overlapping bands with other aromatic hydrocarbons making it challenging to perform quantitation via FID

Classification of sulfur species using GC×GC–SCD/FID

Flow modulation

Thermal modulation

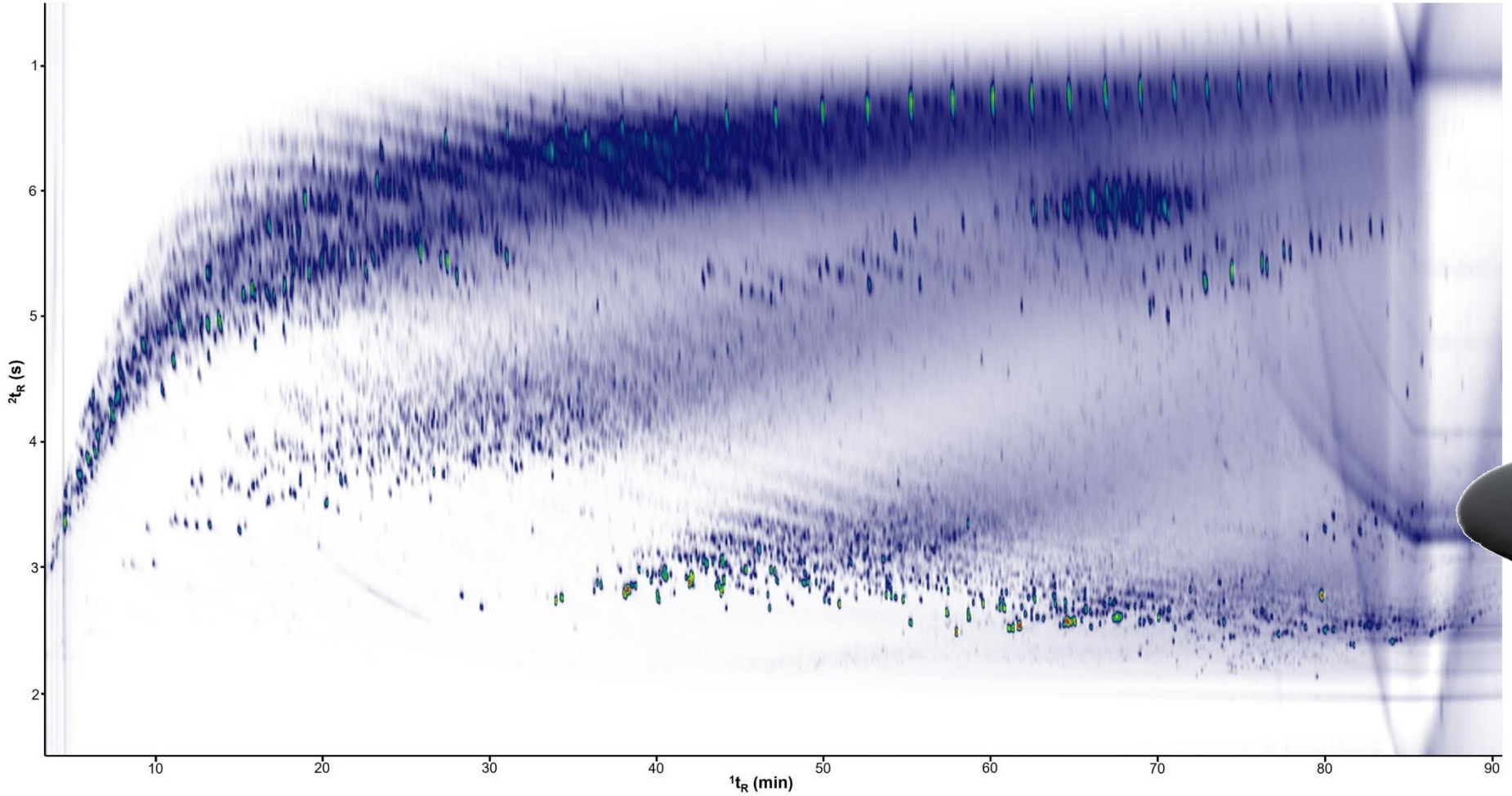


Sulfurs that elute alongside other aromatic hydrocarbons can be confidently quantified on SCD

Example application: Crude oil fingerprinting

Flow modulation

Thermal modulation

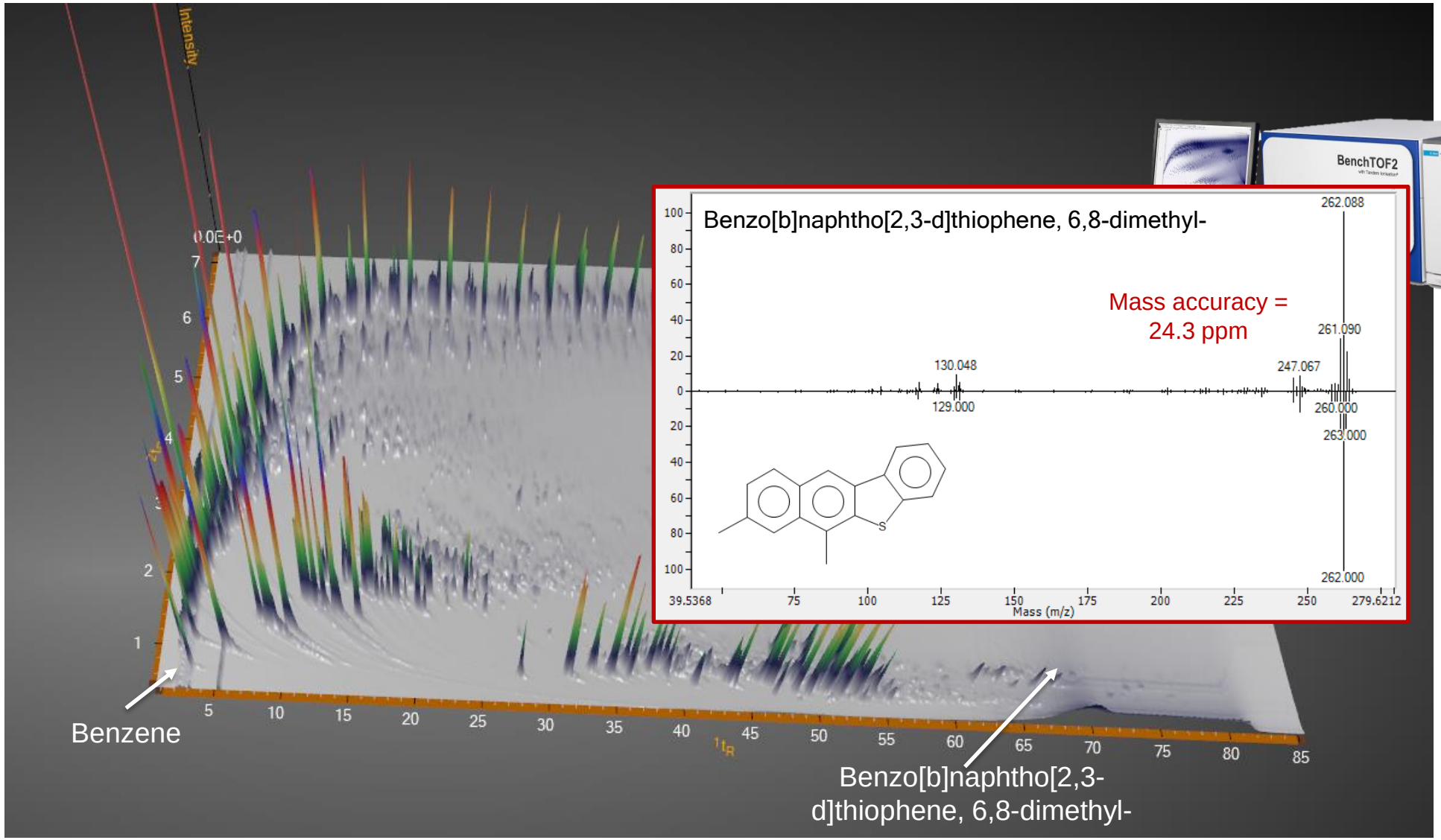


- We can help to optimise your method and make the most of the separation space

Example application: Crude oil fingerprinting

Flow modulation

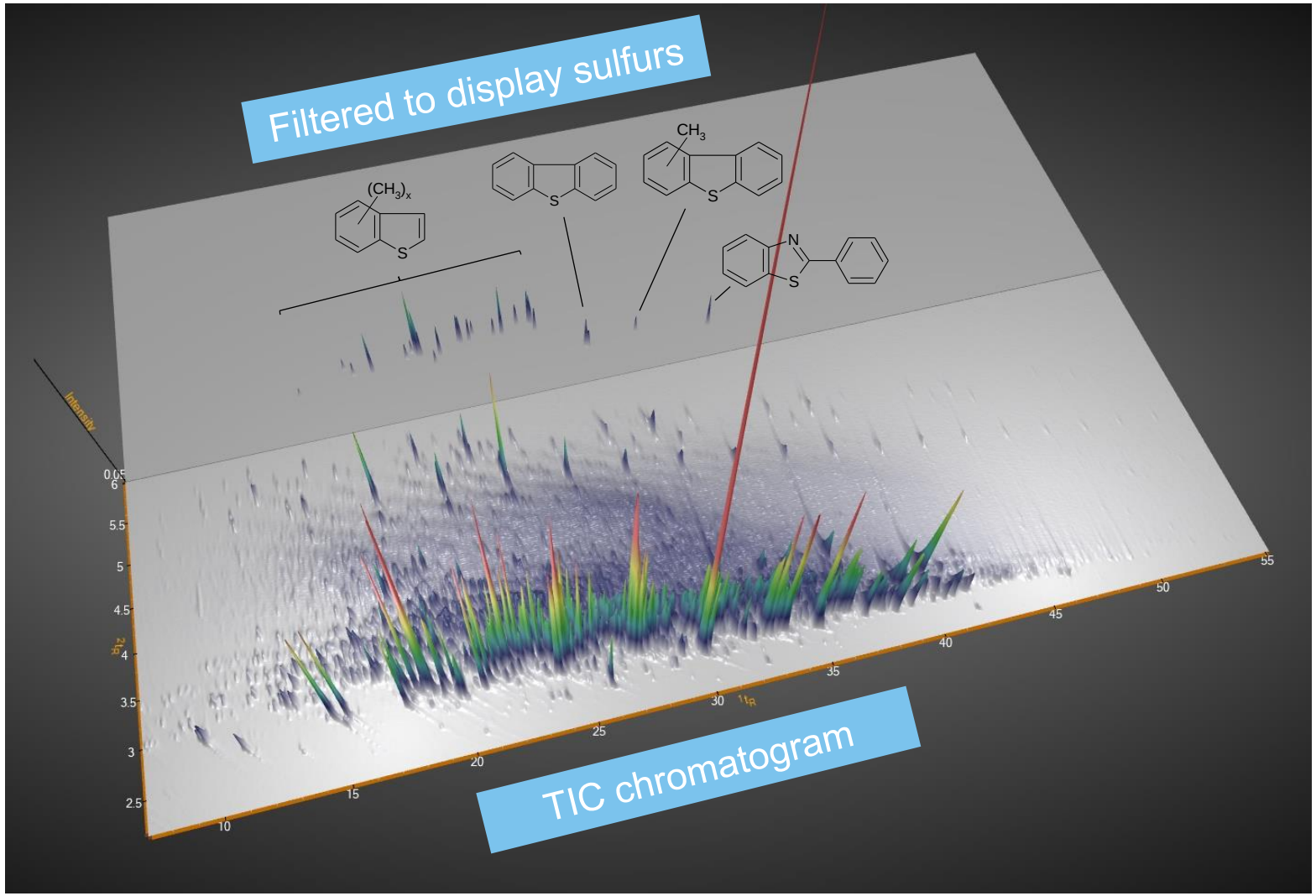
Thermal modulation



Example application: Analysis of pyrolysis oils

Flow modulation

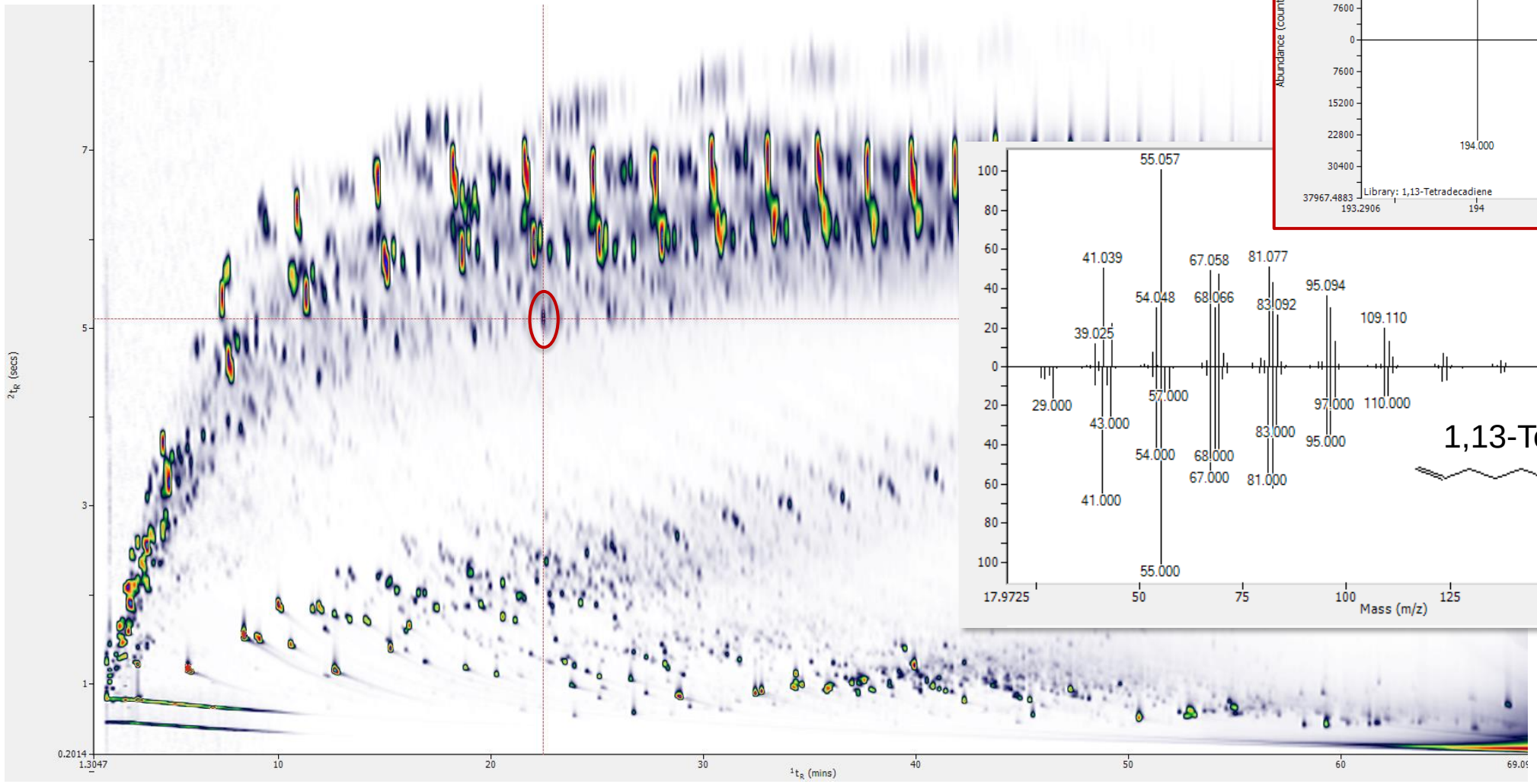
Thermal modulation



Samples kindly supplied by Dr Miloš Auersvald (University of Chemistry and Technology Prague, Czech Republic)

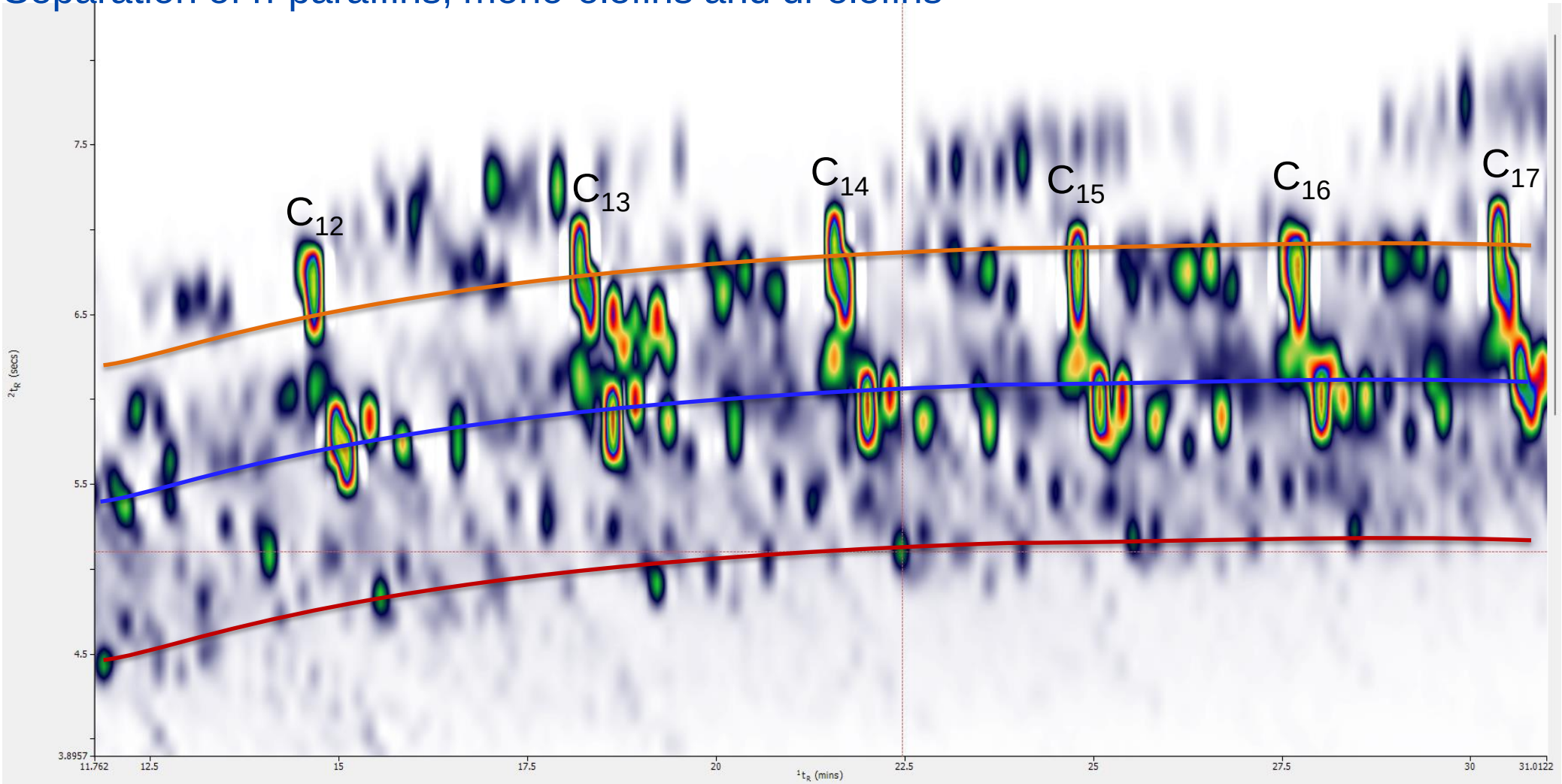
Example application: Analysis of pyrolysis oils

Separation of n-paraffins, mono-olefins and di-olefins

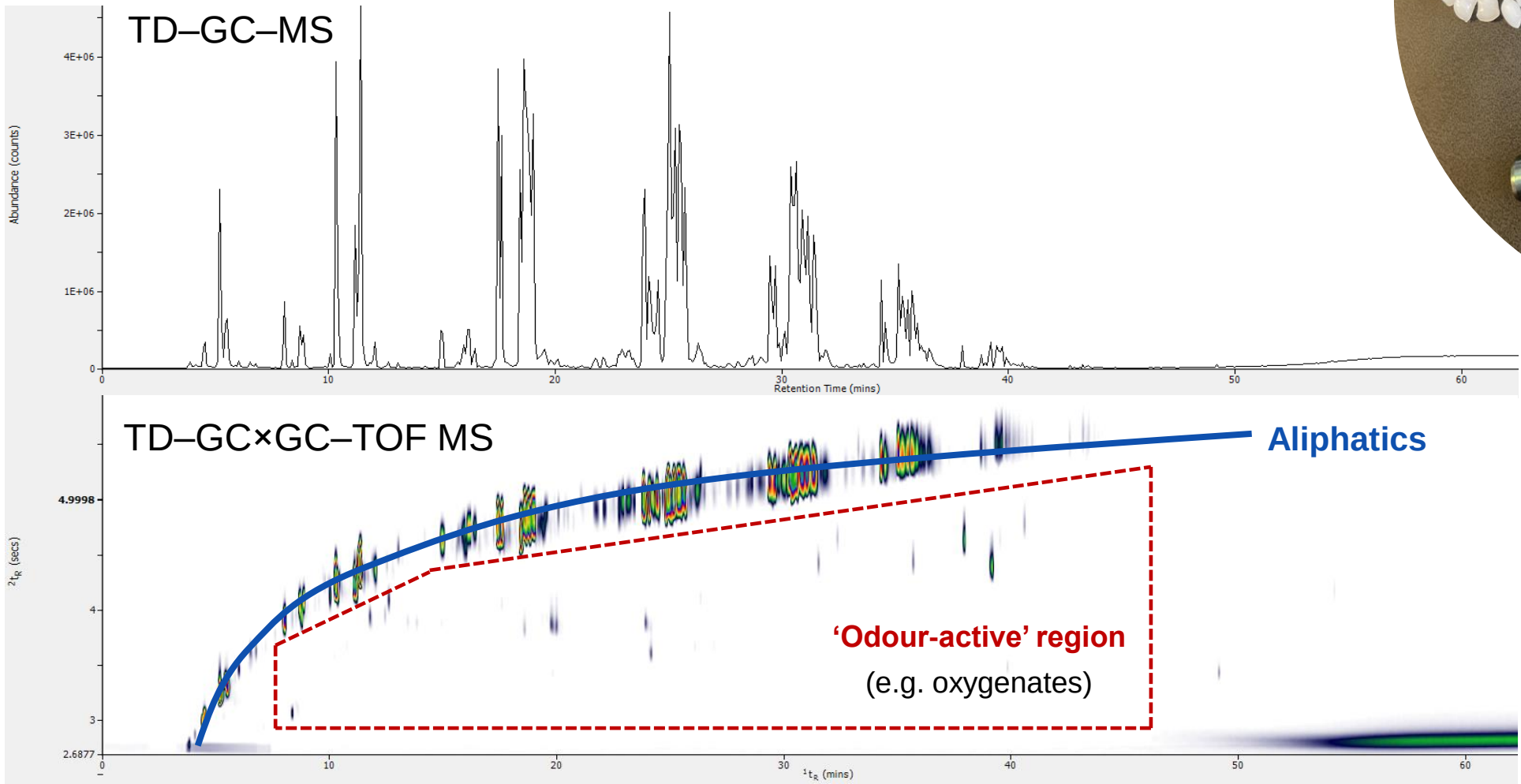


Example application: Analysis of pyrolysis oils

Separation of n-paraffins, mono-olefins and di-olefins



Odours in polymer pellets



What about potential migrants?

Analysis of packaged beverages

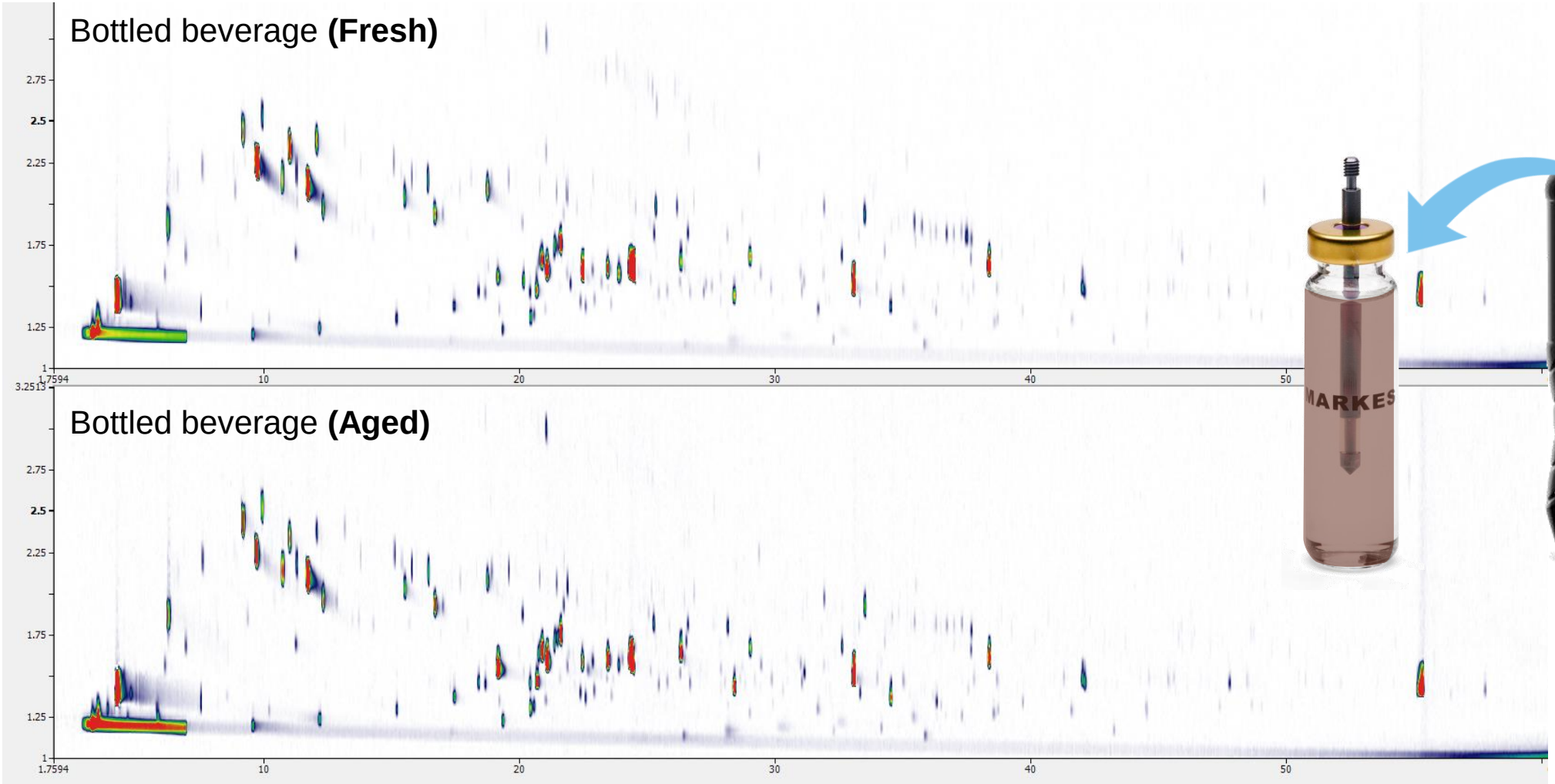
25% recycled/75% virgin PET bottle containing a popular soft drink

HiSorb™
sorptive extraction probe

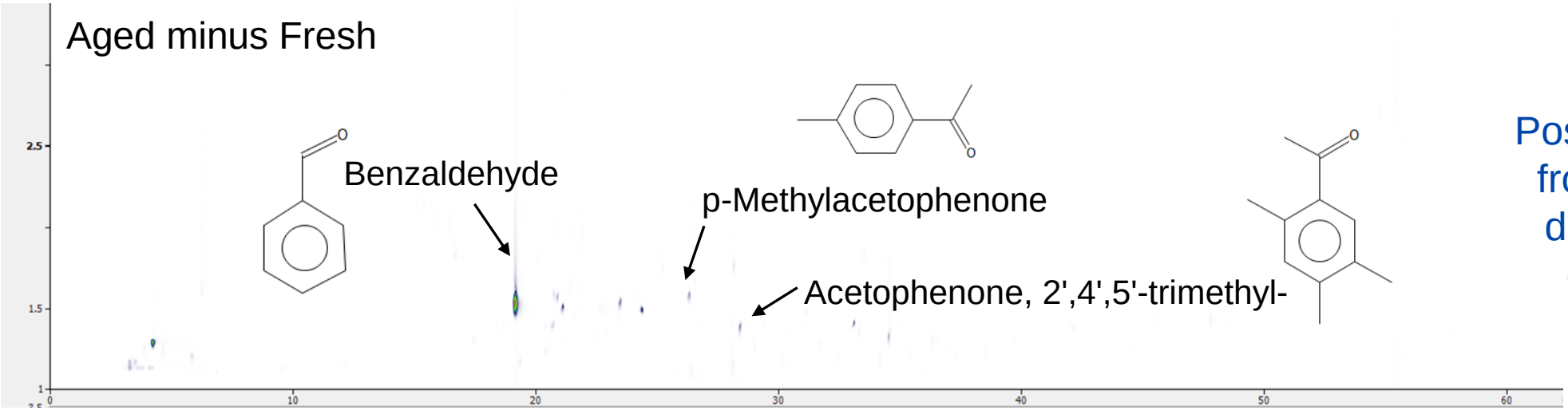
‘Aged’
Exposed to heat & direct sunlight for 8 weeks

‘Fresh’
Refrigerated for 8 weeks

Impact of packaging on beverages



Impact of packaging on beverages



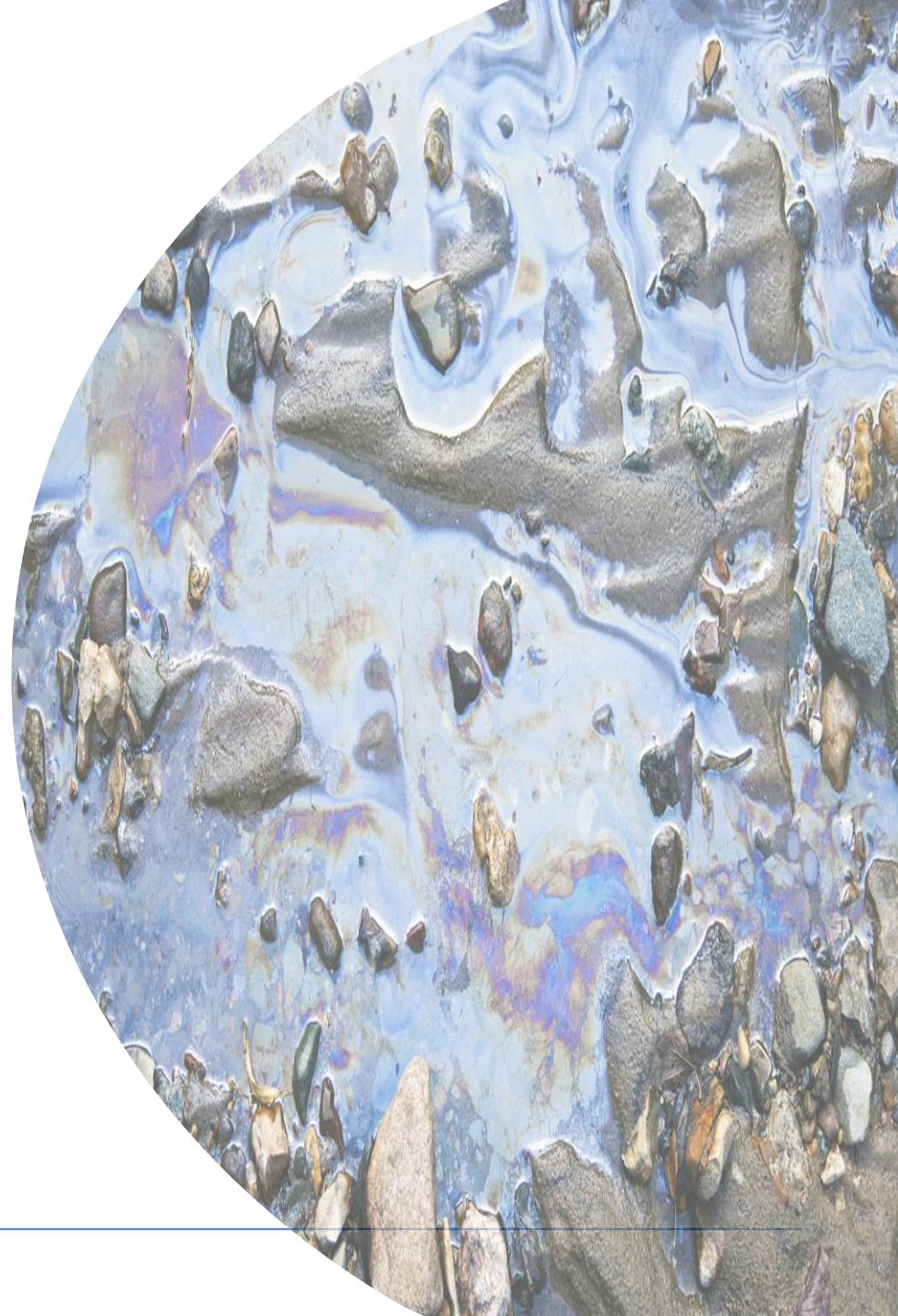
Possible migrants from the plastic due to thermal degradation

Total Petroleum Hydrocarbons (TPH)

- Commonly split into:
  - **Volatile** Petroleum Hydrocarbons (VPH) ~C_5-C_{10}
  - **Extractable** Petroleum Hydrocarbons (EPH) ~C_8-C_{40+}

- For environmental fate and risk-based analysis the aliphatic and aromatic hydrocarbons must be separated

- Compounds are reported as groups (>C_8-C_{10}, >C_{10}-C_{14}…etc) rather than individually



A new approach to EPH…

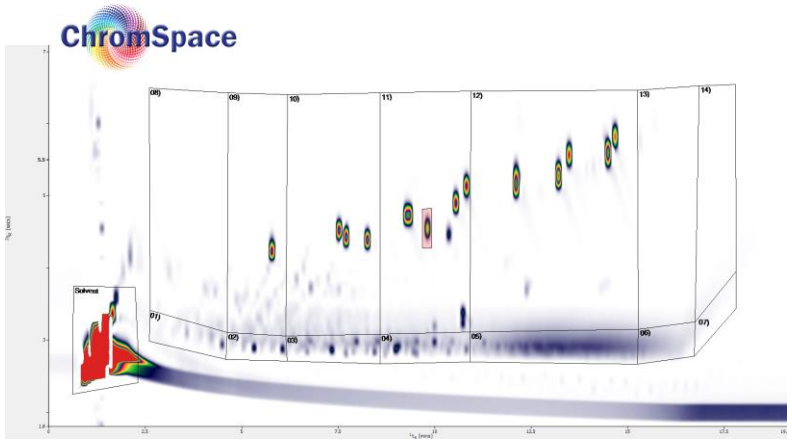
…using GC×GC–FID

- Chromatographic separation of aliphatic and aromatic hydrocarbons in a single run, reducing processing time

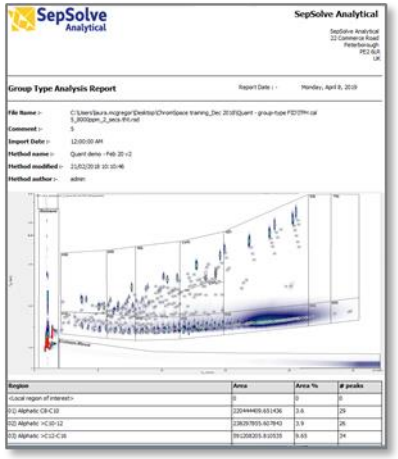
Sample

Traditional solvent extract

Single transfer



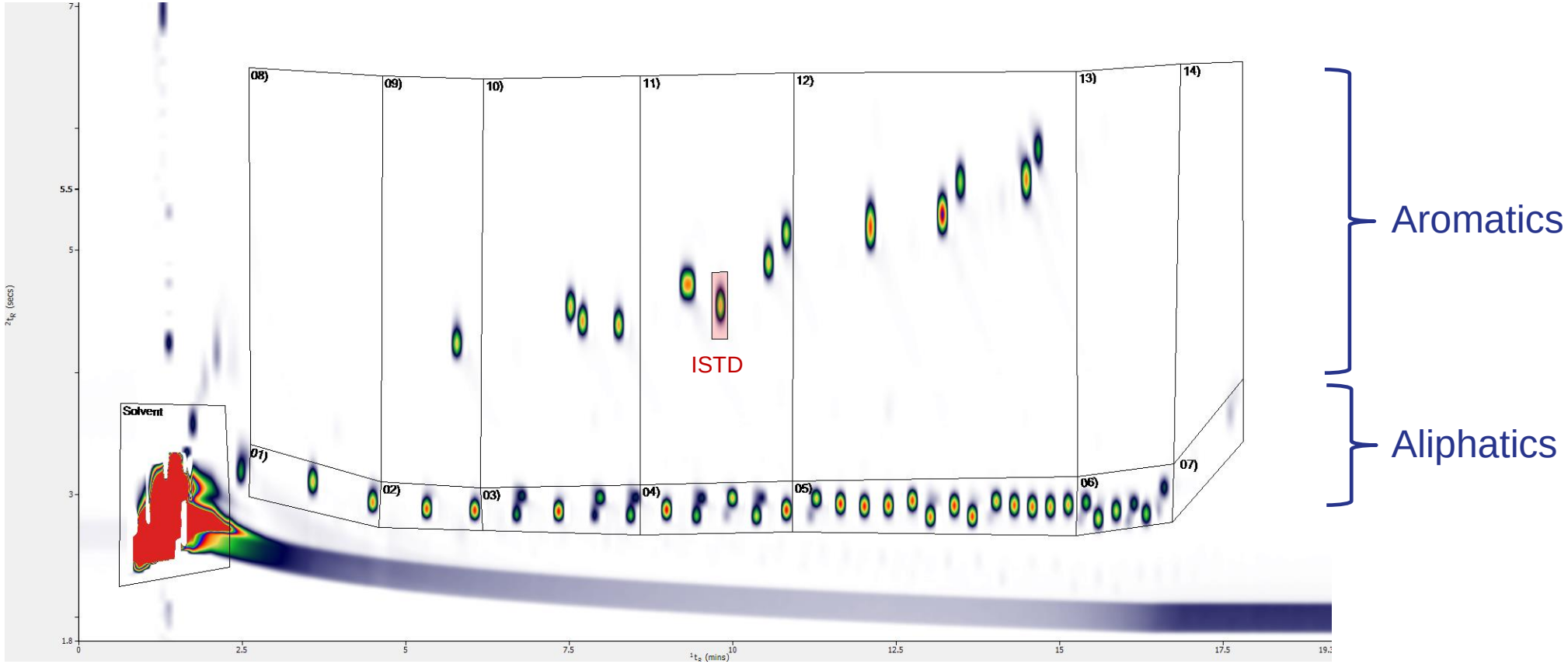
Single analysis AND simple data processing using stencils



Automated reporting

Simple data processing…

…using stencils

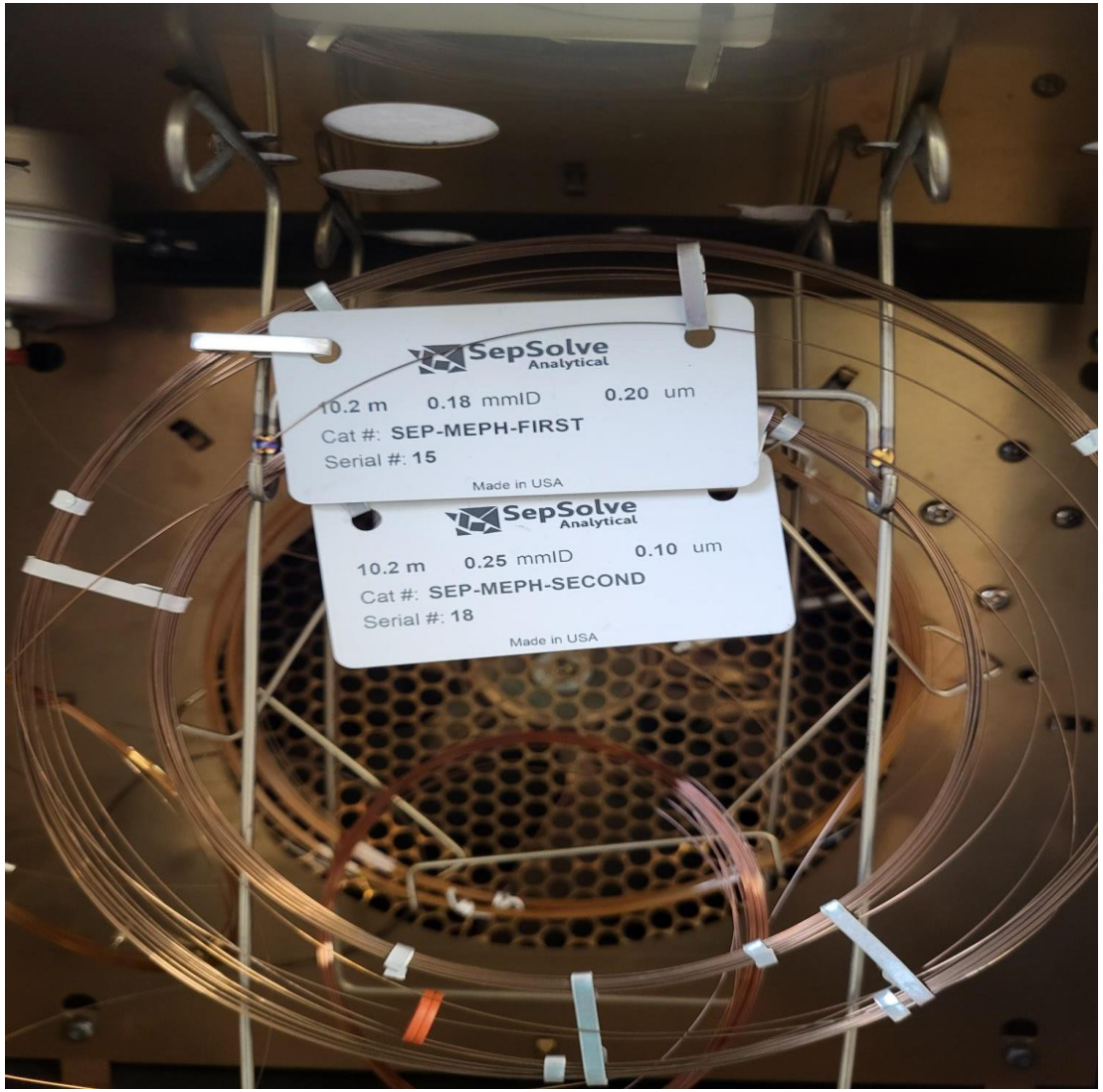


- Regions of interest (Aliphatic >C_{10}-C_{12}….etc) are identified using a banding standard
- Internal standard and surrogate regions can also be added

Enhanced method robustness…

…via metal analytical columns

- Robust metal design provides extended lifetime
- Typically, 3500 – 4000 analytical runs before replacement



The TPH product package

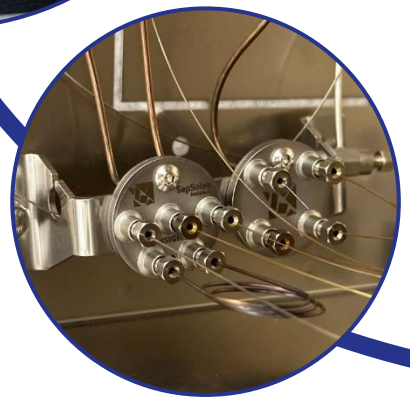
What's available?

We provide everything you need for routine TPH analysis

- INSIGHT-Flow modulator
  - And optional second GC×GC channel
- ChromSpace GC×GC software
  - Full instrument control and data processing
- Method statements
- Column sets
  - EPH analysis
  - VPH analysis
- Standards
  - Required to build stencils and calibrations

Summary

- GC×GC–TOF MS provides detailed sample characterisation for even the most complex petrochemicals
- Flexible GC×GC–TOF MS configurations:
  - Robust and repeatable INSIGHT-Flow reverse fill/flush flow modulator
  - Cryogen-free INSIGHT-Thermal with unbeatable productivity and performance
- Unattended analysis within easy-to-manage sequences
- BenchTOF2 provides confident identifications, with excellent spectral quality and powerful mass accuracy (<50 ppm)
- Automated processing workflows with fast and efficient group-type analysis using customisable stencils in ChromSpace.
- Flexible method development and full applications support



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