Sniff smarter: Empowering GC–O with trap-based enrichment and GC×GC for advanced aroma profiling

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Global Food, Flavour and Fragrance Sector Manager

Who are we?

MARKES international

SepSolve Analytical

Sampling technologies

Thermal desorption

Sample enrichment

Separation technologies

Unique identification

Data analysis

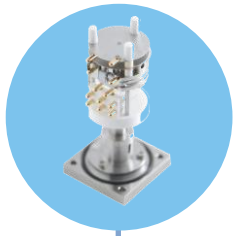
Our history in separation technologies

2008

Launch of first generation **BenchTOF** mass spectrometers

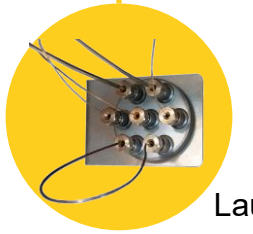
2016

Launch of **Tandem Ionisation**



2017

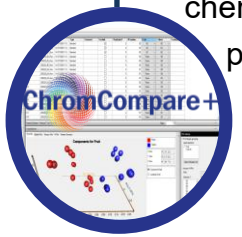
Launch of **INSIGHT®-Flow** reverse fill/flush modulator…



…and **ChromSpace** GC×GC software

2020

Launch of **ChromCompare+** chemometrics platform



2021

Launch of **BenchTOF2** with improved mass accuracy

Next generation **INSIGHT-Flow** modulator

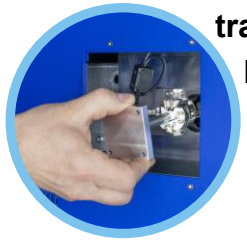
2023

Launch of the **INSIGHT®-Thermal** cryogen-free modulator

2024

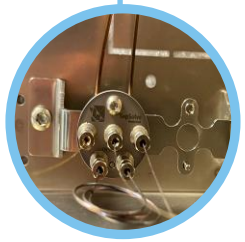
HyperChrom acquired by SepSolve

Redesigned **ion source and transfer line** for BenchTOF2

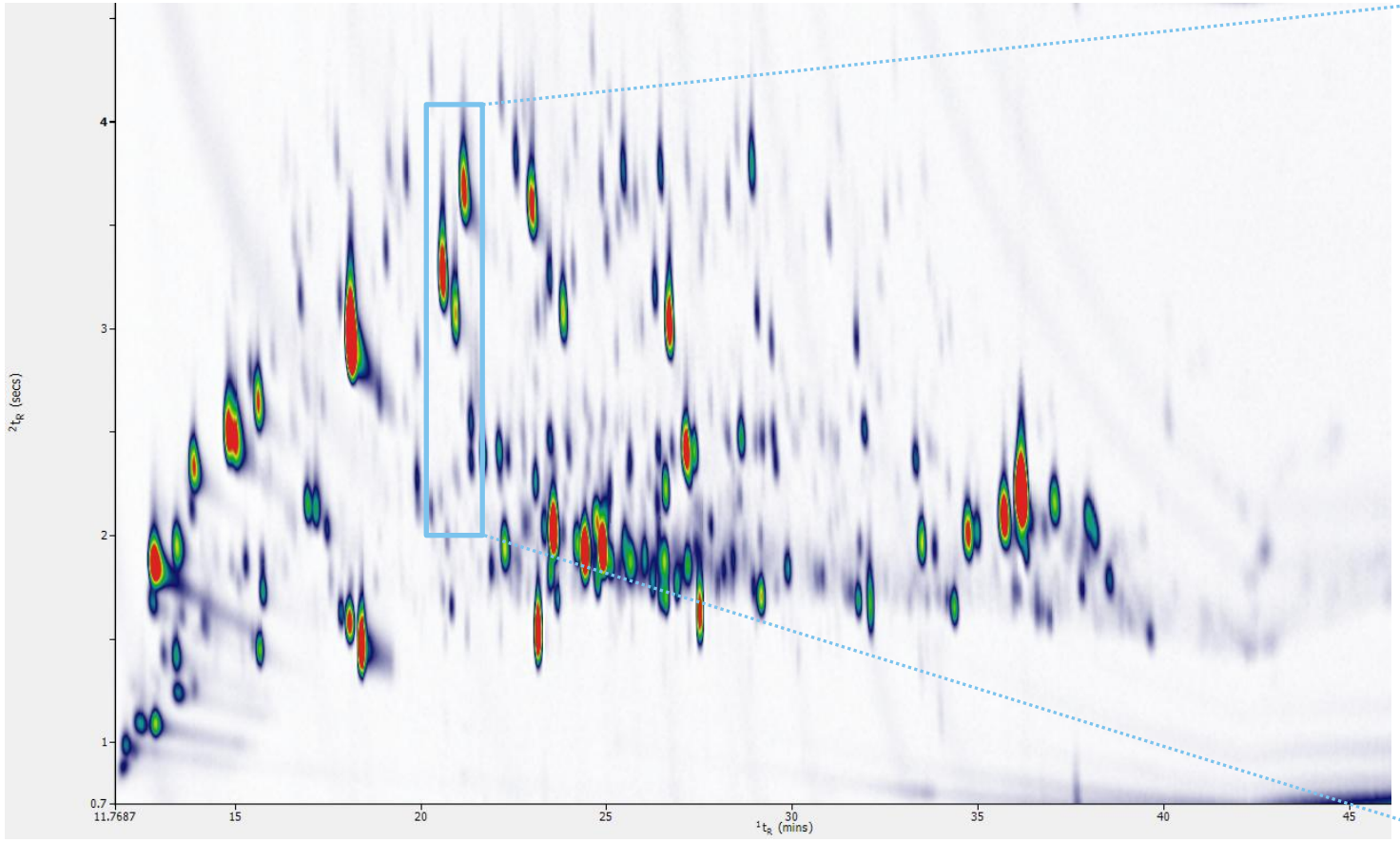


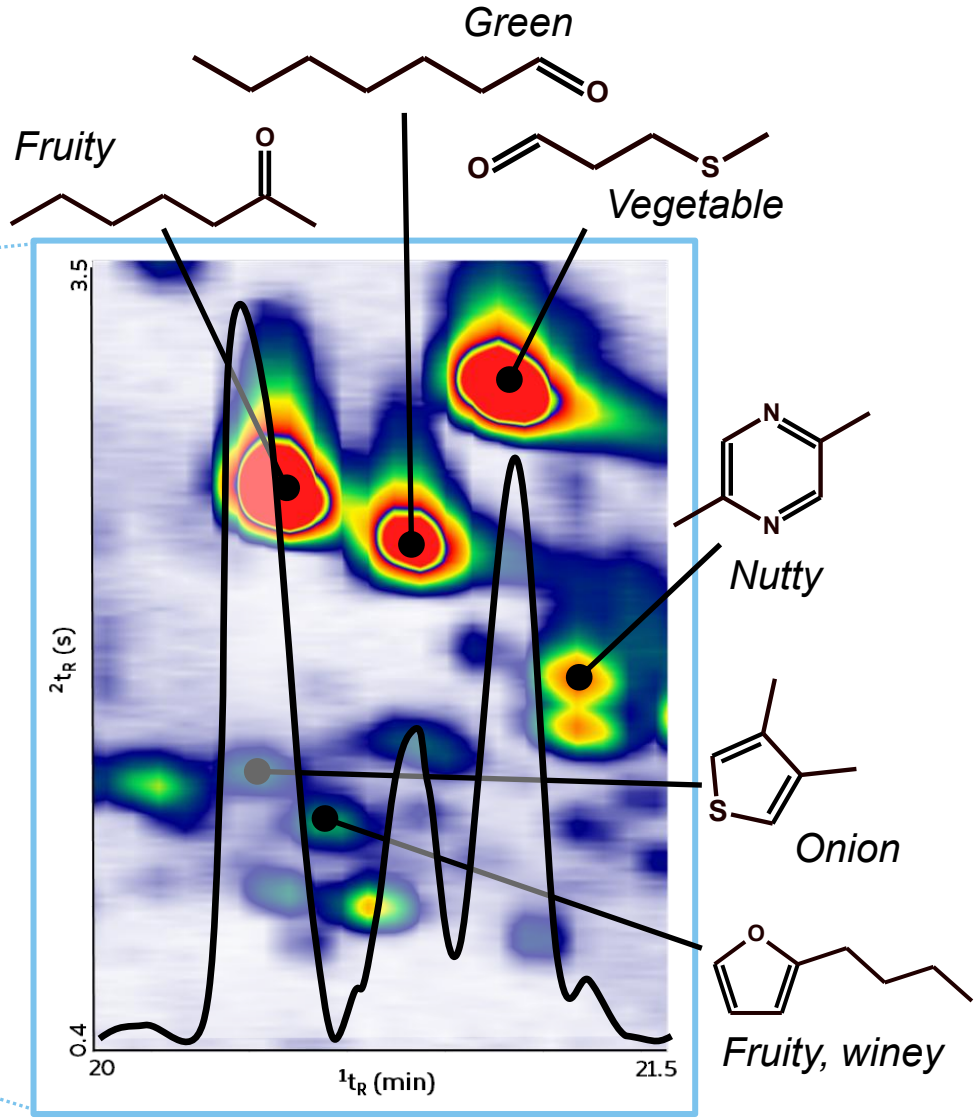
2025

Launch of **Smart Subtract®**



GC×GC for advanced aroma profiling





Correlating chemical data and sensory experience

Correlating chemical and sensory data

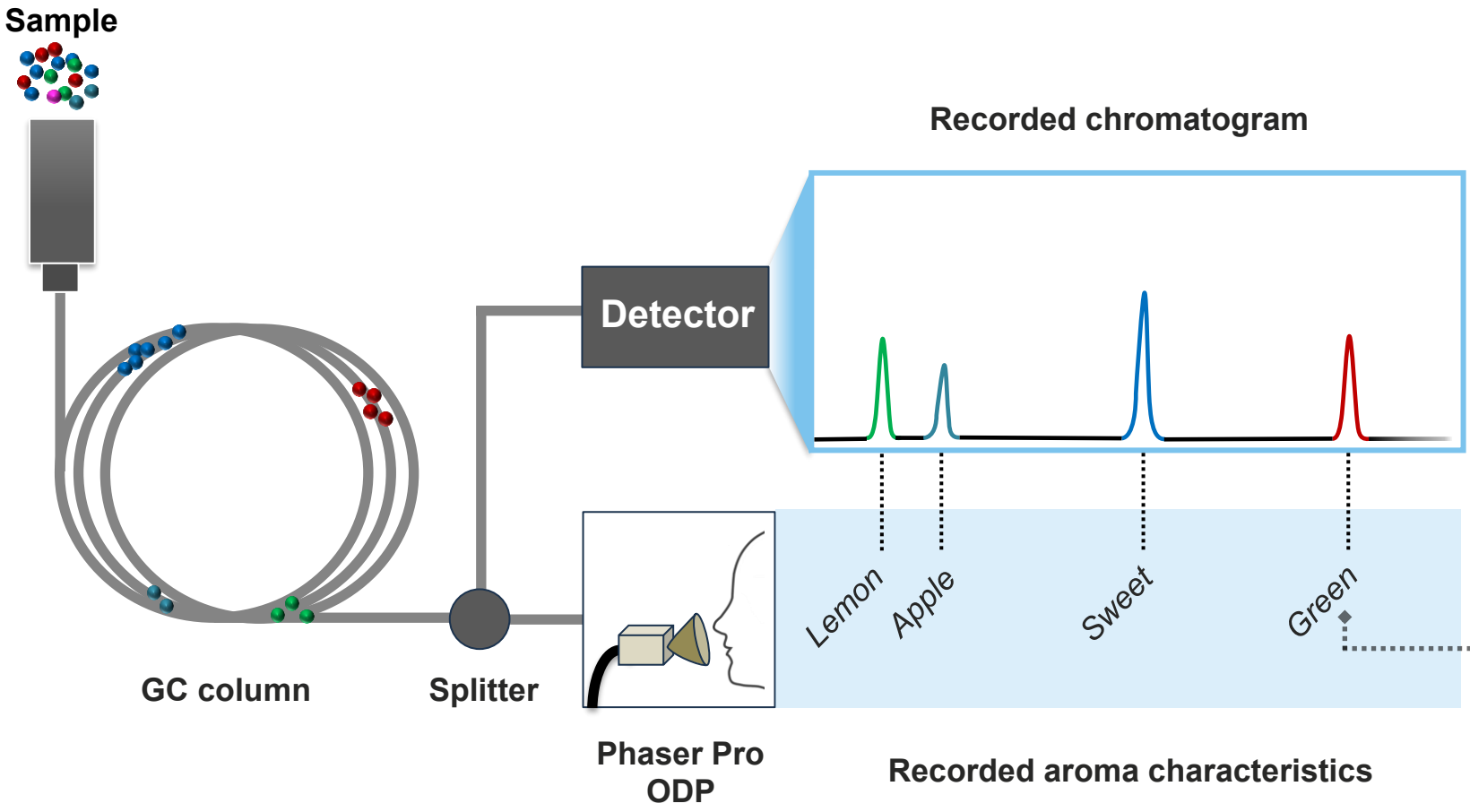
The challenges in traditional GC–O analysis

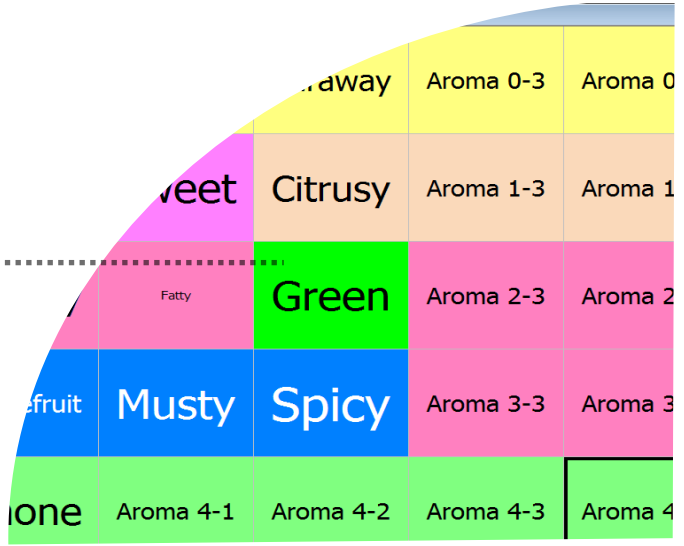
- **Trace-level odorants:** low odour detection thresholds (ODT) mean our noses may detect what the mass spectrometer can’t

- **Co-eluting compounds:** make it difficult to identify the specific compound(s) responsible for a perceived odour

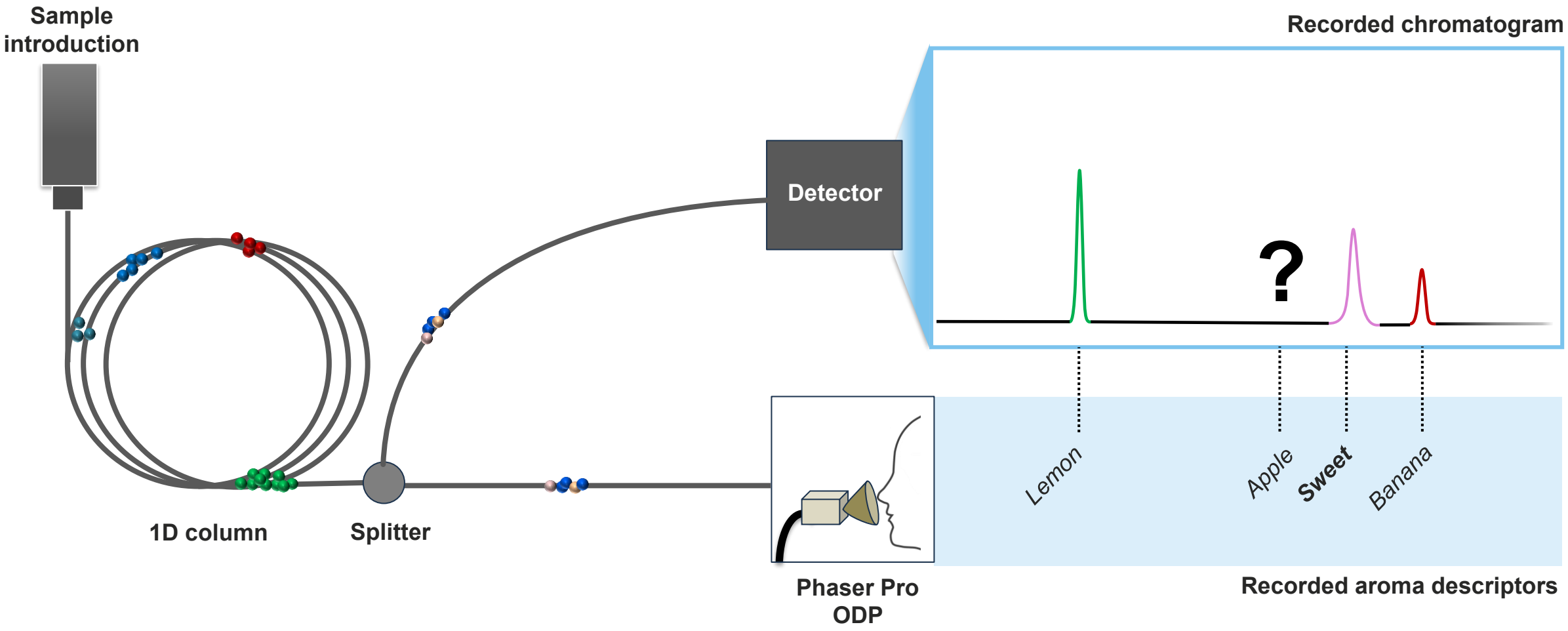
Integrating sensory analysis into workflows

Phaser Pro odour detection port (ODP)





Challenges in sensory evaluation with GC(O)–MS



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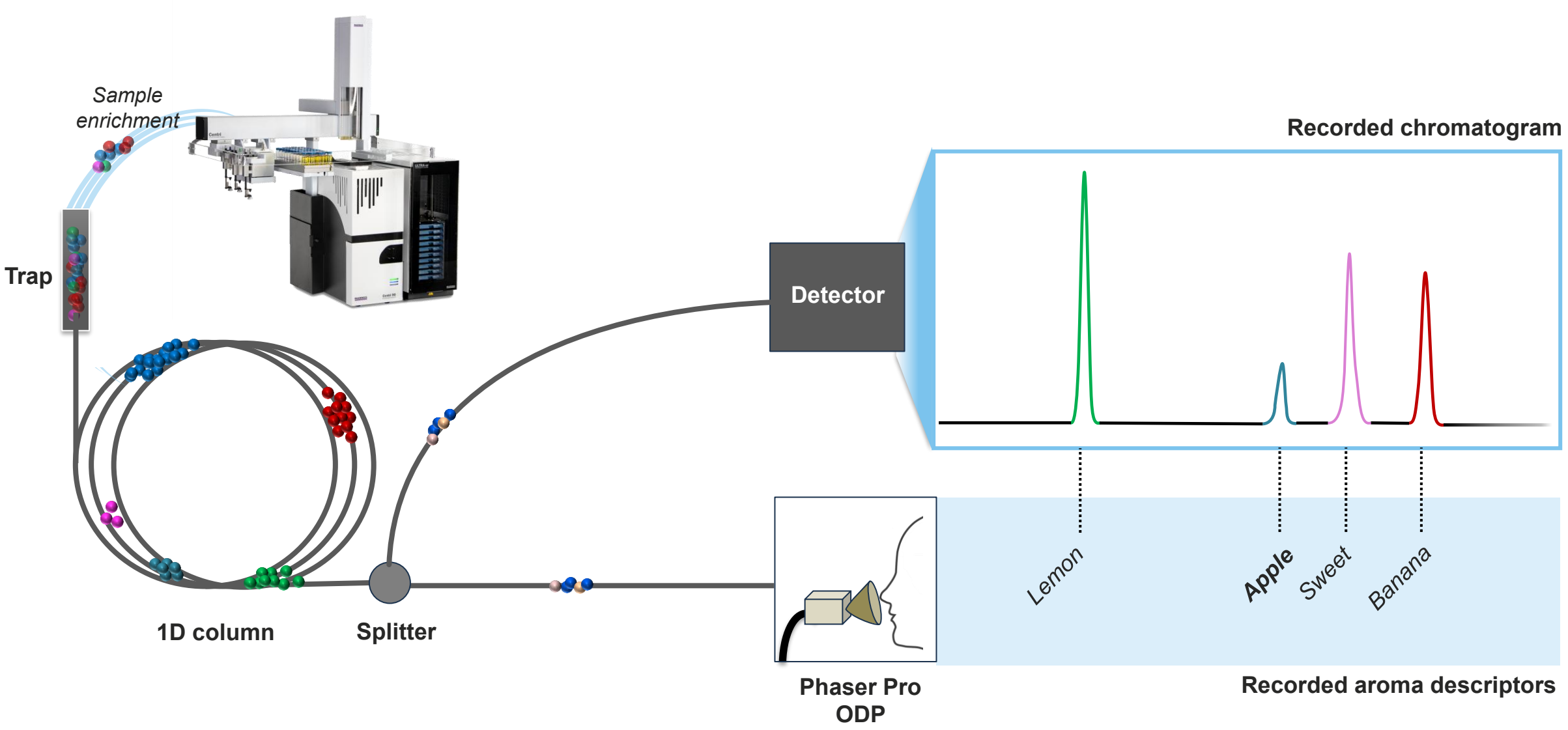
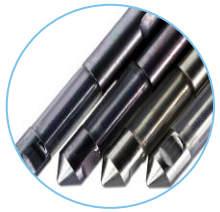


Enrichment using trap focusing

Step 1: Desorption of sampled analytes and focusing of VOCs



HiSorb

SPME

Headspace

Tube-based TD

Interferents such as water and air can be **selectively purged** prior to trap desorption

Trapping uses **electrical cooling** rather than cryogen

Analytes enter the electrically-cooled trap

Enrichment using trap focusing

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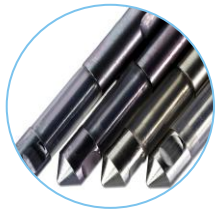

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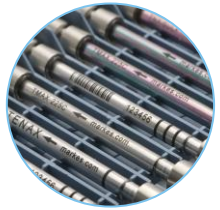

Tube-based TD

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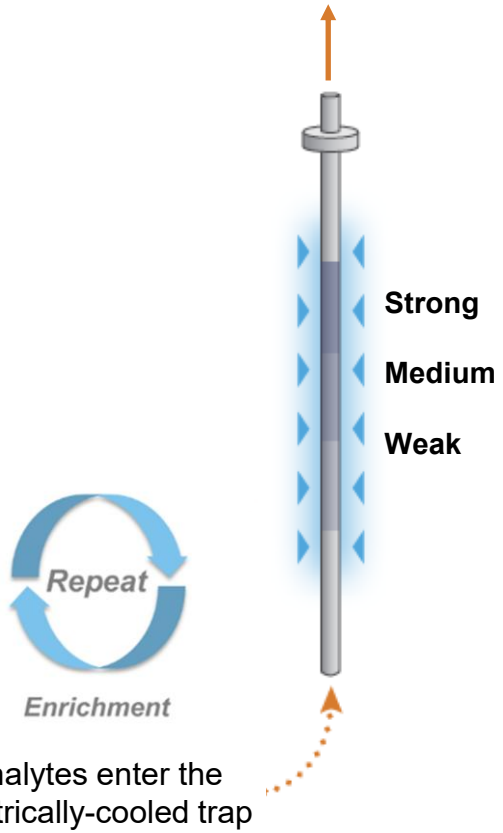
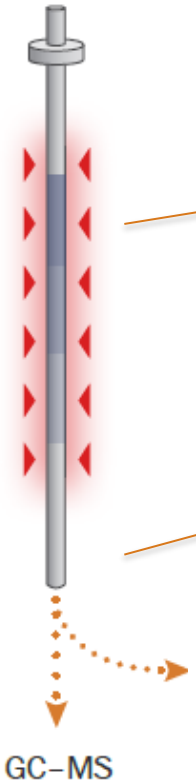


Analytes enter the electrically-cooled trap

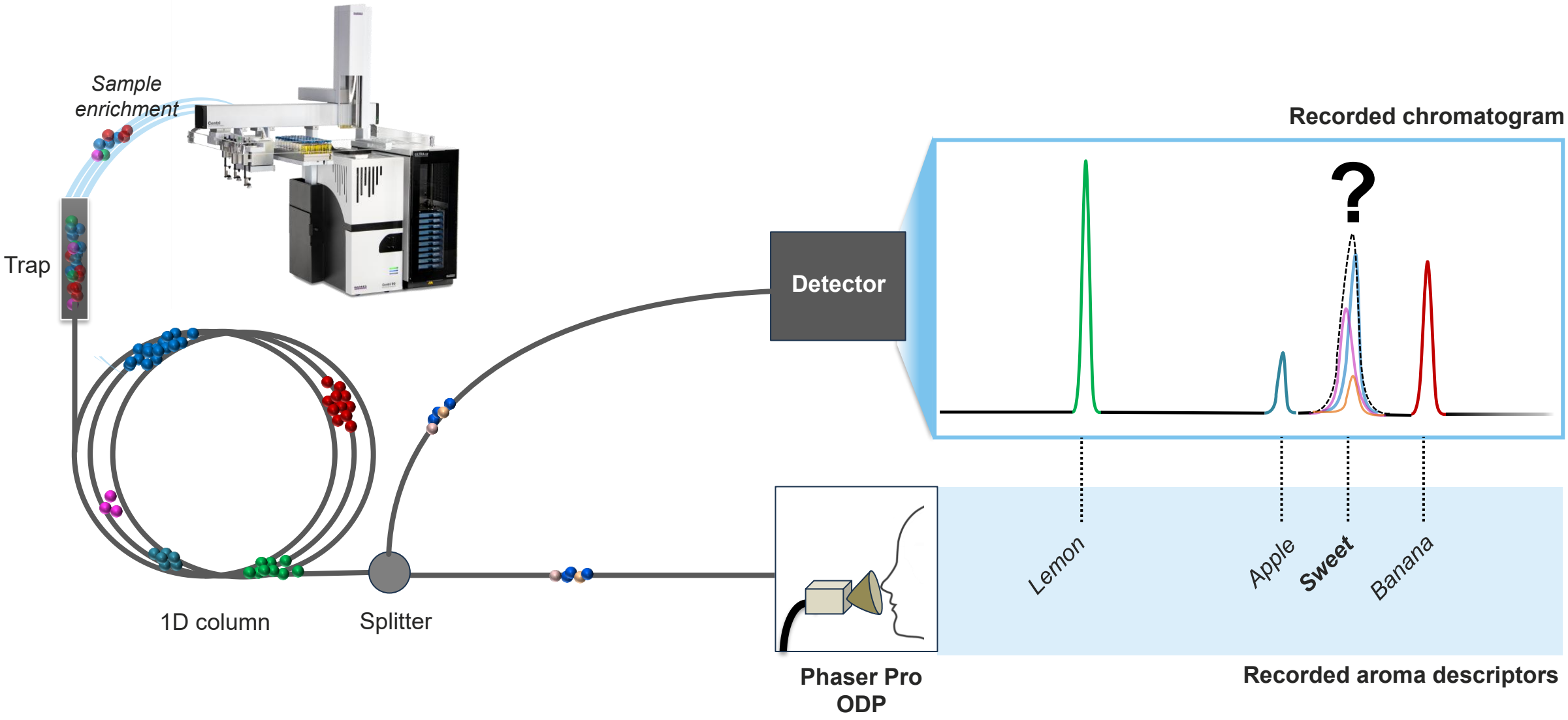


The trap is heated rapidly, up to 100ºC/s, during desorption

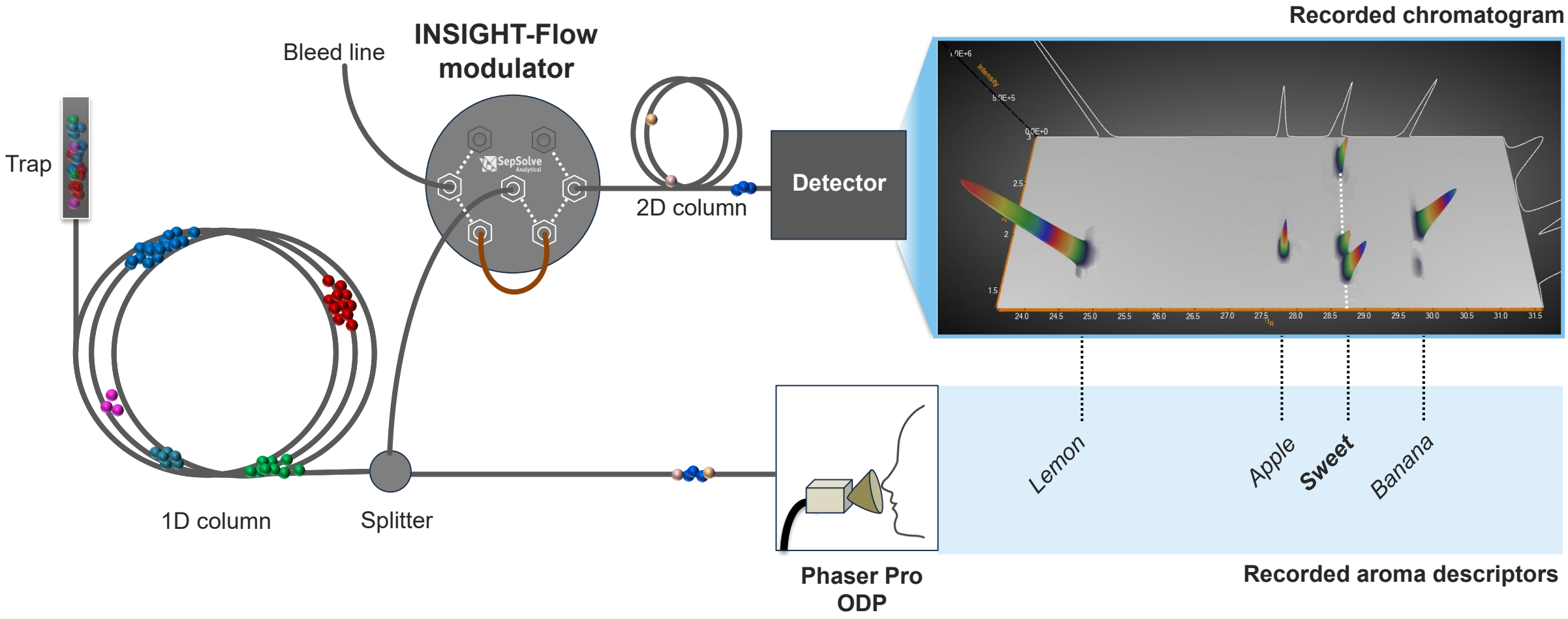
Analytes enter and leave the trap at the same end **('backflush desorption')**

Automated re-collection **–** optional split

Challenges in sensory evaluation with GC(O)–MS



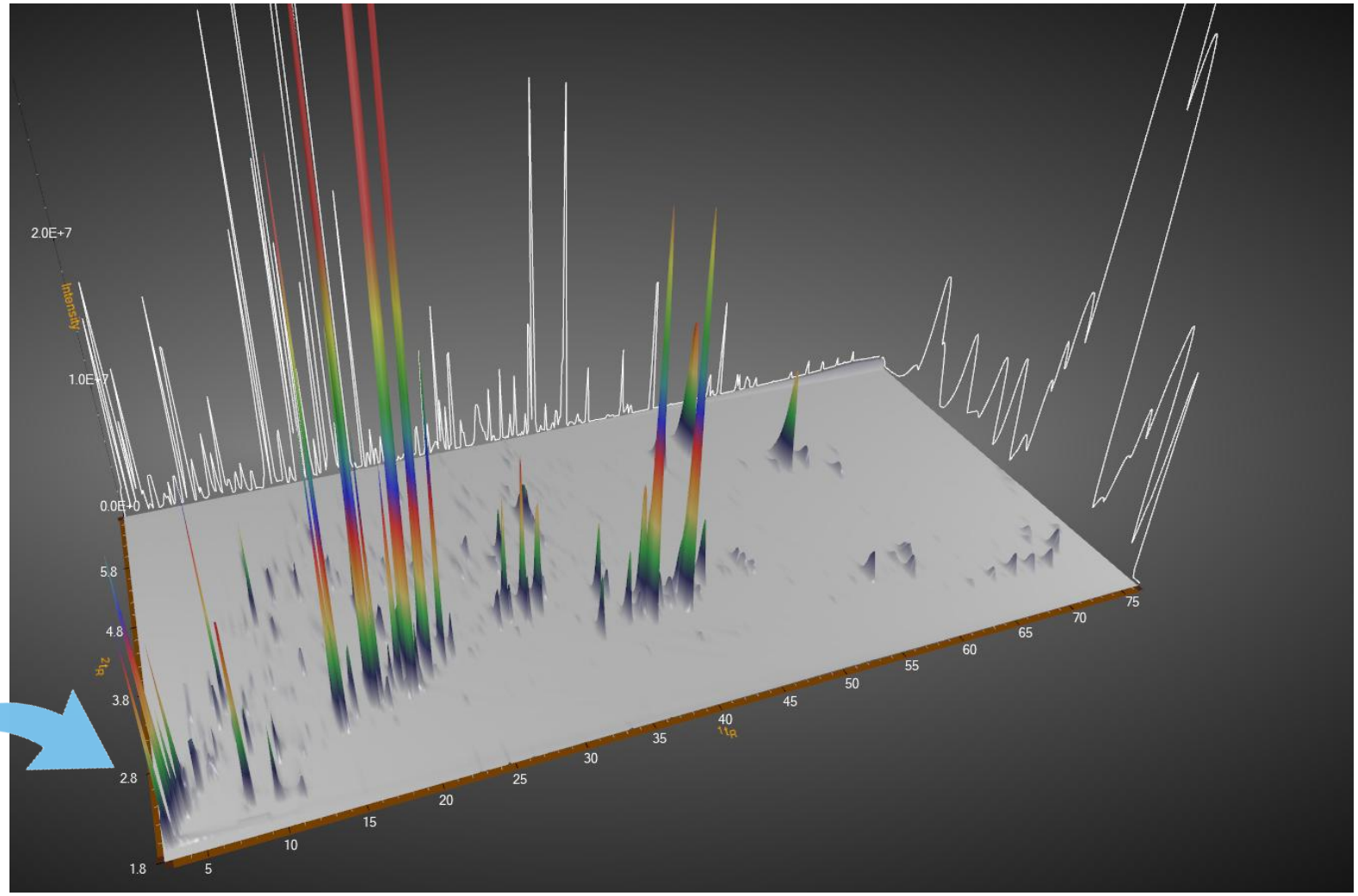
Enhanced sensory evaluation with GC×GC–TOF MS



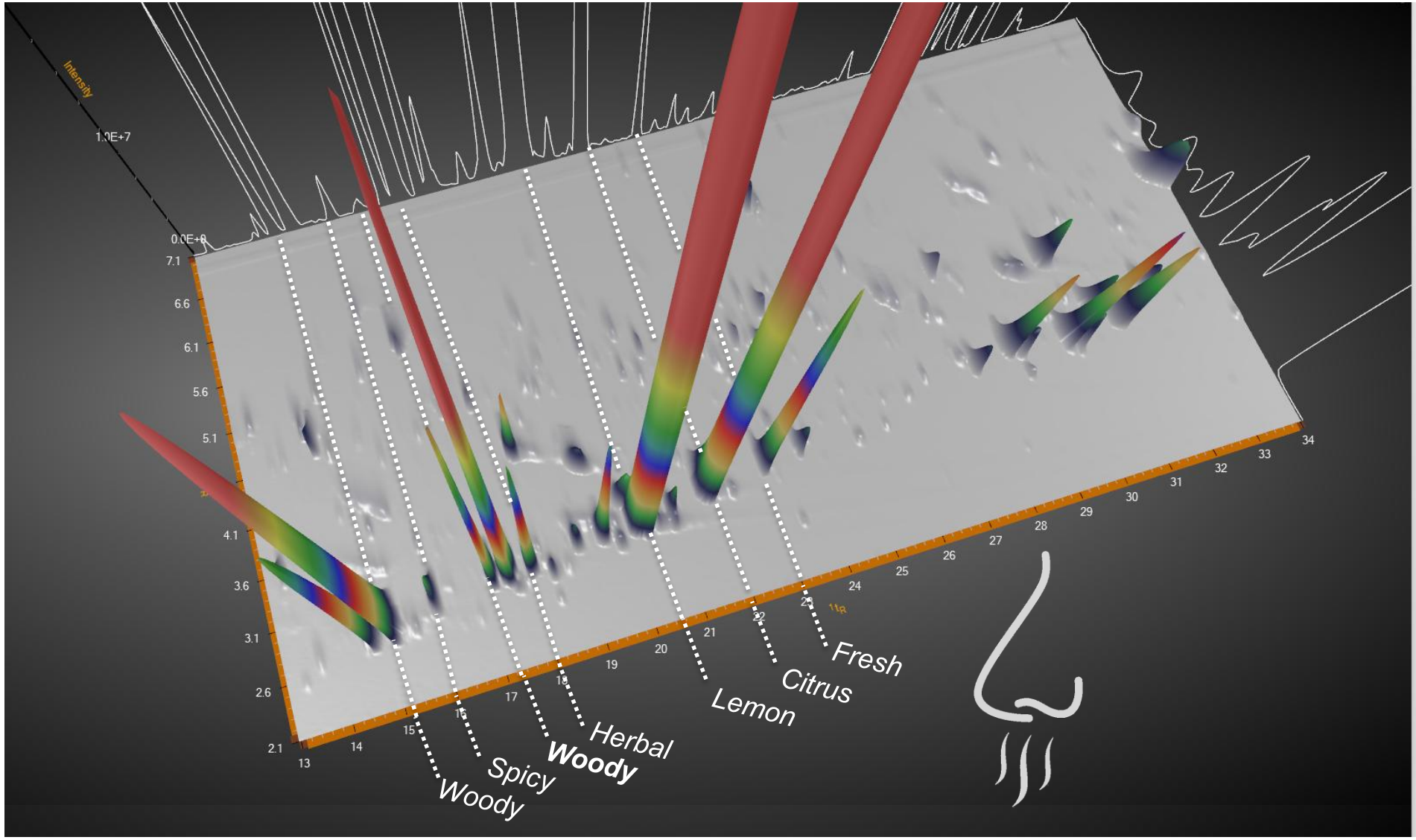
Preliminary study

Direct desorption of citrus rinds

Citrus rinds (~50 mg)
in empty TD tube



Analysis of citrus rinds by TD–GC(O)×GC–TOF MS



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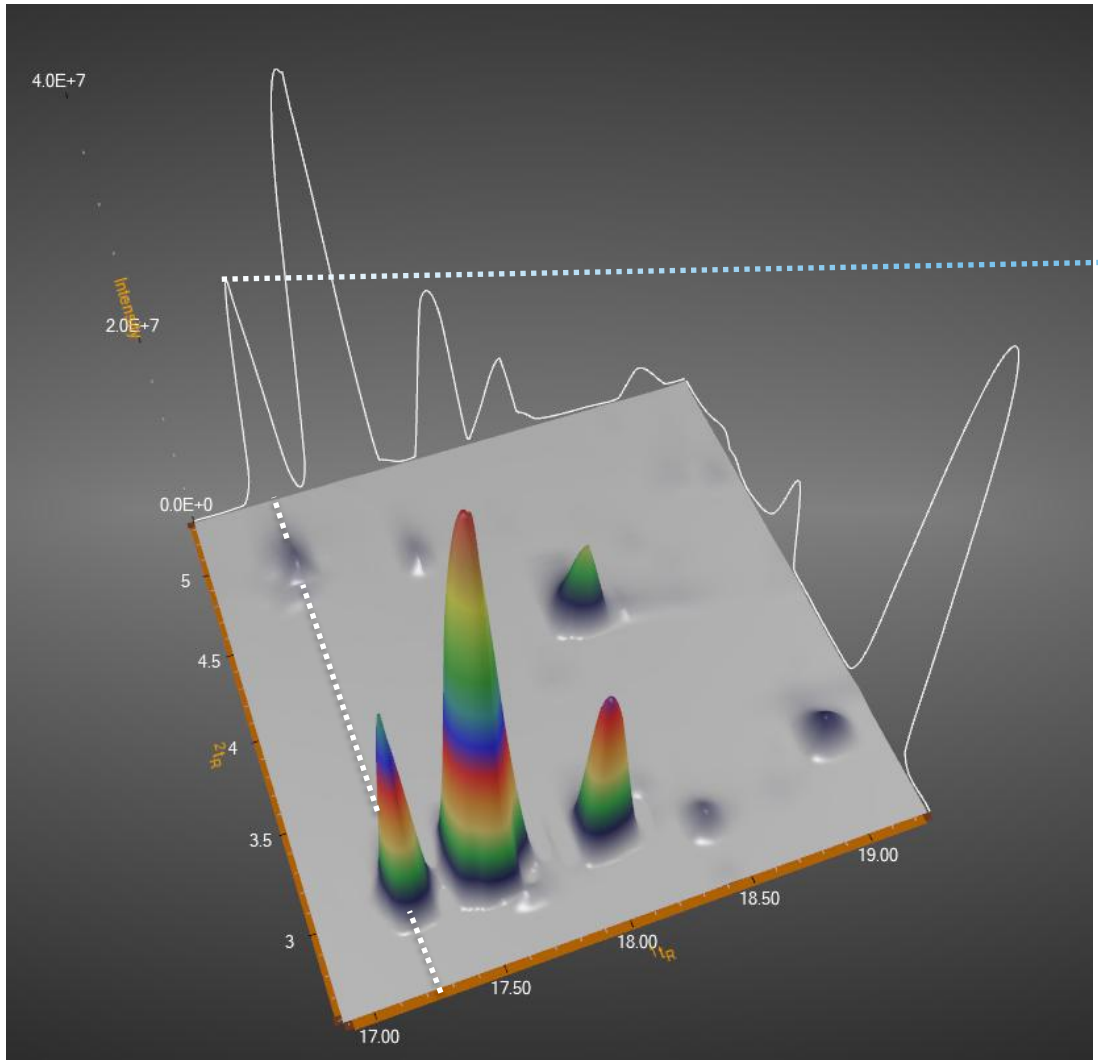
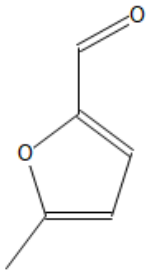


To ODP

Woody odour recorded

Analysis of citrus rinds by TD–GC(O)×GC–TOF MS

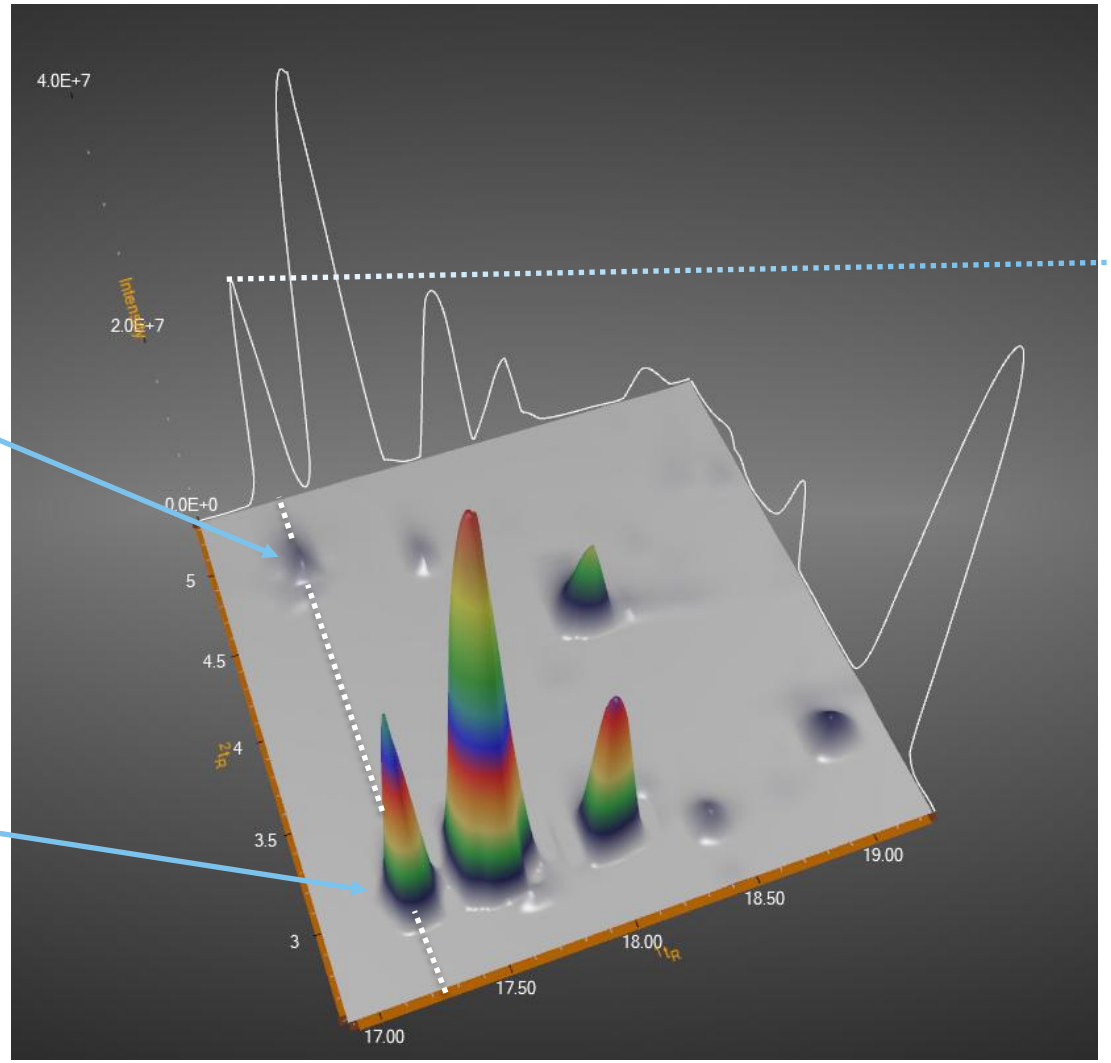


5-Methylfurfural

'Caramellic'

β-Pinene

'Herbal, woody'



To ODP

Woody odour recorded

Sensory evaluation of orange juice

Headspace sorptive extraction and GC×GC–(O)–TOF MS

VS

With pulp

Without pulp

Experimental conditions

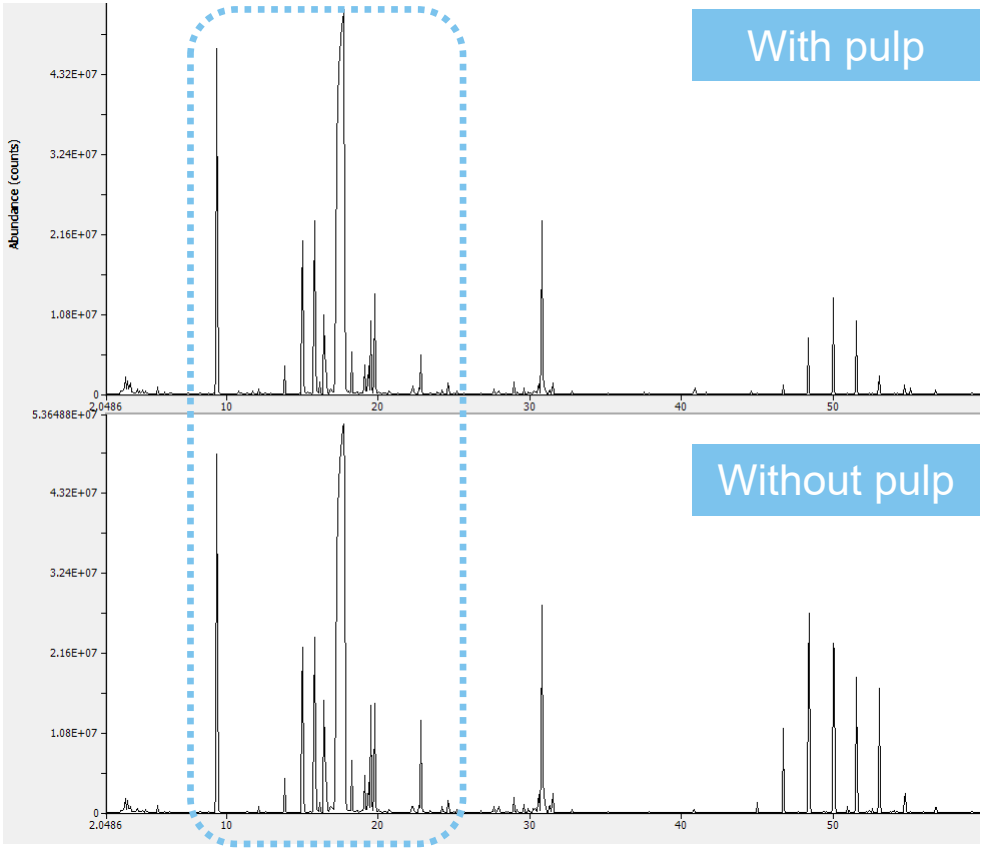
Sampling: Headspace Hisorb sorptive extraction

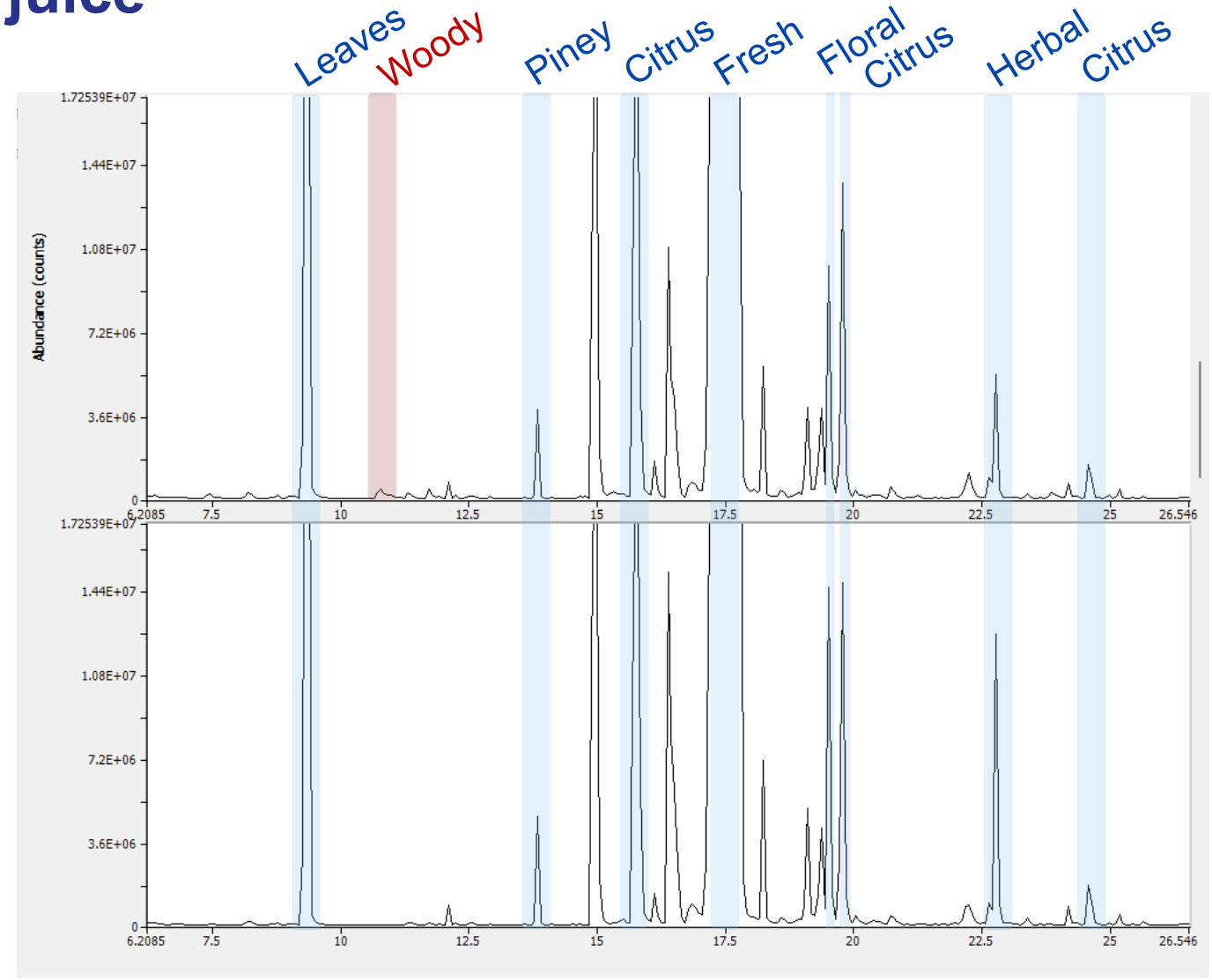
Sample: 10 mL orange juice in 20 mL vial

Sorptive phase: Car/PDMS

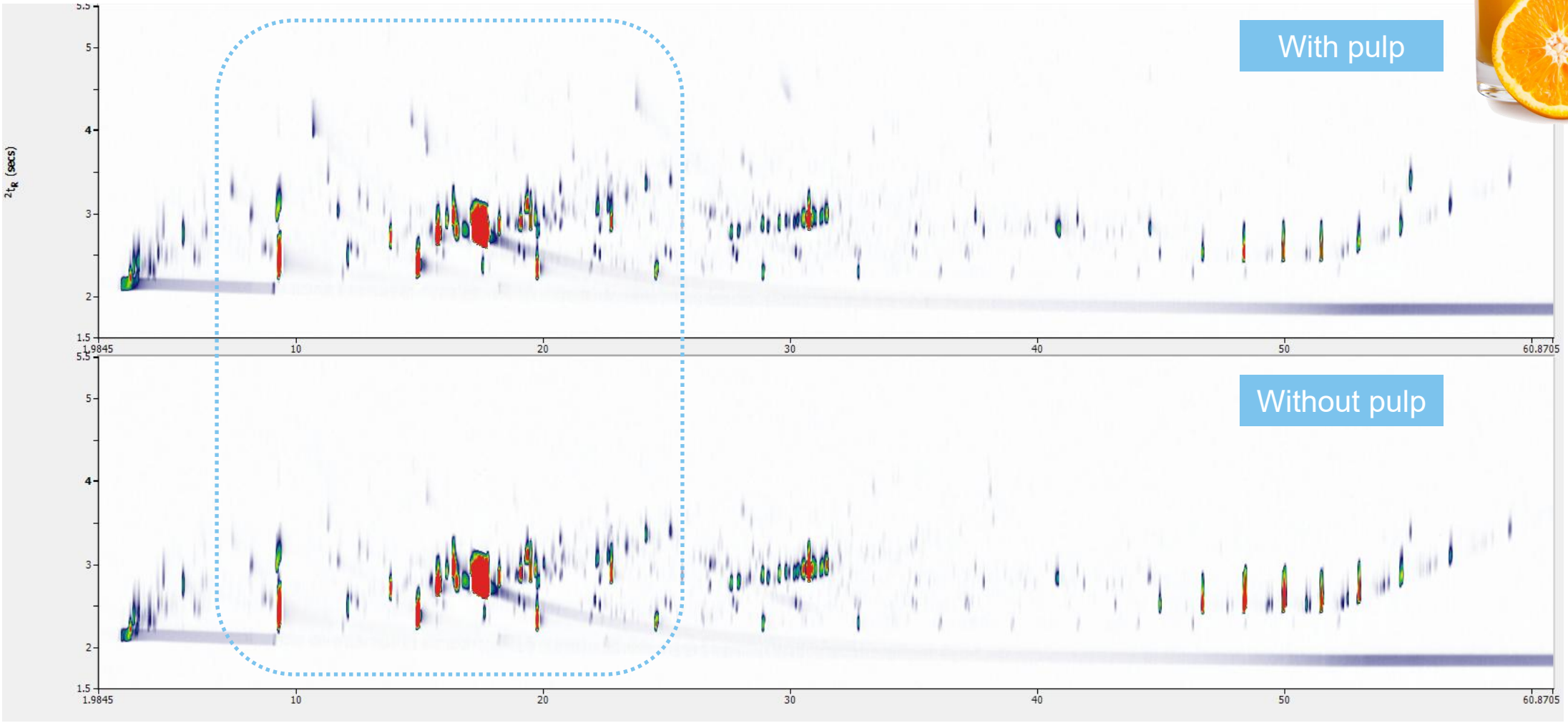
Extraction: 30 min at 40 °C and 300 rpm

Sensory evaluation of orange juice





GC×GC–(O)–TOF MS of orange juice



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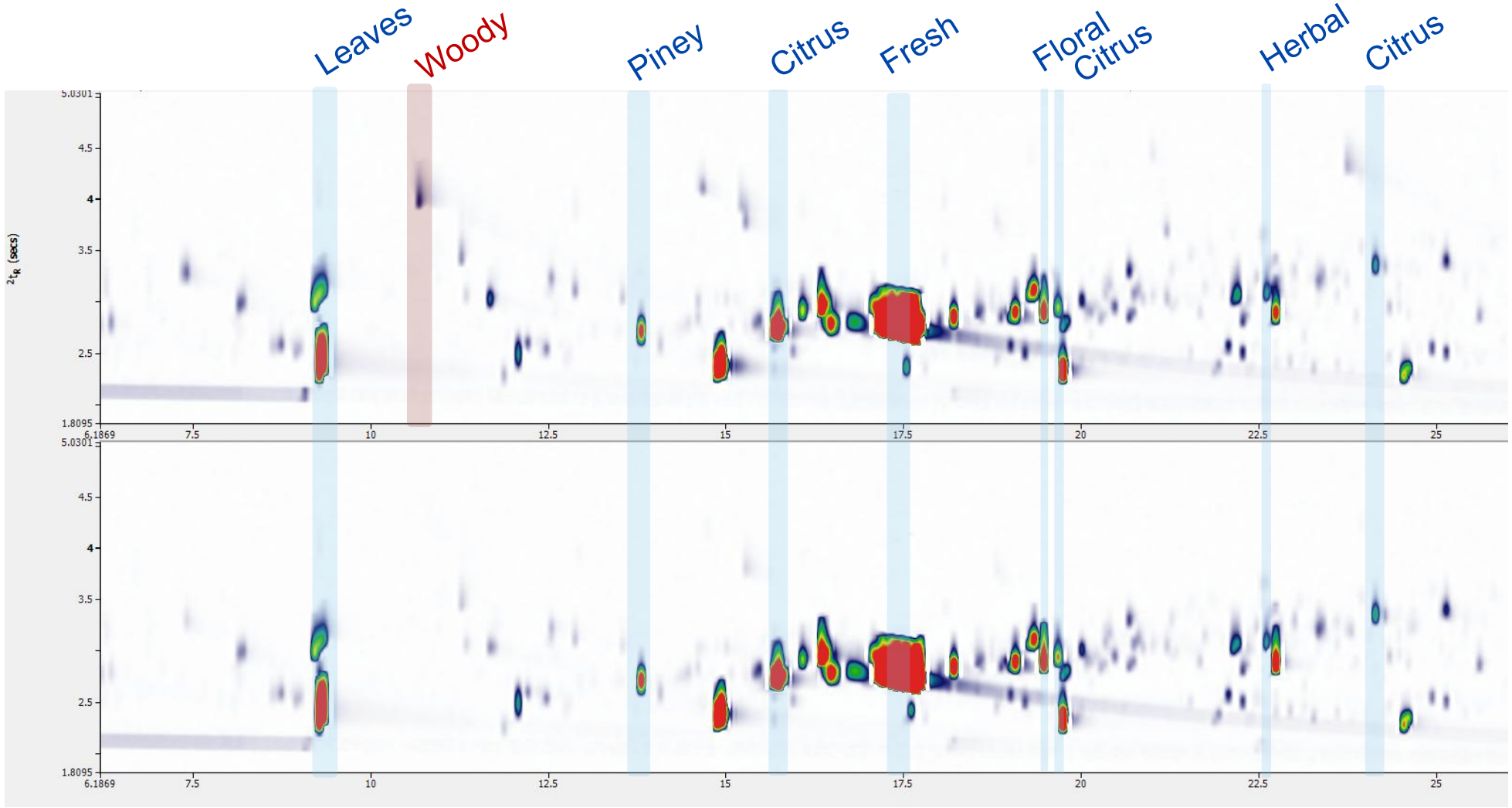

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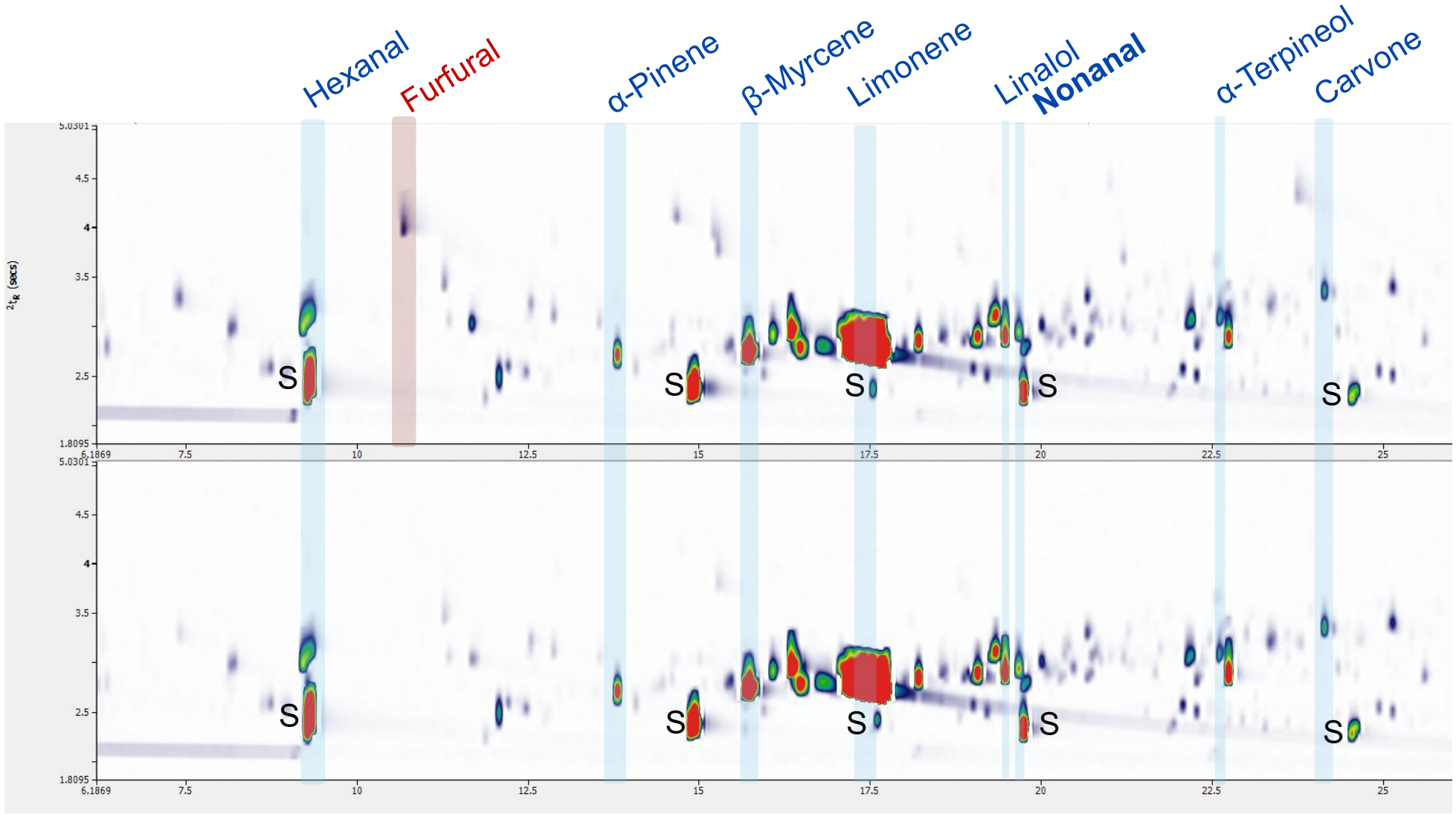
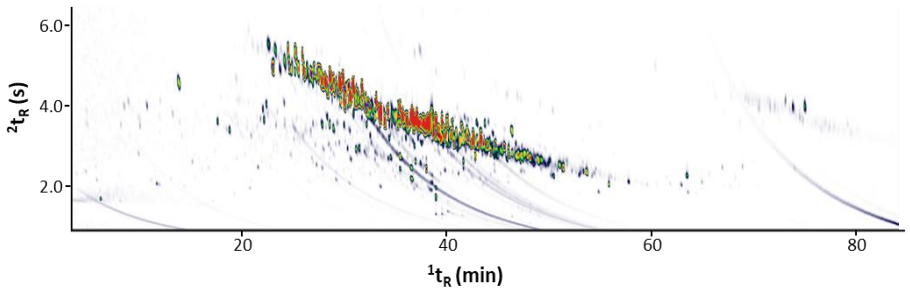
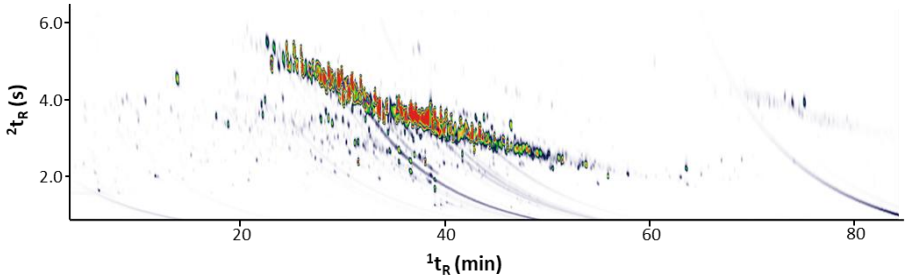


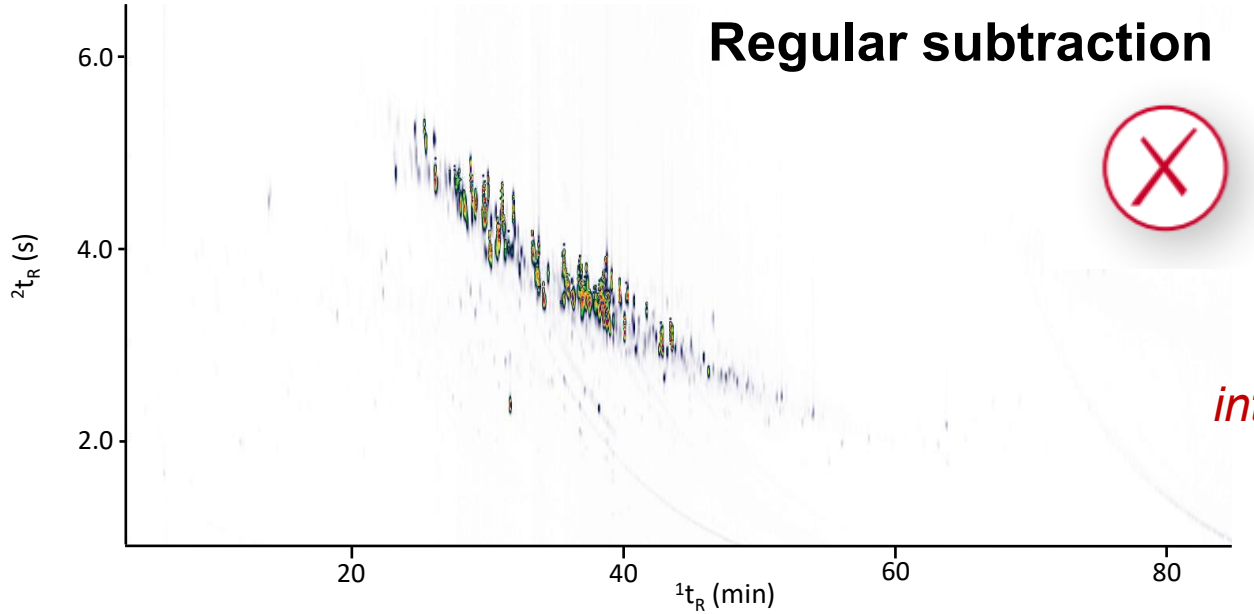
S = Siloxane

Comparison of GC×GC chromatograms



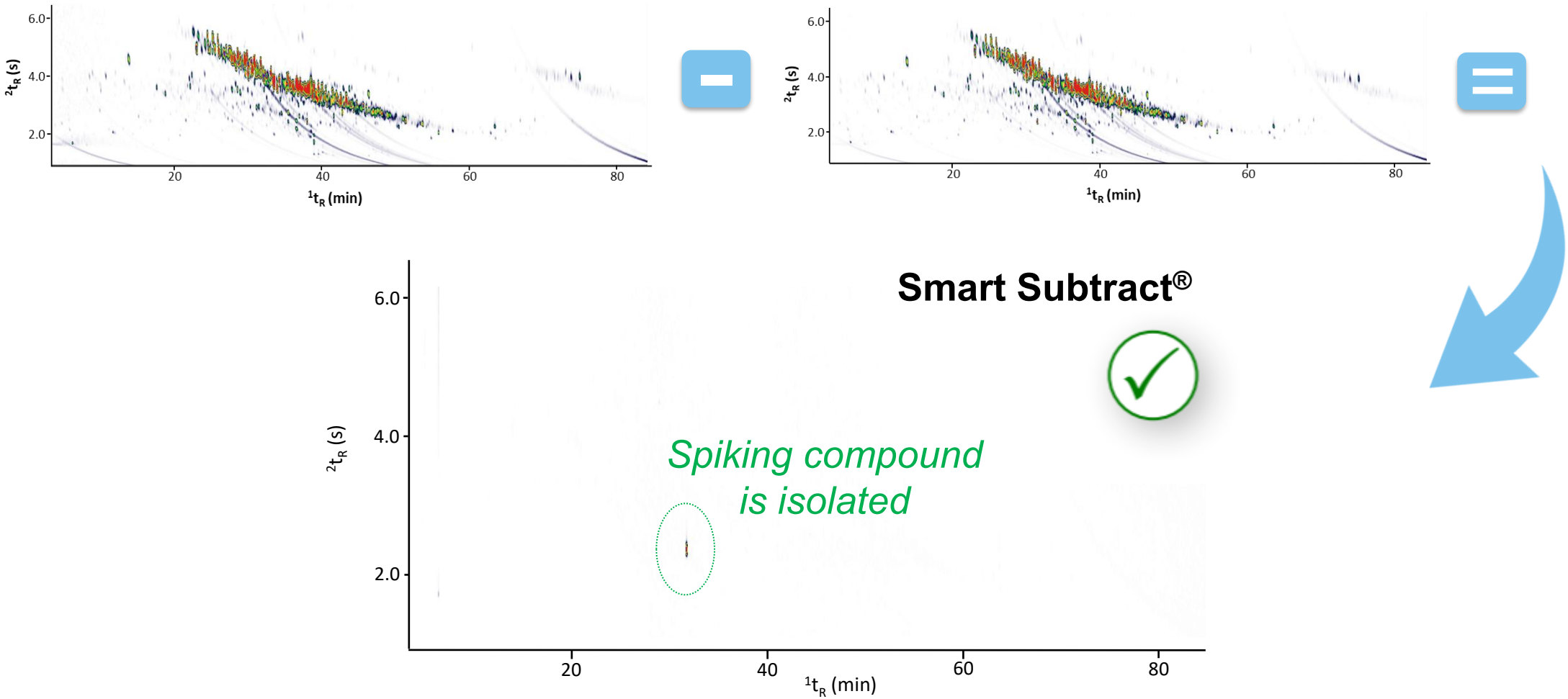


Regular subtraction



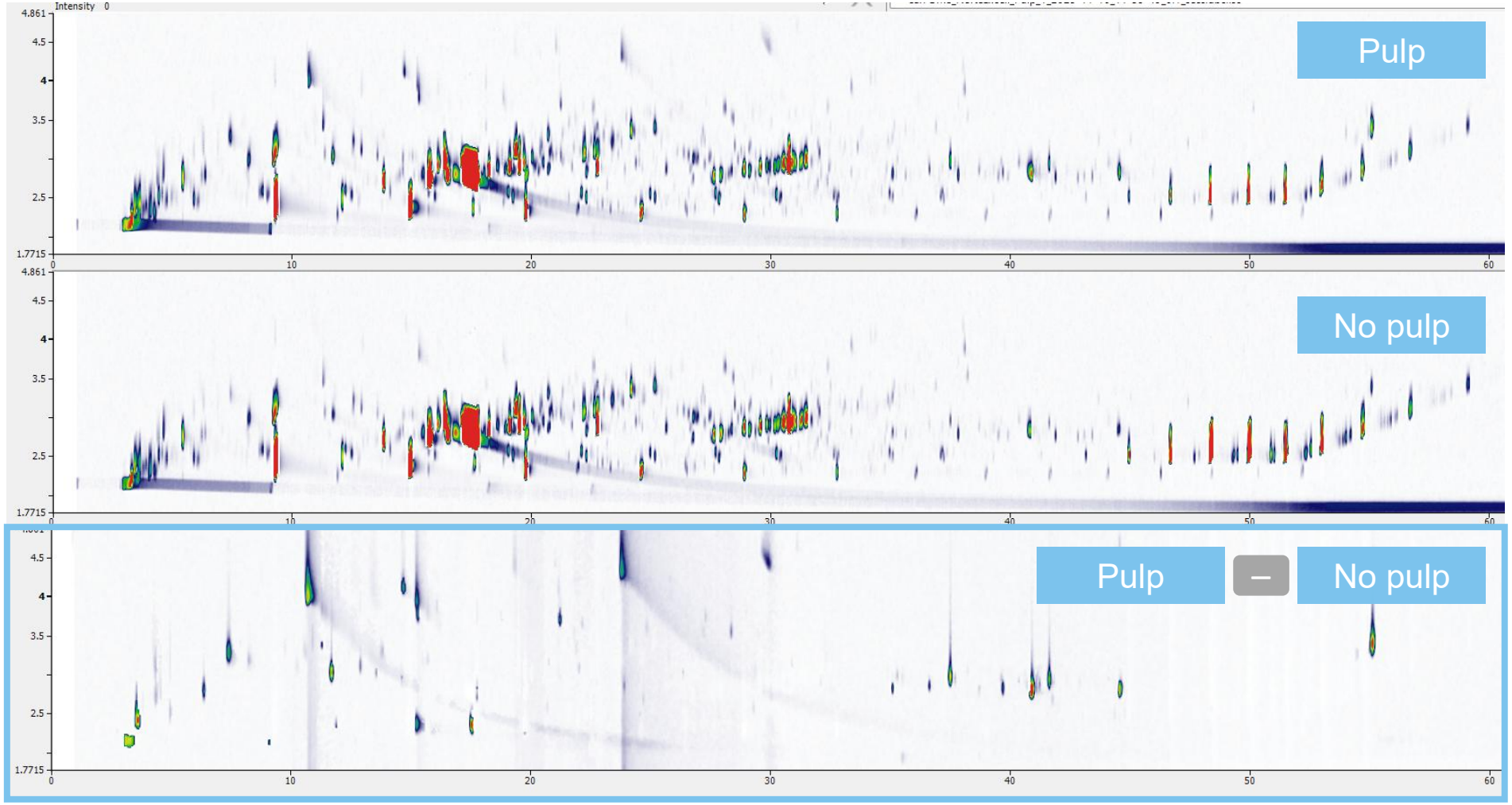
Small differences in intense peaks dominate the chromatogram

Comparison of GC×GC chromatograms



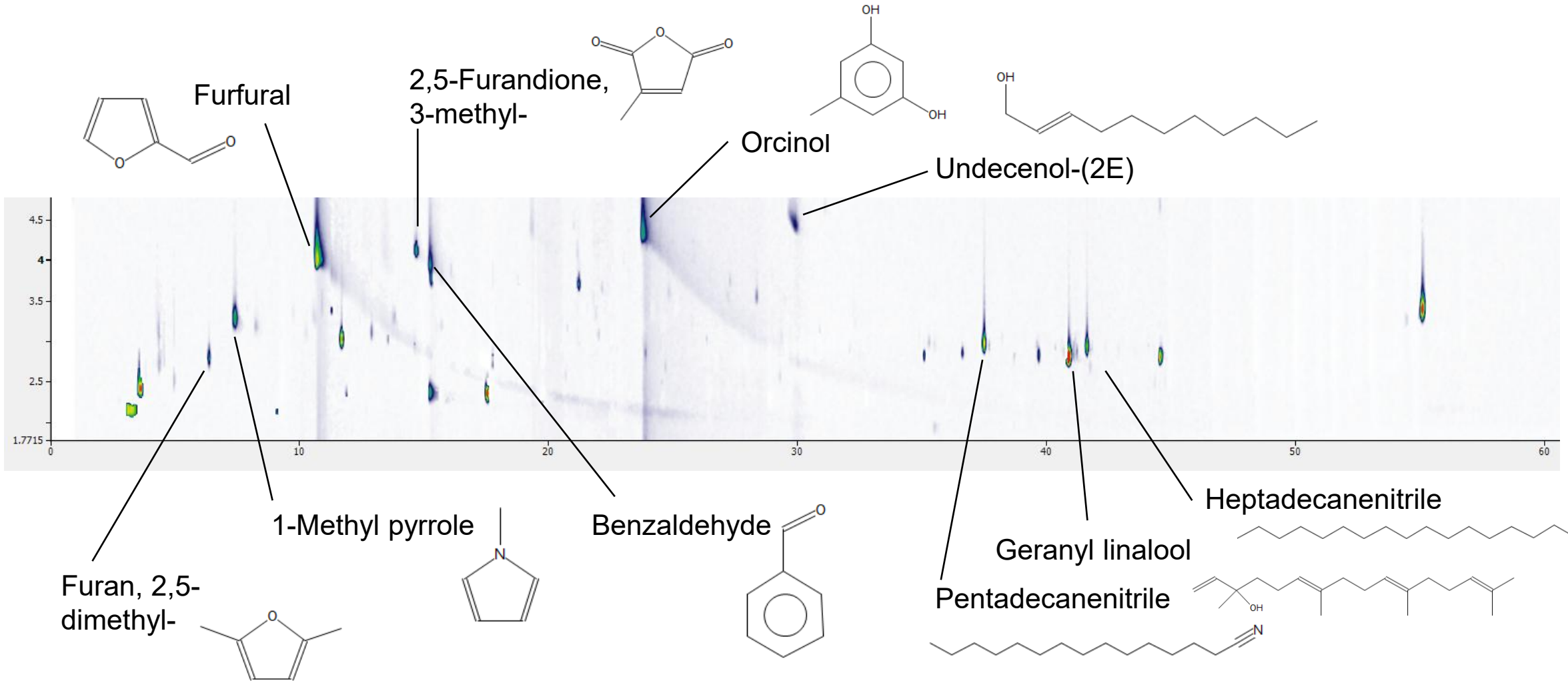
Comparison of orange juice

Pulp vs No pulp



Comparison of orange juice

Smart Subtract: ‘Pulp’ minus ‘no pulp’

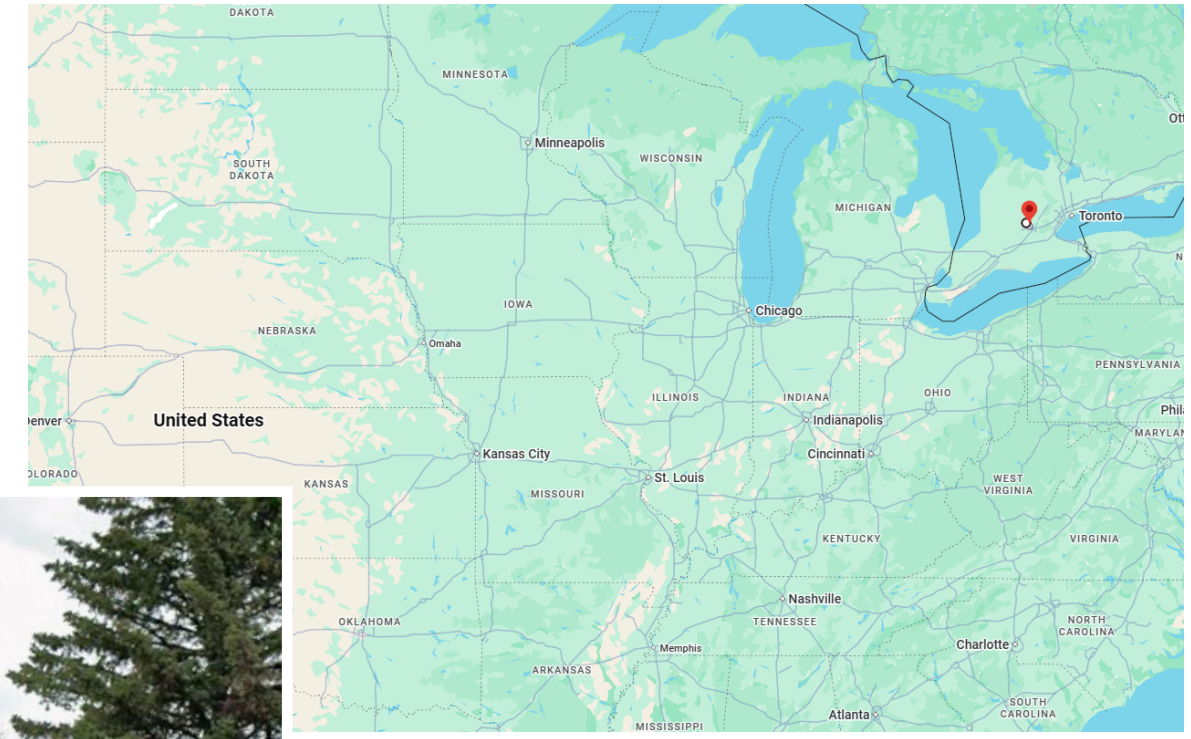


Summary

- GC–O is an indispensable tool in sensory evaluation, bridging the gap between chemical analyses and the subtleties of human olfaction.
- Trap-based enrichment boosts sensitivity to aid detection of trace-level odourants.
- GC×GC effectively resolves co-elutions, improving confidence in the identification of the compound(s) responsible for a perceived odour.
- GC×GC–(O)–TOF MS combined with smart software enabled comprehensive profiling of citrus volatiles, providing insights that help link chemistry with sensory evaluation

We’re moving!

Stay tuned for more info



New site in **Kitchener, Ontario** being kitted out with our full product portfolio

Thanks for listening! Any questions?

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