

# HS-GC-IMS: a rapid technique for assessing quality, safety and integrity of foods

**Marco Arlorio**

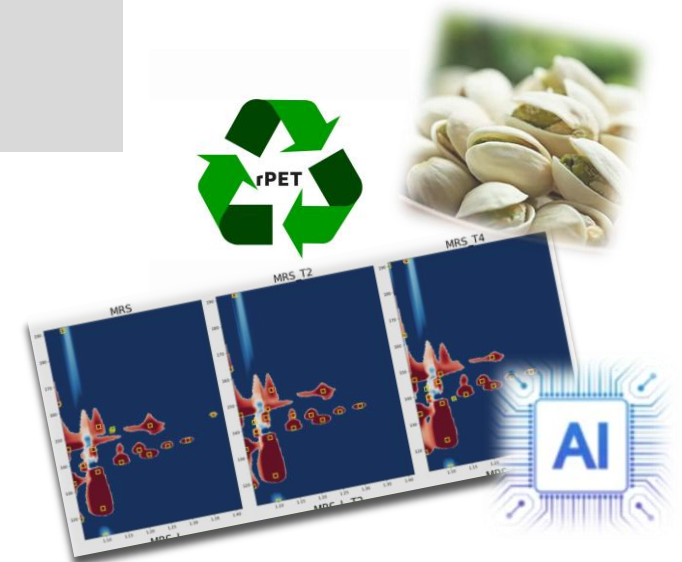
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Dipartimento di Scienze del Farmaco, UPO “Amedeo Avogadro” – Novara (Italy)

Food Chemistry, Biotechnology and Nutrition Unit



Second Italian User Meeting  
Bologna 22-04-2026



# Agenda

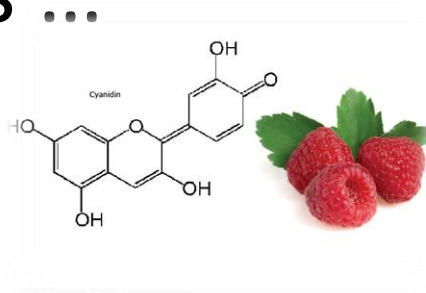
- 1. Interplays among quality, safety, integrity and rapid targeted/untargeted analysis: a need...
- 2. HS-GC-IMS (FlavourSpec<sup>®</sup>): three case studies
- 3. Conclusions and perspectives

# Agenda

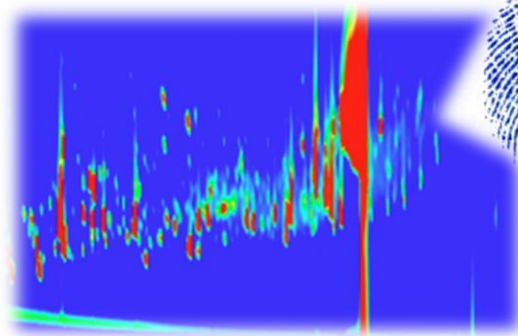
- 1. Interplays among quality, safety, integrity and rapid targeted/untargeted analysis: a need...
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Targeted analysis ...



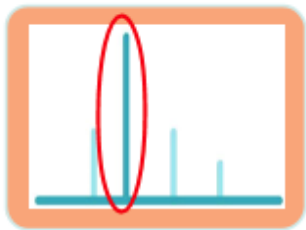
... or non-targeted







non-targeted → First level (screening...)



targeted → Second level (confirmatory method...)



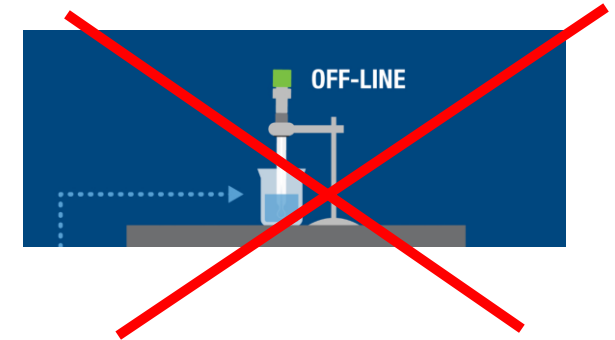
**RAPID METHODS**

# PROCESS MONITORING: RAPID METHODS AND AT-LINE MEASUREMENTS

**AT-LINE:** *sample is transferred from the process solution to an analytical instrument in **close physical proximity to the process** and returns analytical result in a **short time cycle**.*

## Requirements:

- ✓ *rapid*
- ✓ *sensitive and reproducible...*
- ✓ *“smart” (no highly-specialized personnel is required)*
- ✓ *possibly low cost*



**INDUSTRIAL  
PLANTS**



**RAPID SAMPLING  
(NO SAMPLE PREPARATION)**



**POST ANALYSIS  
PROCESSING**



## A recent trend...

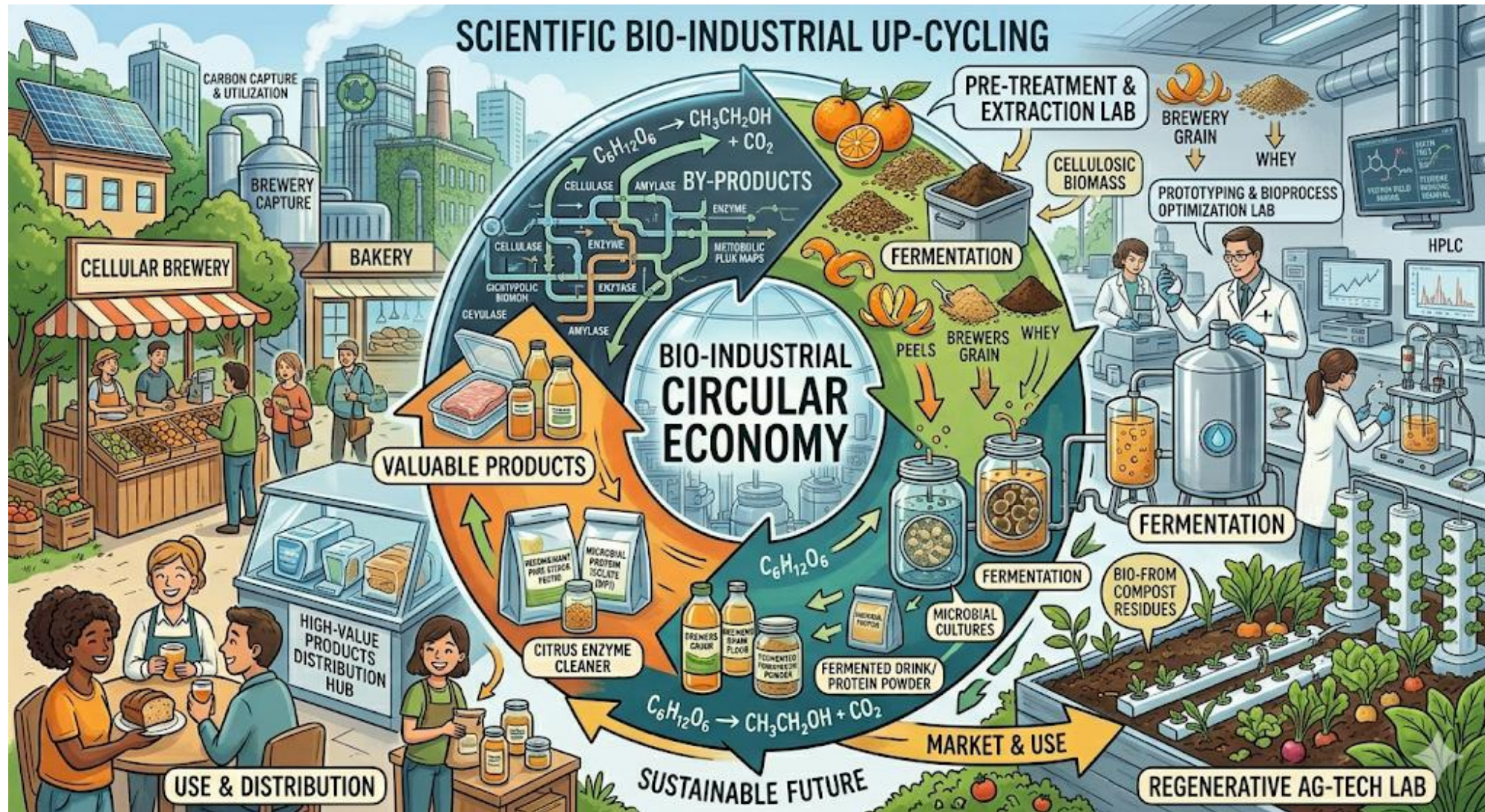
*fermentation*



- “Traditional” fermentation (winemaking, brewery...)
- “New trendy” food products (*kombucha*...)
- Microbial biomasses (probiotics)

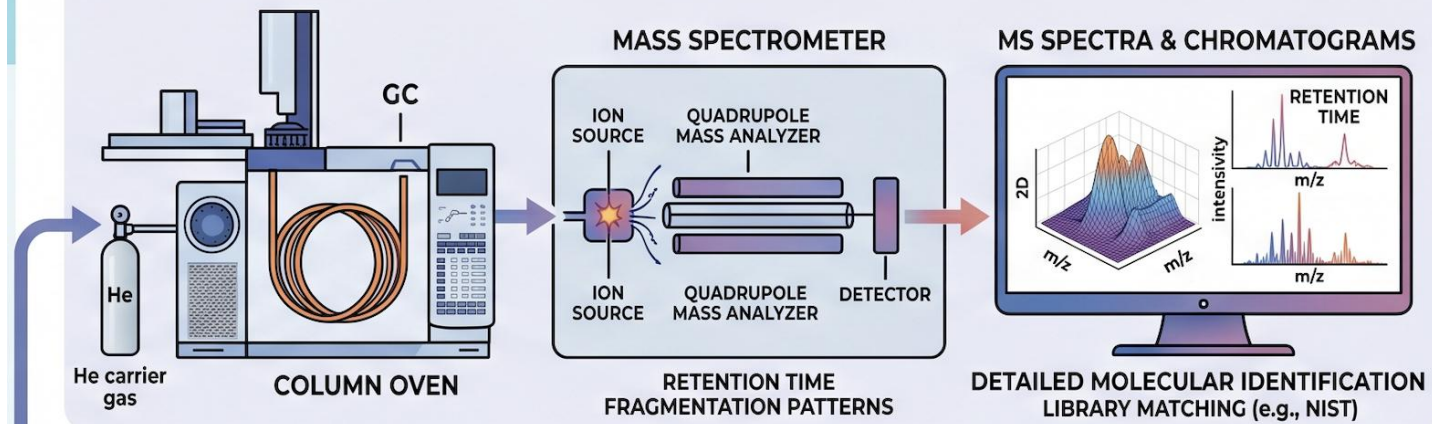


# Bioeconomy, upcycling...and more

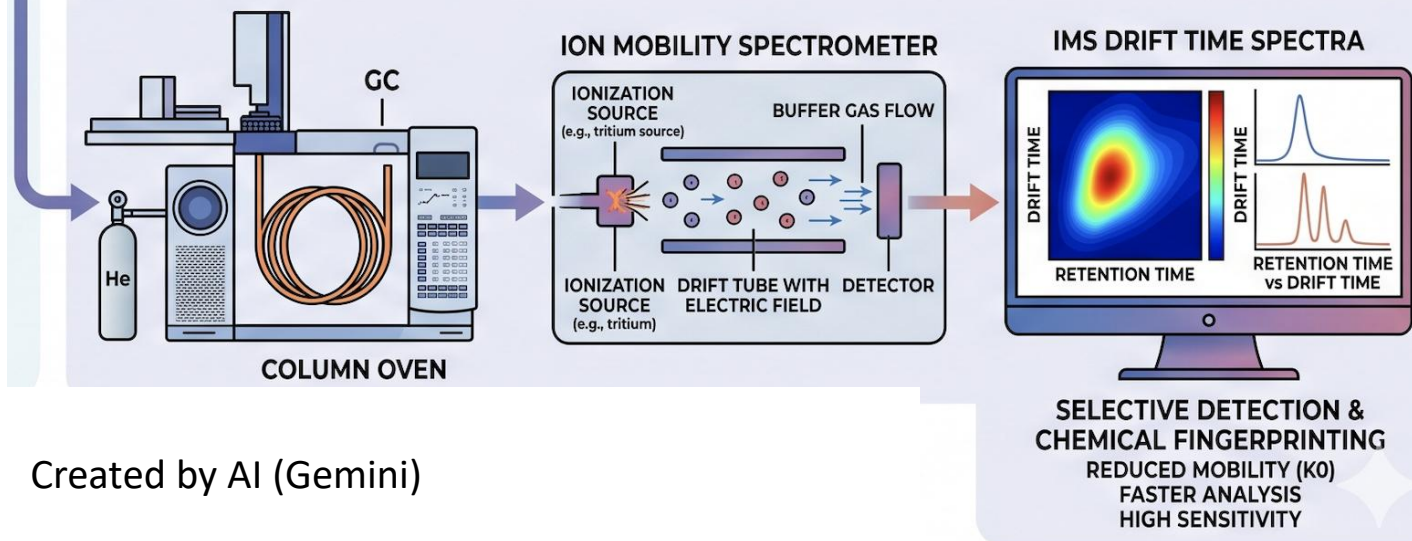




## GC-MS (GAS CHROMATOGRAPHY-MASS SPECTROMETRY)



## GC-IMS (GAS CHROMATOGRAPHY-ION MOBILITY SPECTROMETRY)



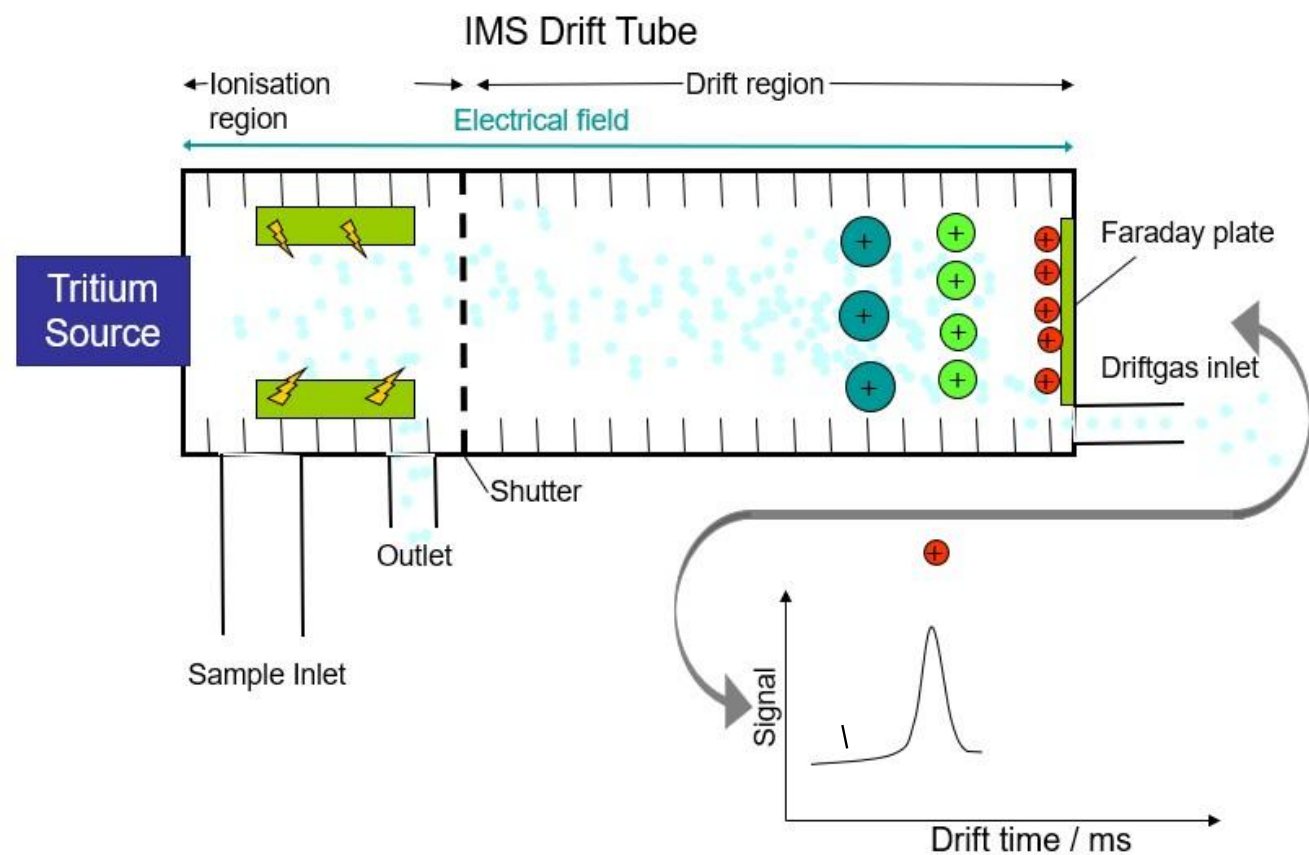
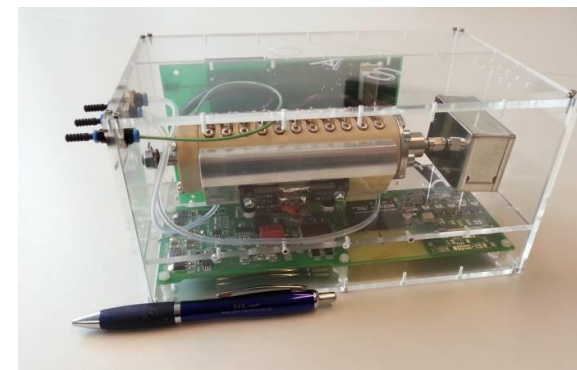
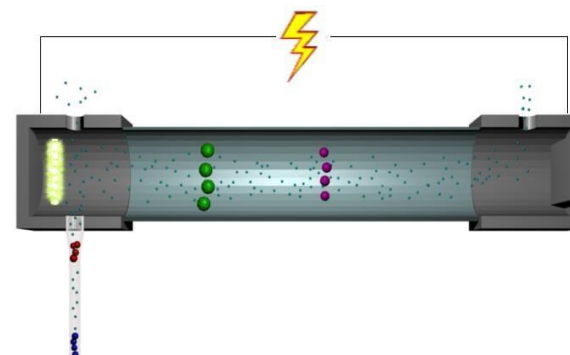
Created by AI (Gemini)

The link:  
exploring the **volatilome**





*...about the principle*

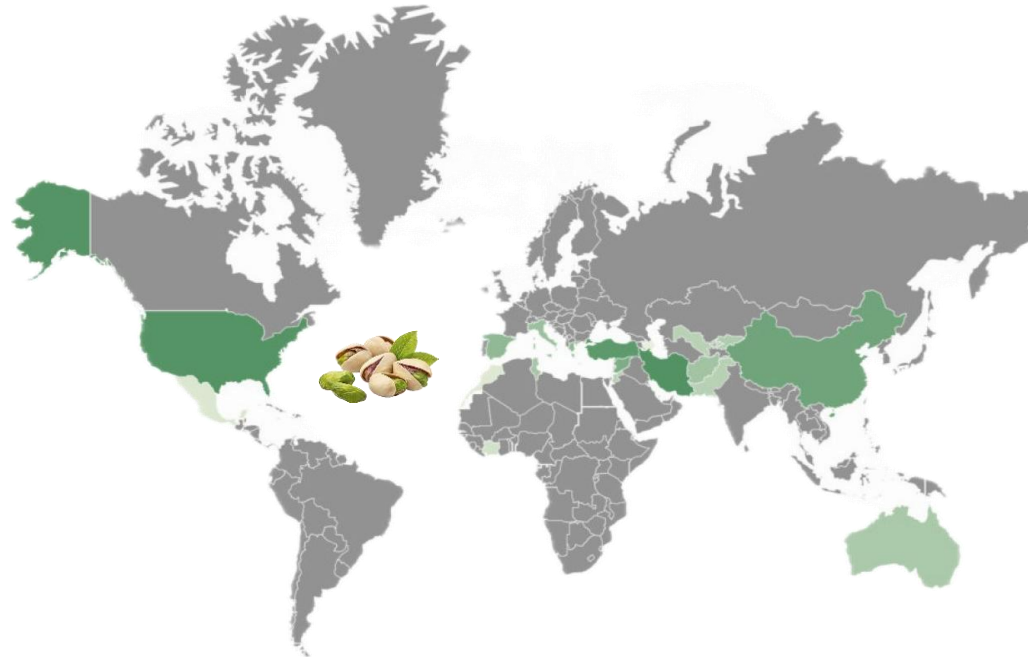


# Agenda

- 1. Interplays among quality, safety, integrity and rapid targeted/untargeted analysis: a need...
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- 3. Conclusions and perspectives



## Case study 1: pistachios (*Pistacia vera*)



- Family: ***Anacardiaceae***
- Origin: western Asia
- Main producer Countries: USA, Iran and Turkey

In collaboration with:

**UNIGRA**



Dr. Giacomo Pedron – DSF UPO



Best Poster Award  
SISTAL 2025



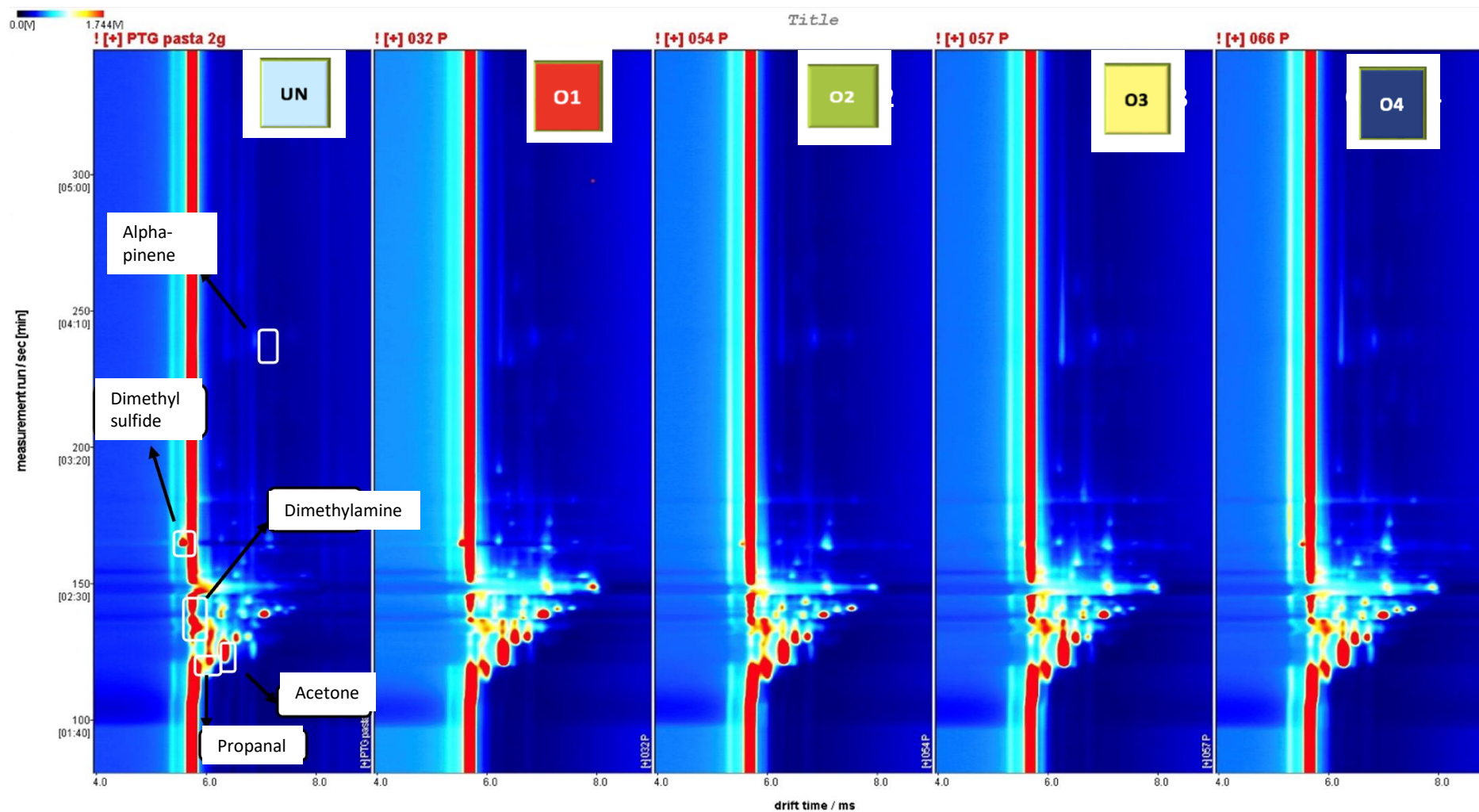
## Case study 1: pistachios (*Pistacia vera*)

In collaboration with: **UNIGRA**

Processing



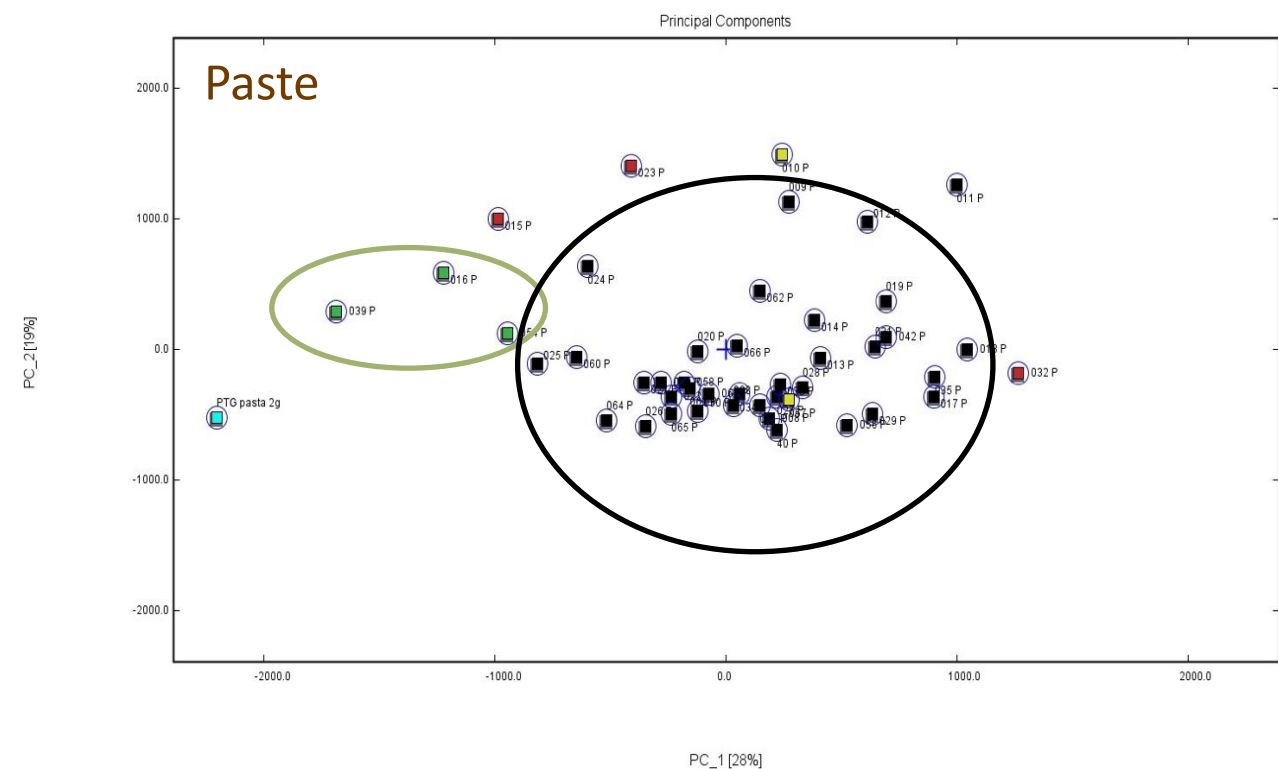
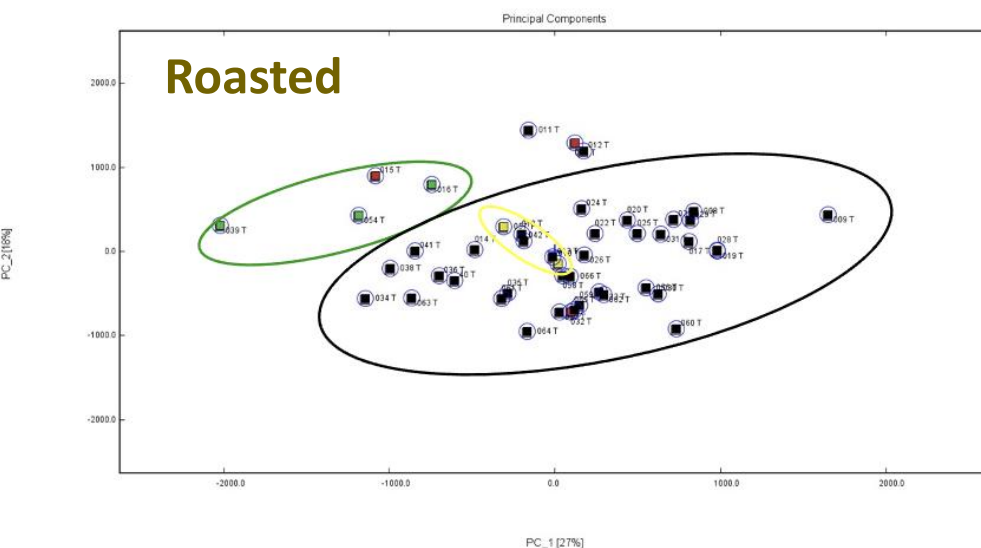
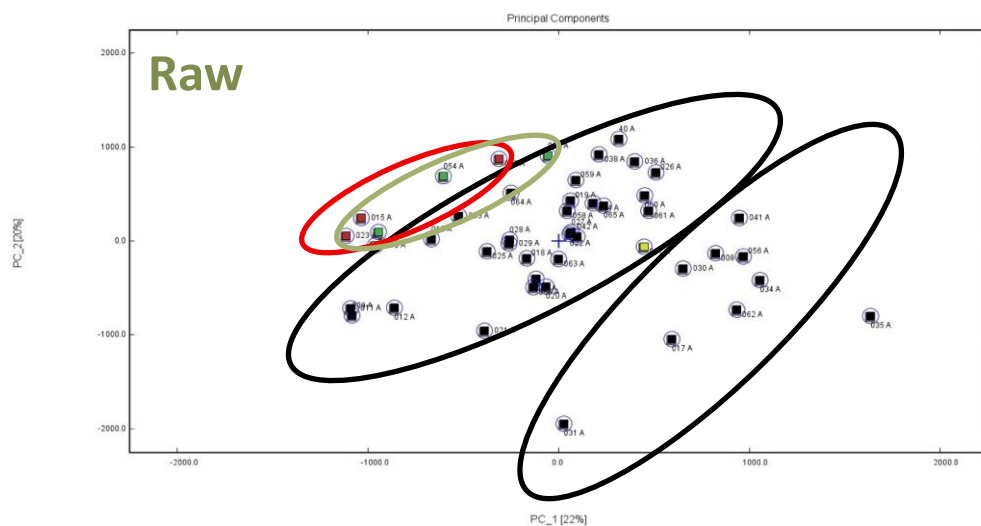
# Case study 1: pistachios (*Pistacia vera*)



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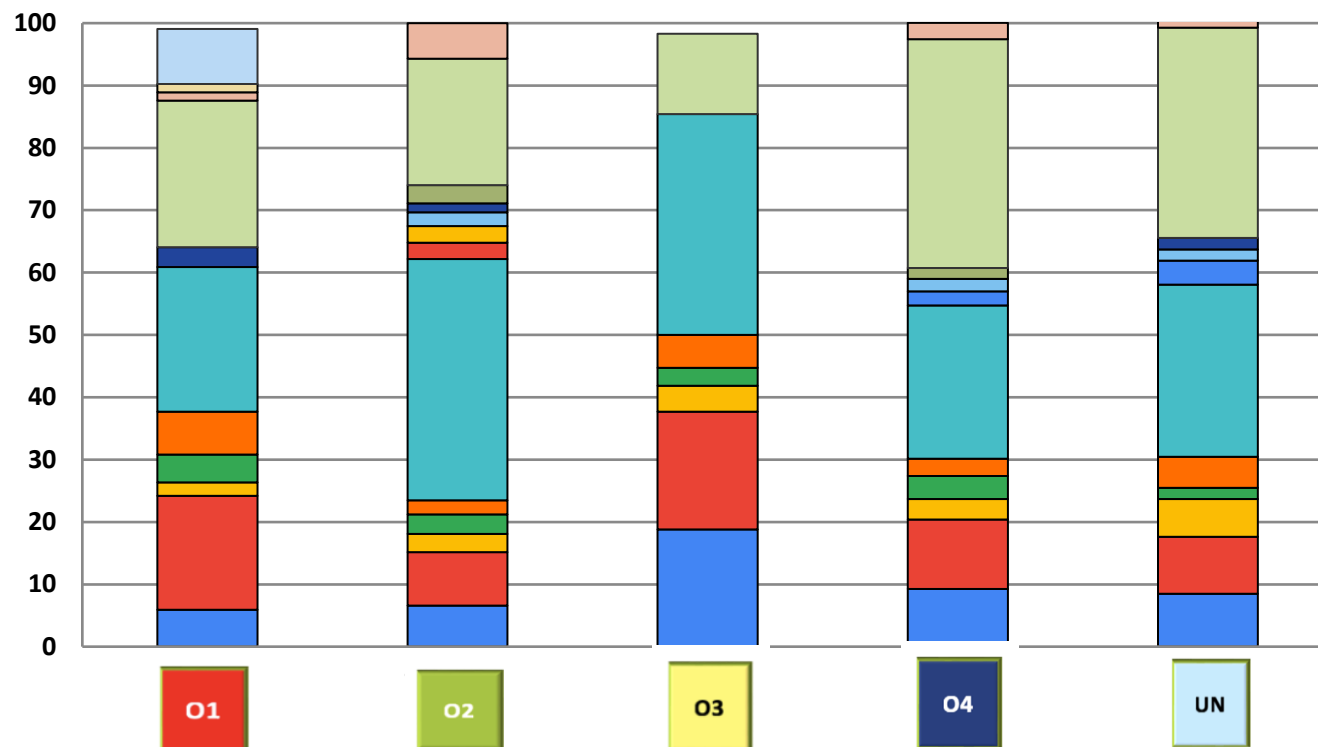
## Non-targeted clustering

■ USA ■ Iran ■ Spagna ■ Turchia

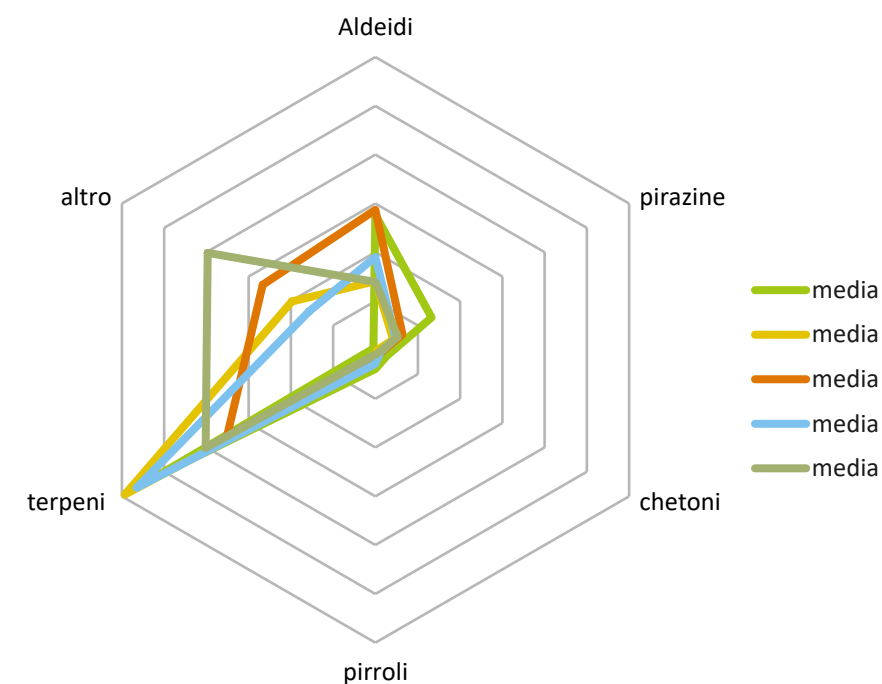


# Case study 1: pistachios (*Pistacia vera*)

## Volatilome (GC-MS)

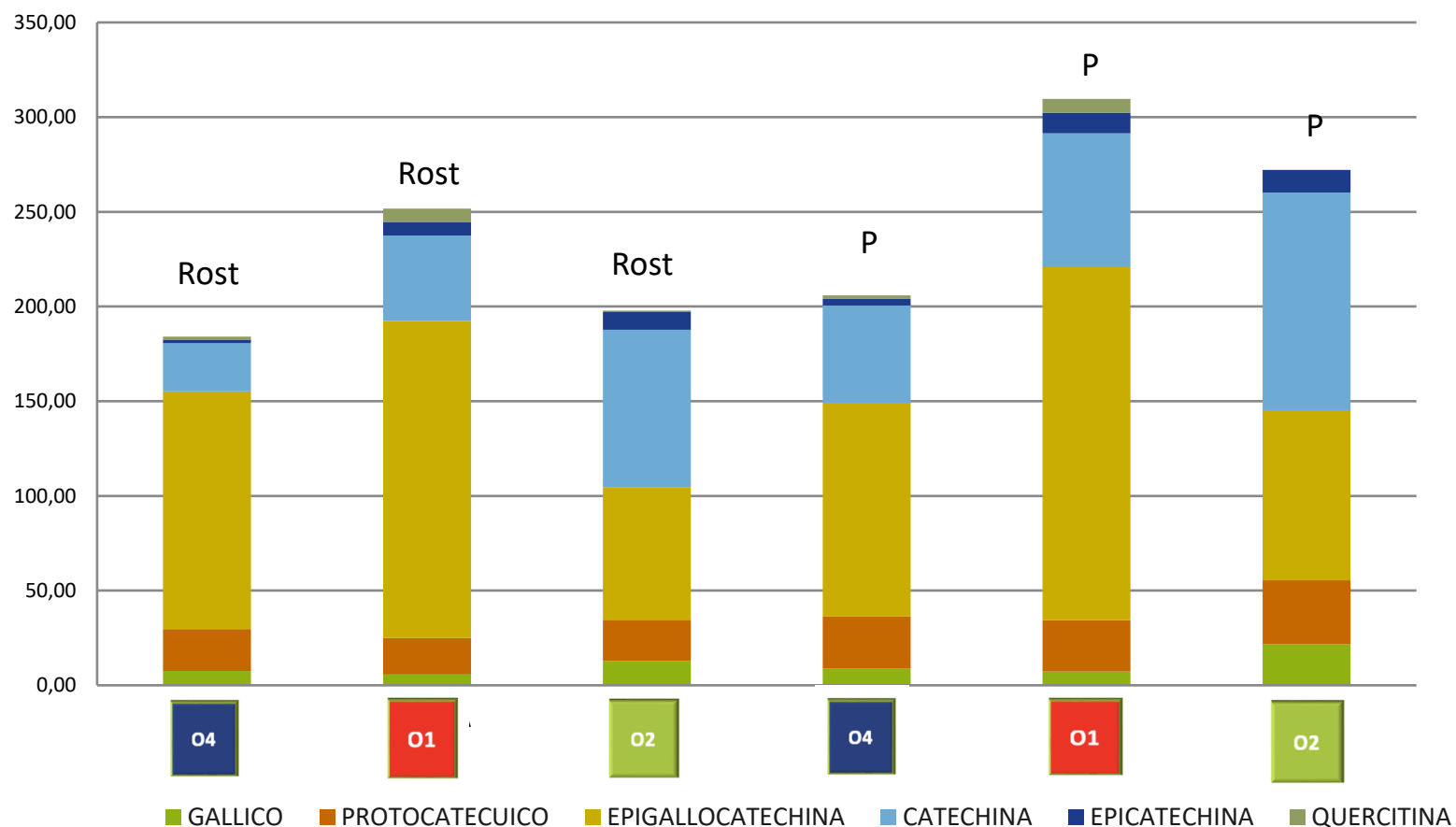


- 3-metilbutanale
- 2-metilbutanale
- Esanale
- 1-metil-1H-pirrolo
- 2,5-dimetilpirazina
- Alpha-pinene
- Alpha-thujene
- Camphene
- Beta-pinene
- Beta-mircene
- 2-etil-3-metilpirazina
- 3-carene
- 3-etil-2,5-dimetilpirazina
- 2-metilpropanale
- D-limonene
- Terpinolene



## Case study 1: pistachios (*Pistacia vera*)

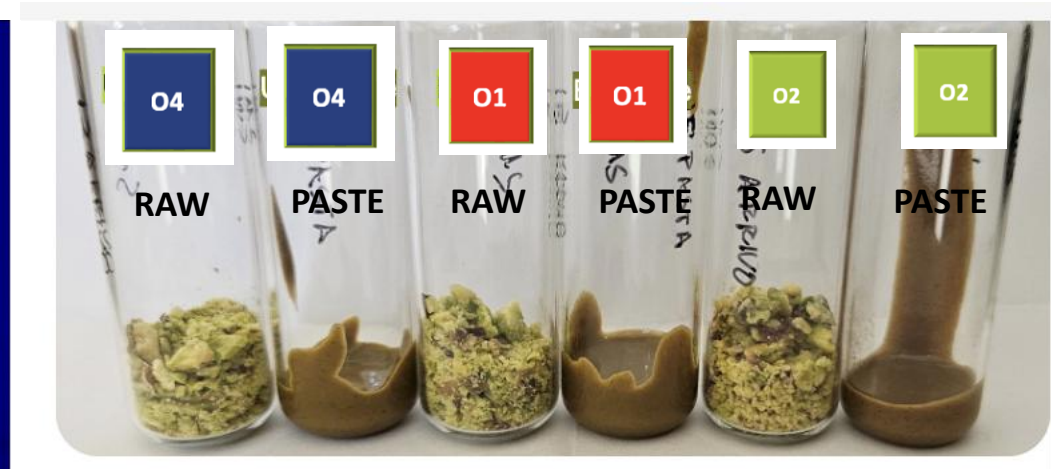
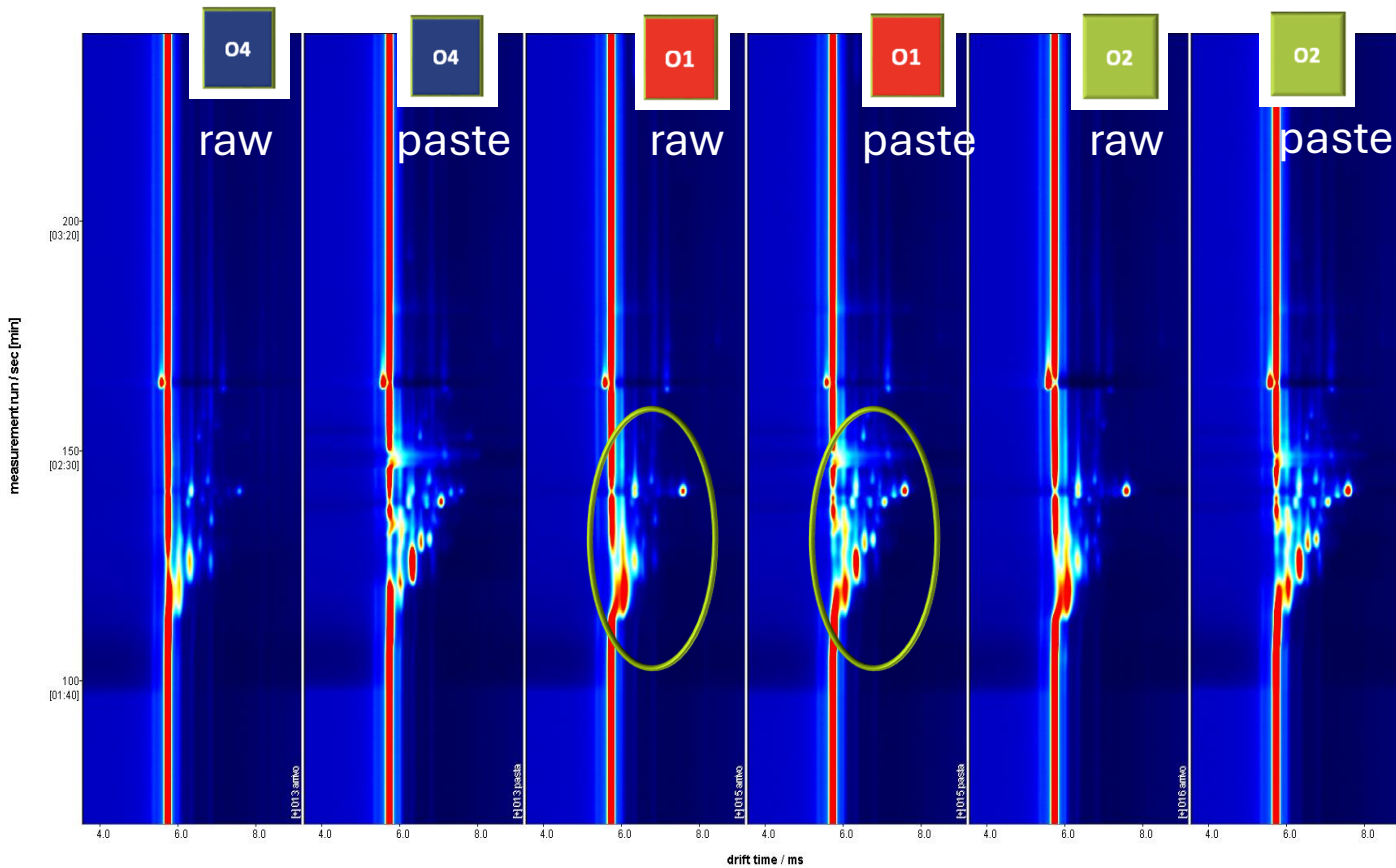
### Polyphenols signature





# Case study 1: pistachios (*Pistacia vera*)

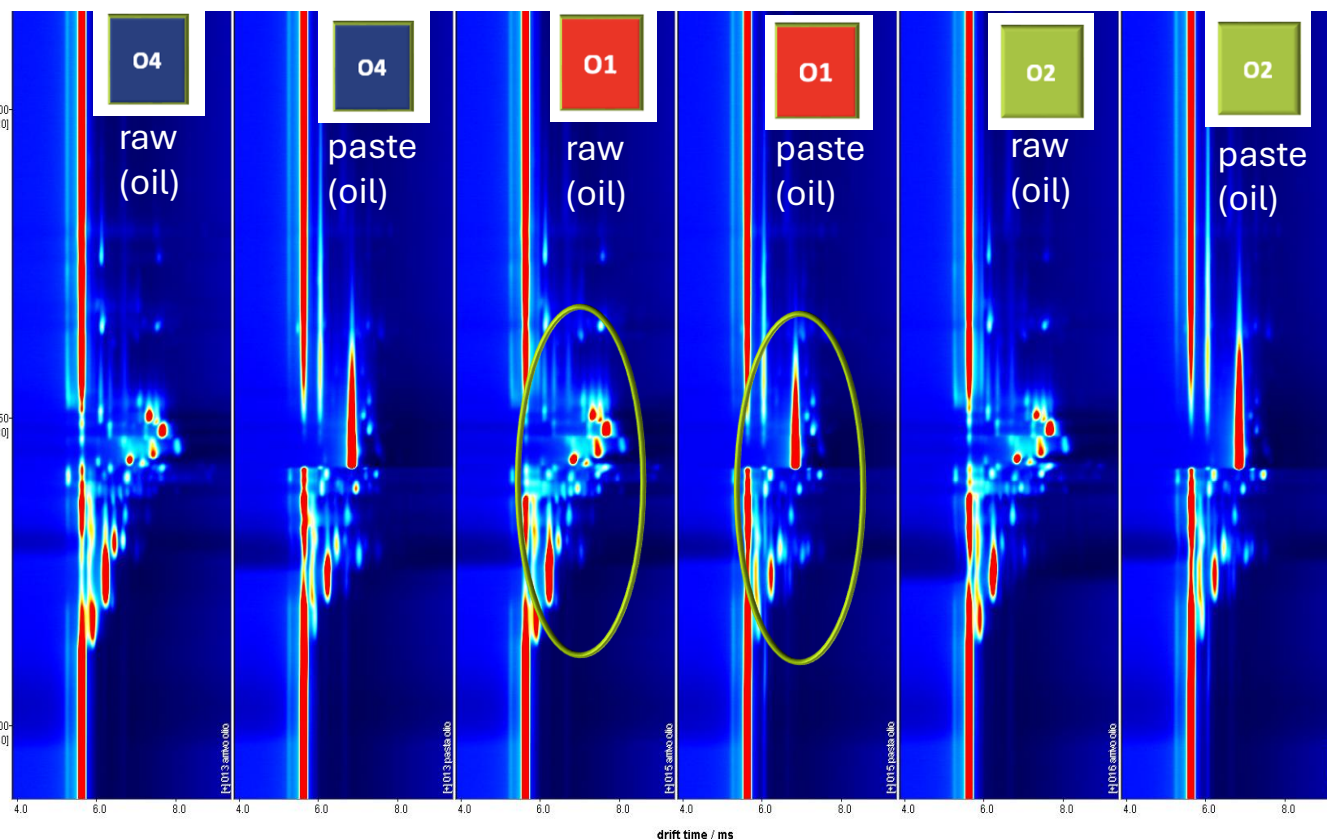
## GC-IMS



Aroma and flavor profile evolution of raw and paste of pistachios analyzed by GC-IMS

## Case study 1: pistachios (*Pistacia vera*)

### GC-IMS profile of pistachio's oils

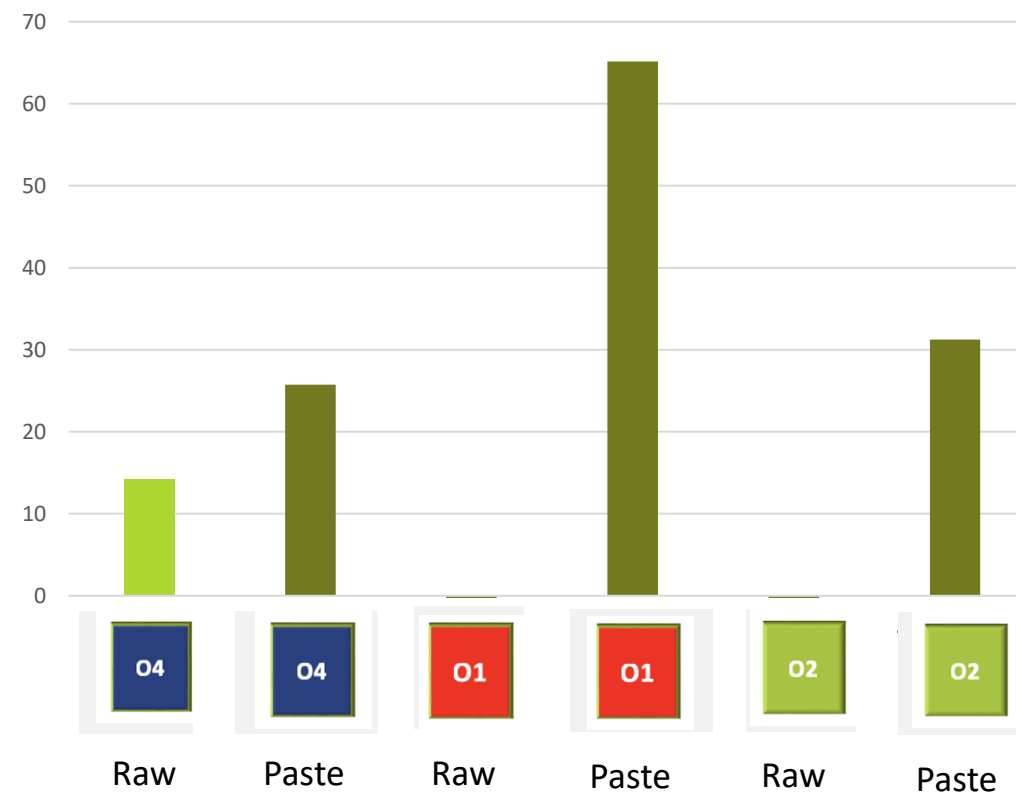


Evolution of volatile aroma and flavor profiles in pistachio oil extracted from raw and paste samples, analyzed by GC-IMS

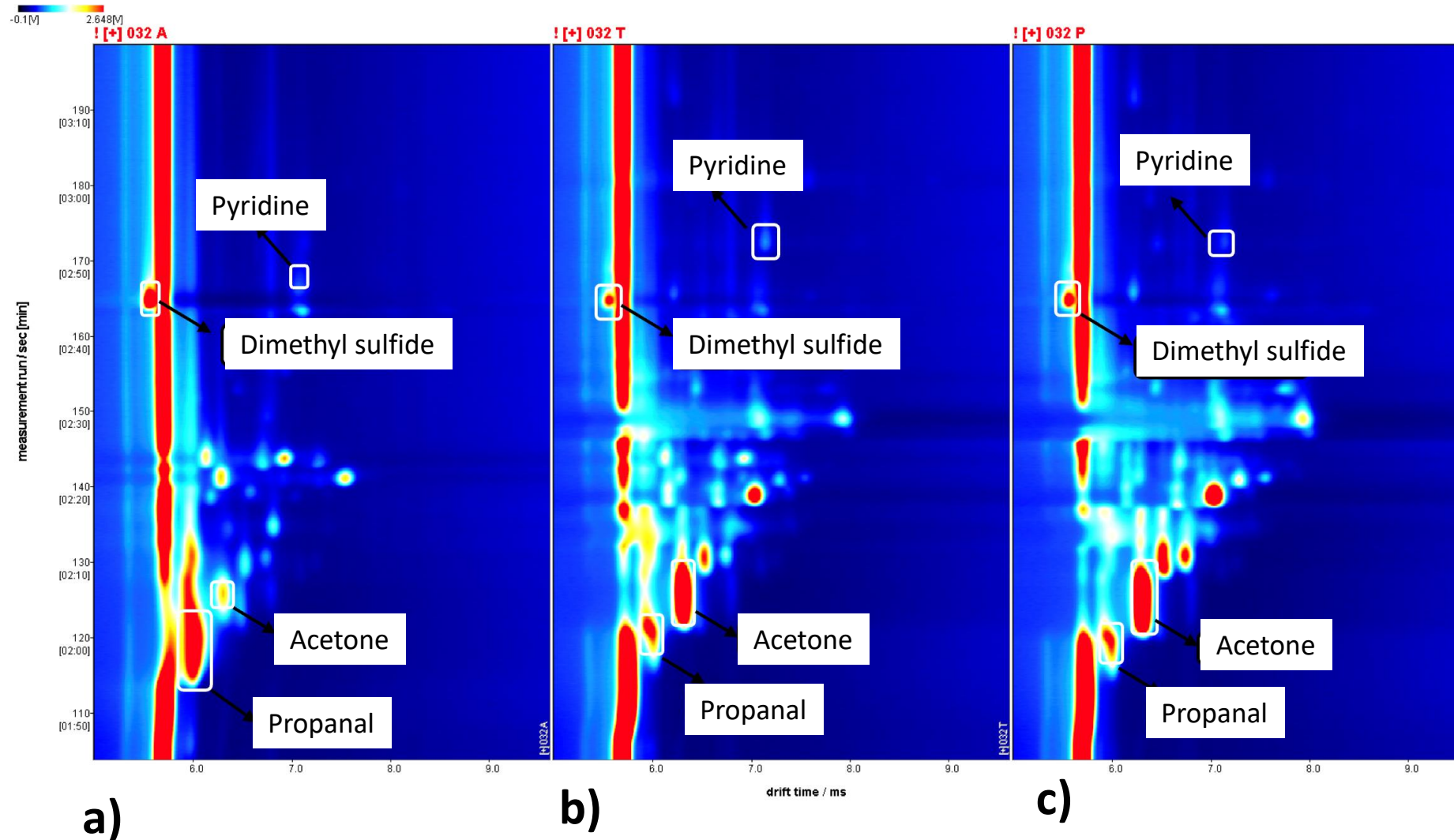


### Hexanal (GC-MS confirmation)

Concentration ng/g



# Case study 1: pistachios (*Pistacia vera*)



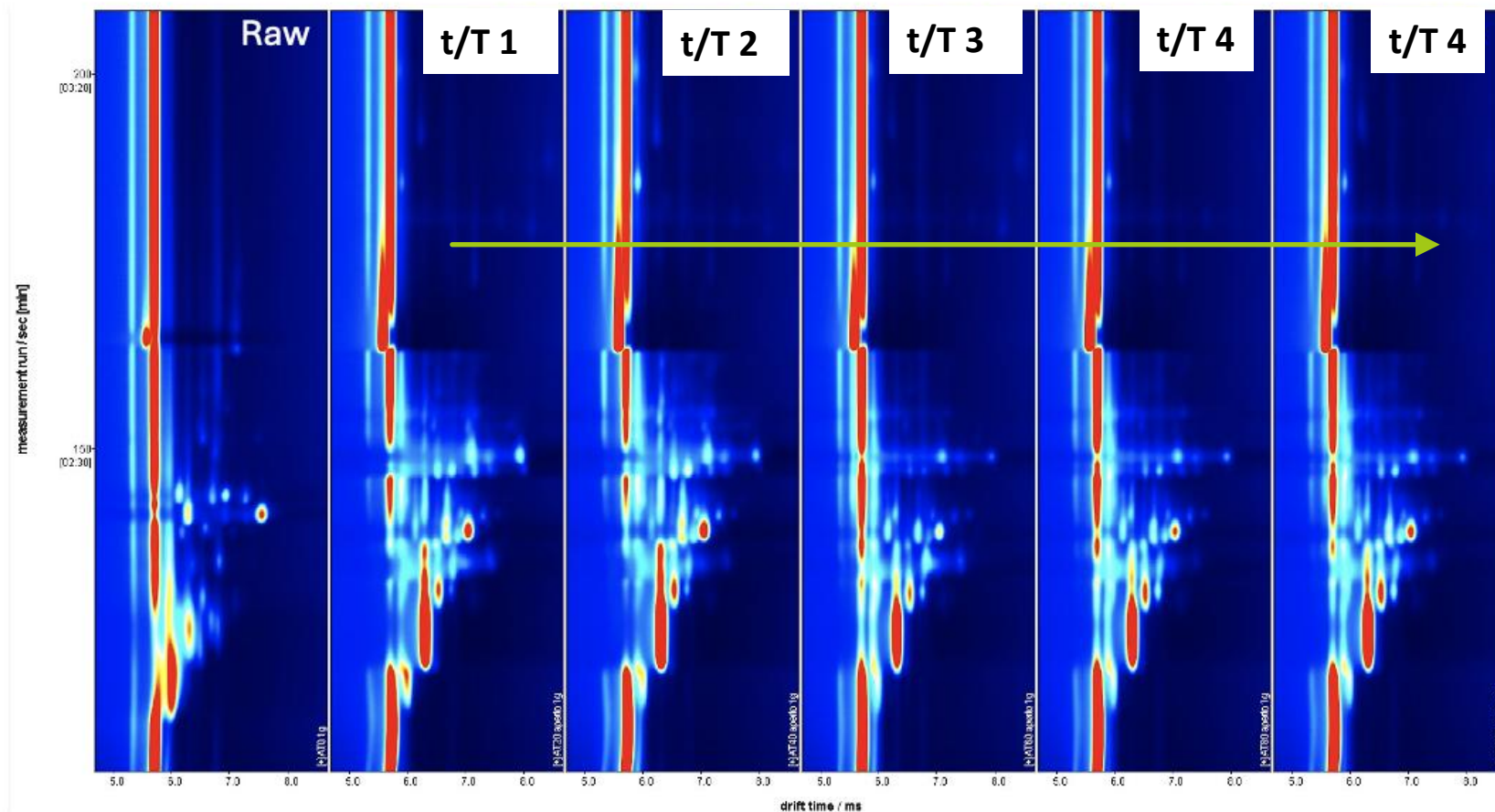
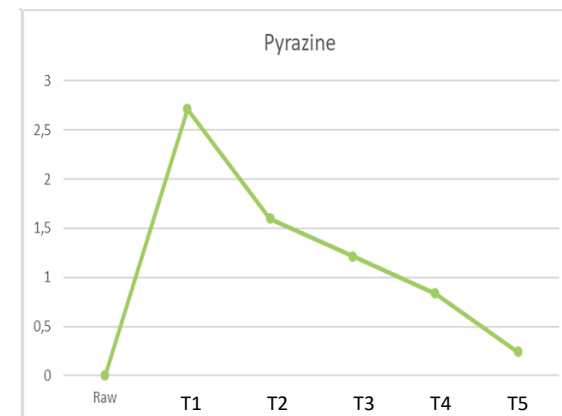
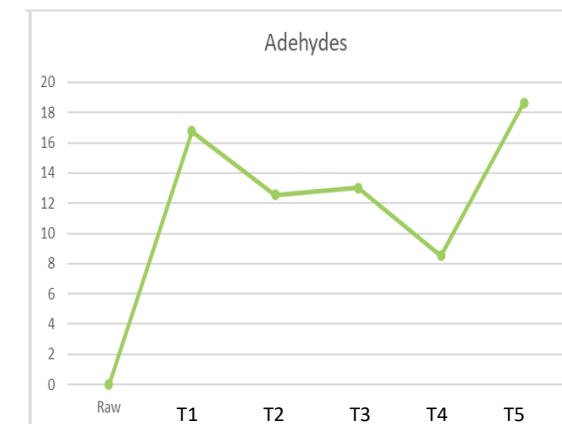
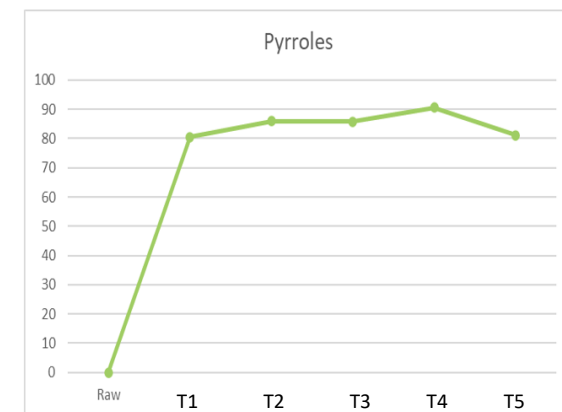
2D GC-IMS profiles ( **01** ) Raw (a); roasted (b); paste (c)





Color evolution (different roasting parameters)

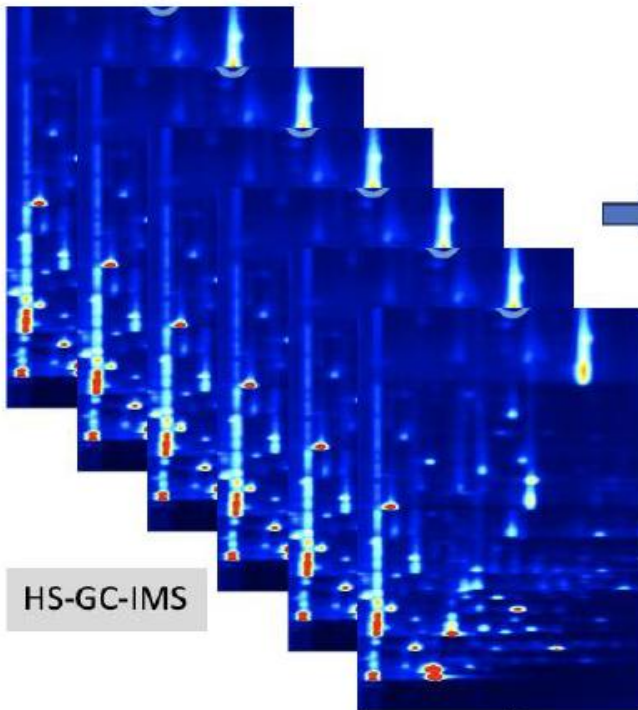
**GC-IMS + GC-MS**



Aroma and flavor profile evolution of roasted pistachios analyzed by GC-IMS.

## Case Study 2: “smart” fermentation monitoring

### NUTRIAGE project (NODES)



HS-GC-IMS

**DIGITAL PROCESSING**  
(Computer Vision  
Image Analysis)

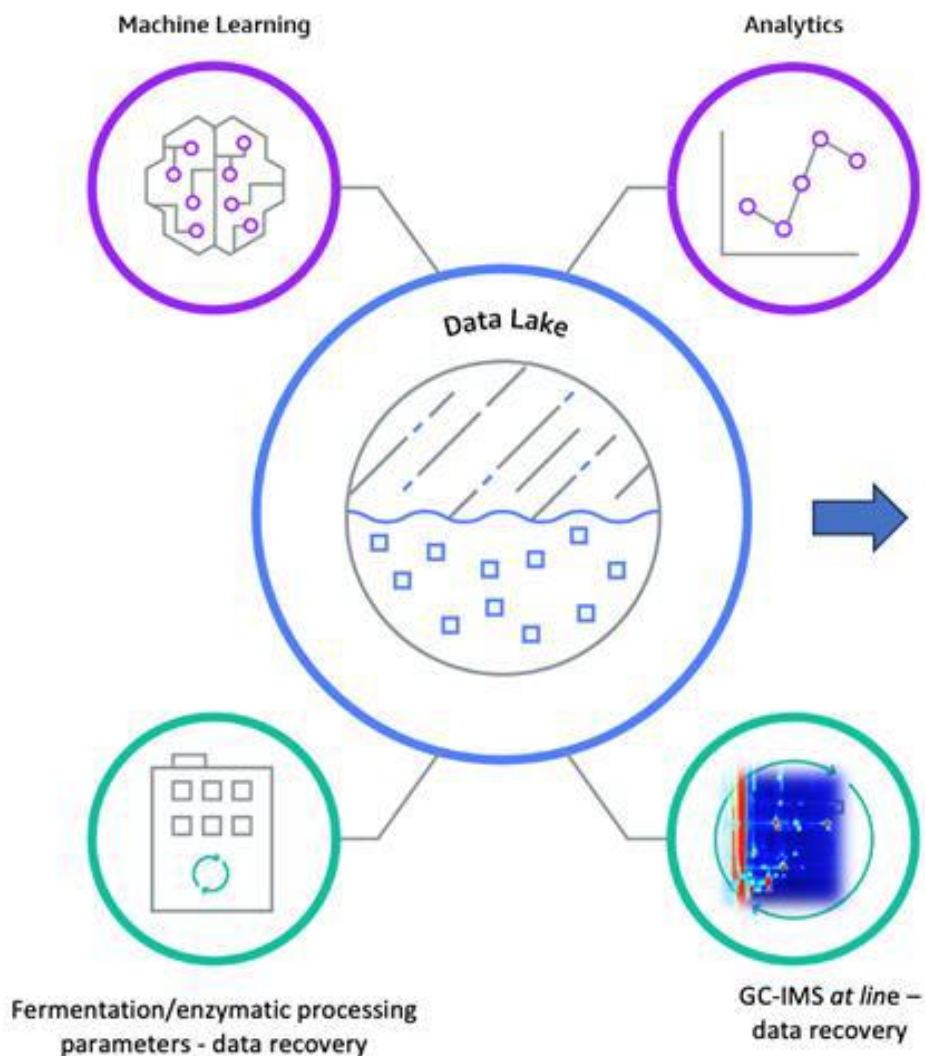
1. Preprocessing
2. Signal “cleaning” (and automatic selection of the best performing markers)
3. Data storage & data mining

#### Preprocessing

1. Alignment (RIP normalization)
2. Signal to noise correction/scaling
3. Data set preparation



## Case Study 2: «smart» fermentation monitoring



1. “Smart” monitoring
2. Database creation (GC-IMS + plant parameters + other analytical techniques: *data fusion*)
3. “Smart” elaboration of the data and process optimisation

## Case Study 2: «smart» fermentation monitoring

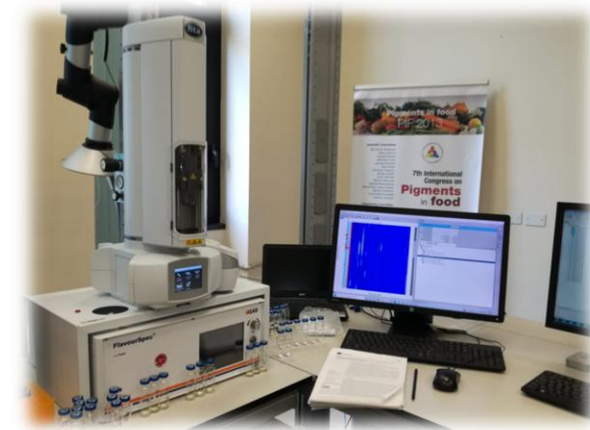


Sample	Code
Culture Medium	(MRS)
Culture Medium + <i>Lactobacillus Paracasei</i>	(MRS + L)
Culture Medium + <i>Lactobacillus Paracasei</i> + <i>Saccharomyces cerevisiae</i>	(MRS + L + S)
Culture Medium + <i>Lactobacillus Paracasei</i> + Contaminated swab	(MRS + L + X)



### Sampling

0, 2, 4, 6, 24 h



## Case Study 2: «smart» fermentation monitoring

### Approach:

Optimisation of the pre-processing steps such as:

1. region of interest (ROI) identification;
2. threshold selection, then combines Persistent Homology and Variable Importance Projection (VIP) scores of PLS-DA
3. Identification of selected descriptive peaks of VOCs generated during the fermentation process (selection of the markers)

➡ *This approach **reduces manual intervention**, improving the efficiency and accuracy of complex data processing*

## Approach:

### □ Pre-processing:

gc-ims-tools (version 0.1.7) Python (Spectrum class; Dataset class; exploratory data analysis, PCA and Supervised learning, PLS-DA)

*Christmann, Joscha; Rohn, Sascha; Weller, Philipp (2022): gc-ims-tools – A new Python package for chemometric analysis of GC–IMS data. In: Food chemistry 224 (4), S. 133476. <https://pypi.org/project/gc-ims-tools/>*

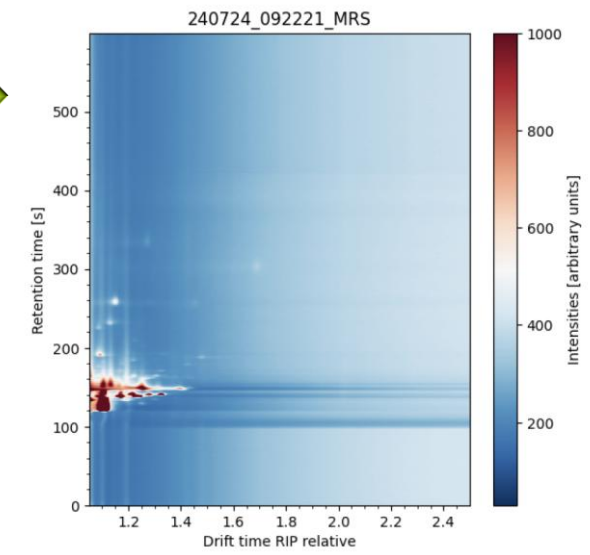
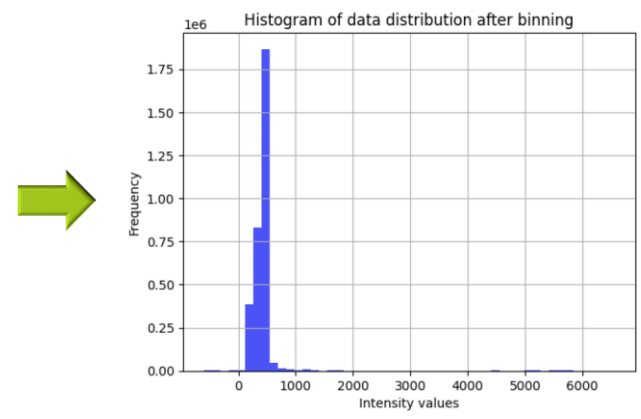
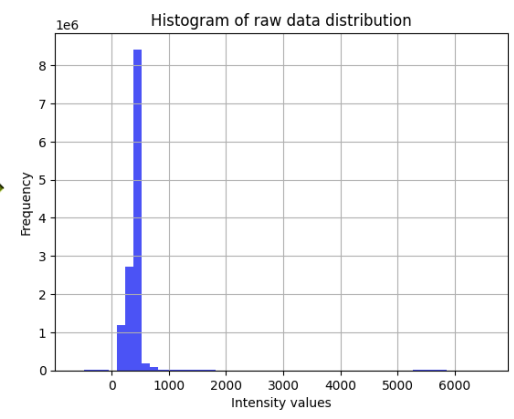
### □ Post-Processing:

**NumPy:** Used for efficient array computations, particularly effective in handling large GC-IMS datasets

**Pandas:** Employed for data input/output (I/O) operations and manipulation of tabular data

**Matplotlib and Seaborn:** Used for data visualization, aiding in the clear representation of the analysis results

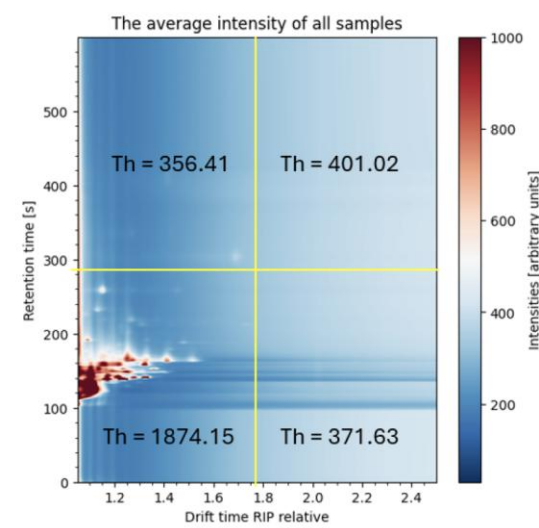
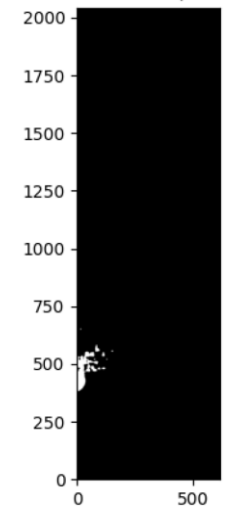
Vocal software  
(G.A.S., Germany)



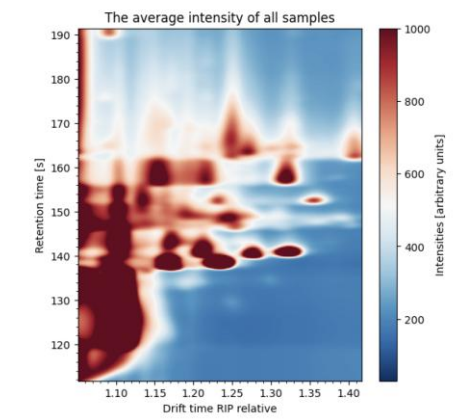
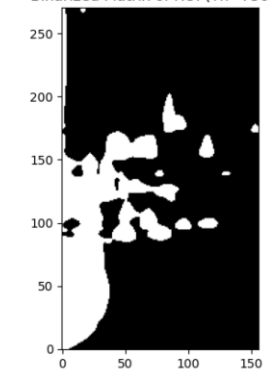
After drift time alignment

Region Of Interest selection;  
threshold value; binarizing

Binarized Matrix (Th=750.8)



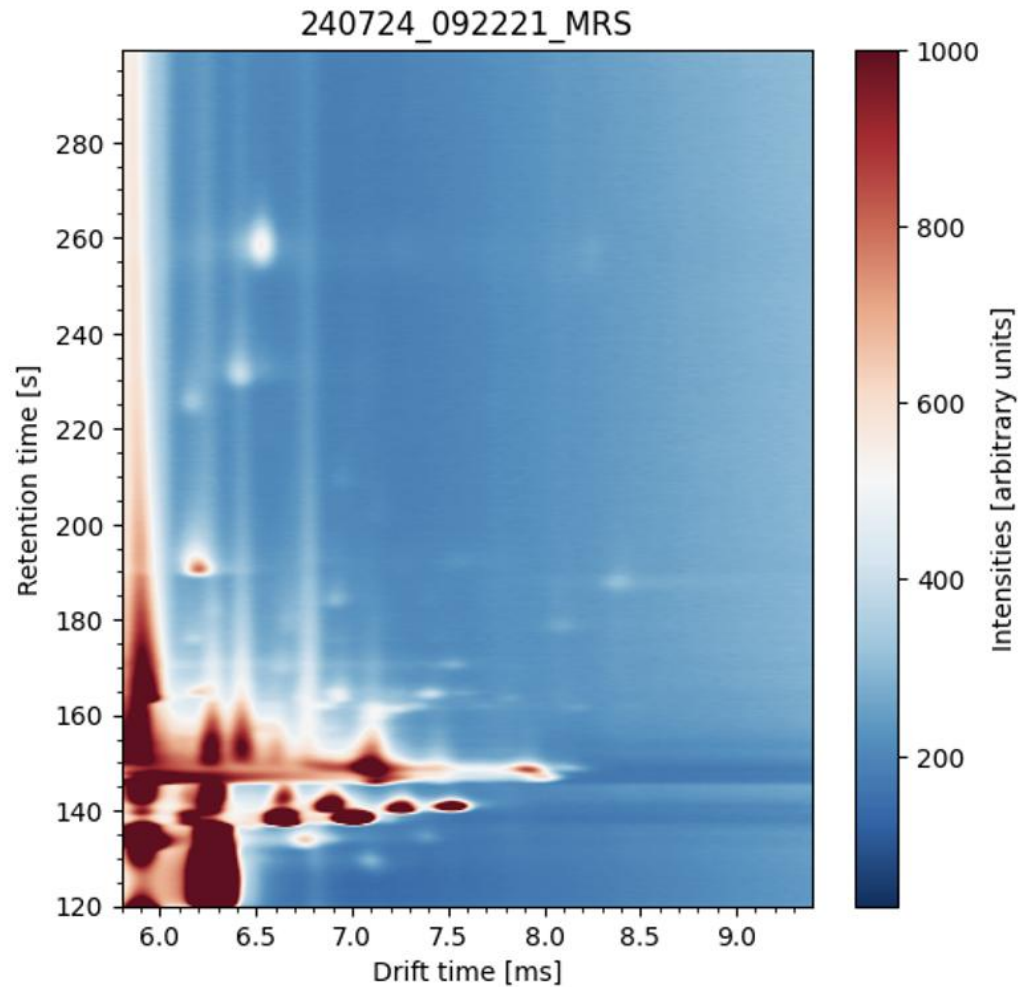
Binarized Matrix of ROI (Th=750.8)



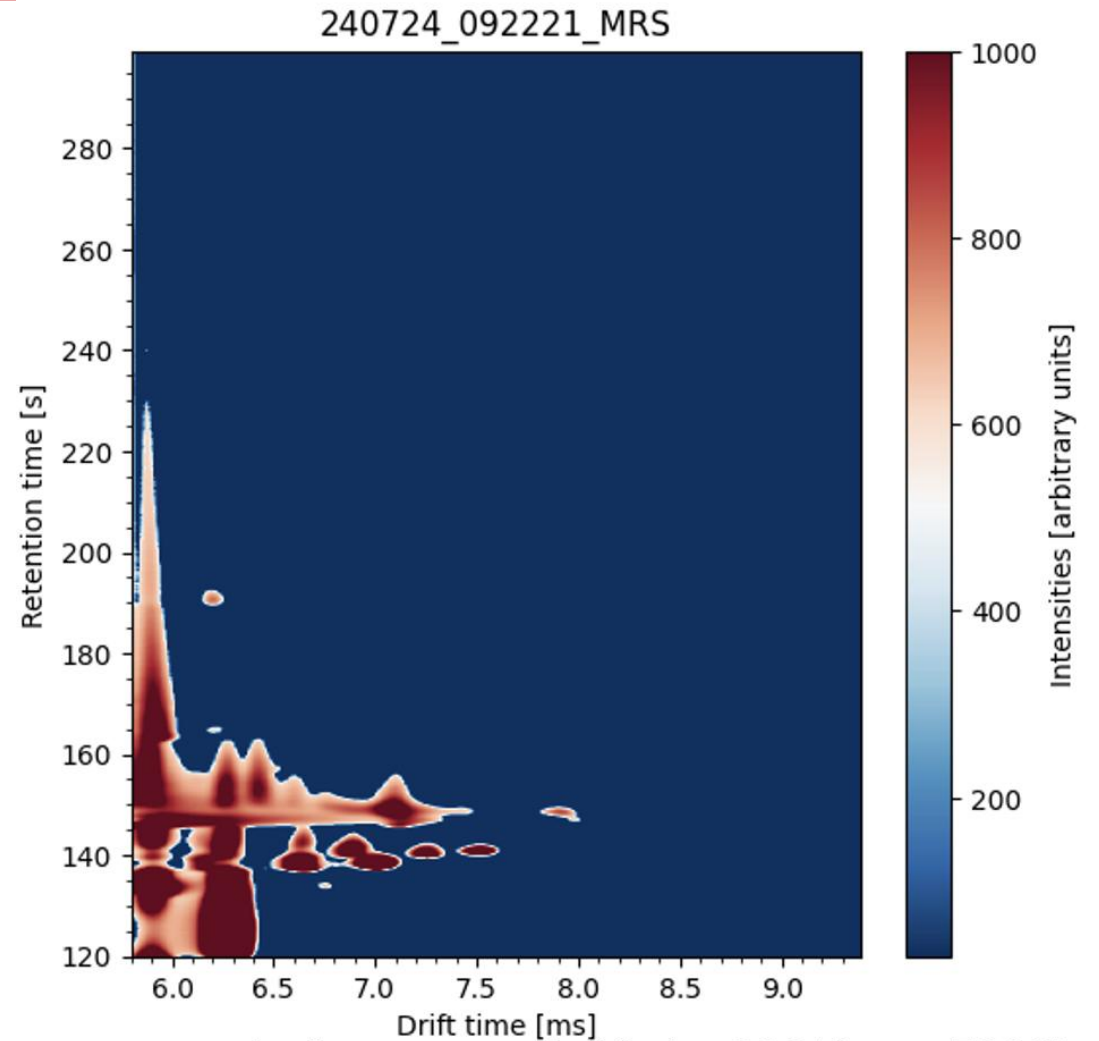
Average intensity matrix with 4 regions



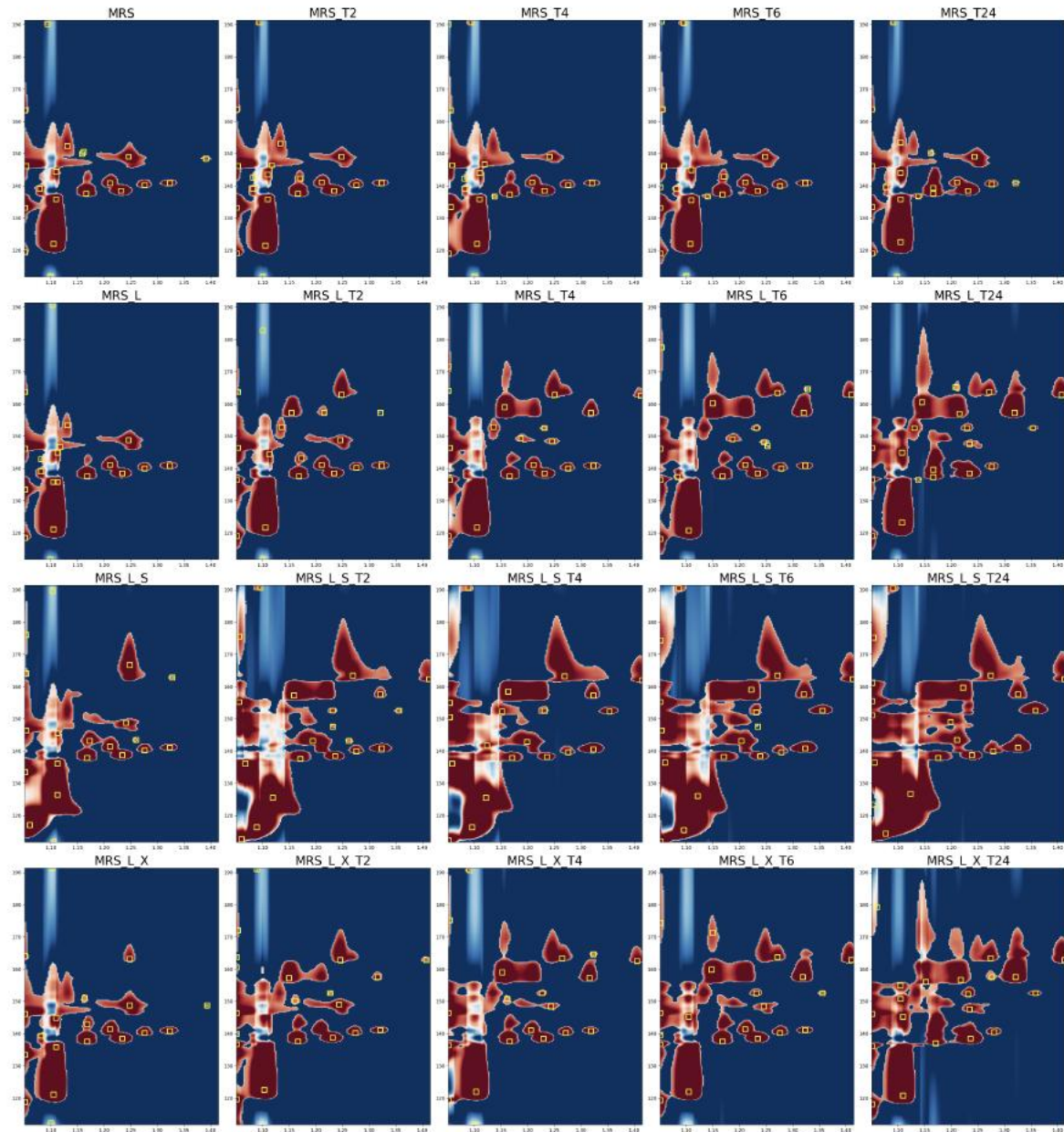
## Quality of “new fermented ingredients”



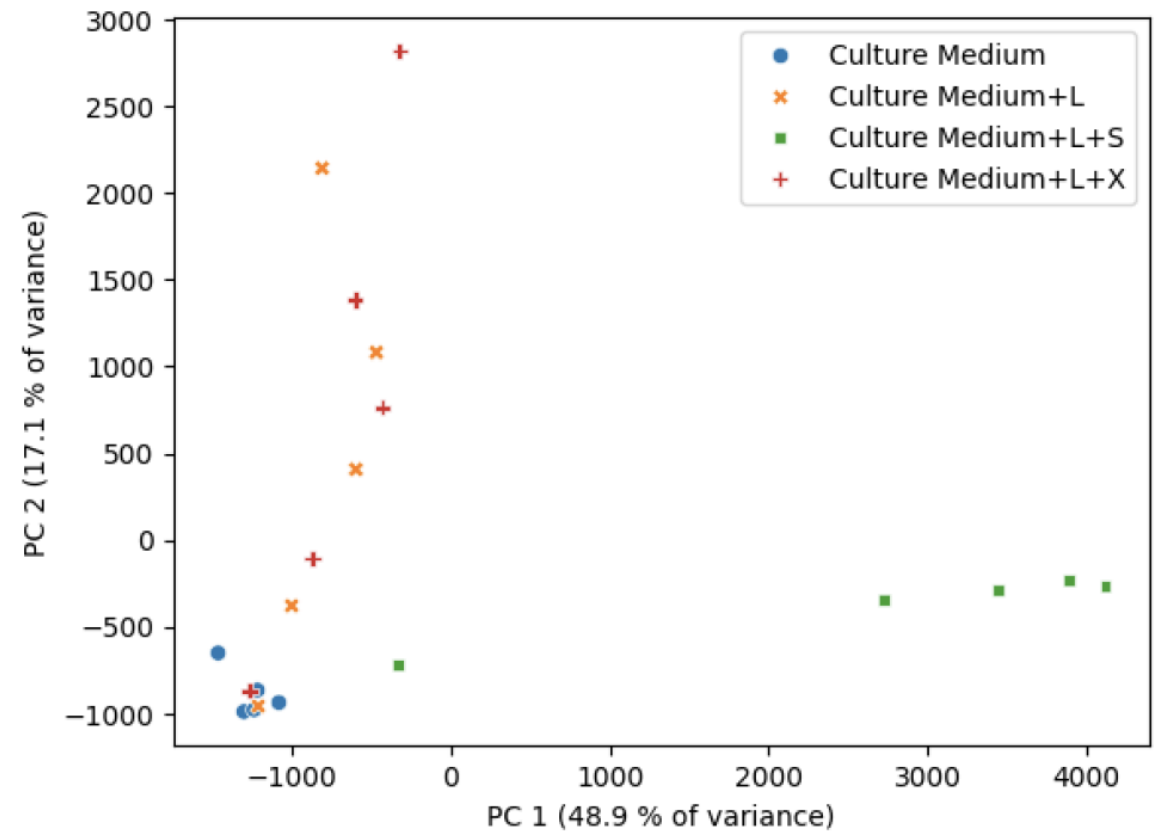
**Before AI processing**



**After AI processing (noise elimination);  
20 significant peaks identified**



20 significant peaks in all the samples  
(not-contaminated vs artificially-contaminated)



PCA score after preprocessing and AI processing

## Case study 3: water (Food Contact Materials: recycled PET)



PET

VS

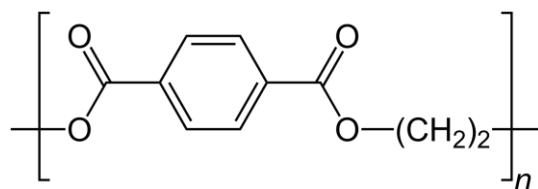


r-PET

VS



GLASS



**In collaboration with: Leader Italian Company  
in bottled mineral water production**

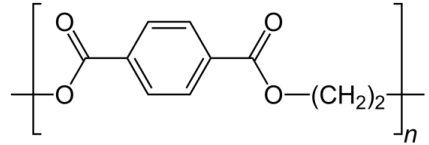
**Impact:**

- ☐ pH
- ☐ Temperature (environment...)
- ☐ Material nature/process (e.g. deodorization)

# Case study: water (Food Contact Materials: recycled PET)

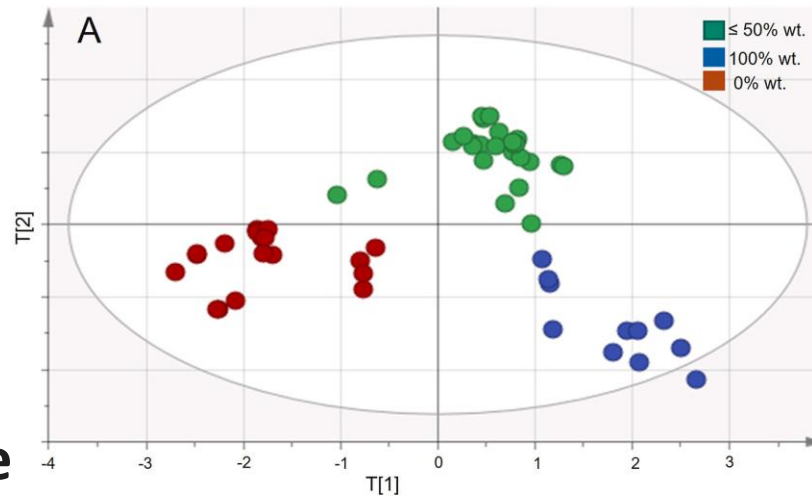


r-PET

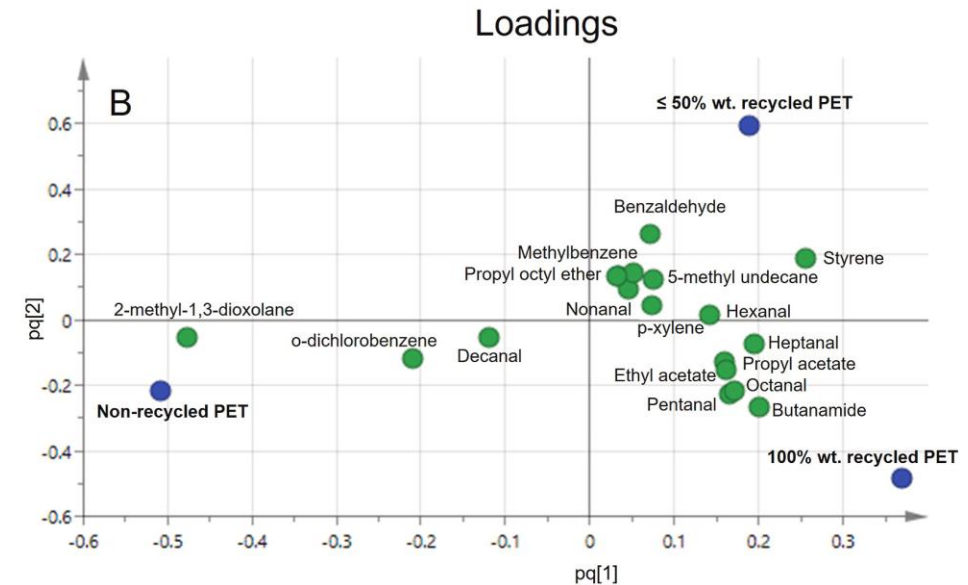


Potential migration of:

- ☐ Benzene
- ☐ Acetaldehyde
- ☐ Benzaldehyde
- ☐ Limonene
- ☐ 2-methyl-1,3-dioxolane
- ☐ 5-methyl undecane
- ☐ Penta...decanal
- ☐ and more...

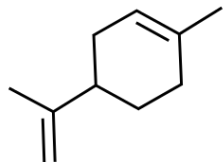


Penalver, Rosa, et al. "Authentication of recycled plastic content in water bottles using volatile fingerprint and chemometrics." *Chemosphere* 297 (2022): 134156.

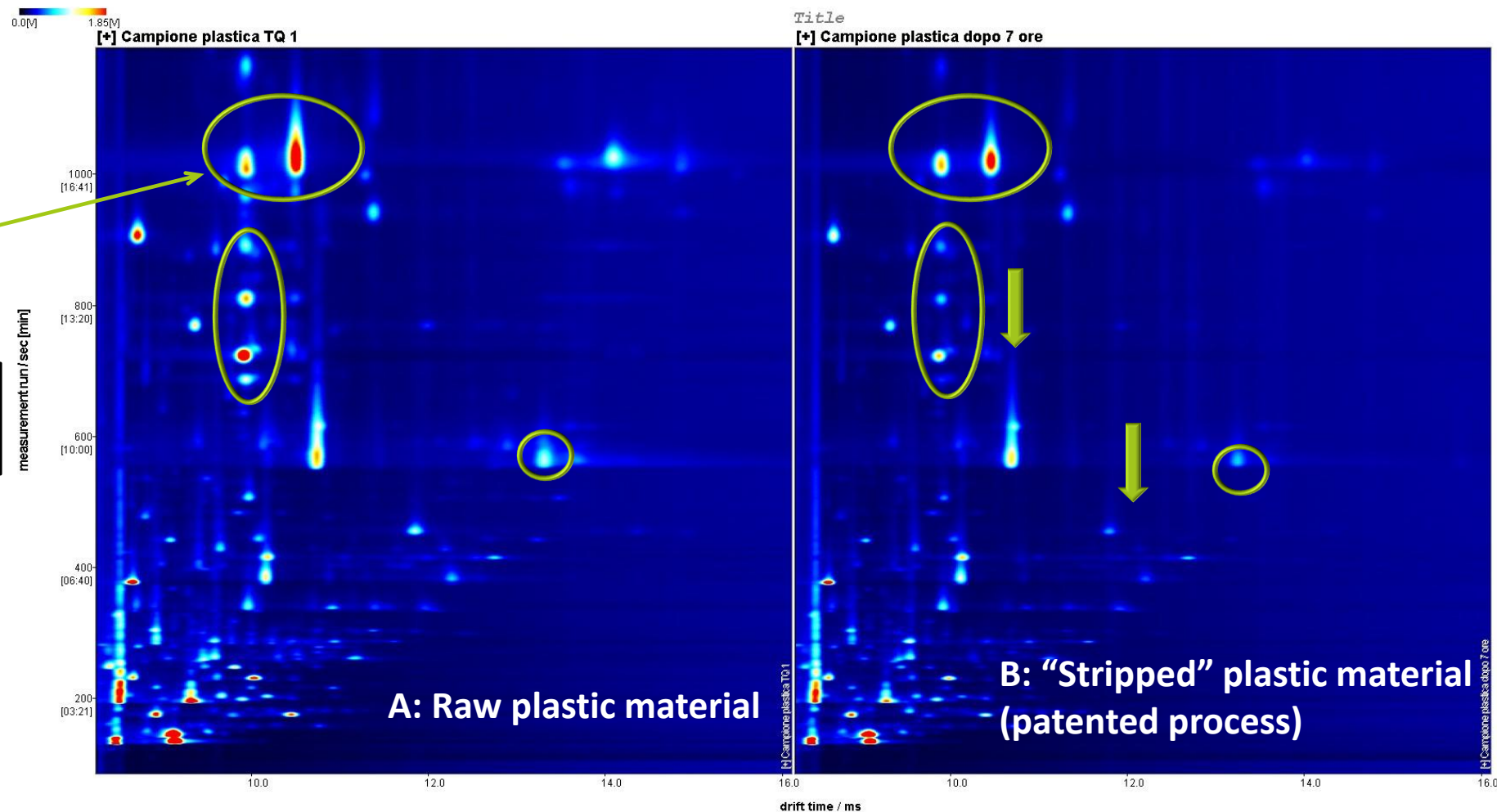




# Case study: water (Food Contact Materials: recycled PET)

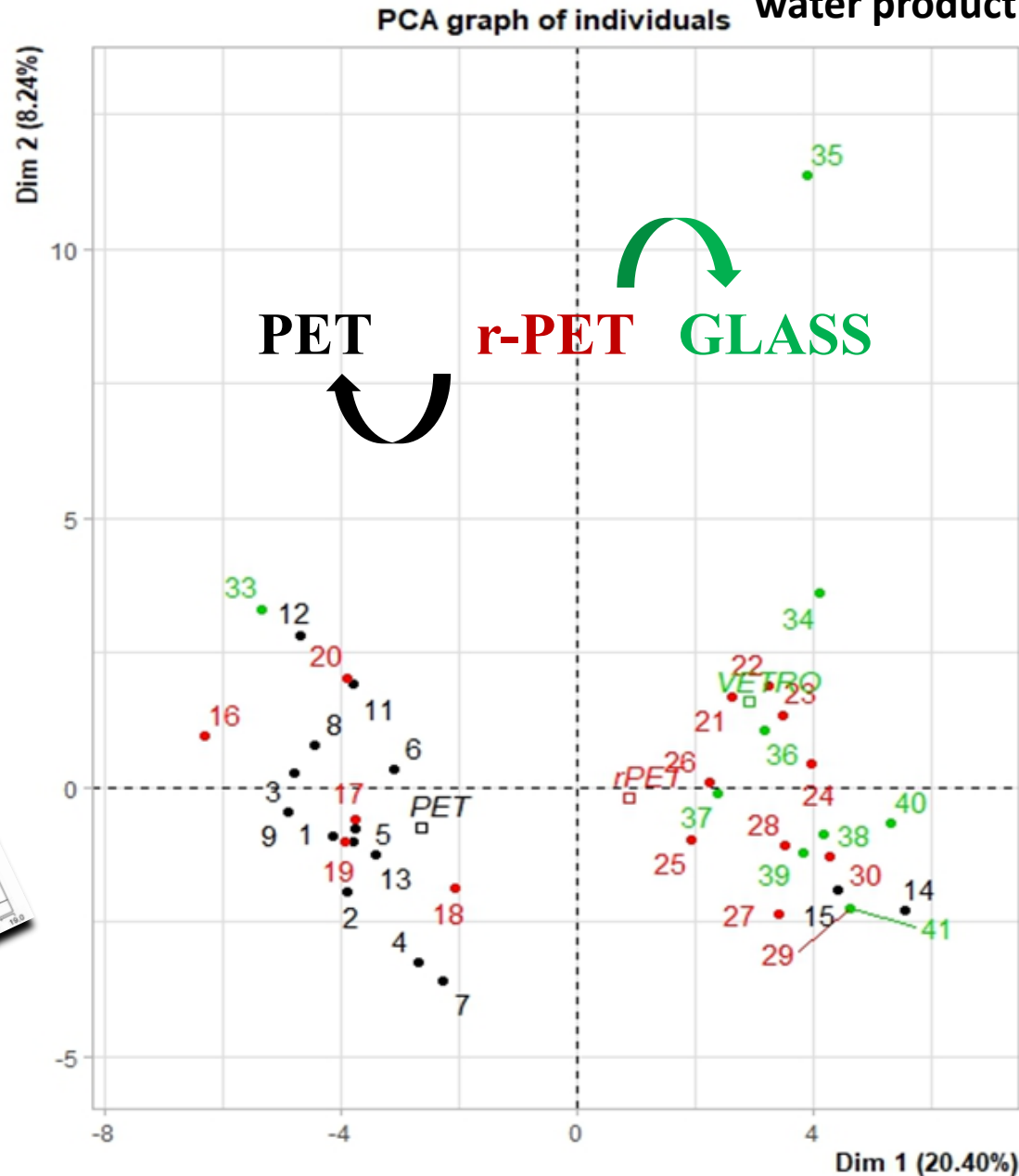
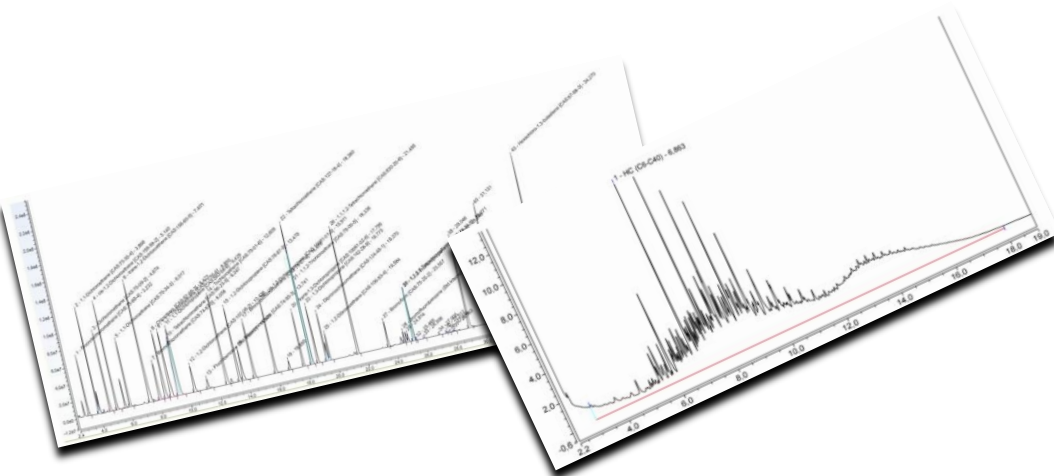


Limonene  
(monomer and dimer)

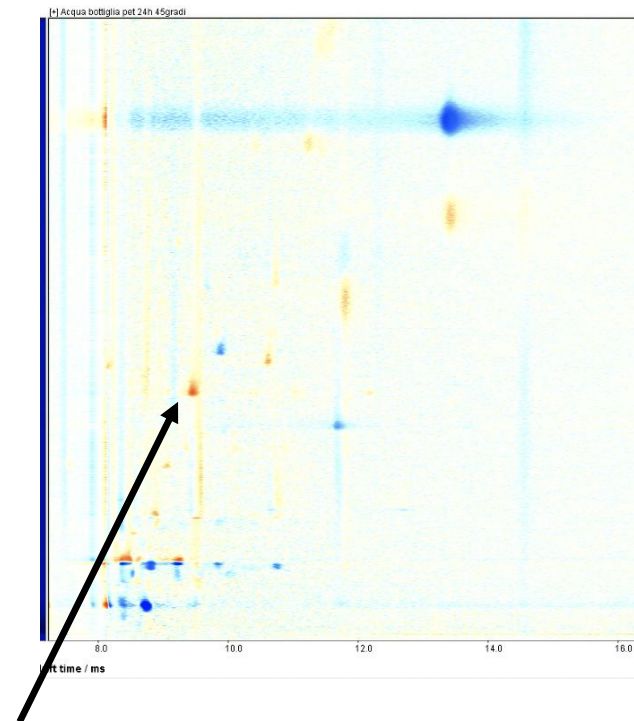
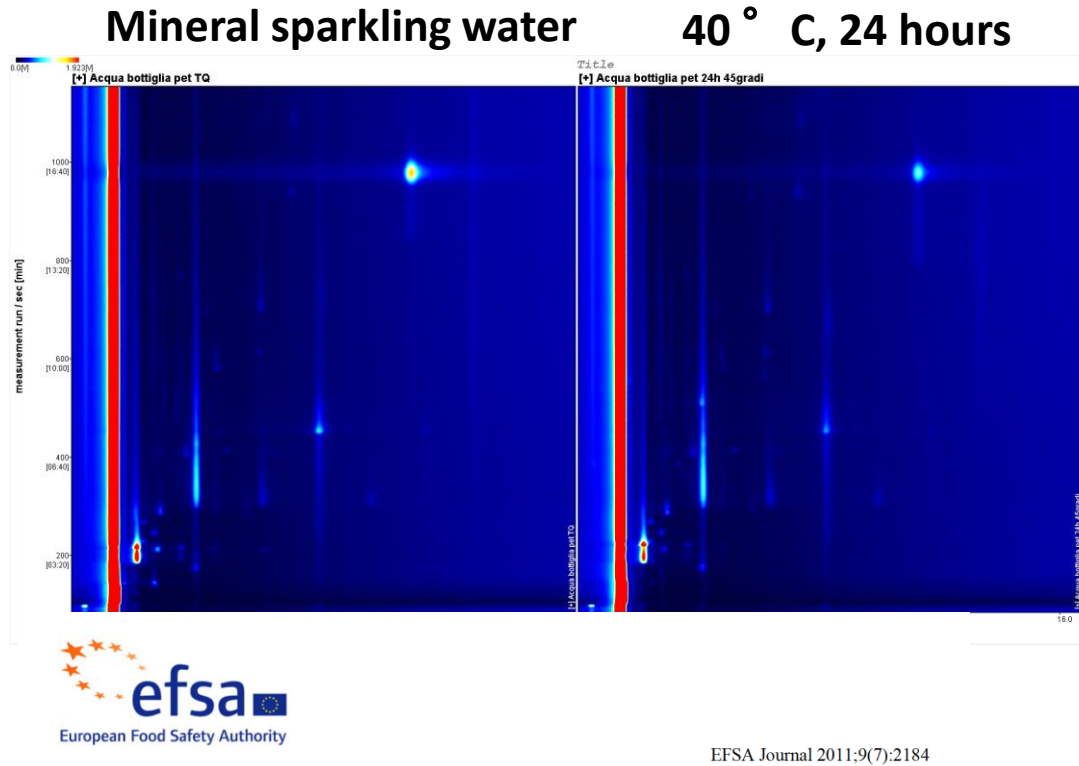


## Water “fingerprint” (different sources; different bottle materials)

- pH
- GC-FID
- GC-MS
- ICP-OES
- IC



# Case study: water (Food Contact Materials: recycled PET)



Benzaldehyde

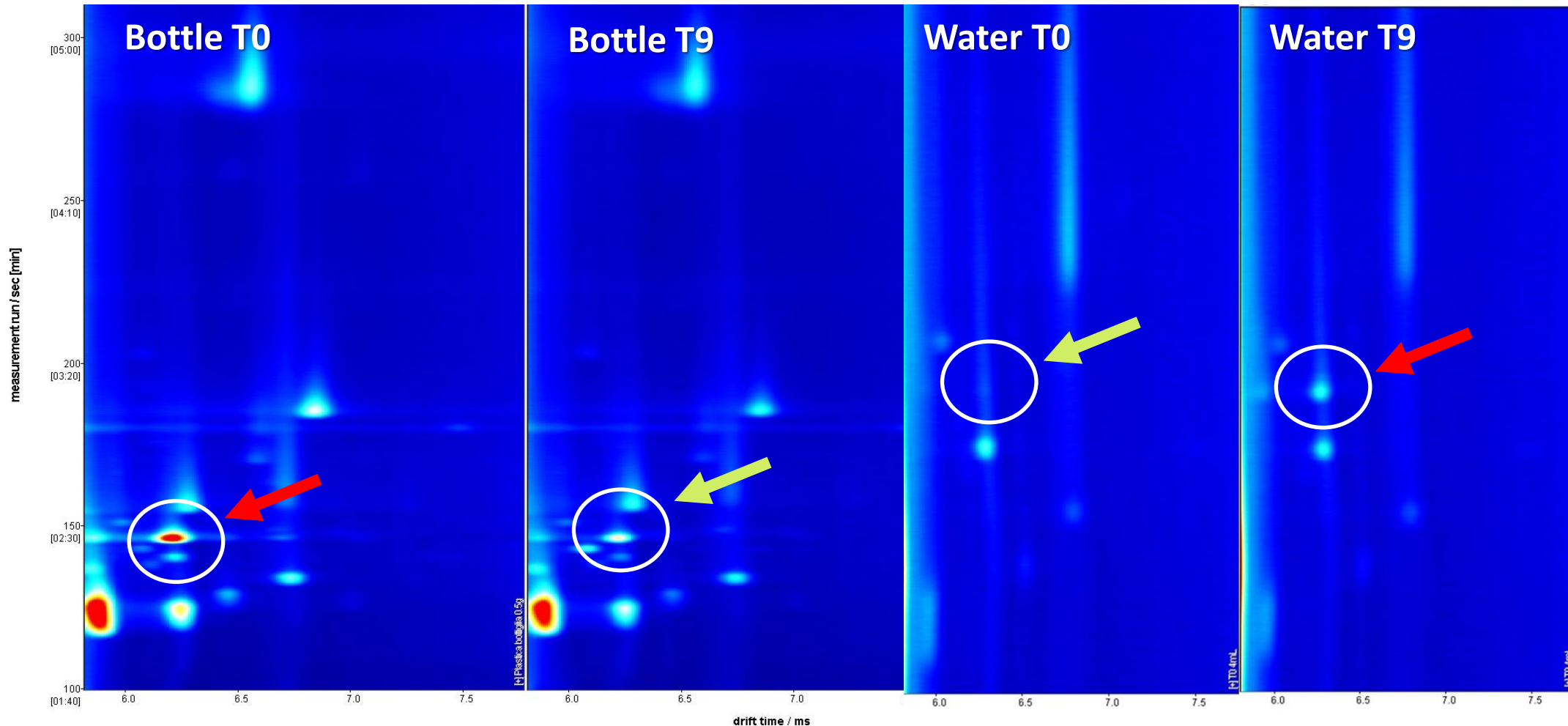
## SCIENTIFIC OPINION

Scientific Opinion on the criteria to be used for safety evaluation of a mechanical recycling process to produce recycled PET intended to be used for manufacture of materials and articles in contact with food<sup>1</sup>

EFSA Panel on food contact materials, enzymes, flavourings and processing aids (CEF)<sup>2,3</sup>

## Non-targeted monitoring of water “integrity”

70 ° C; 9 days



Ongoing work...



## Conclusions

- **GC-IMS is a powerful tool to distinguish among samples (non-targeted or targeted approach)**
- **The data fusion (including sensorial analysis) is a natural development of the GC-IMS analysis**
- **The development of rapid methods (at line/on line) will permit a more performing quality/safety control**
- **AI will permit further optimisation of this technique...**

# Acknowledgements

**Prof. Matteo Bordiga**  
(DSF-UPO, Italy)  
Food Chemistry Group



**IS** Lab Service  
analytica Analytica



G.A.S. Gesellschaft für  
analytische Sensorsysteme mbH

A special thanks for collaboration and support:



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**Thanks for your kind attention...**

