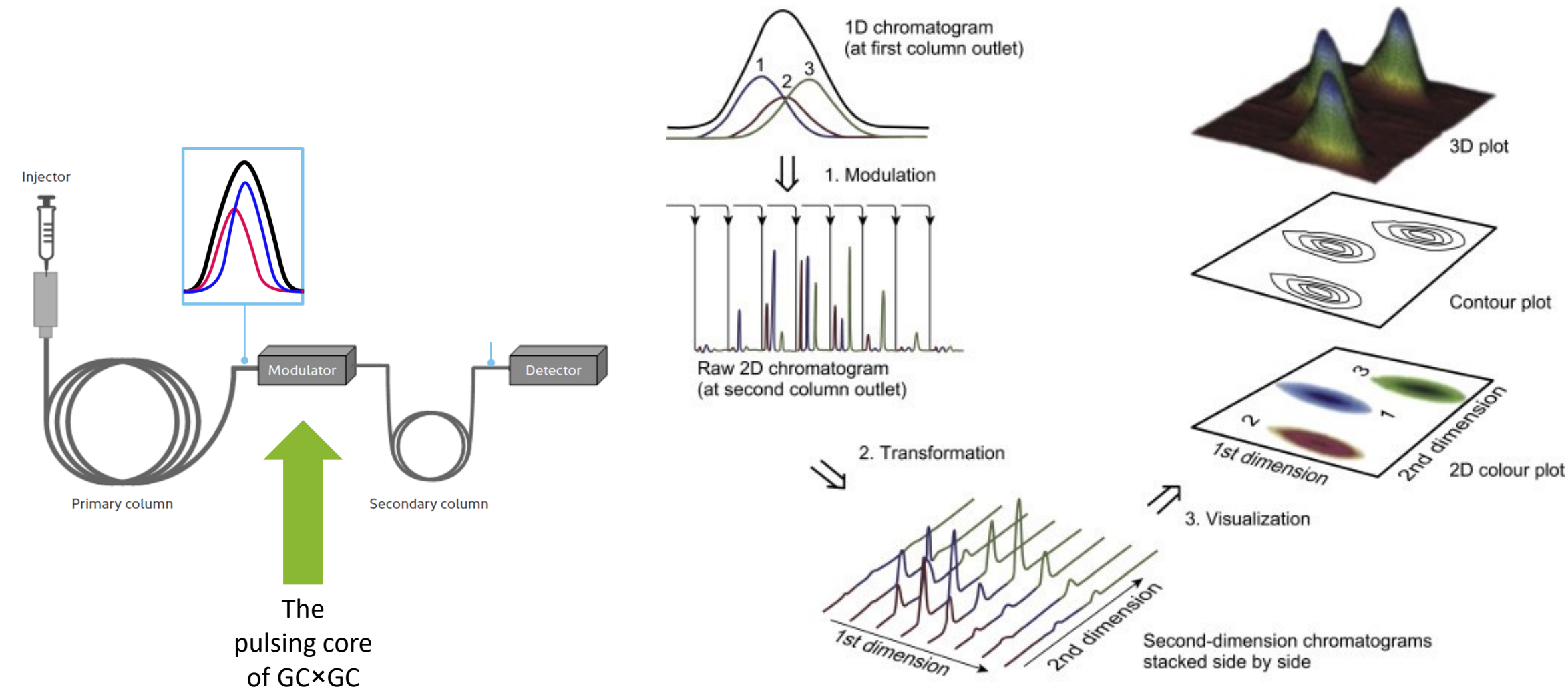


GC×GC, a powerful tool to unravel sample identity

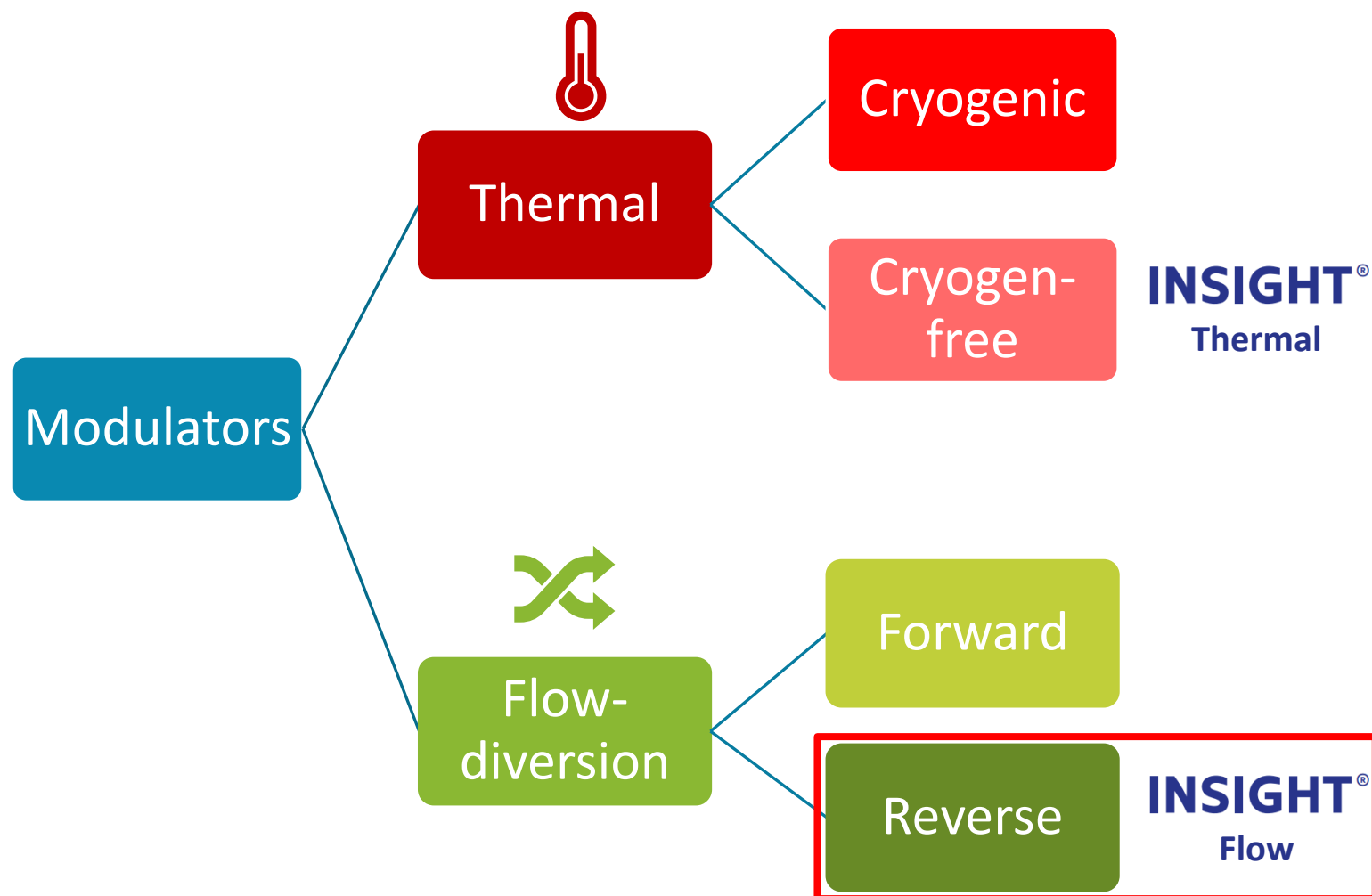
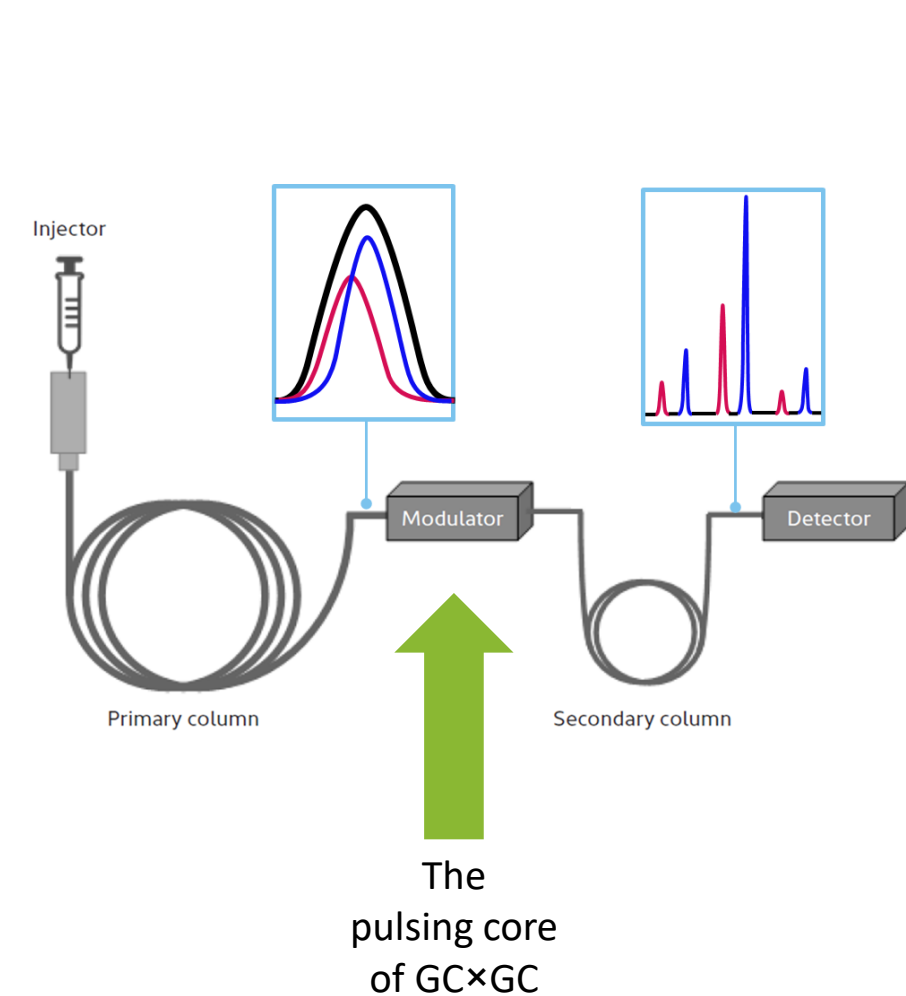
Damien Eggermont



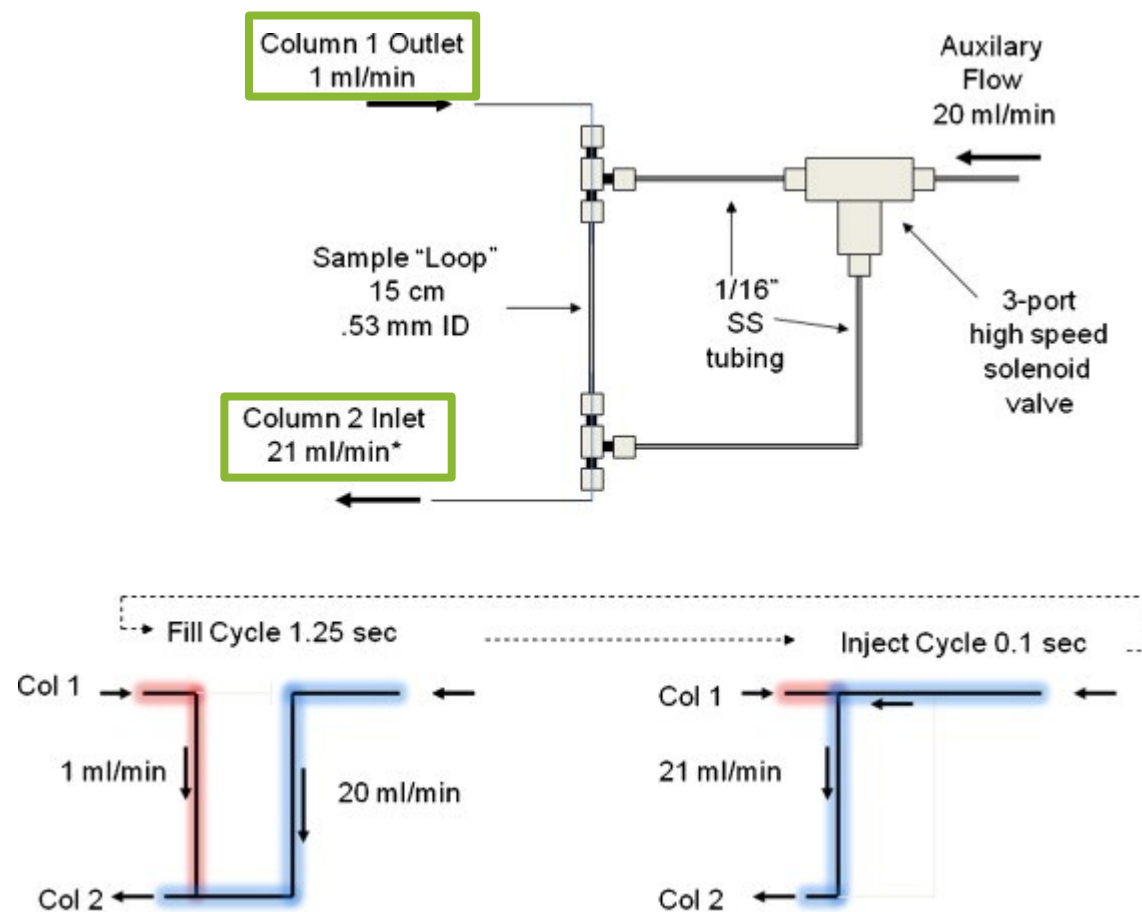
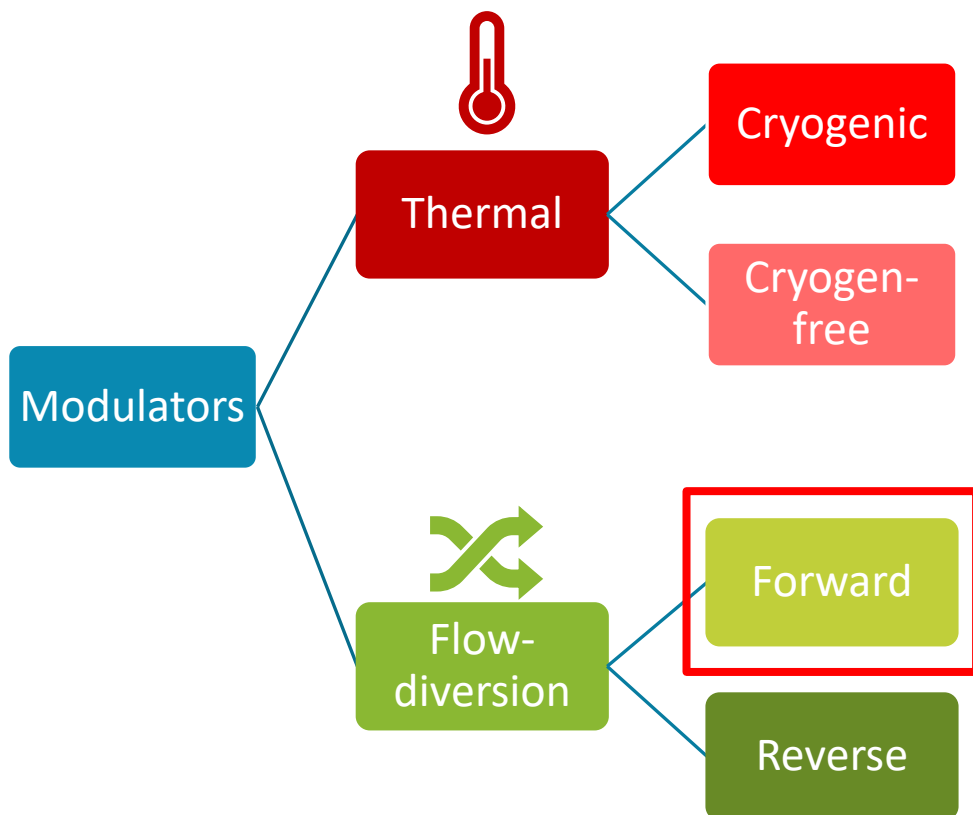
Introduction: Data visualisation



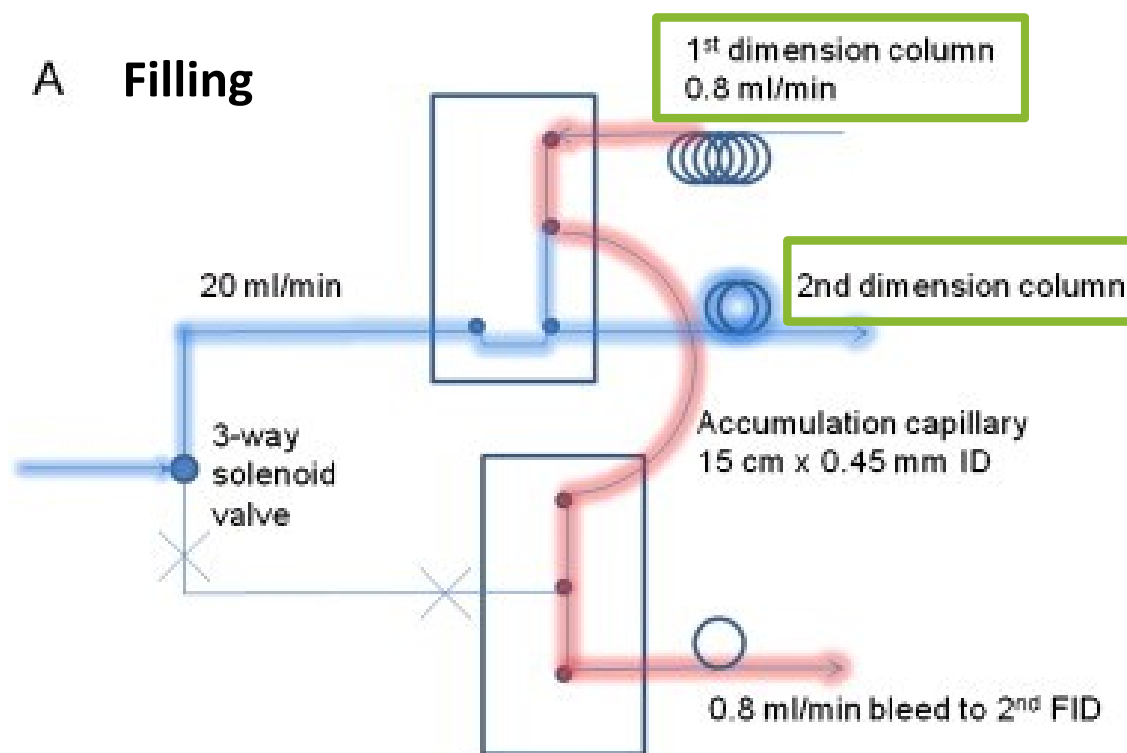
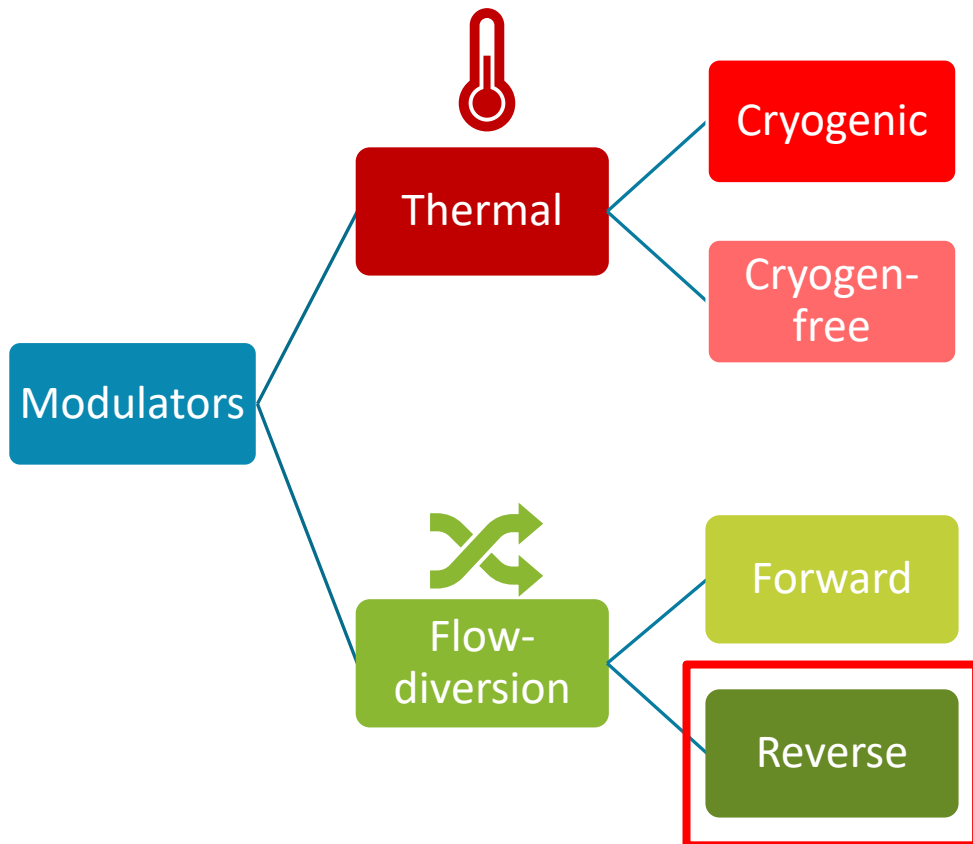
Introduction: Modulators



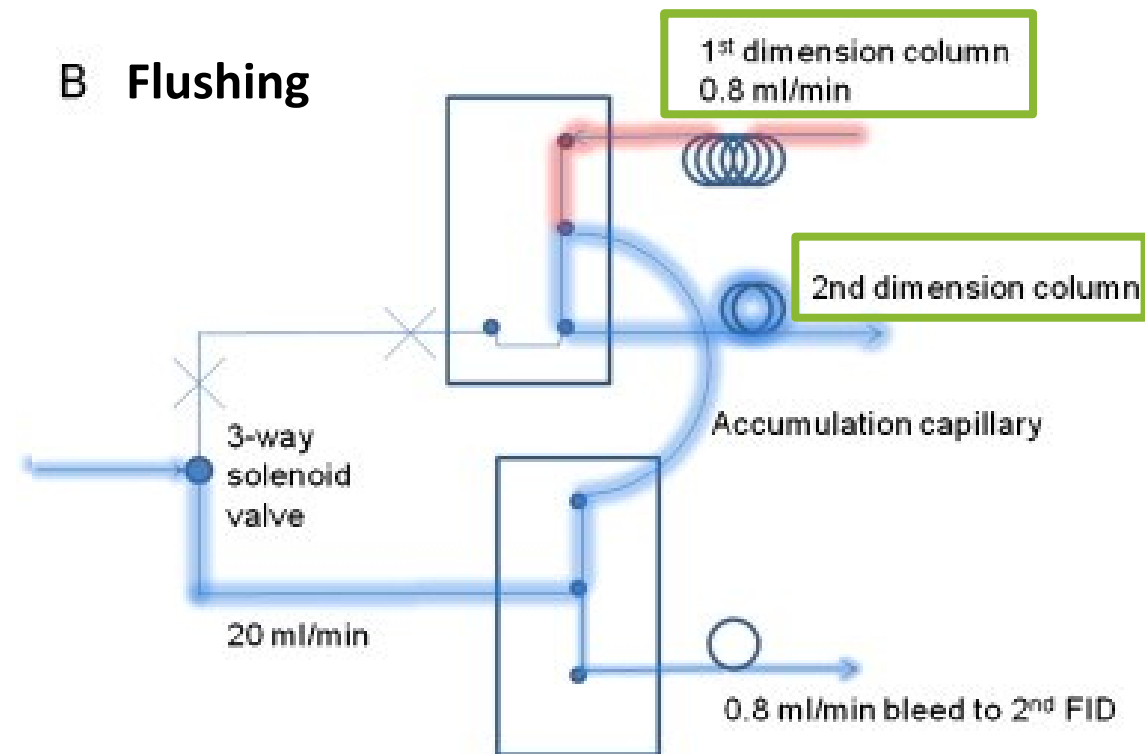
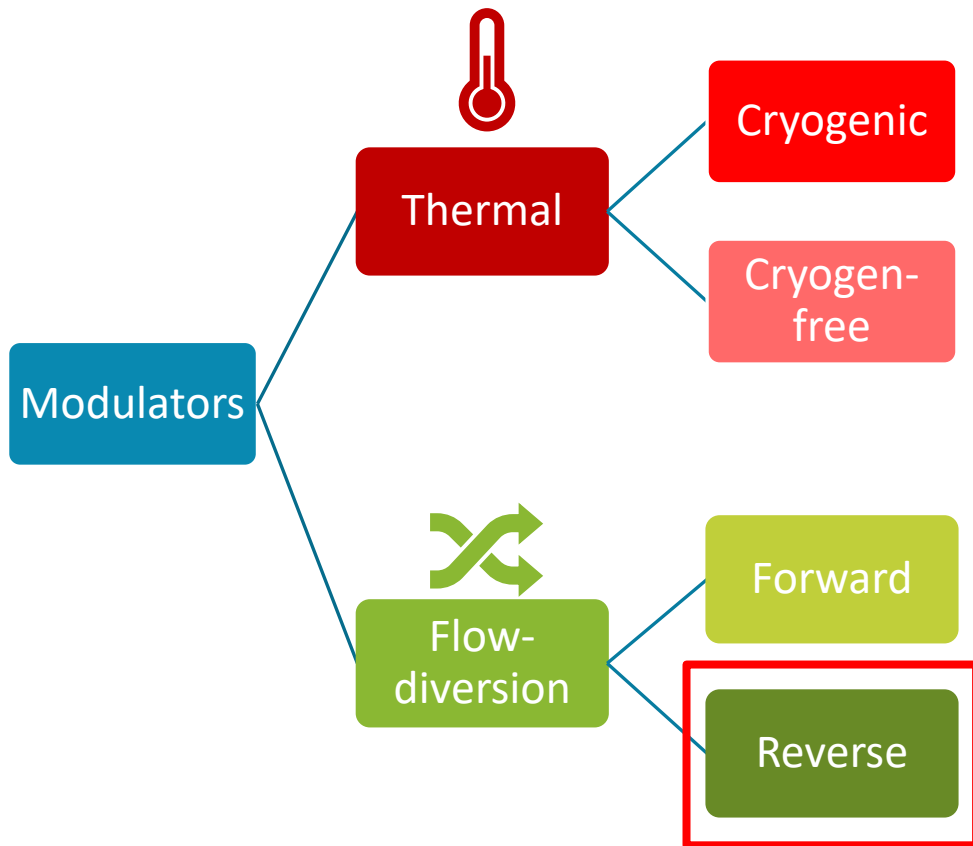
Introduction: Flow Modulators



Introduction: Flow Modulators

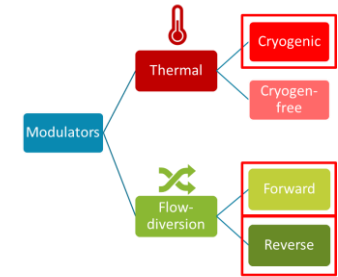
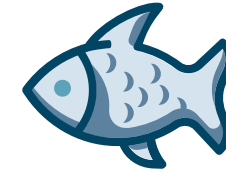


Introduction: Flow Modulators

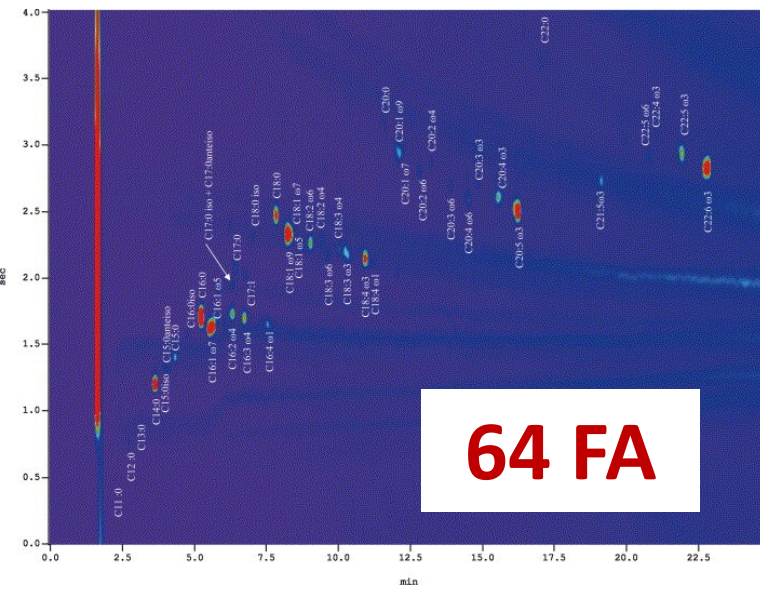


Introduction: Modulators

Menhaden oil fatty acid analysis FAMES derivatization

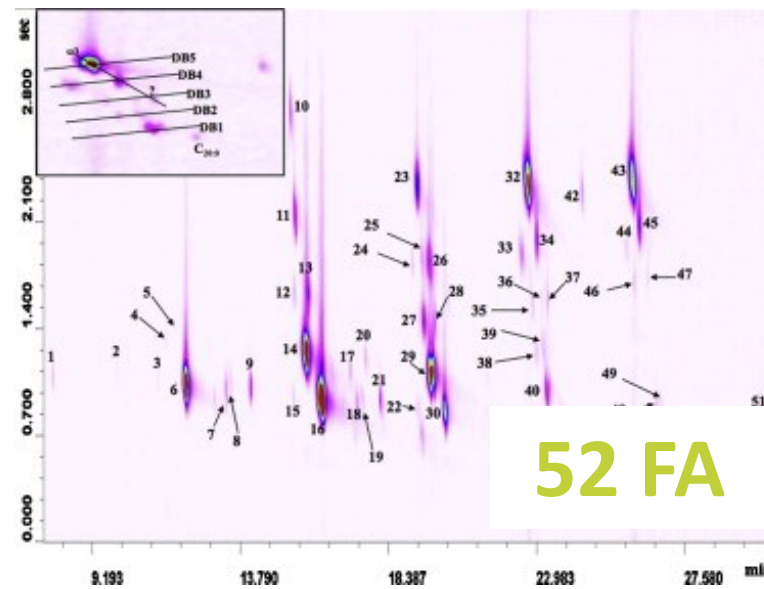


Cryogenic



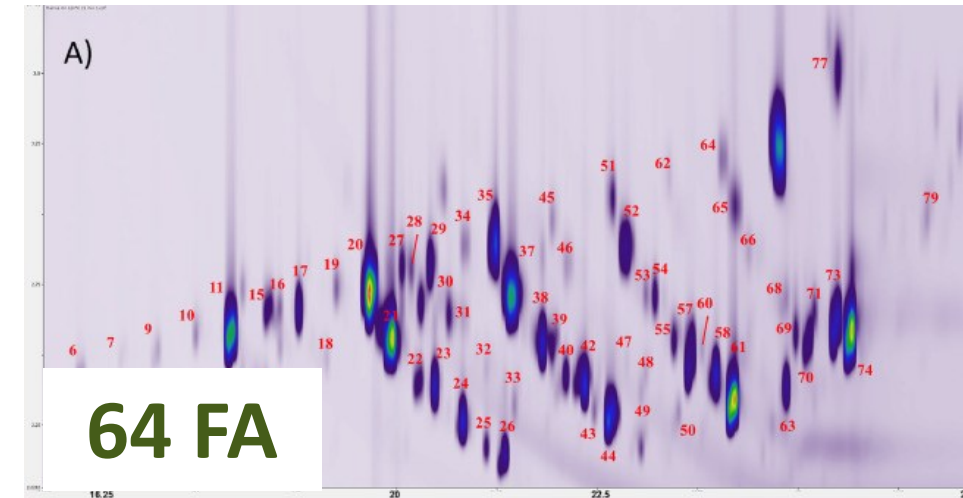
Mondello (2003)

Forward-FF



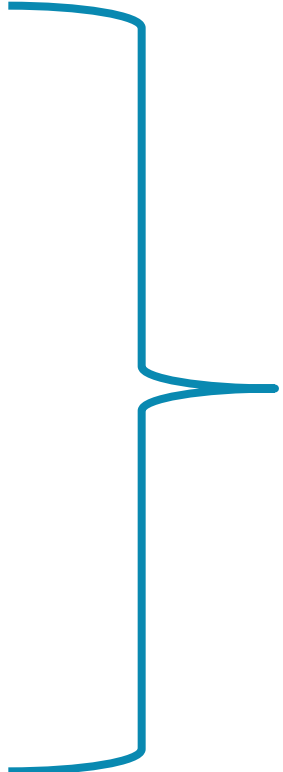
Tranchida (2012)

Reverse-FF



Fina et al. (2022)

Advantages of GC×GC

- 
- Better Representativity
 - Solving Co-elution
 - Supporting Identification
 - Higher Throughput
- Defining a fingerprint
 - Multi response analysis

Advantages of GC×GC

- Better Representativity

- Solving Co-elution

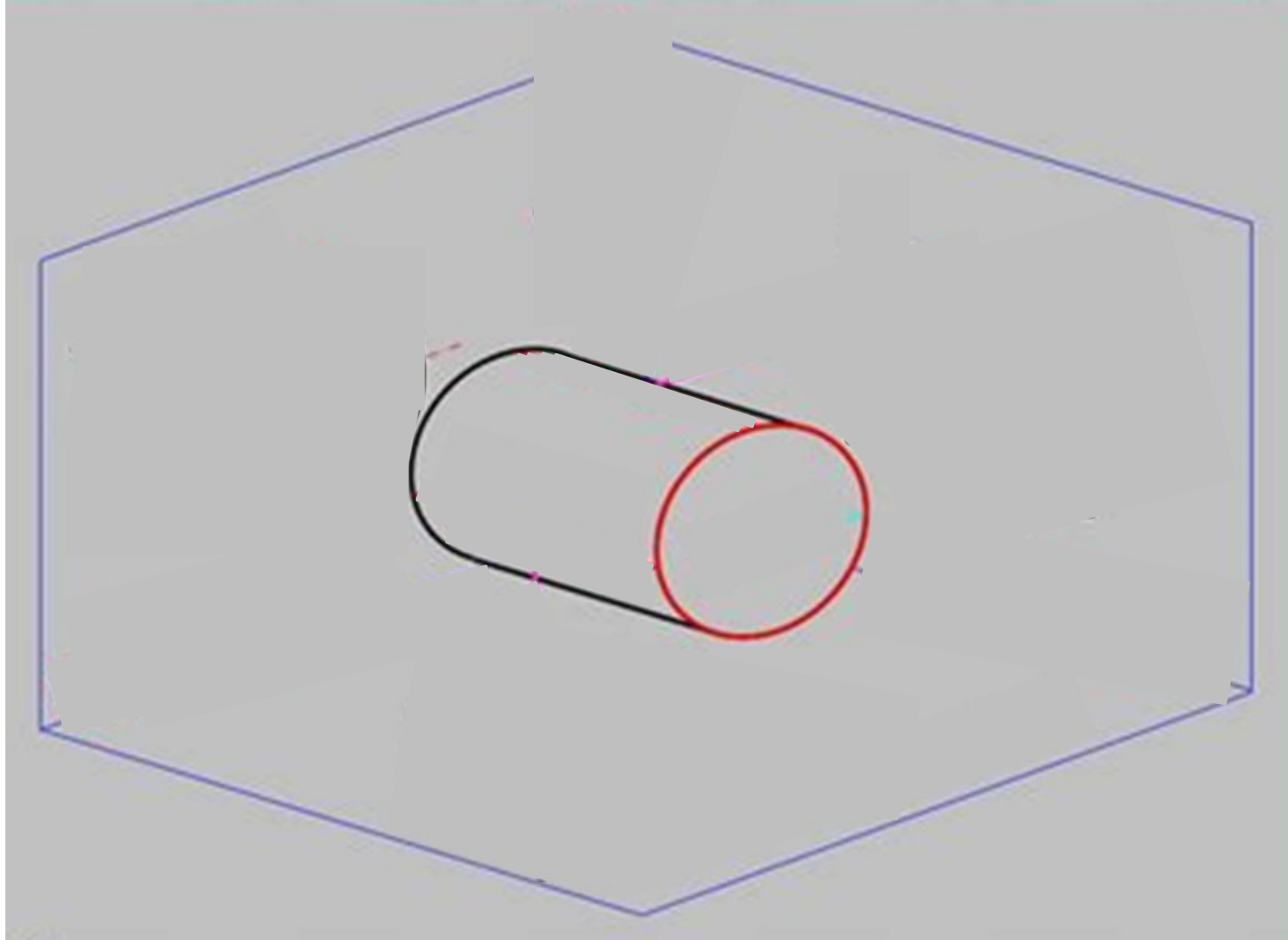
- Supporting Identification

- Higher Throughput

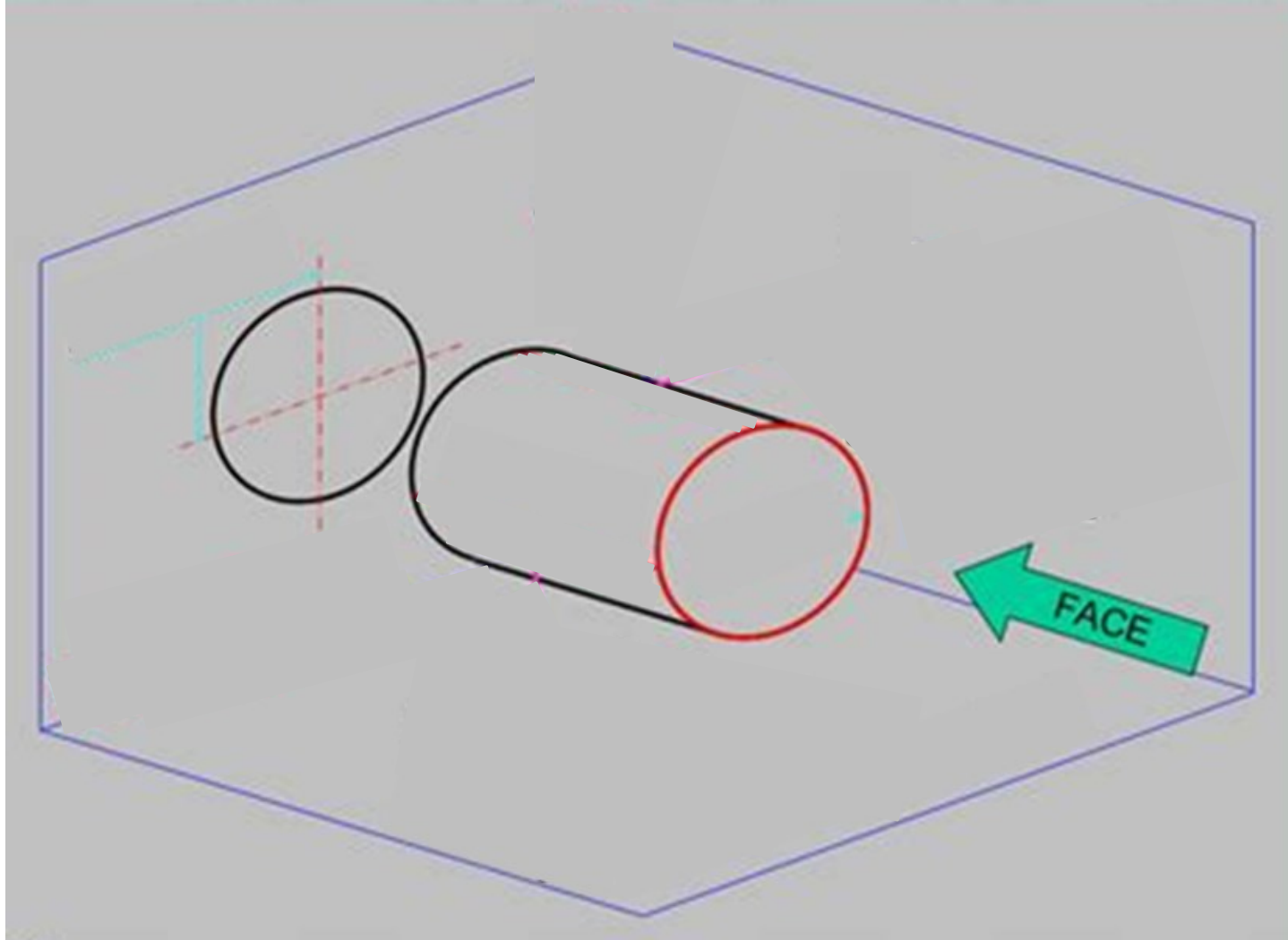
- Defining a fingerprint

- Multi response analysis

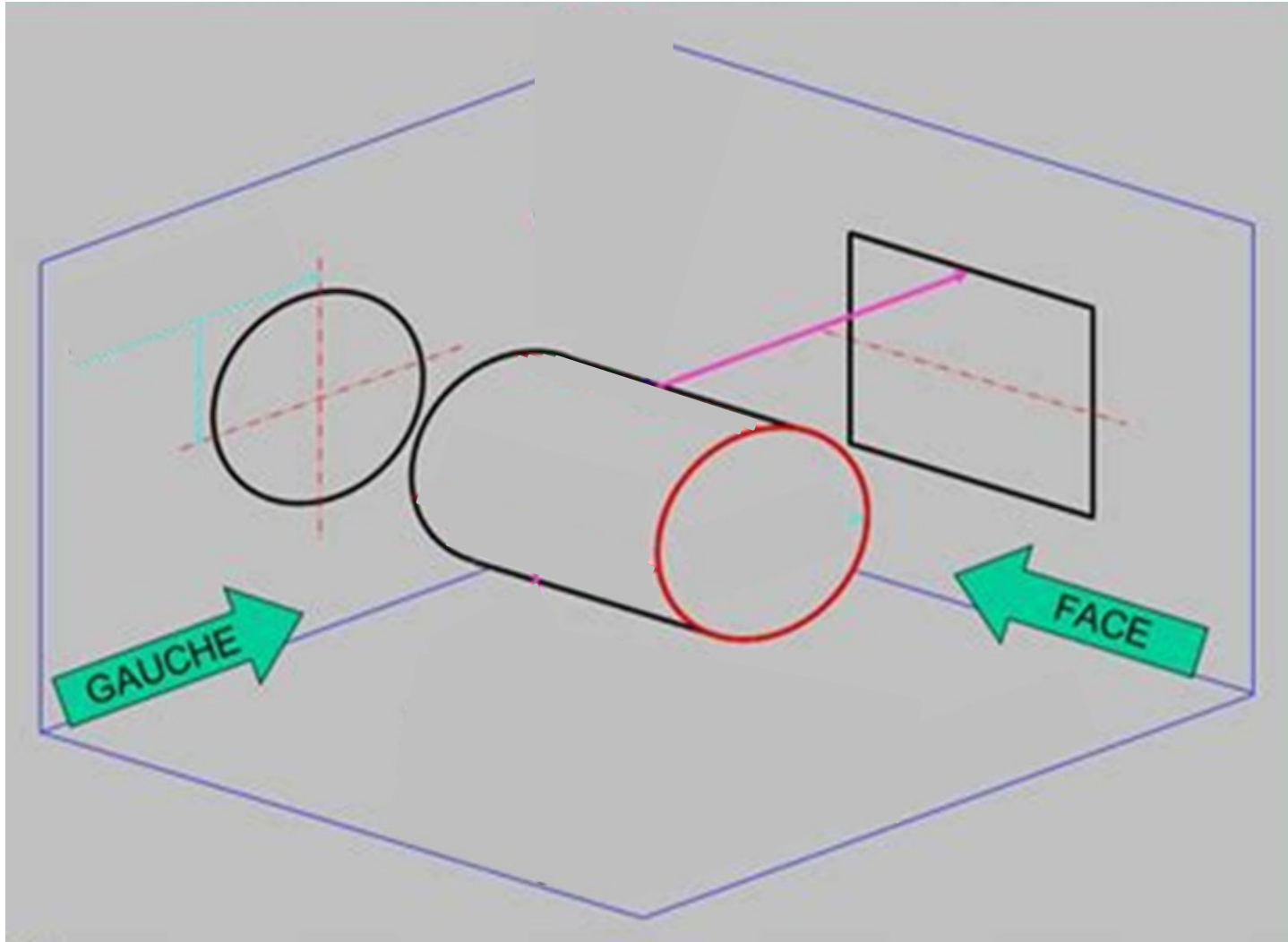
GC×GC: Better Representativity



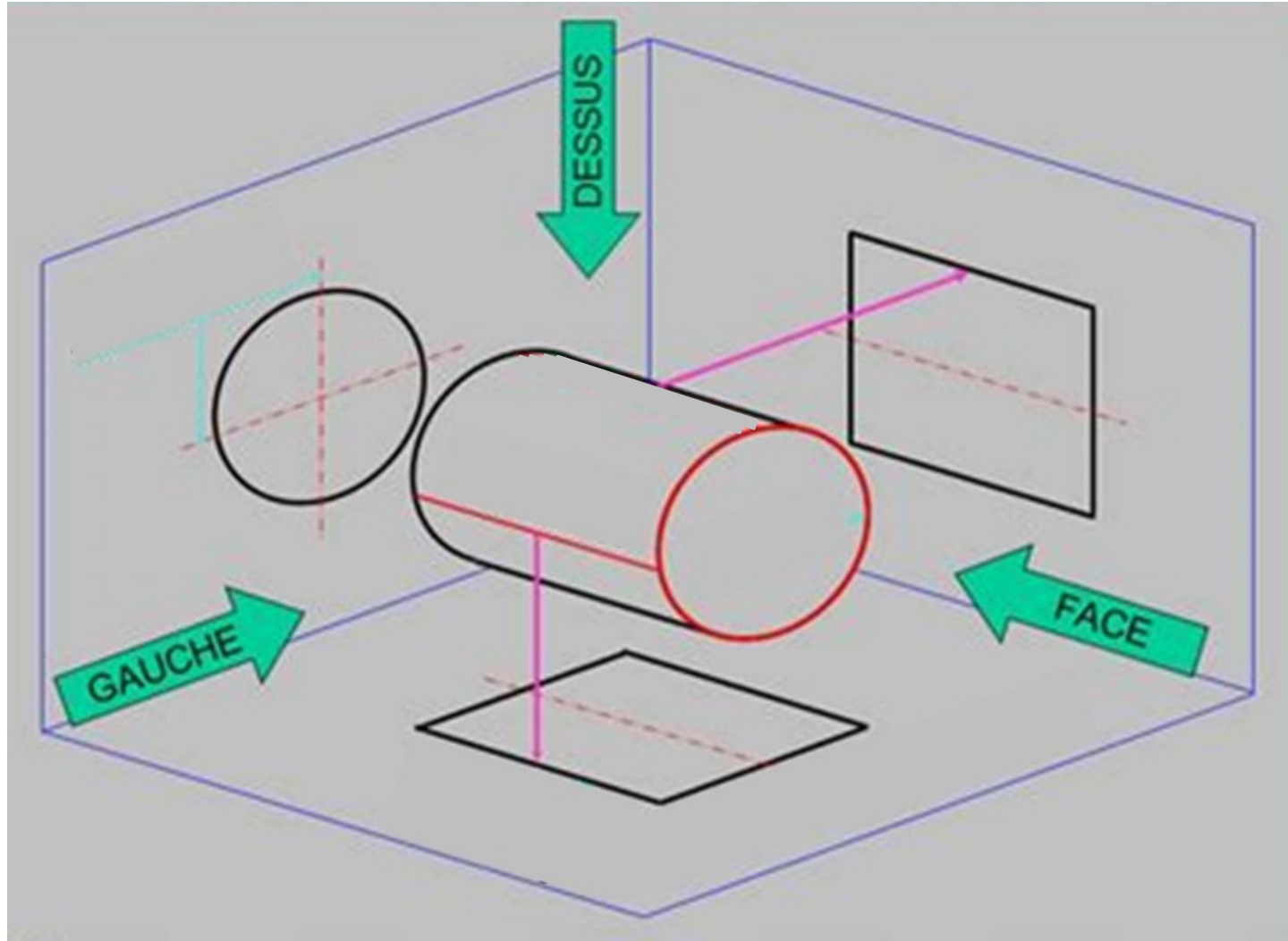
GC×GC: Better Representativity



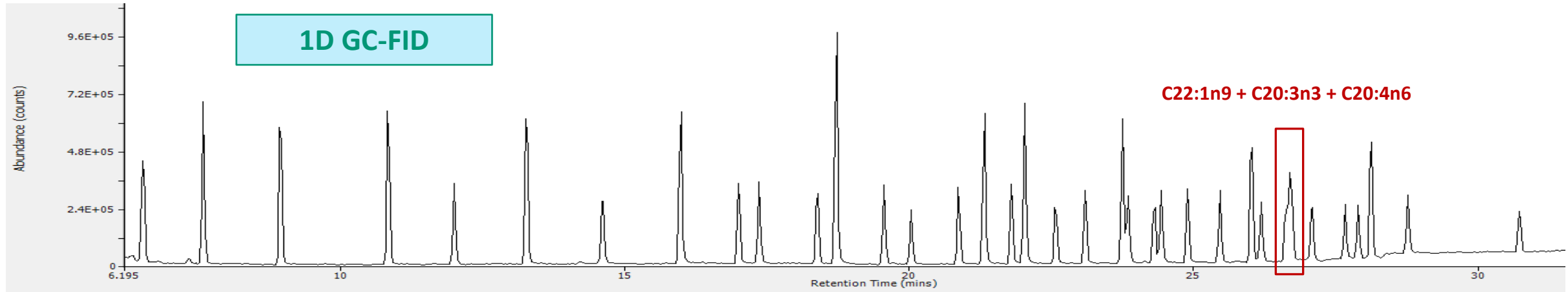
GC×GC: Better Representativity



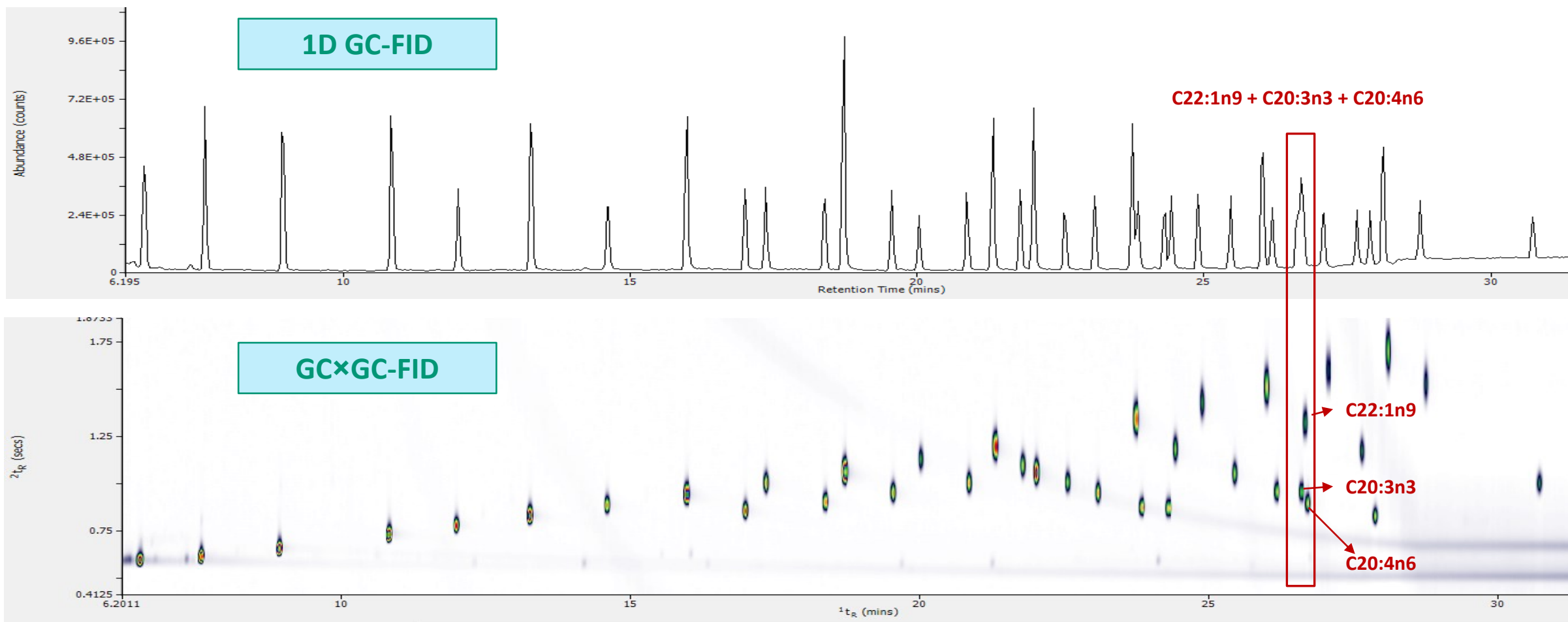
GC×GC: Better Representativity



GC×GC: Solving Co-elution



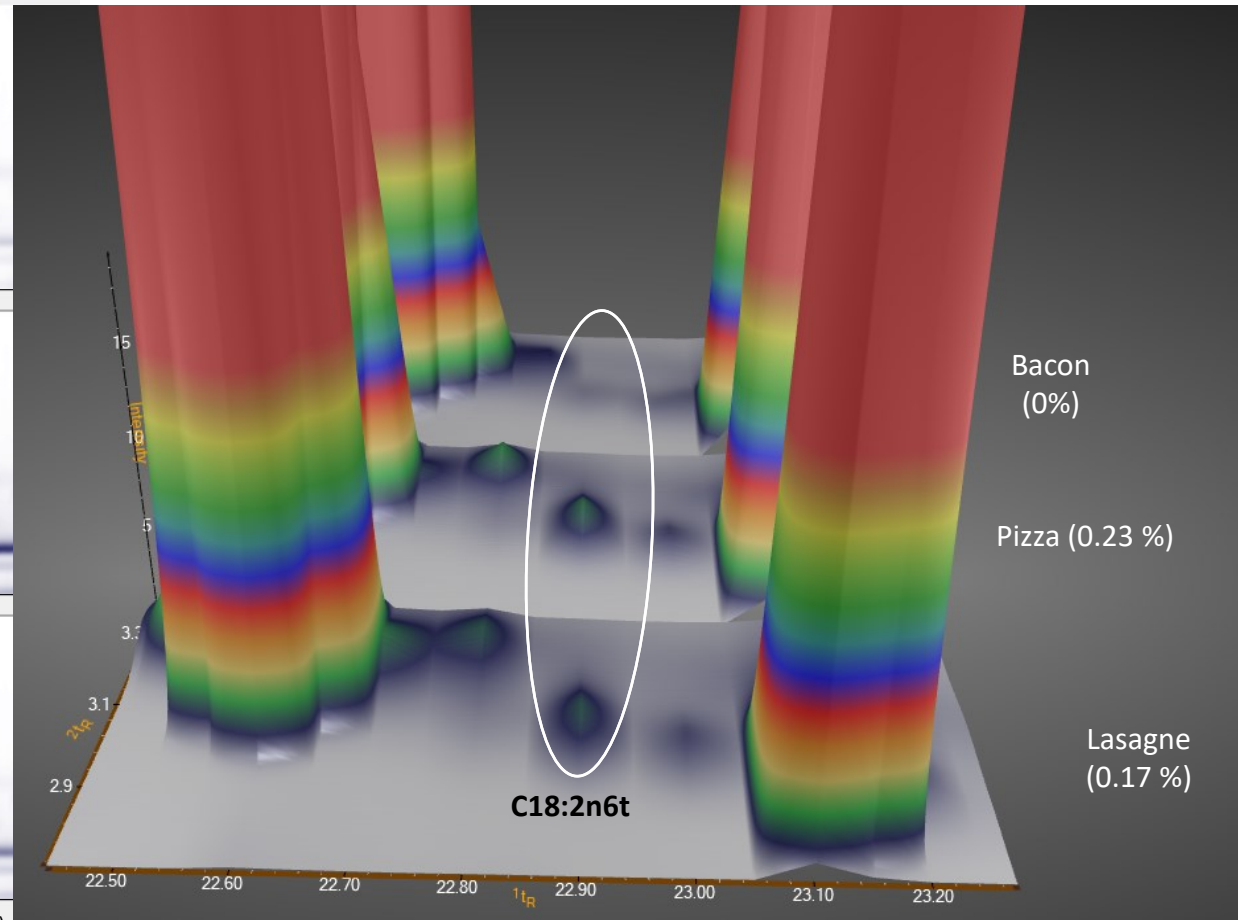
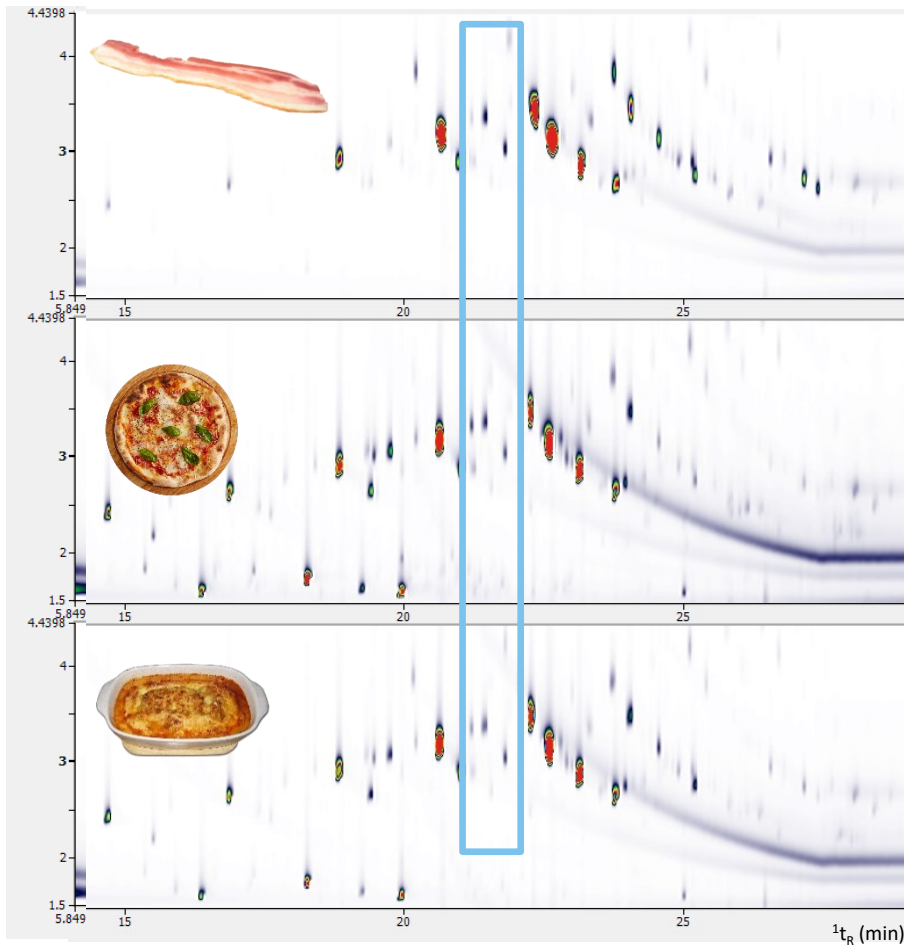
GC×GC: Solving Co-elution



GC×GC: Solving Co-elution

GC×GC-FID

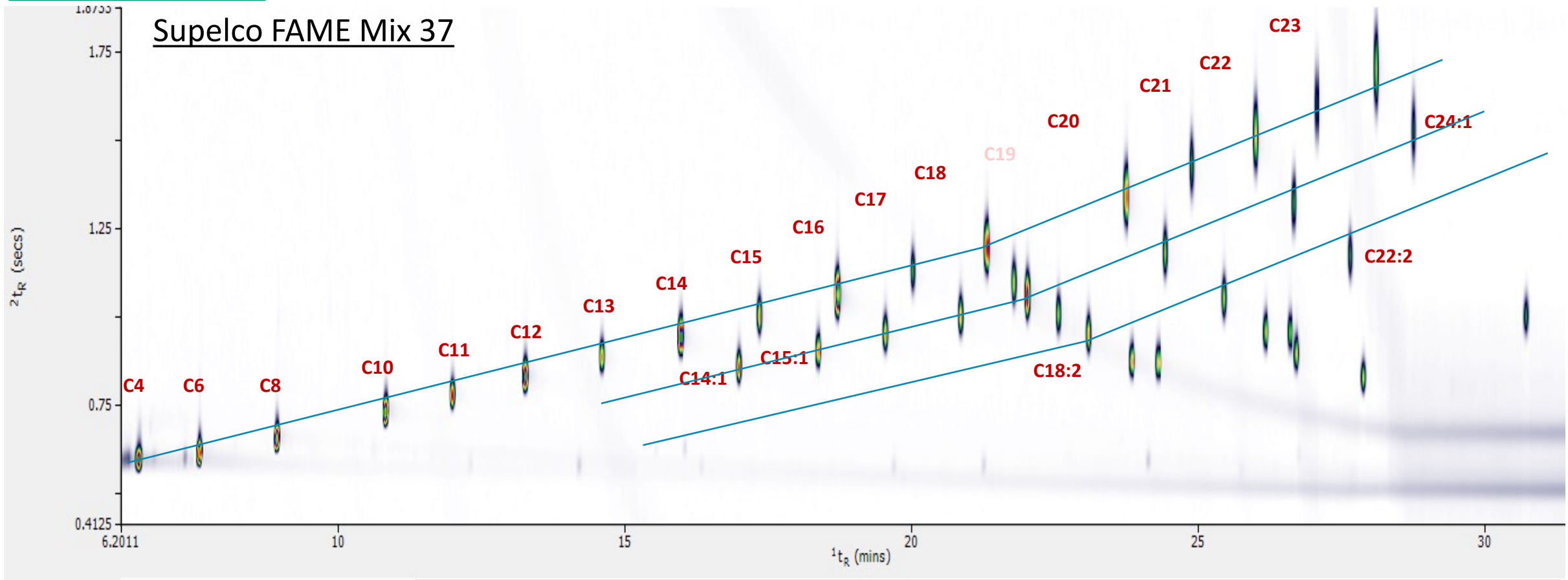
Food fatty acid analysis



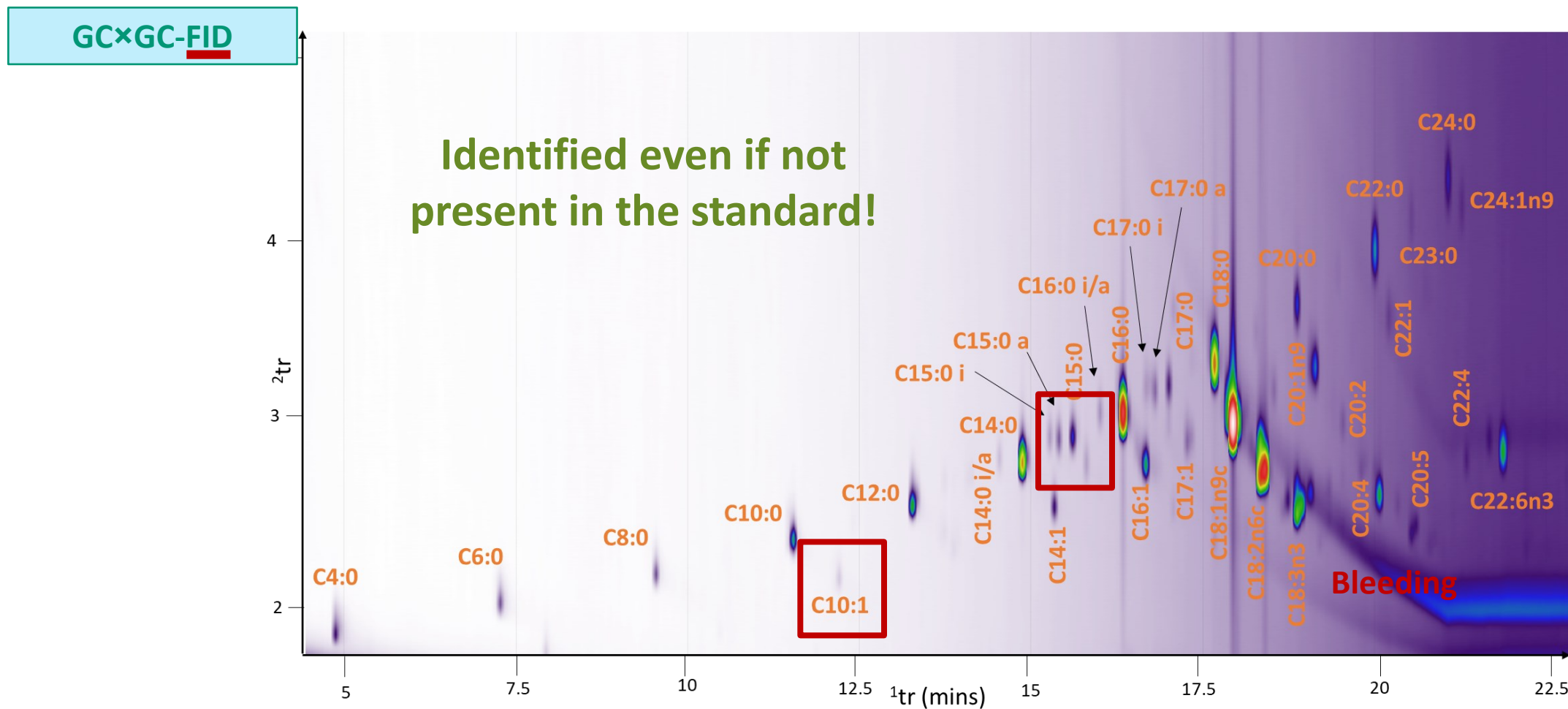
GC×GC: Supporting Identification

GC×GC-FID

Supelco FAME Mix 37



GC×GC: Supporting Identification

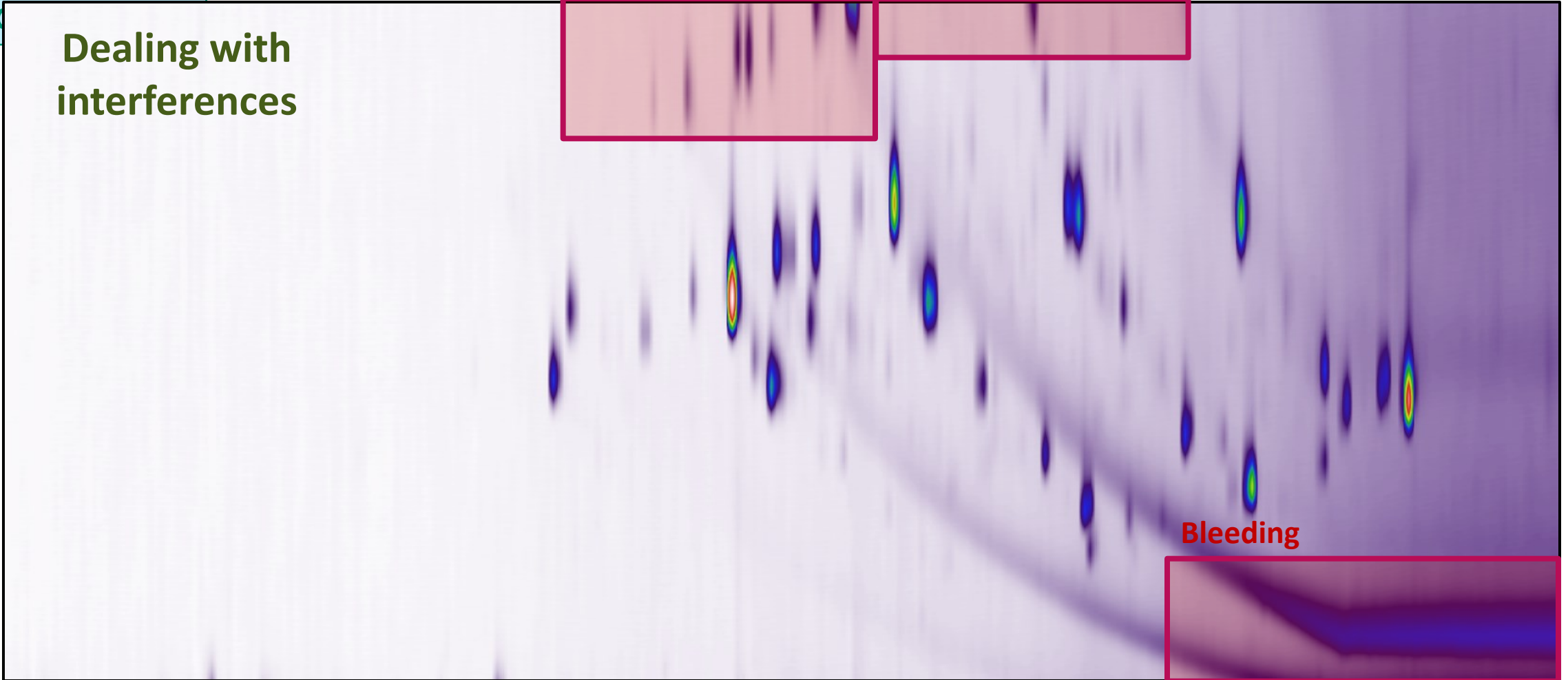


GC×GC: Supporting Identification

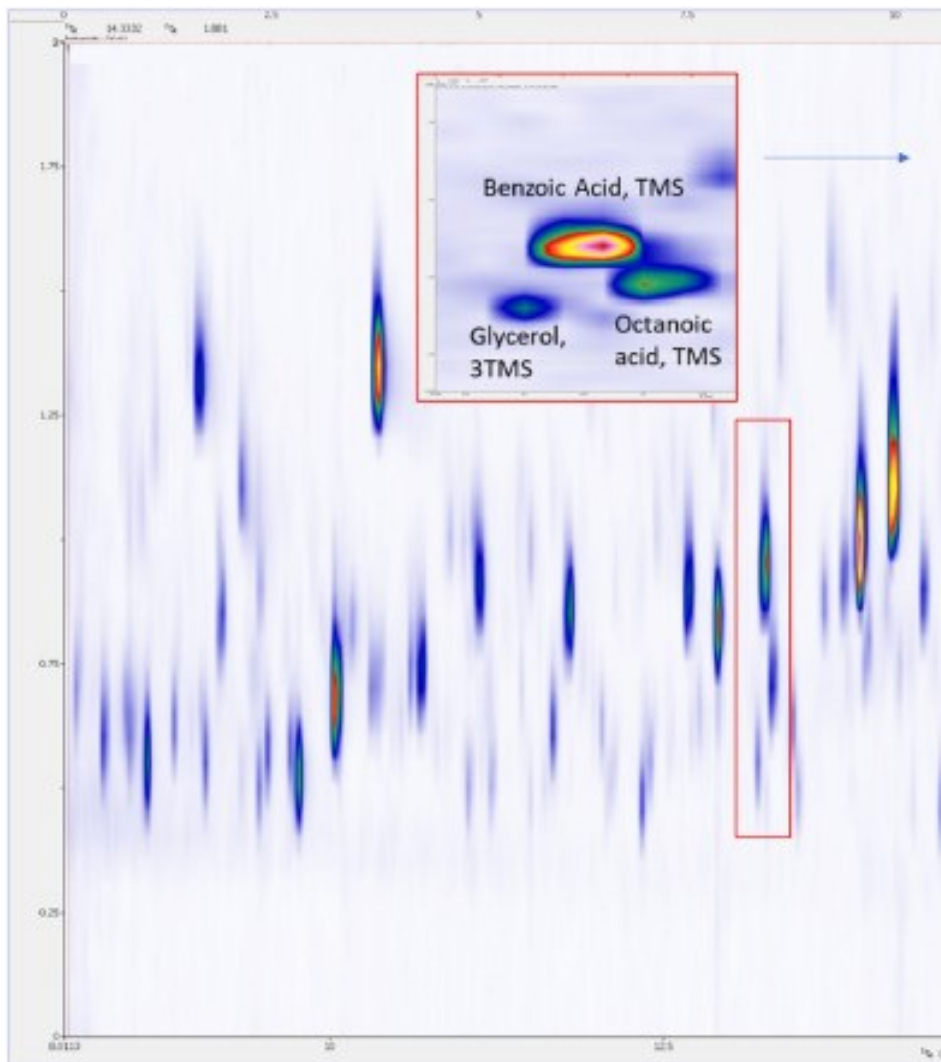
Dealing with
interferences

Alkanes

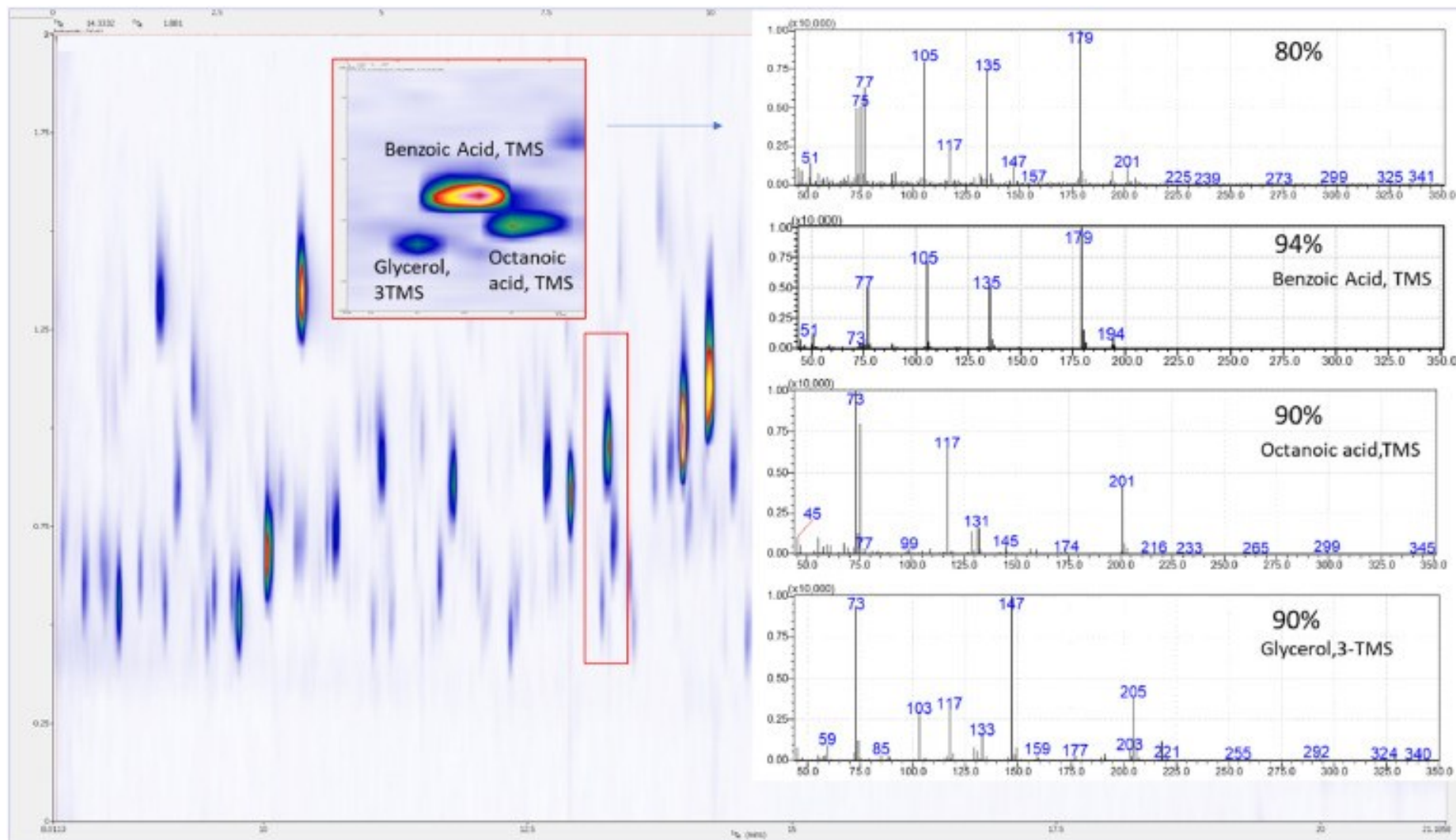
Bleeding



GC×GC: Supporting Identification



GC×GC: Supporting Identification



1D Peak

2D Peaks



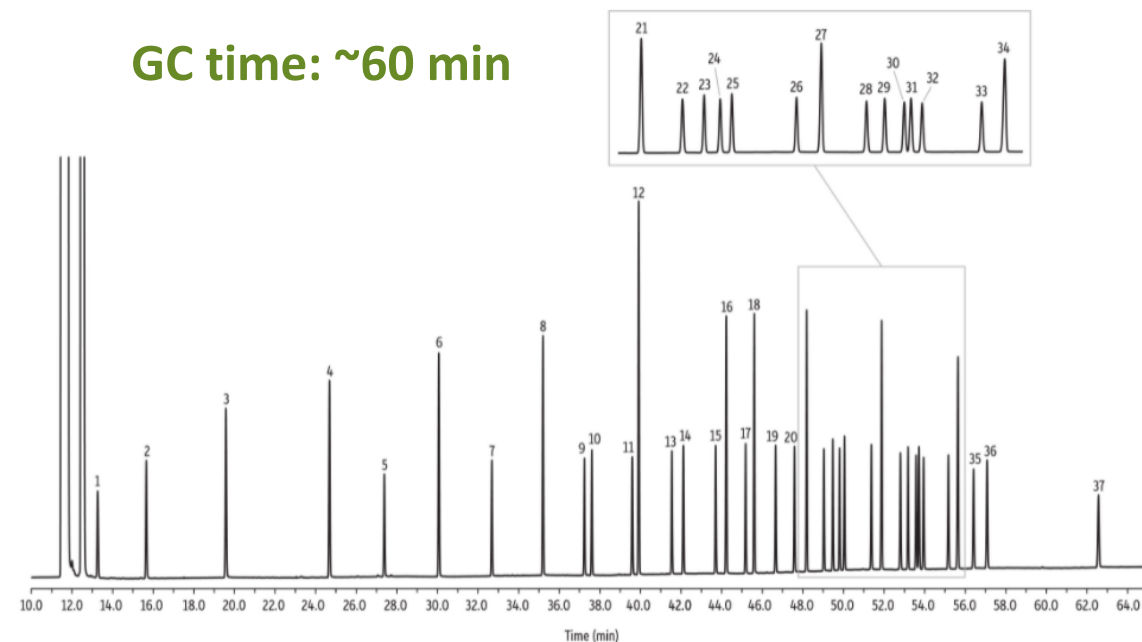
GC×GC: Higher Throughput

Fatty acids analysis of fat and oil

Official Methods:

- AOAC official method 996.06
- AOCS official method Ce 1j-07

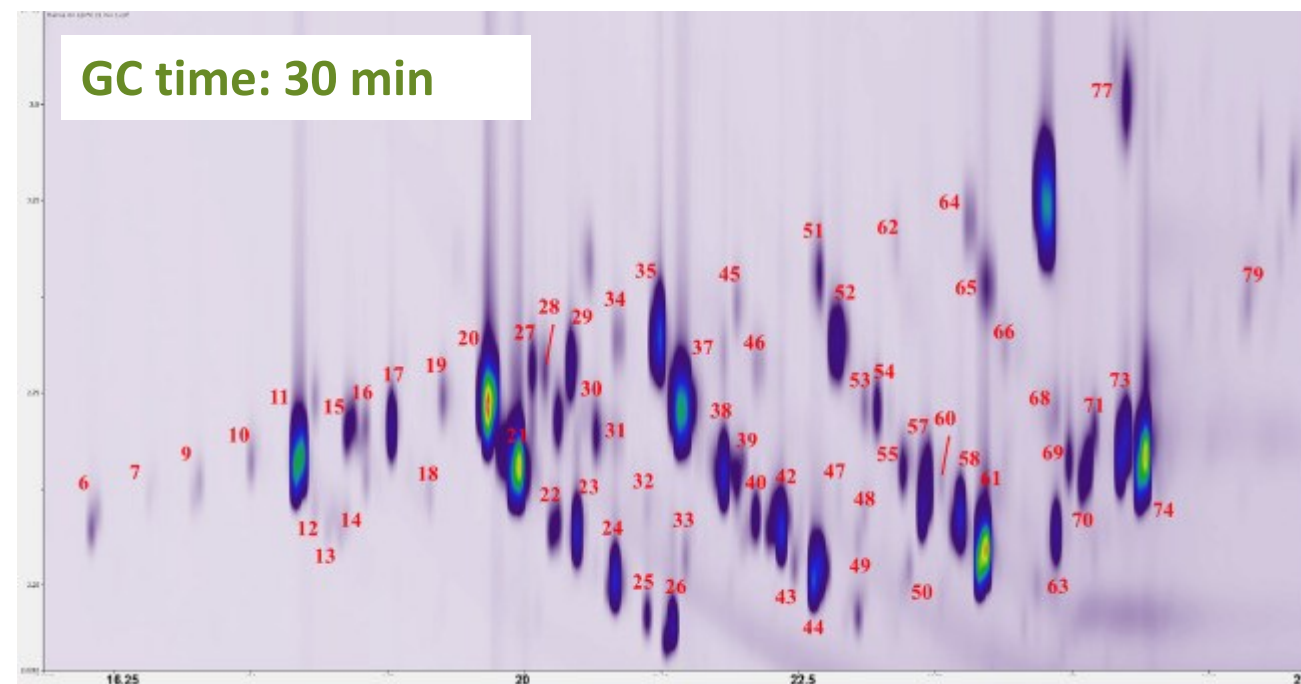
GC time: ~60 min



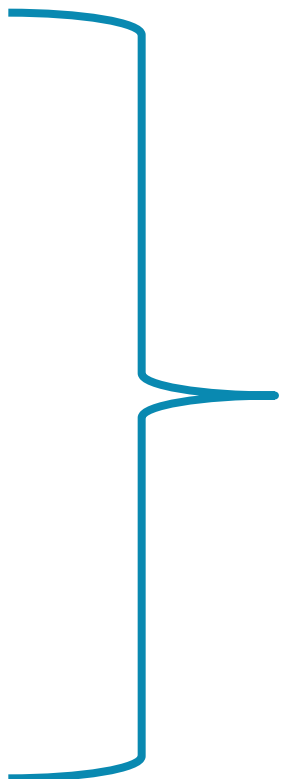
Developed GC×GC Methods

Similar performances than official methods!

GC time: 30 min



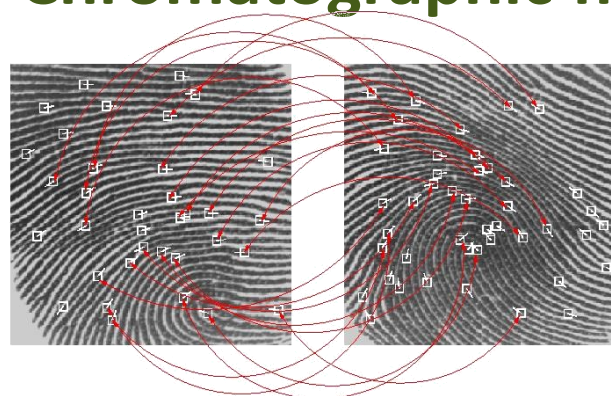
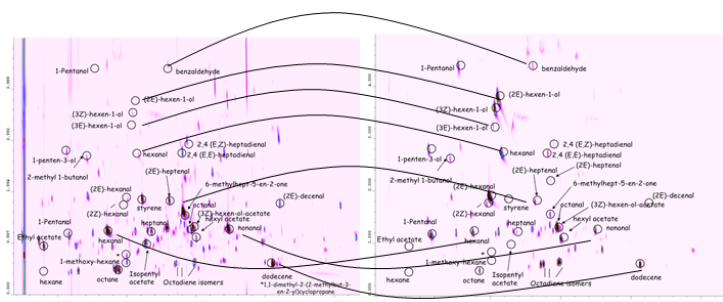
Advantages of GC×GC

- 
- Better Representativity
 - Solving Co-elution
 - Supporting Identification
 - Higher Throughput
- Defining a fingerprint
 - Multi response analysis

- Detailed analysis
- Compounds-centred
 - Qualitative
 - Quantitative

- High throughput analysis
- Extraction of relevant information

GC×GC Chromatographic fingerprint

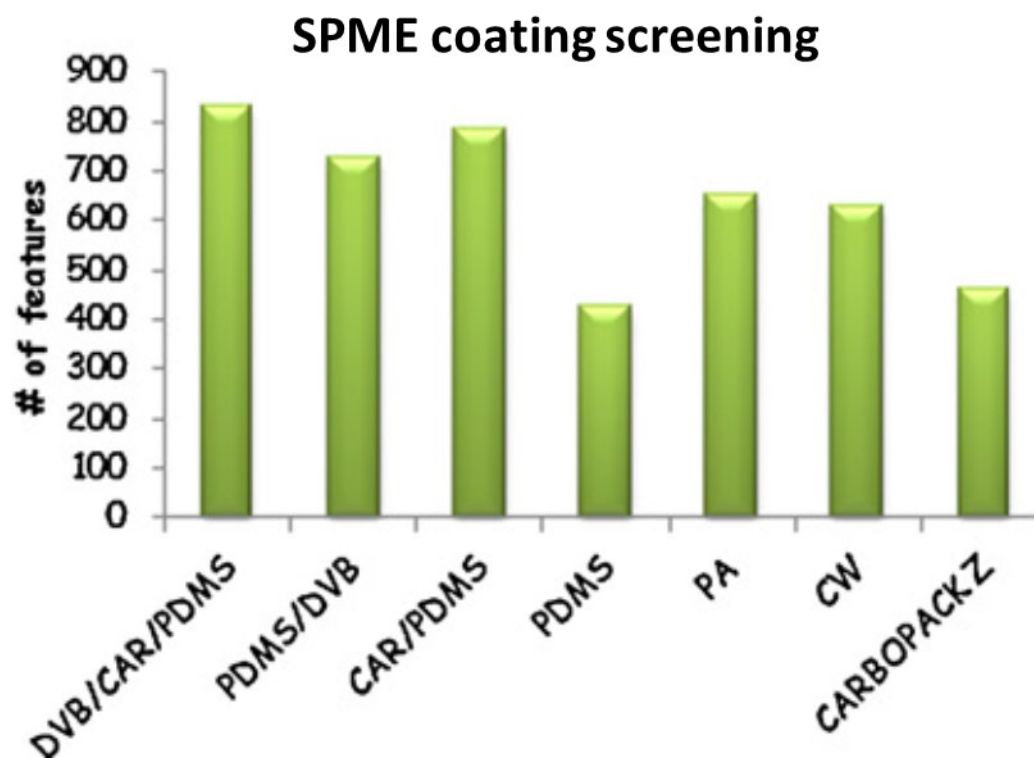


Both approaches available!
Multi-level information



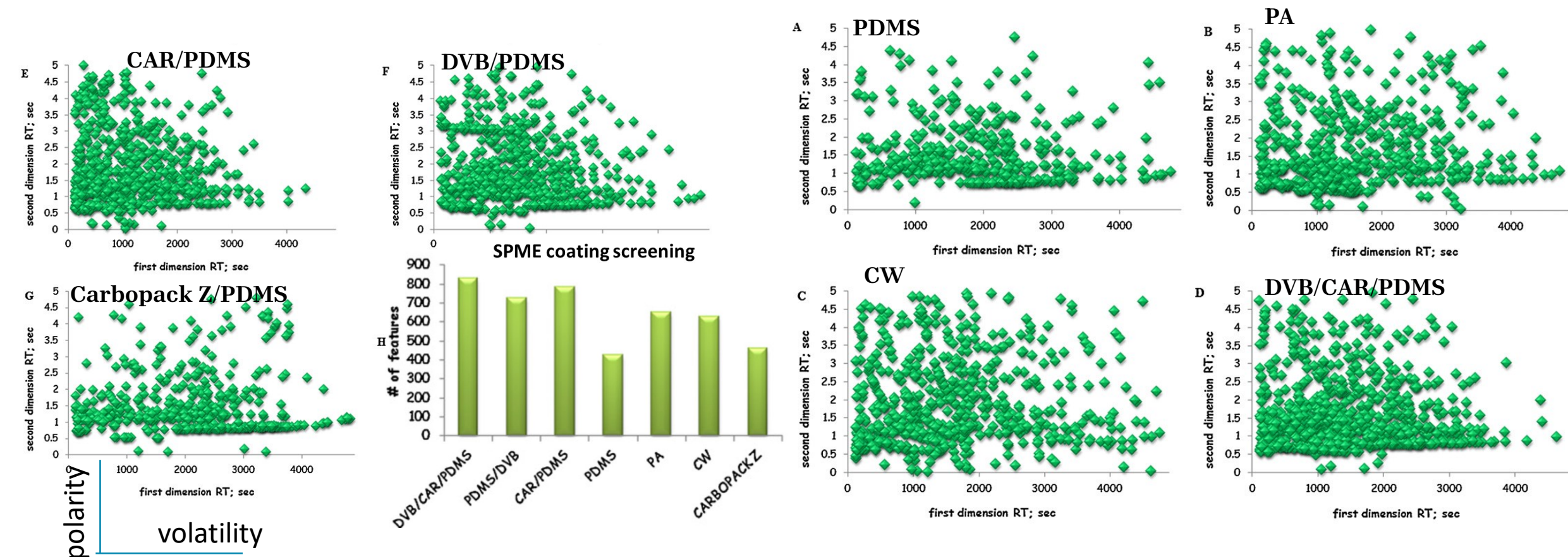
Chromatographic Fingerprint

Metabolites analysis optimisation



Chromatographic Fingerprint

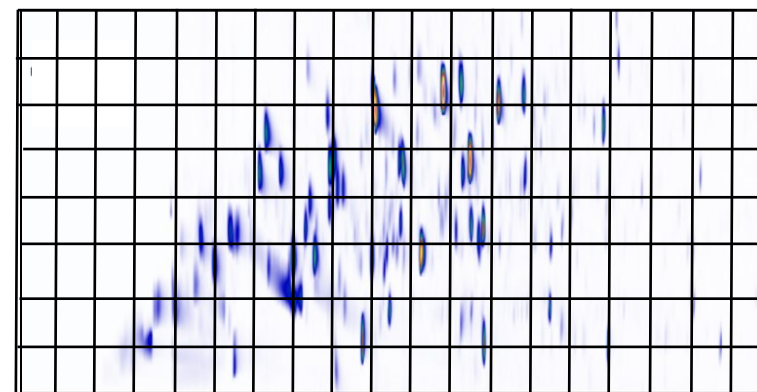
Metabolites analysis optimisation



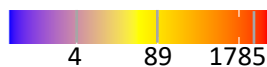


Chromatographic Fingerprint

Chocolate aroma analysis optimisation



Area

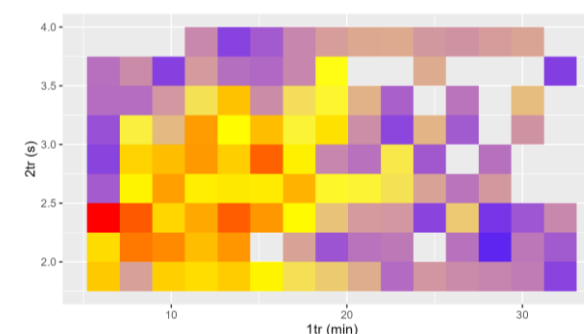
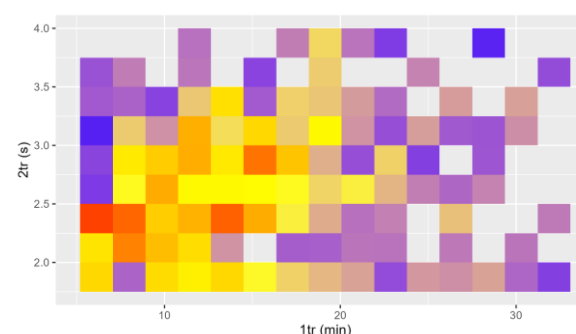
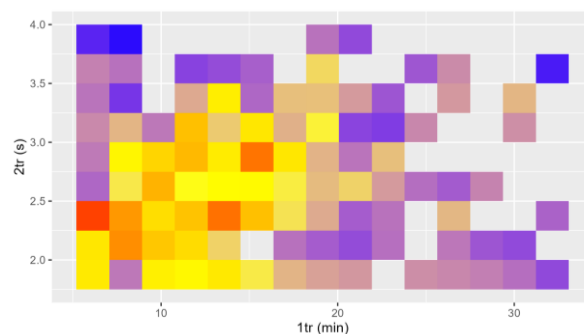
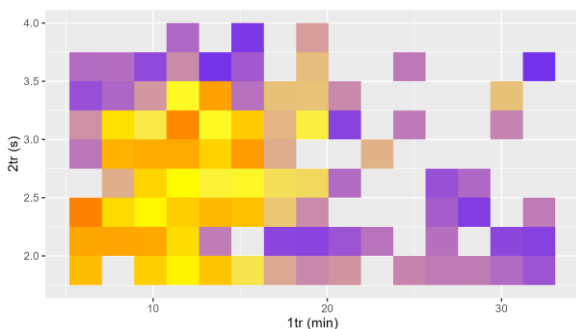


10 min

25 min

35 min

50 min



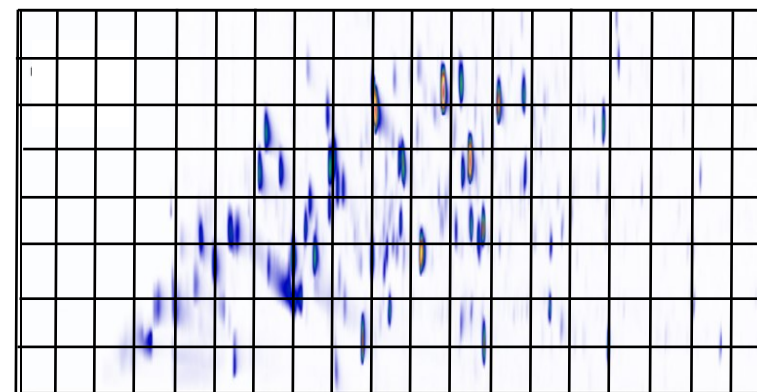


Chromatographic Fingerprint

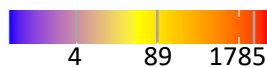
Chocolate aroma analysis optimisation



“Maps of improvement”



Area



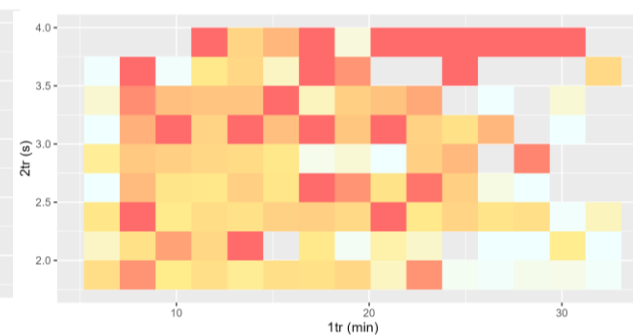
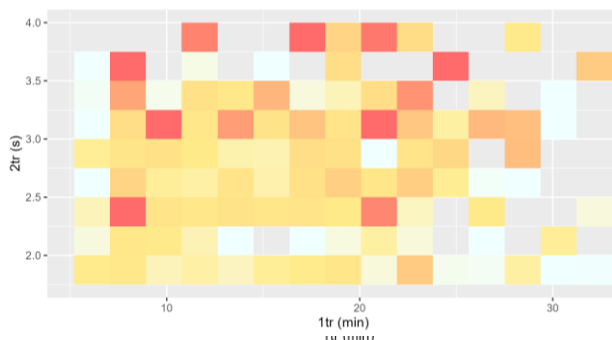
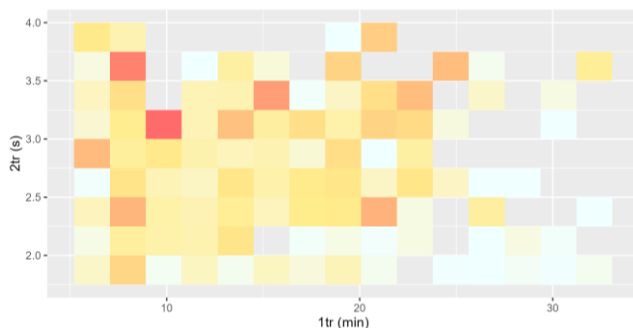
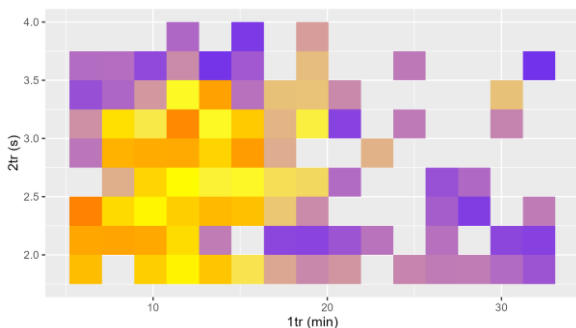
10 min

Ratio over 10 min

25 min

35 min

50 min

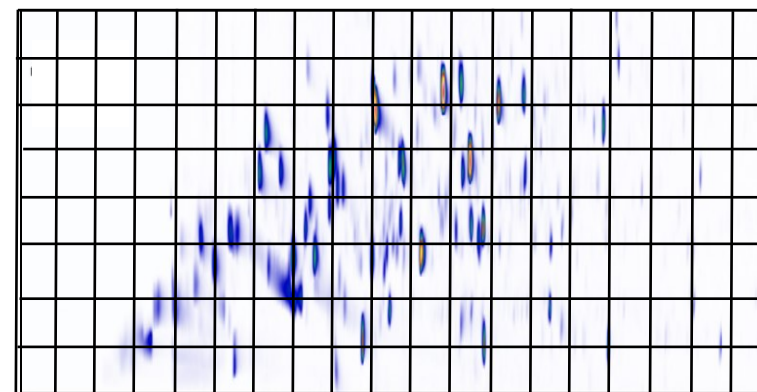


Chromatographic Fingerprint

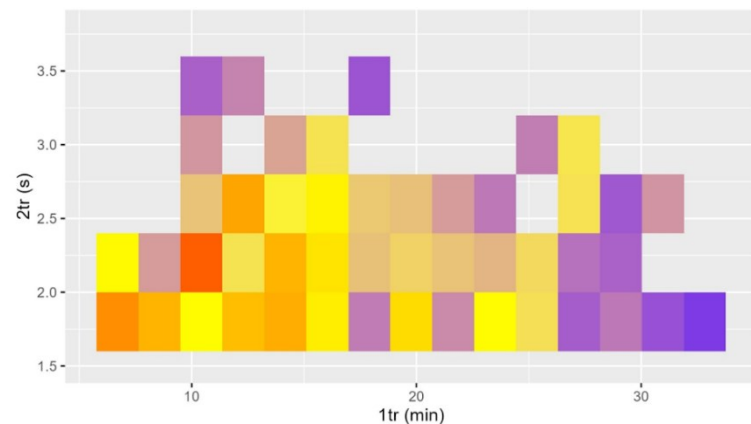
Chocolate aroma analysis optimisation



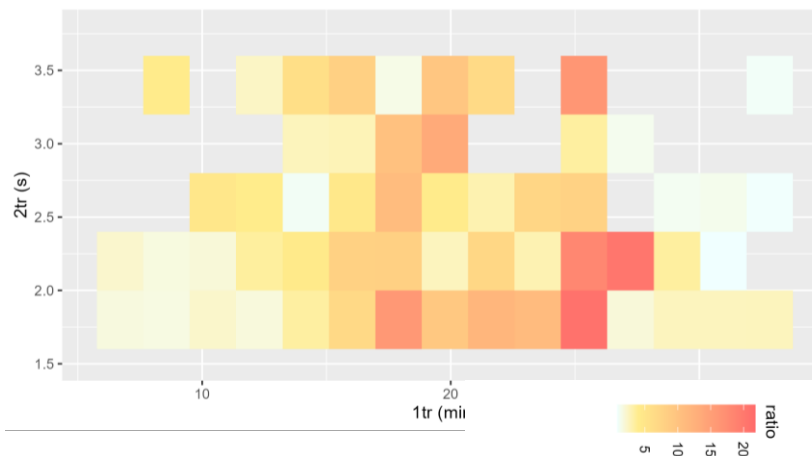
“Maps of improvement”



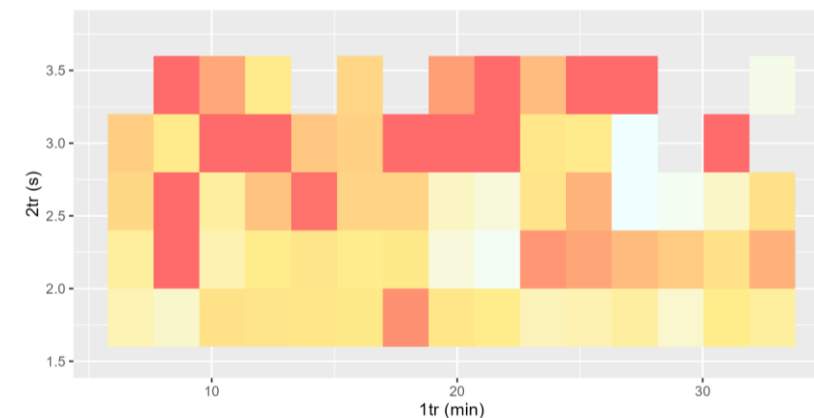
HS-SPME



Ratio Vac-HS-SPME/HS-SPME



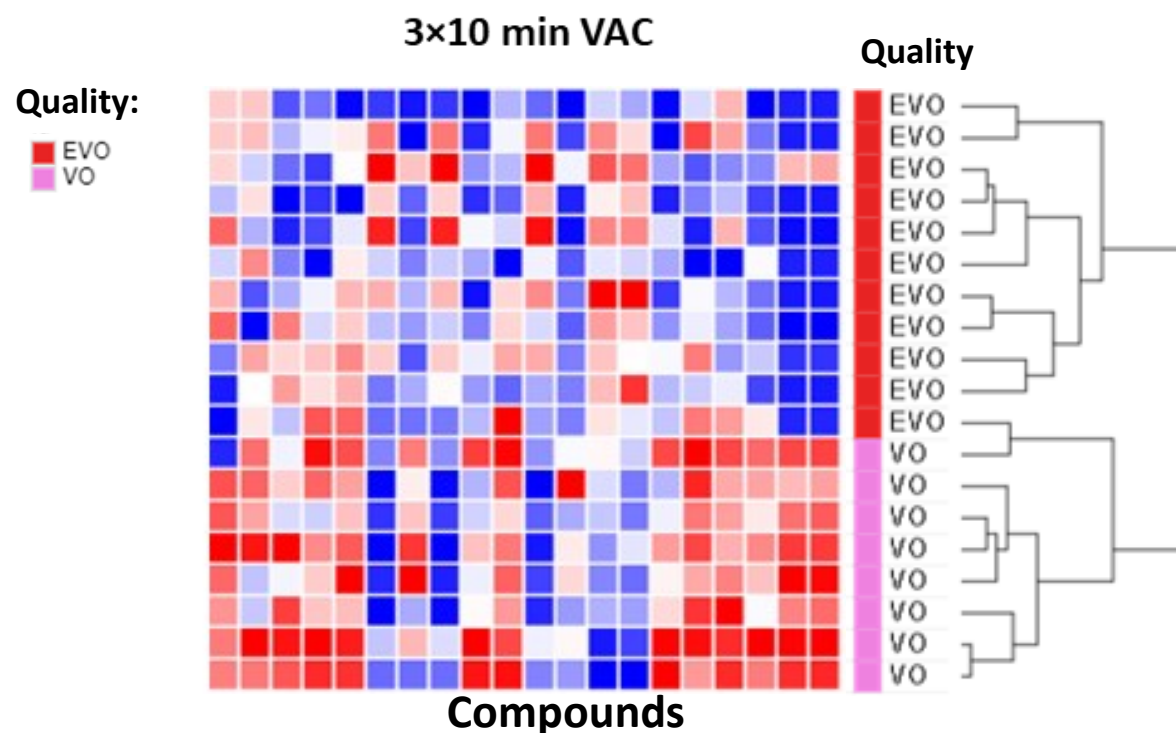
Ratio HiSorb/HS-SPME





Fingerprint: multiple case study

Olive oil quality assessment: Extra Virgin (EVO) vs. Virgin olive (VO) oil



Then:

- Further markers identification
- Monitoring of identified markers
- Identifying practice improvements
- Use of model for prediction
- ...

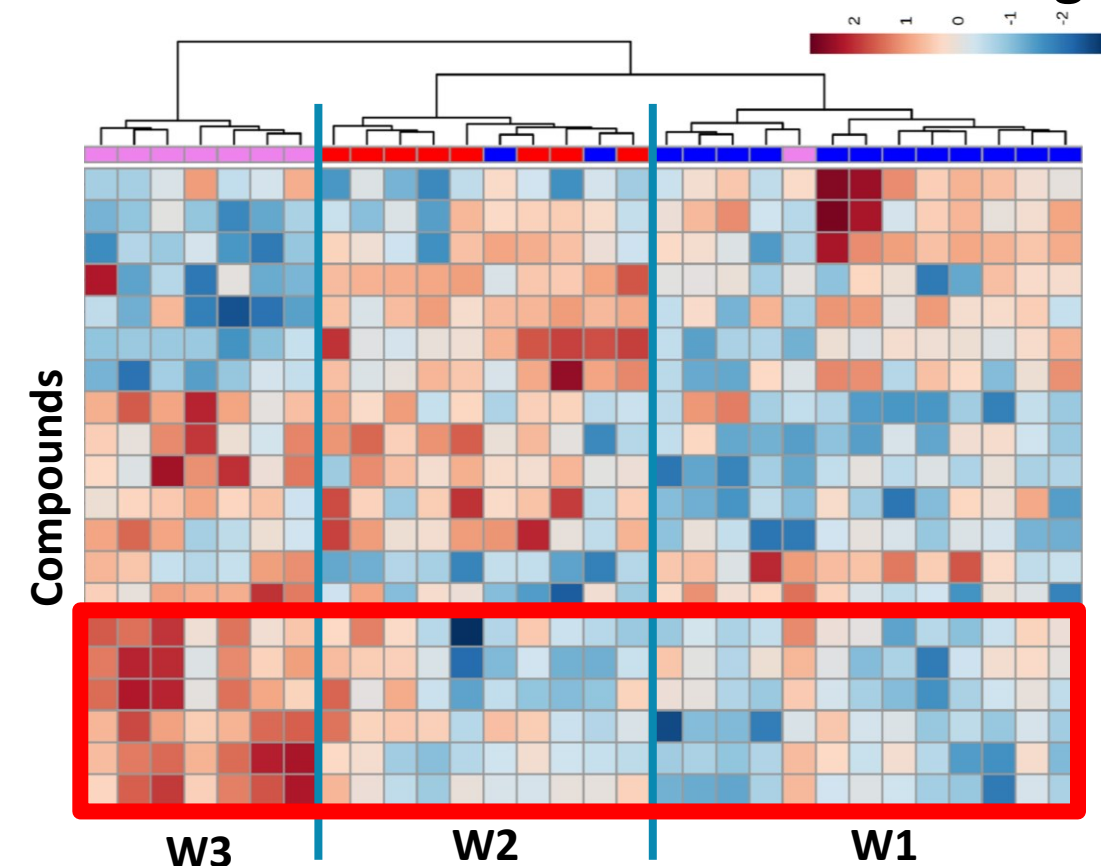




Fingerprint: multiple case study

Answering specific question : *Silene nutans* speciation

How scent is different between lineage ?



- VOCs implied in bugs-plants interaction
- Significant difference of VOCs confirmed by transcriptomics

➔ Confirm the speciation scenario between W3 and W1/W2

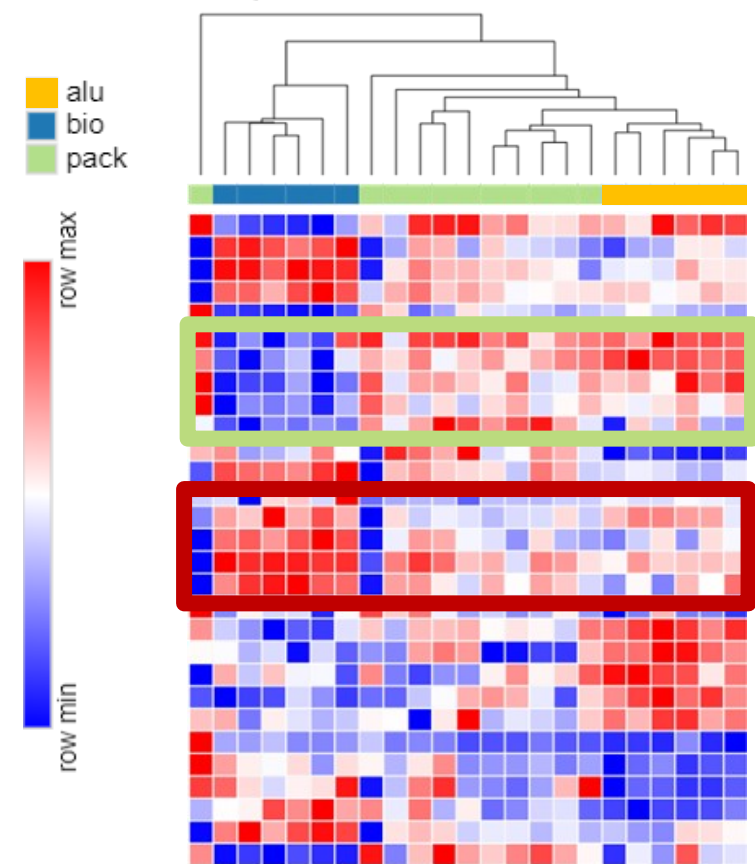




Fingerprint: multiple case study

Answering specific question : Coffee aging

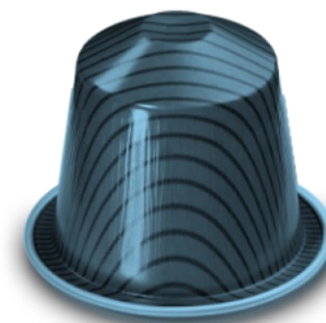
What give that coffee a bad aroma ?



- Loss of key odorant compounds
- Increase in oxidation markers



Compostable barriers to be improved



Aluminium



Compostable



Aluminium bag



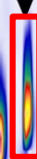
Fingerprint: Multi-response Analysis



From limited number of analytes

A) Vac

5-HMF

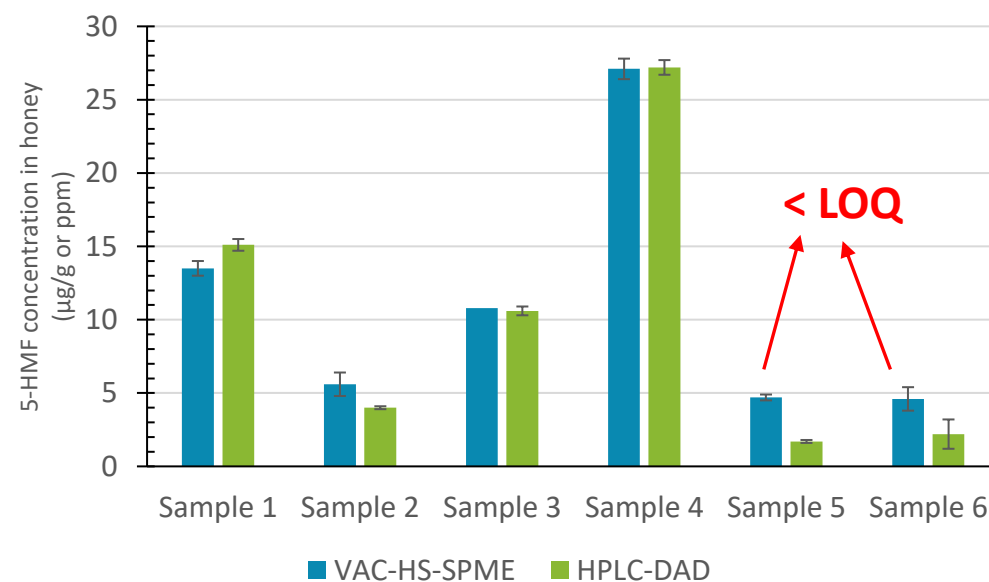


LoD : 1.6 $\mu\text{g/g}$

LoQ : 4.7 $\mu\text{g/g}$

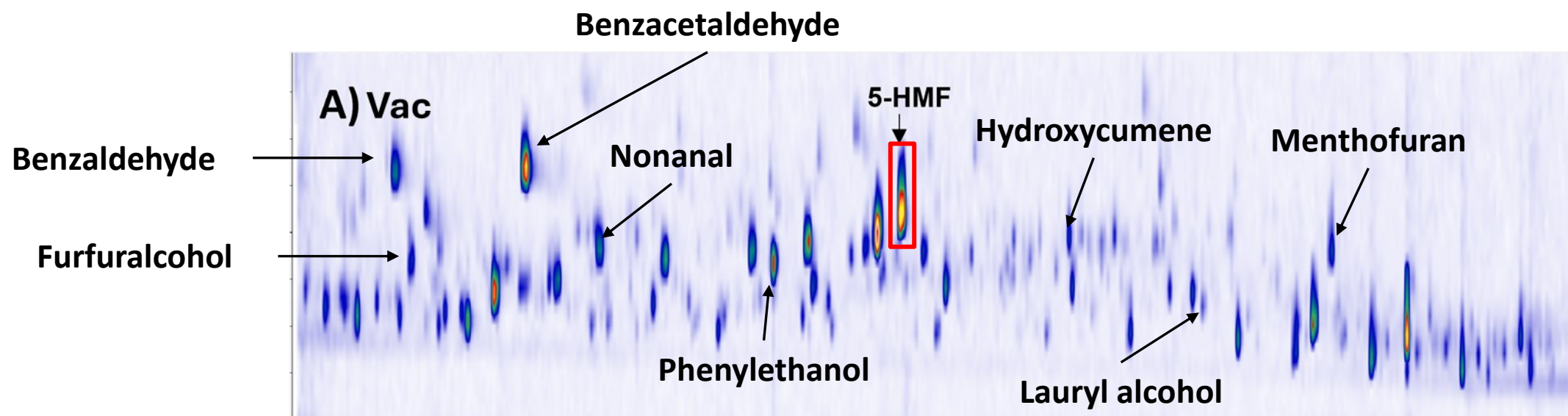
Biais against HPLC method : 6 %

Methods comparison



🎯 Fingerprint: Multi-response Analysis

👤 From limited number of analytes to multi-response analysis



Geographical, botanical, mono/multifloral, etc. determination



Natasha's presentation PM

Take home message

Gaining perspective to better comprehend



Thank you for your attention !



Analytical Chemistry GxABT :

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Paula Albendea

Damien Eggermont

Aleksandra Gorska

Donatella Ferrara

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Carlo Bellinghieri

Nicolas Ruin