SepSolve Analytical

15TH Multidimensional Chromatography Workshop

A holistic view of river water quality using passive sampling and GC×GC–TOF MS

Presented by: Dr Jonathan Grandy
Sampling performed by Natural Resources Wales and Analysis in conjunction with Sepsolve Peterborough

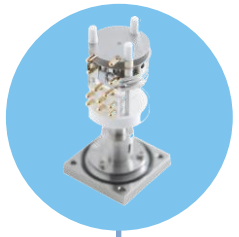
GC×GC at SepSolve Analytical

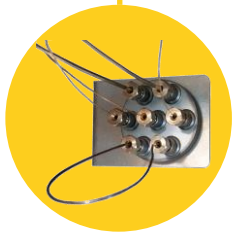
Launch of first generation BenchTOF mass spectrometers

2008

2016

Launch of Tandem Ionisation

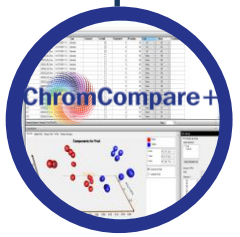




2017

Launch of INSIGHT® comprehensive reverse fill/flush modulator…

…and ChromSpace GC×GC software

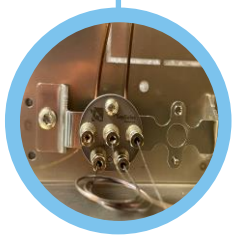


2020

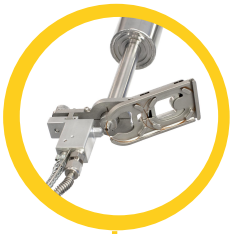
Launch of ChromCompare + chemometrics platform

2021

Launch of BenchTOF2 mass spectrometers



Second generation of INSIGHT-Flow modulator

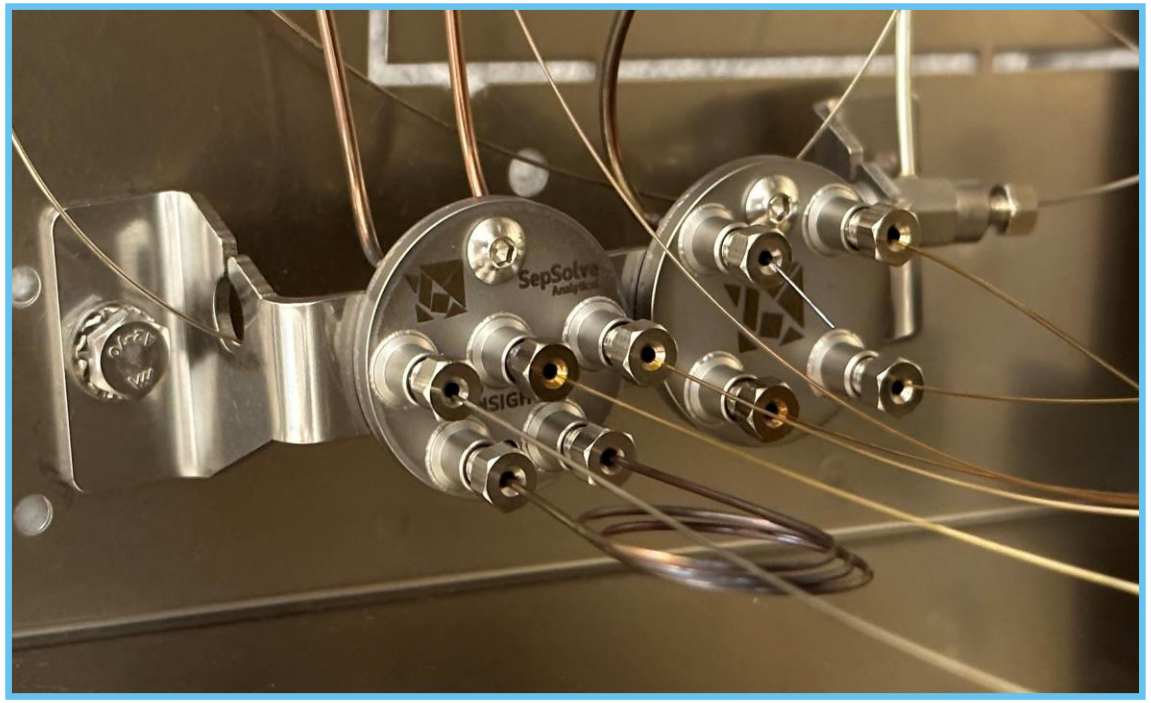


2023

Launch of the INSIGHT-Thermal cryogen-free modulator

The INSIGHT® modulator series

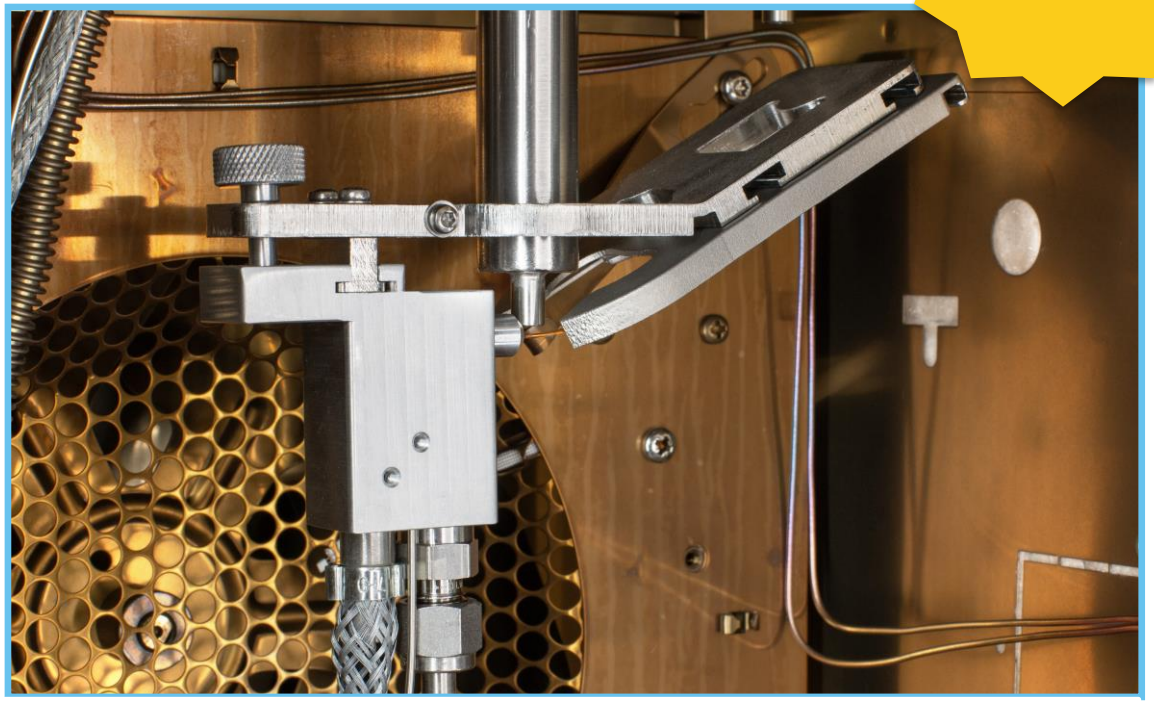
INSIGHT-Flow



- Reverse fill/flush (RFF) flow modulator
- Bleed line control kit for greater flexibility in method development
- Optional 4-port purged splitter

INSIGHT-Thermal

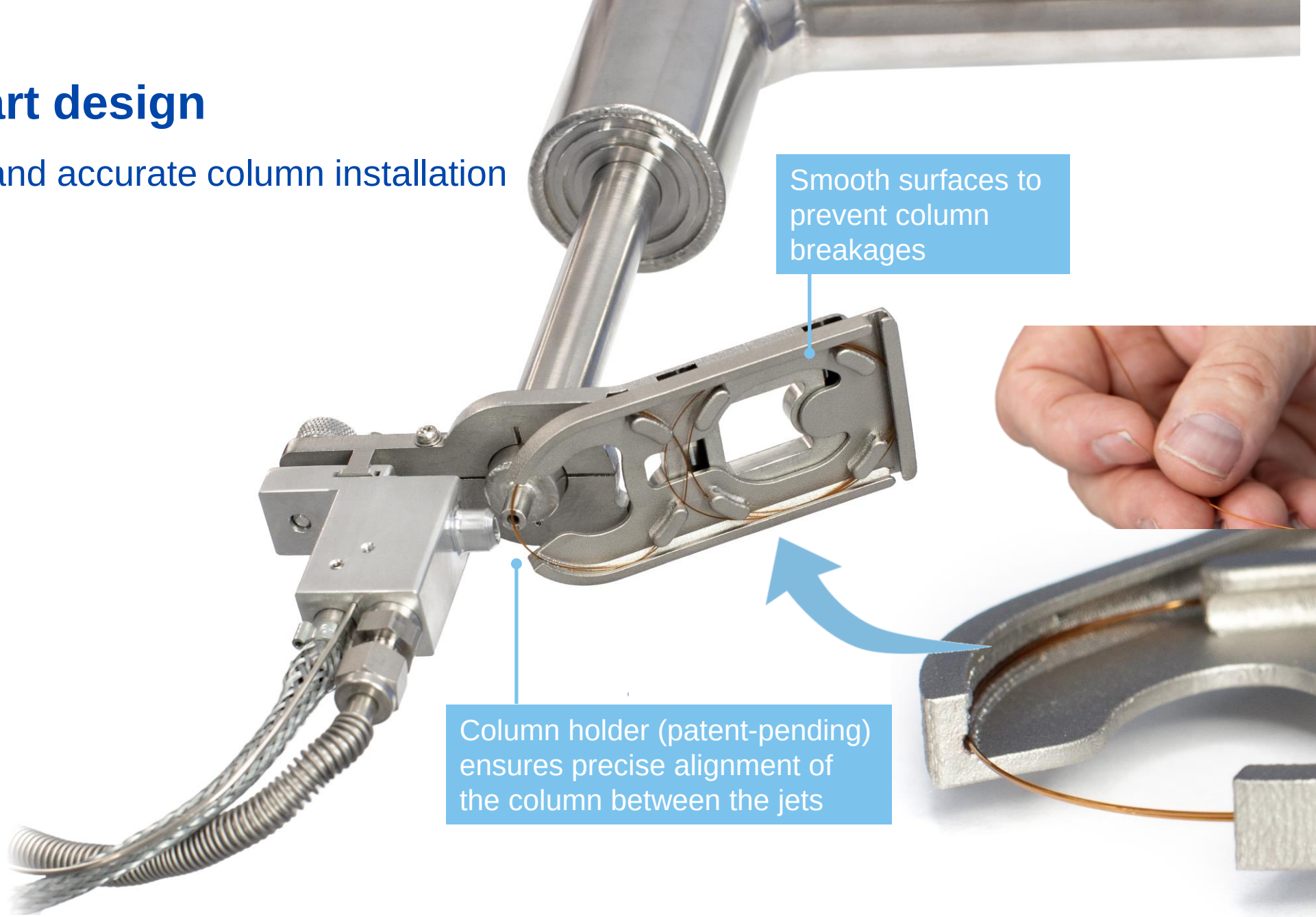
NEW!



- Cryogen-free thermal modulator using delay loop technology
- Advanced control of cold jet flow rate
- Smart column holder design for easy set-up

Smart design

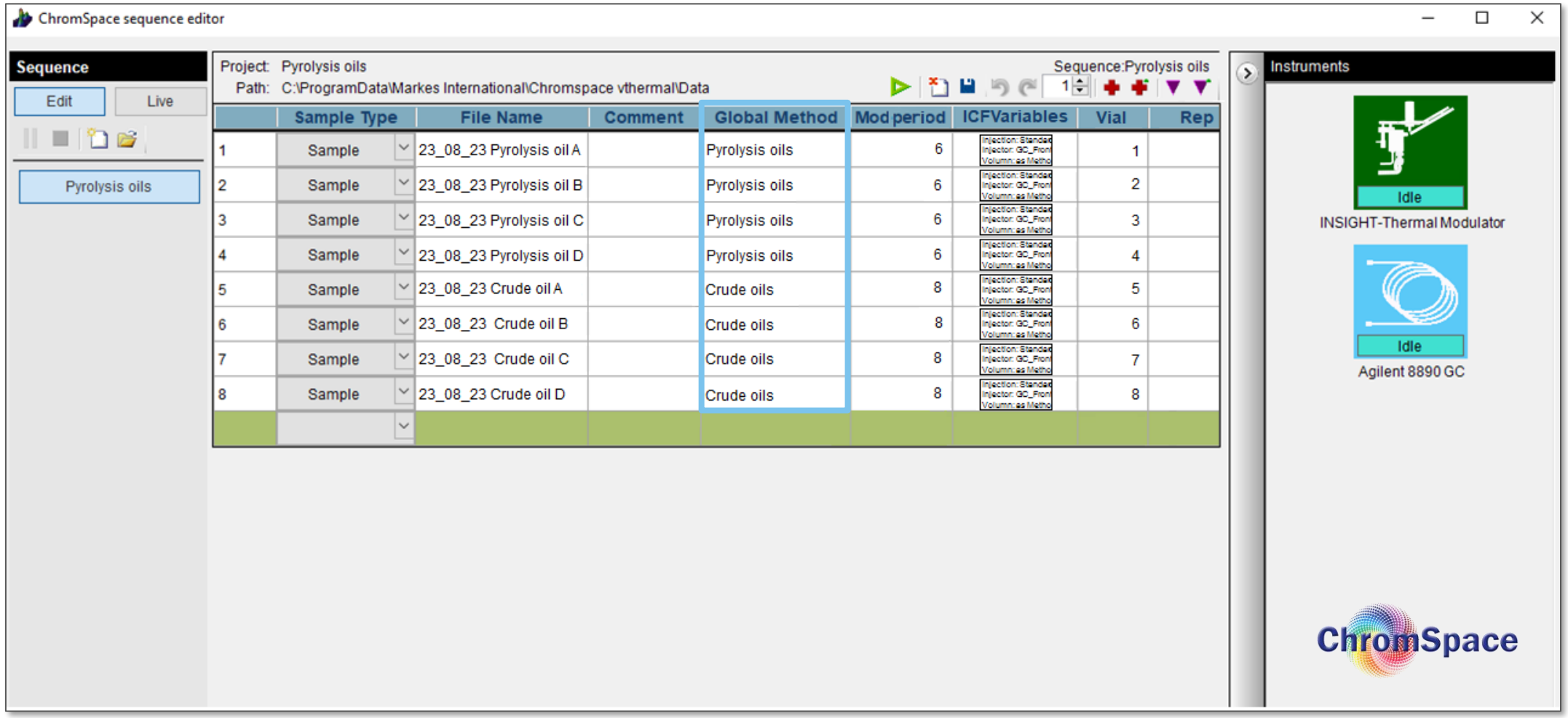
Fast and accurate column installation



Smooth surfaces to prevent column breakages

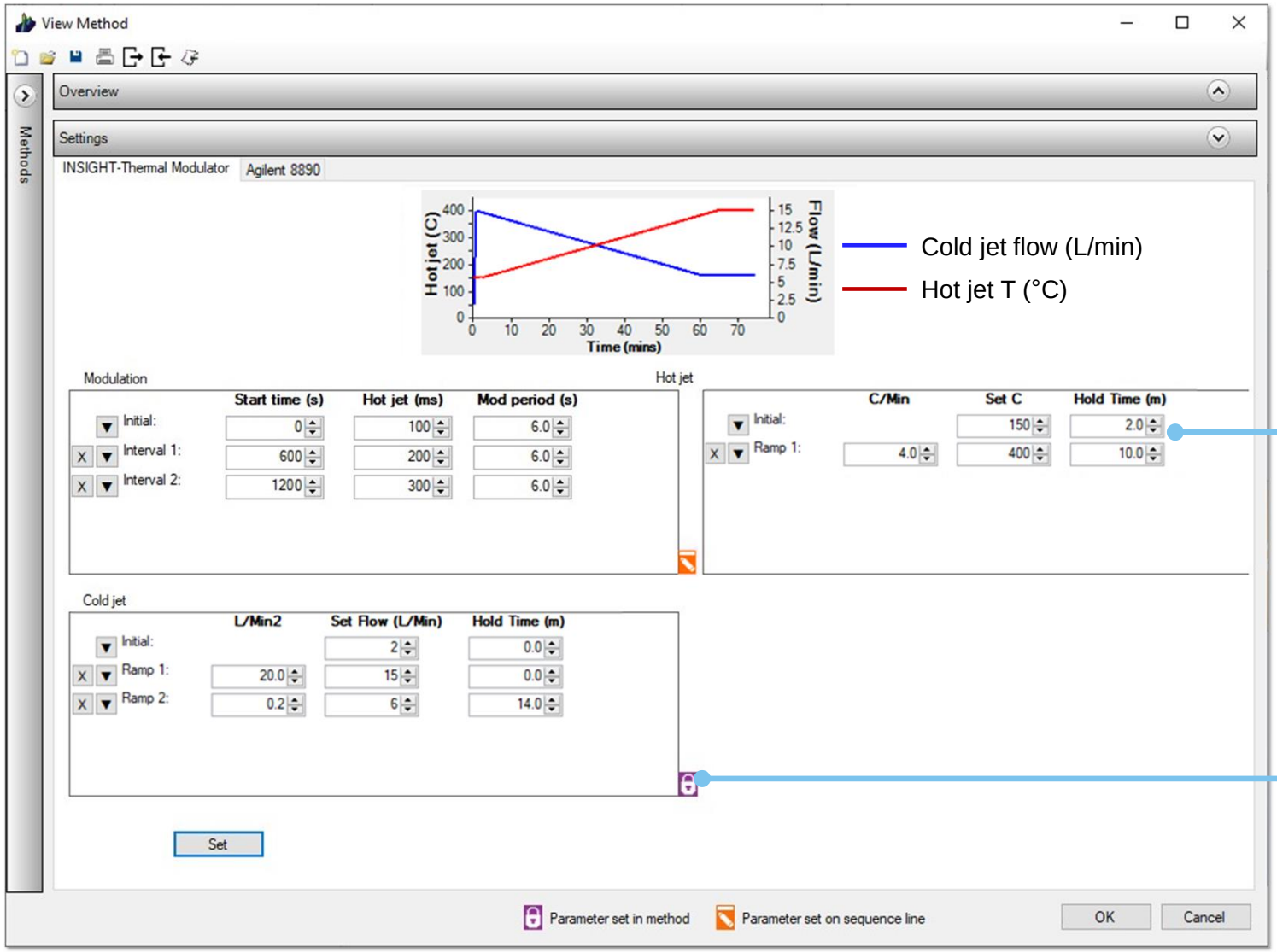
Column holder (patent-pending) ensures precise alignment of the column between the jets

Fully unattended analysis to maximise sample throughput



- Full control of all jet parameters and easy sequencing of instrument methods

Fully unattended analysis to maximise sample throughput

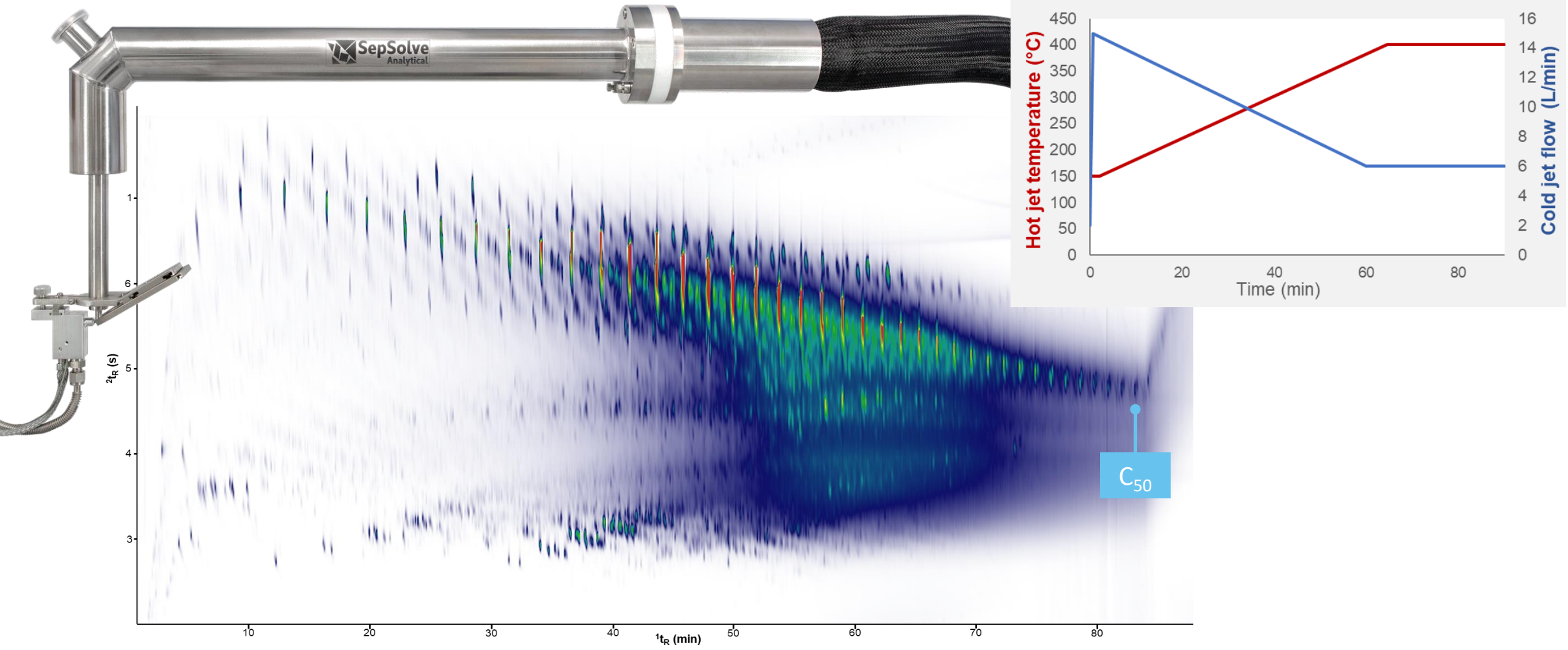


Apply linear ramp rates to cold jet flow

Unlockable parameters for fast method development

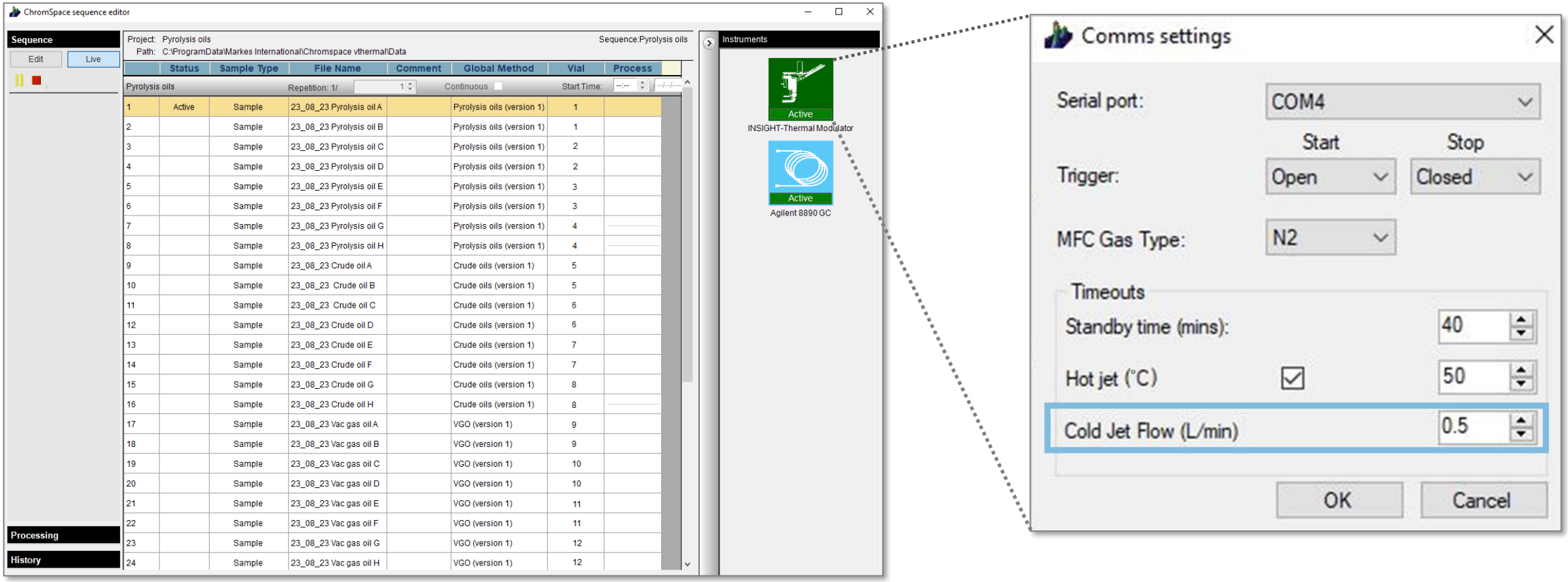
Extending the analyte range

Efficient modulation of C_7 to C_{50+}



Standby flows to prevent icicle formation

Have the confidence to leave your samples running unattended



- Cold jet flow defaults to 0.5 L/min between runs and sequences to prevent issues, such as icicle formation, previously experienced during unattended operation or over weekends

Monitoring river water quality

What are the challenges?

- Constantly seeking lower detection limits
- New sampling techniques (e.g., passive sampling) deliver extracts with greater complexity
- Focus is typically on “priority”(organochlorines) substances, but what about those of emerging concern?

What are the emerging contaminants?

Pharmaceuticals and hormones

Personal care products and fragrances

Industrial additives and by-products

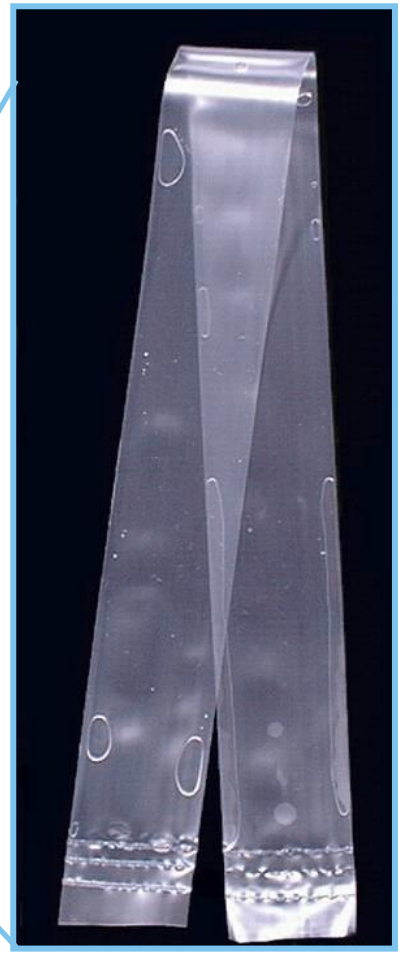
Water treatment by-products

Caffeine and nicotine
(and their metabolites)

Flame/fire retardants and surfactants

Experimental

Semi-permeable membrane device (SPMD)



- May pick up temporal contaminant releases overcoming a limitation of grab sampling
- Designed to concentrate hydrophobic chemicals (with log Kow > 4), more sensitive to heavier VOC's and SVOC's
- Extraction for 4 weeks, stored at -18 C under argon, desorbed with hexane cleaned by SEC and reconstituted to 1 mL

Samples kindly supplied by Dr Anthony Gravell (Natural Resources Wales, UK)

Experimental

- **Samples:** Passive sampling extracts from 2 sampling locations in a UK river
- **GC×GC:** INSIGHT-Thermal modulator; Modulation period (P_M): 6.0 s.
- **MS:** Instrument: BenchTOF2™; Mass range: m/z 30–600; Acquisition rate: 100 Hz in Tandem Ionisation® mode at 70 eV and 14 eV.
- **Software:** Full instrument control and data processing by ChromSpace®

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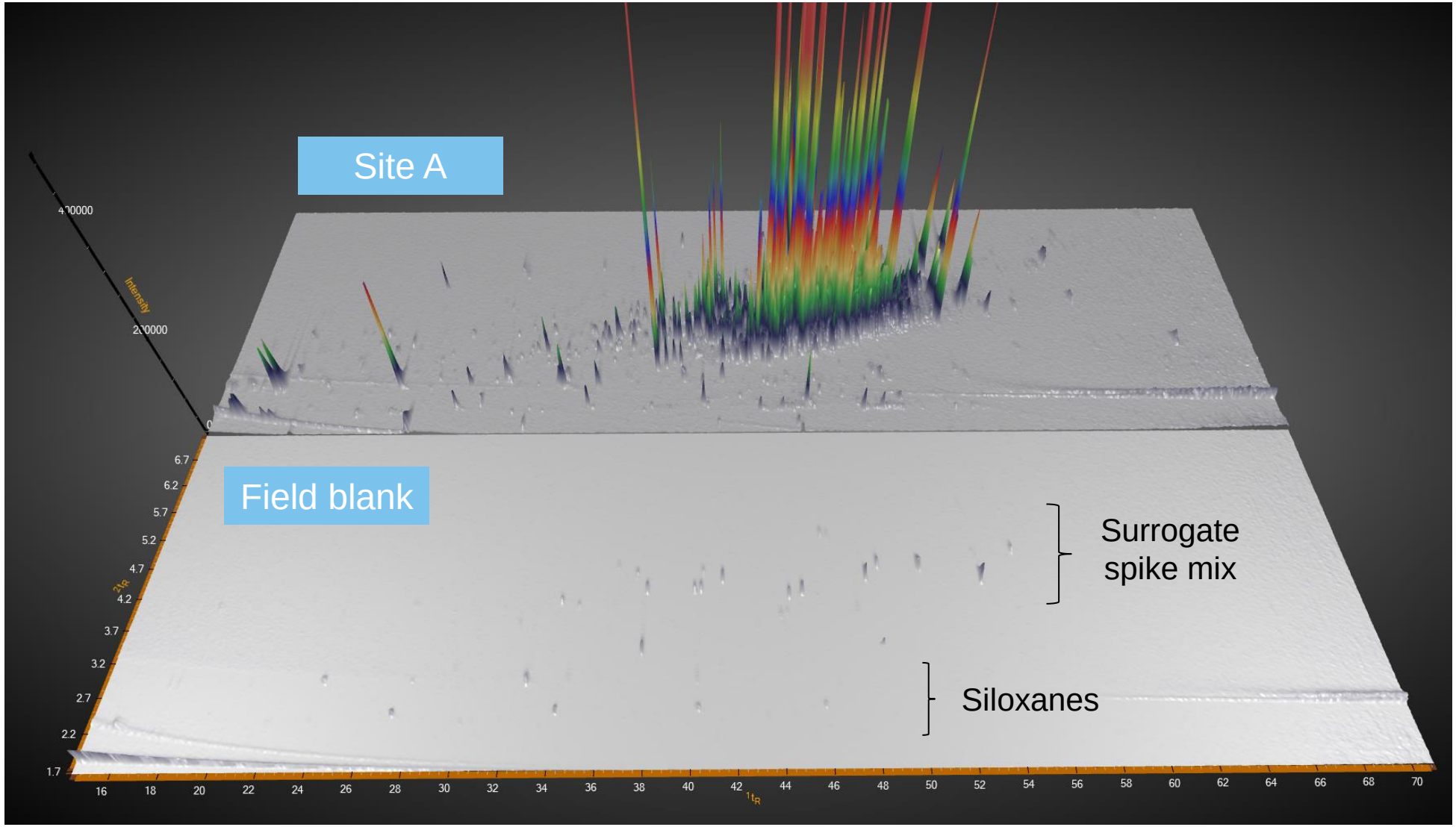
Passive sampling of a UK river with GC×GC–TOF MS



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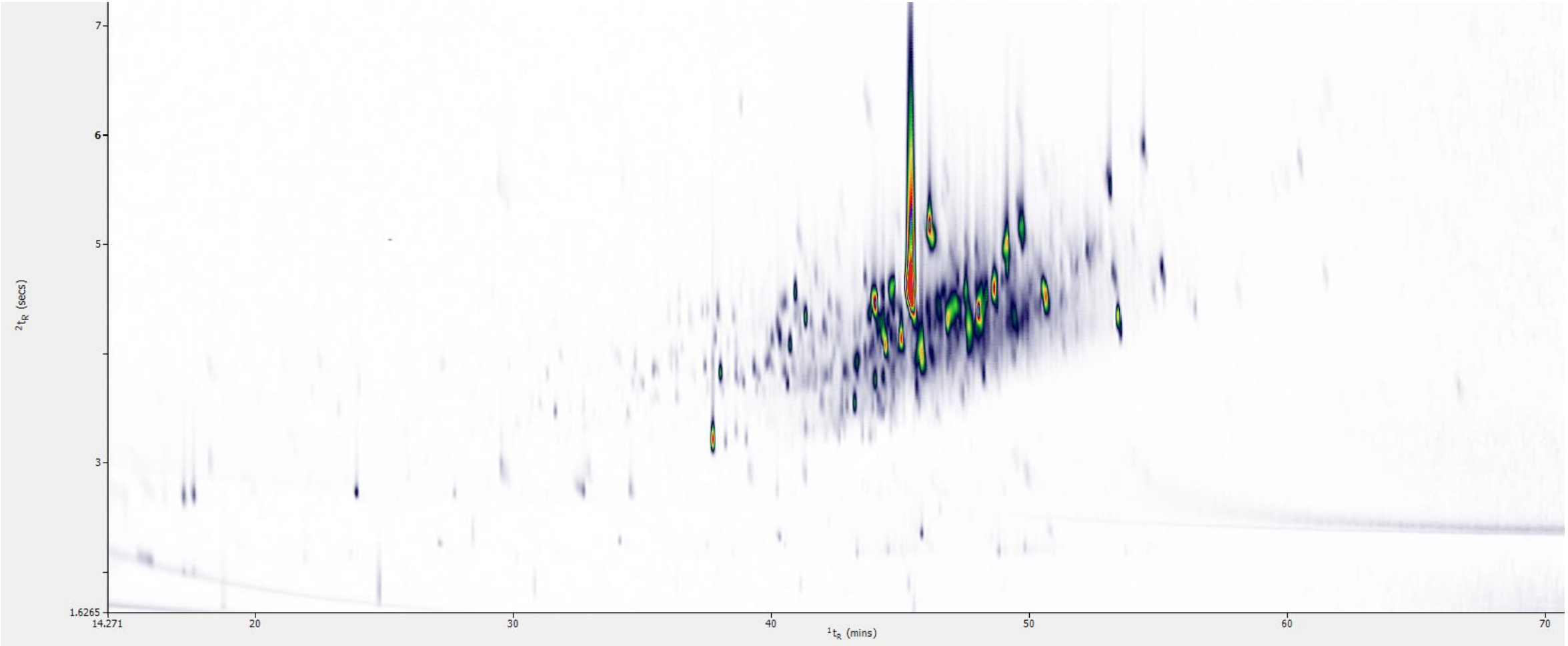
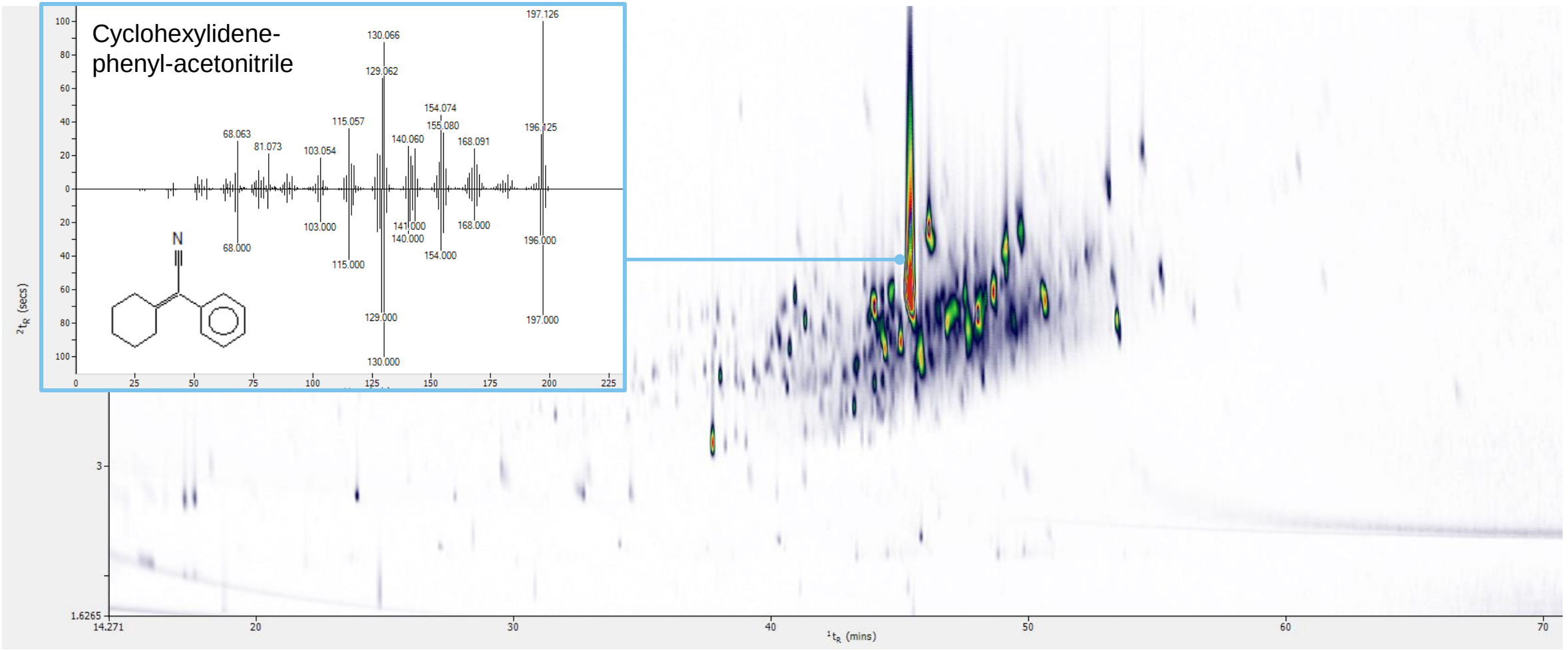


Screening for emerging contaminants



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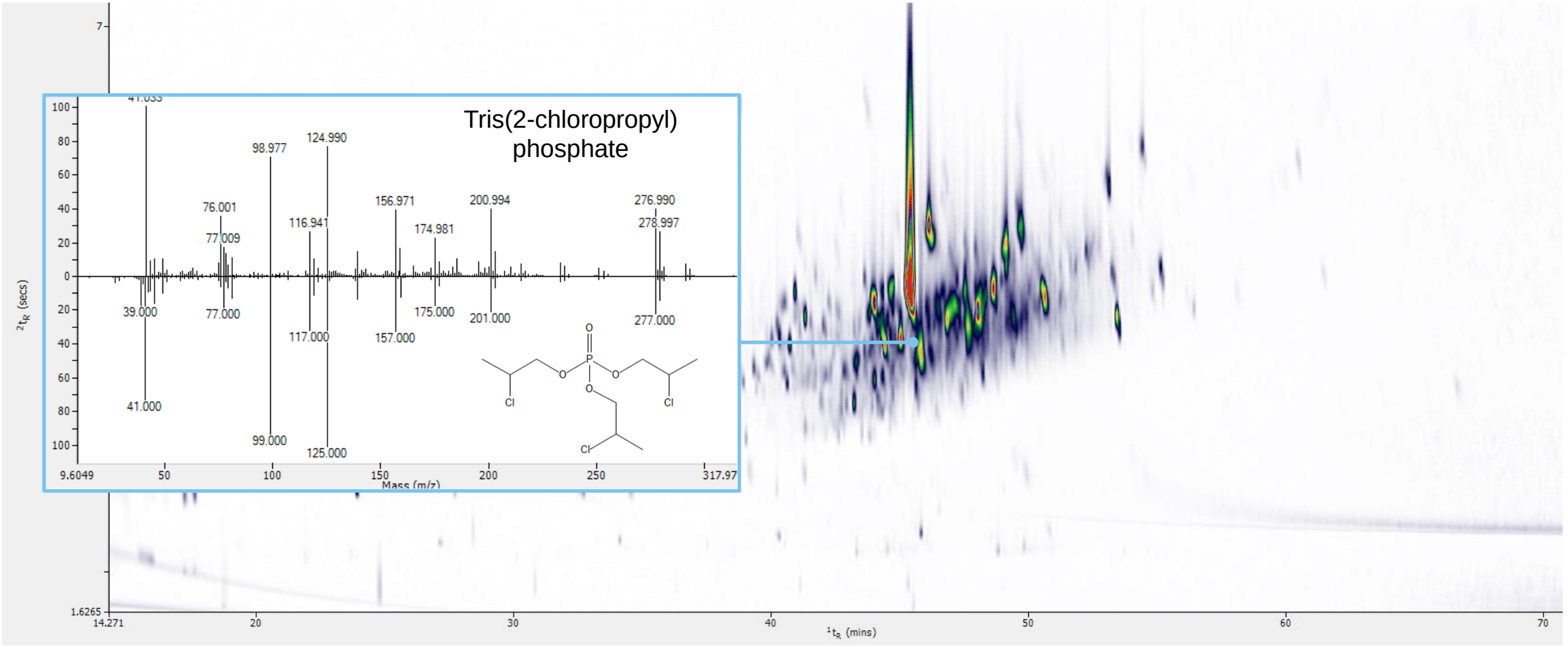
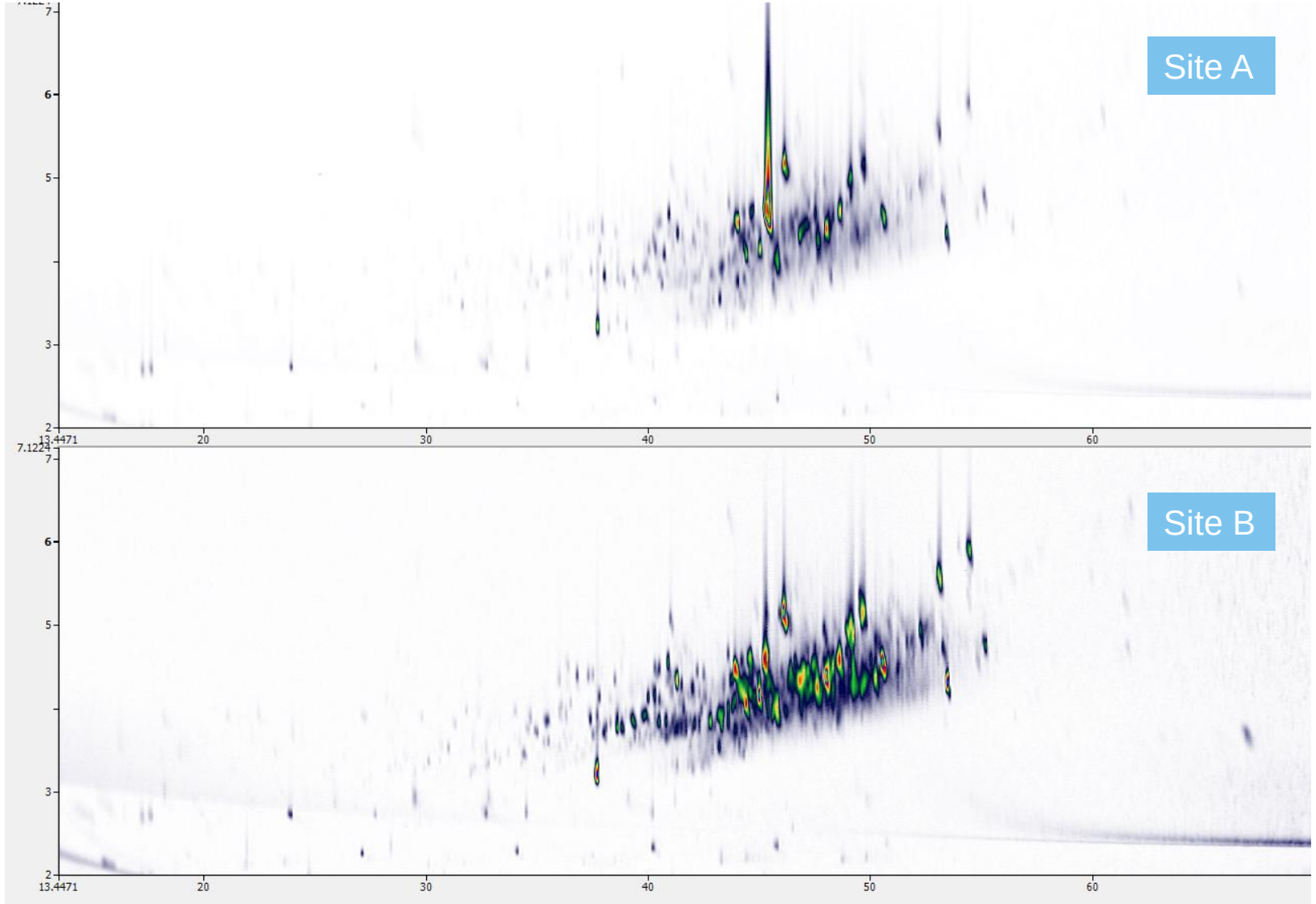


Comparison of sampling sites



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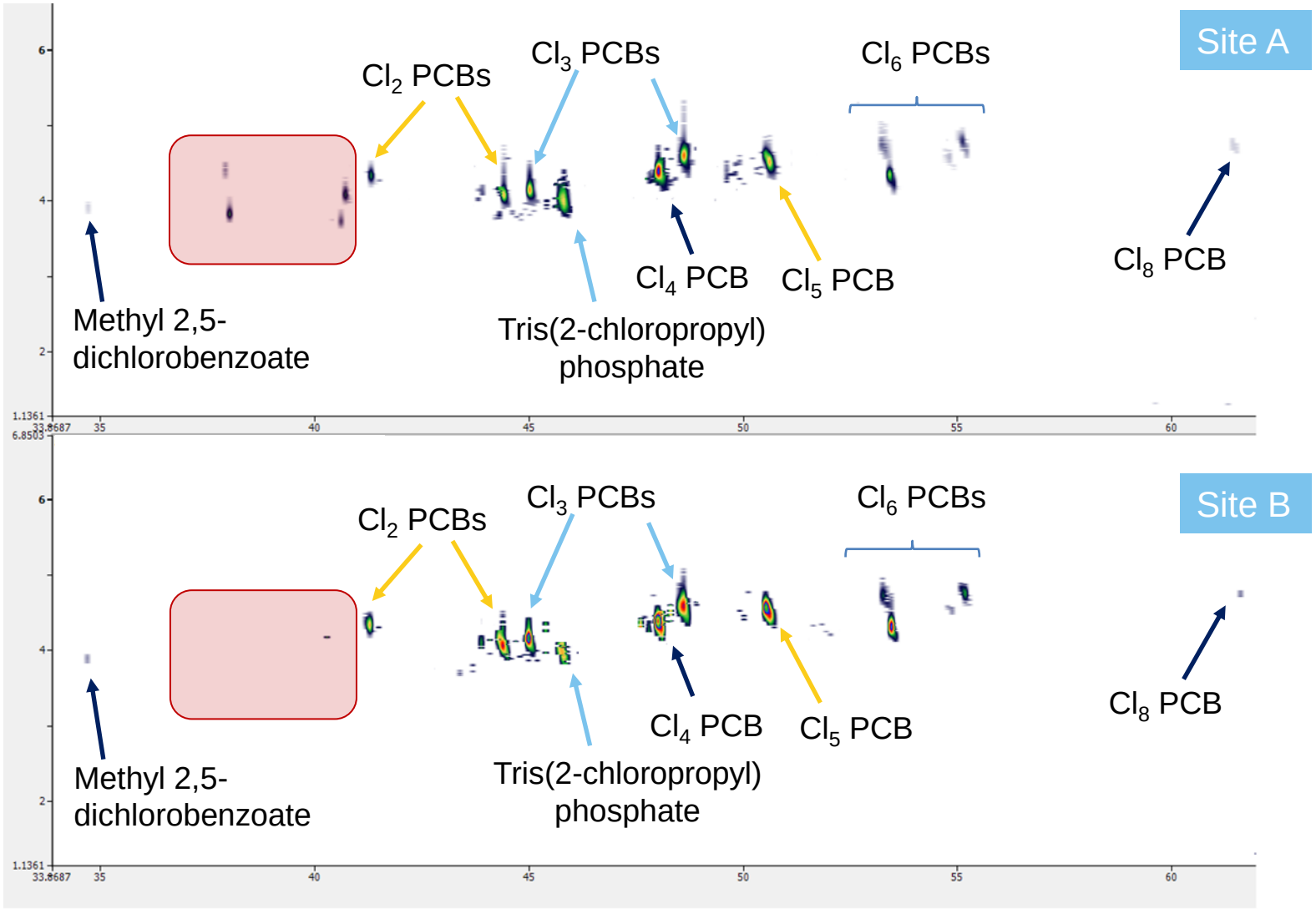
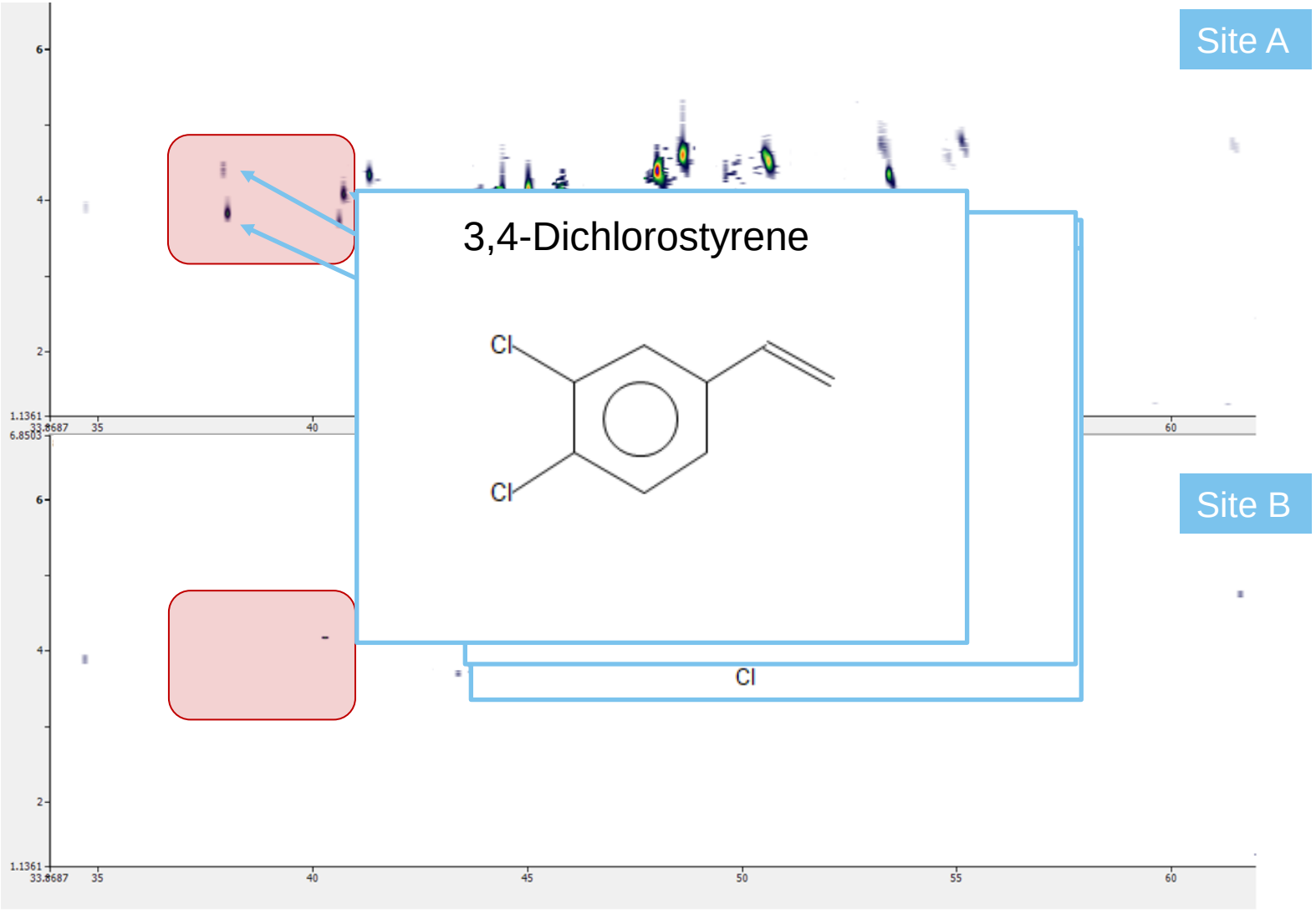


Filtered for organochlorines

ChromSpace

SepSolve Analytical

Comparison of sampling sites



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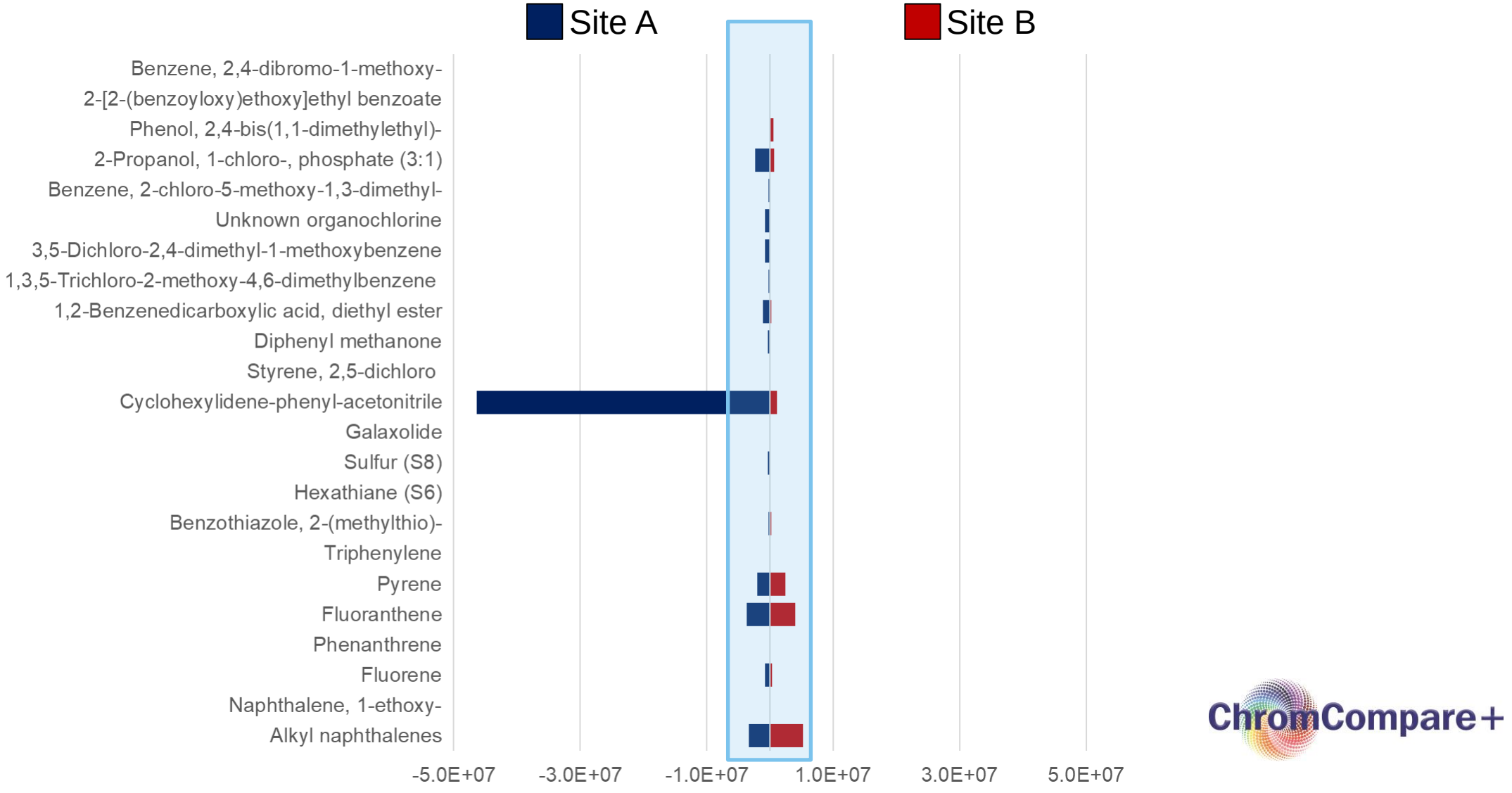
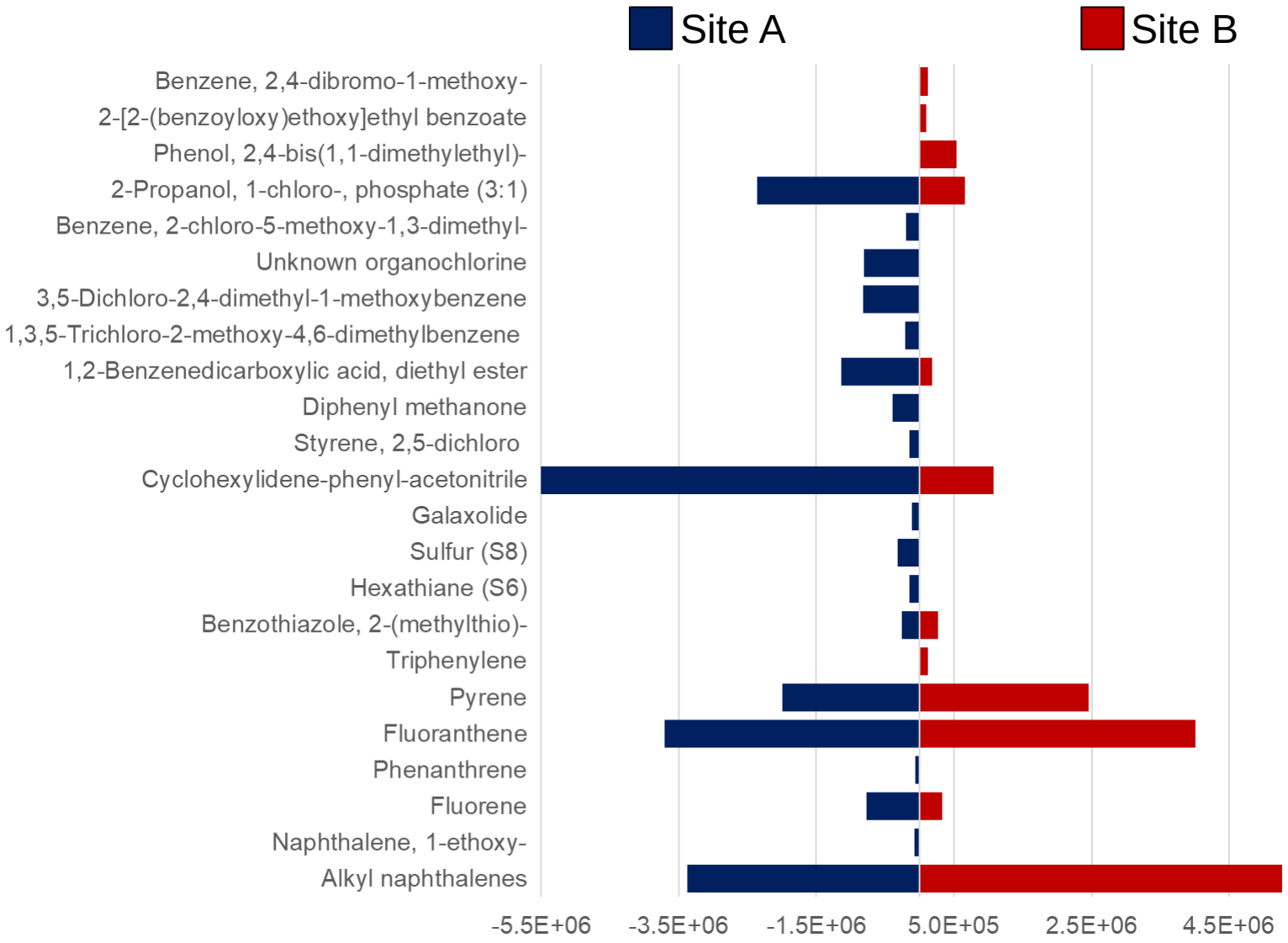


ChromCompare+

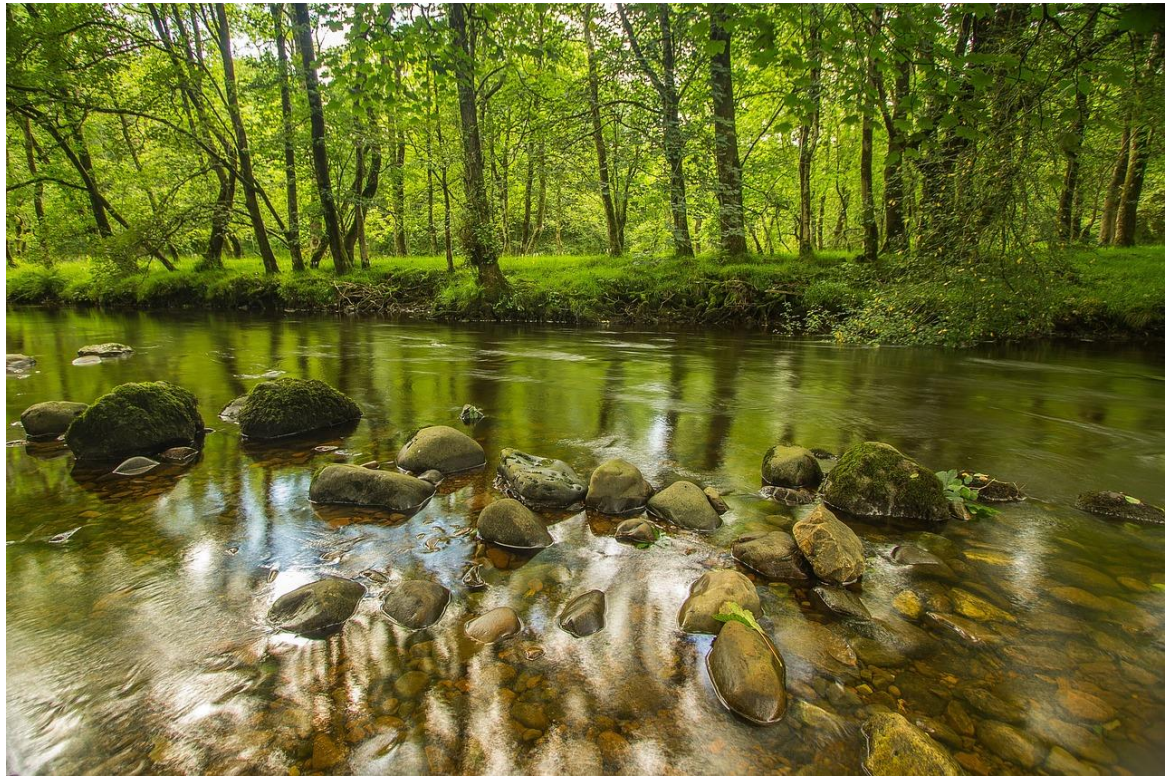
Comparison of sampling sites



ChromCompare+

Future work

- 11 sampling sites in total
- Field blanks performed at each site
- Apply new processing workflows to compare the sites



Summary

- Passive sampling coupled with GC×GC–TOF MS
  - Minimises the risk of missing pollution events
  - Gives greater insight into river quality

- The new INSIGHT-Thermal modulator provides improvements in productivity and performance for thermally modulated GC×GC
  - Ramped cold jet flow rates for efficient modulation of high boilers.
  - Easy to configure column holder for simple set-up and repeatable results
  - Retrofittable to all popular GCs

- Further work on-going to compare multiple sampling sites along a UK river using GC×GC–TOF MS

Thanks for listening! Any questions?

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