Creation of a database of fermented product volatilomics

Analysis of VOCs by dynamic headspace
combined with extraction by magnetic bar sorption (Twister SBSE)

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Maud Lemois – INRAE *Ferments du futur*

Summary

- About Sayfood unit & « Ferments du Futur » program
- MetaVolFood platform
- Project Overview: Study of Commercial Fermented Products
  - Water Kefir : Method comparison
  - Water Kefir : Product comparison
  - Perspectives

About SayFood unit

SayFood Joint Research Unit – INRAE / AgroParisTech / Université Paris-Saclay

A leading research unit dedicated to food engineering and bioproducts.

- **Location:** Based at the Paris-Saclay campus (Palaiseau, France).
- **Mission:** To design sustainable food systems and innovative transformation processes.
  - Interdisciplinary approach: food science, microbiology, analytical chemistry…

Ferments du Futur program

A public-private partnership supported by

INRAE *National Research Institute for Agriculture, Food and the Environment*

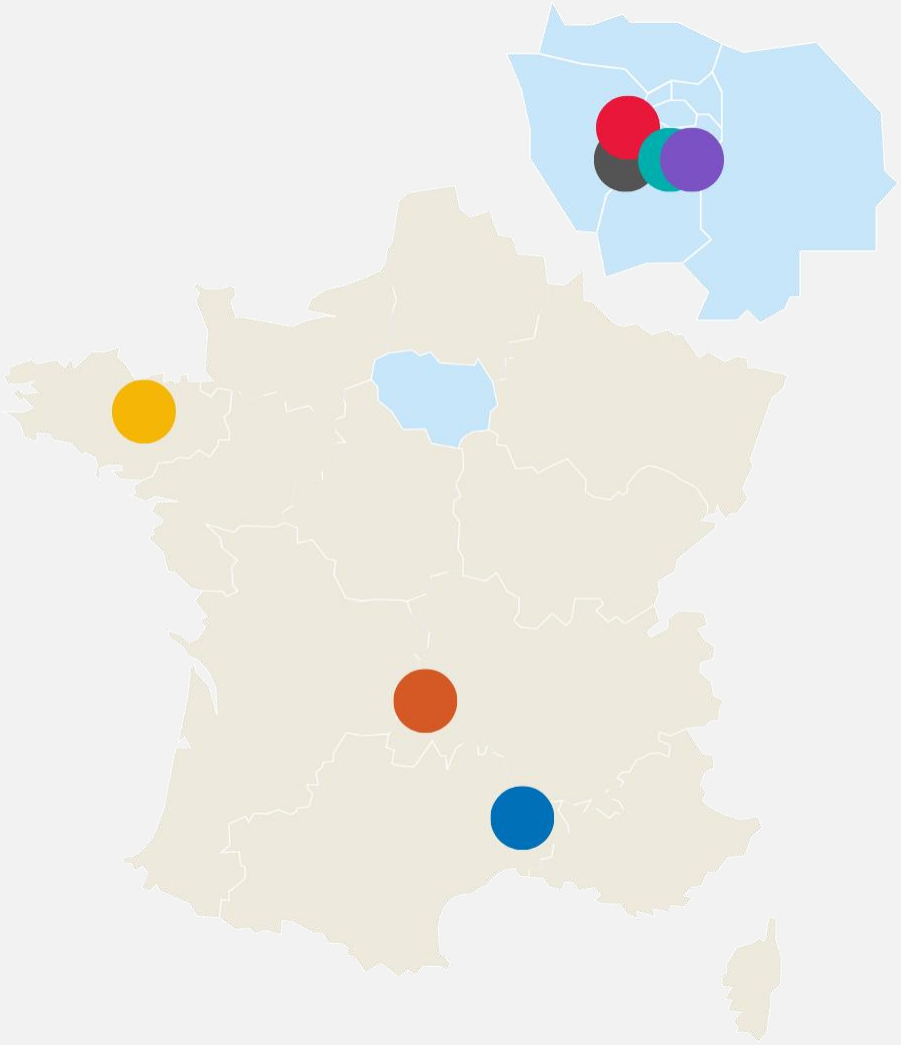
ANIA *National Food Industries Association*

Accelerate research and innovation in the field of ferments and fermented foods

Ambition:

- Enhance food safety and shelf-life.
- Improve nutritional and organoleptic qualities.
- Develop new plant-based fermented products.

Ferments du Futur program : the distributed platform



SPO: Sciences pour l'Œnologie
@Montpellier; INRAE, Univ. Montpellier, Institut Agro; 28 scientists

STLO : Science et Technologie du Lait et de l'Œuf
@Rennes; INRAE, Institut Agro; 35 scientists

UMRF: Unité Mixte de Recherche sur le Fromage
@Aurillac; INRAE, Univ. Clermont-Auvergne, VetAgro Sup; 5 scientists

MICALIS: MICrobiologie de l'ALImentation au service, de la Santé
@Jouy en Josas; INRAE, AgroParisTech, Univ. Paris-Saclay; 109 scientists

SAYFOOD: Ingénierie des aliments et bioproduits
@Palaiseau; INRAE, AgroParisTech, Univ. Paris-Saclay; 25 scientists

MGP: MetaGenoPolis,DPI analyse du microbiote
@Jouy en Josas; INRAE; 9 scientists

MAIAGE: Mathématiques et Informatique Appliquées du Génome à l'Environnement
@Jouy en Josas; INRAE; 37 scientists

About MetaVolFood platform

- Platform dedicated to the analyses of metabolites originating from fermented food matrices.

What is the metabolomics ?

Analyzing the complete set of metabolites in a system to characterize biochemical transformations driven by microbial fermentation.

- Part of ***Ferments du Futur*** program.
- Hosted at SayFood unit – CoMiAl team (Food Microbial Communities).
- Closed collaboration with academic research and industrial partners.

About MetaVolFood platform

MetaVolFood
Food Metabolomics & Volatilomics Platform

Metabolomics

UHPL-HRMS Orbitrap 240
(ThermoFisher)

Untargeted metabolomics and volatilomics

Targeted qualitative and quantitative analyses

Elucidation of metabolic pathways

Volatilomics

GC 8890-MS/MS 7010C (Agilent)
MultiPurpose Sampler (Gerstel)

RIC group

Project Overview: Study of Commercial Fermented Products

Establish a metabolomics and volatilomics database
on a wide range of commercial fermented products

Kefir

Cheese

Kimchi

Natto

Project Overview: Study of Commercial Fermented Products

1st Step : Define analytical parameters in GC-MS

2nd Step : VOC analysis

3rd Step : Determine correlations between LC and GC results

Kefir

Cheese

Kimchi

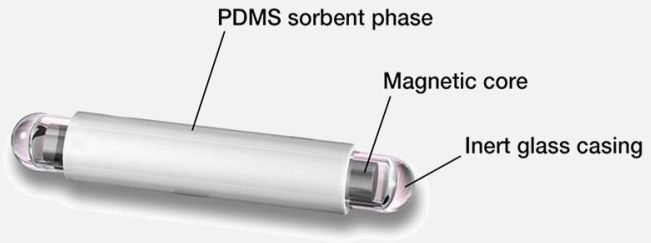
Natto

Project Overview: Study of Commercial Fermented Products

Untargeted analysis
Flavour Profiles (Qualitative)

SBSE

Stir bar sorbtive extraction

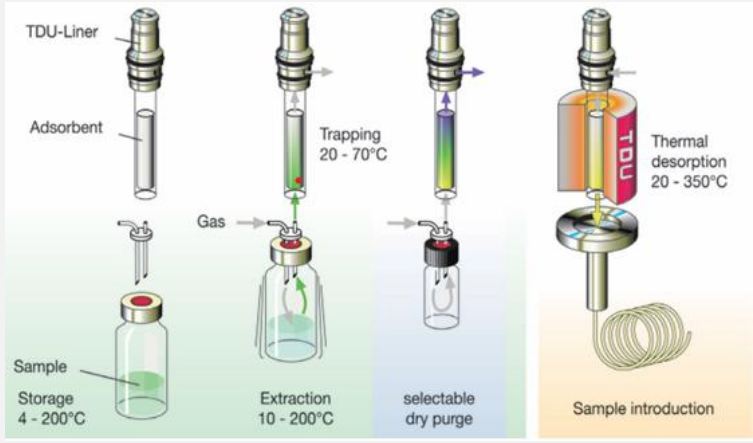


Reference : Gerstel

Extract volatile & semi-volatile retained in the matrix

DHS

Dynamic HeadSpace

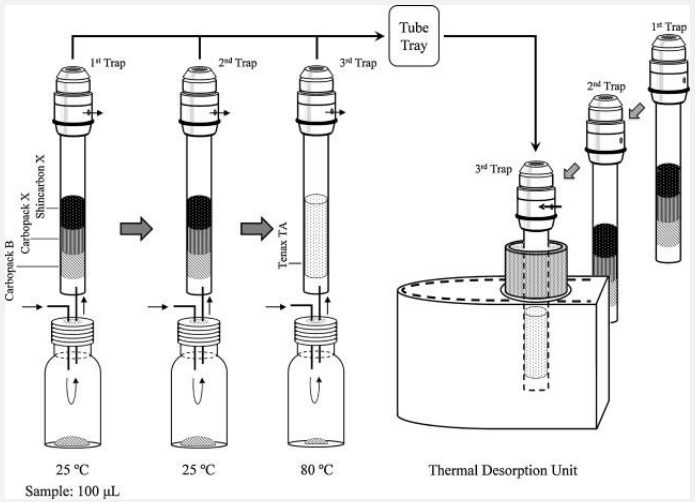


Reference : Gerstel

Aroma profiling and highly volatile fermentation products

MVM

Multi-Volatile Method



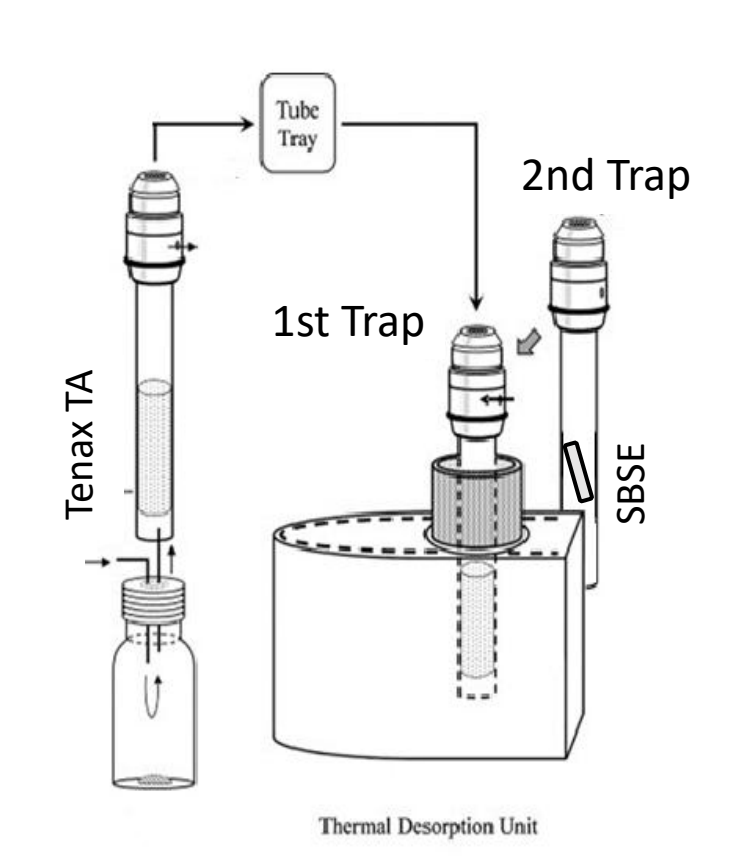
Reference : N. Ochiai et al. / J. Chromatogr. A 1371 (2014) 65–73

Project Overview: Study of Commercial Fermented Products

DHS x SBSE by MVM

1st Desorption - Dynamic Head Space (DHS) : Tenax TA

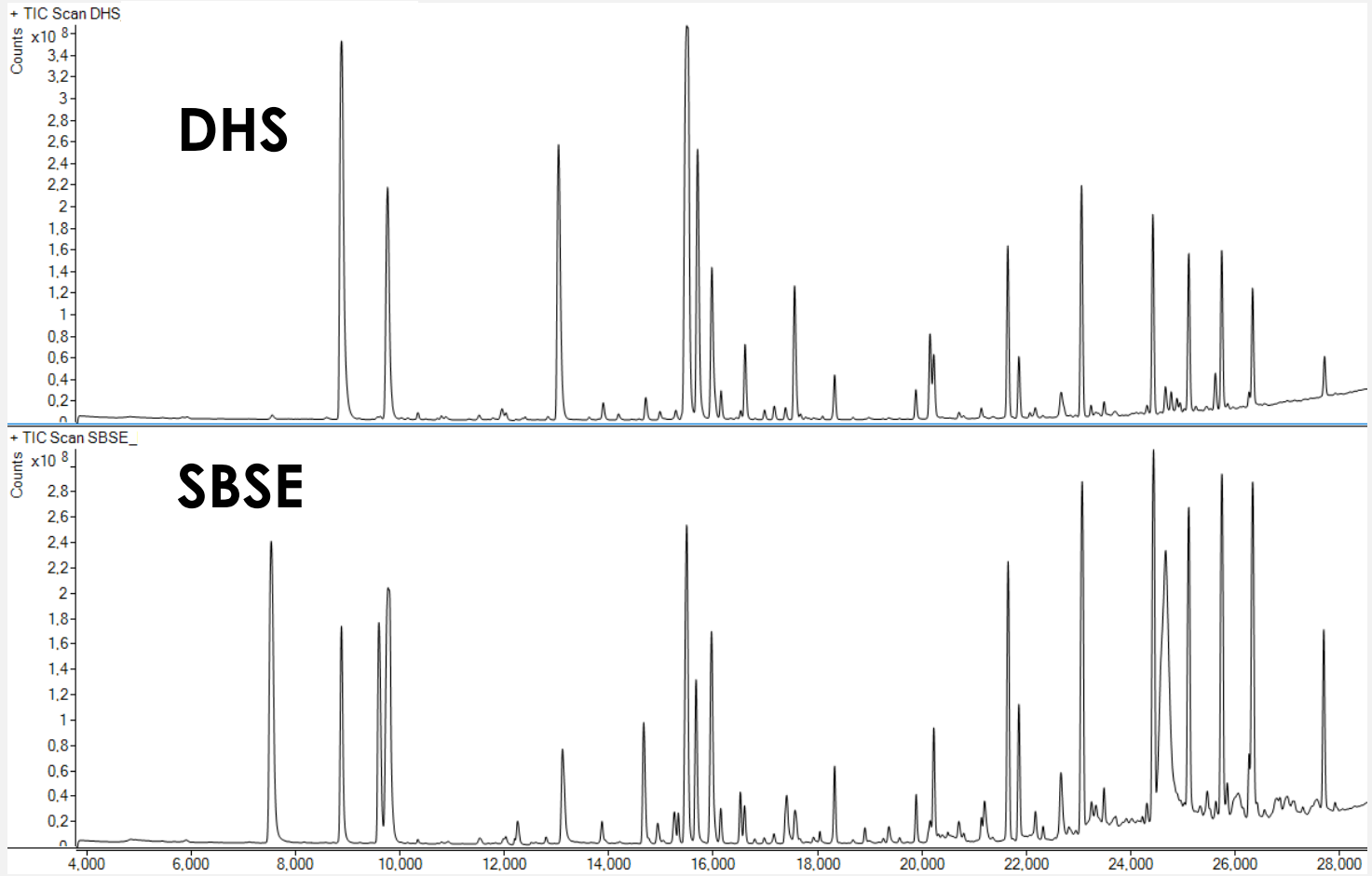
2nd Desorption - Stir bar sorptive extraction (SBSE) : Twister® PDMS 1cm - film 10mm



Project Overview: Study of Commercial Fermented Products

MassHunter Unknown : Deconvolution & Blank Subtraction

R Studio : Statistics & Graphical Representation



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U.S. DEPARTMENT OF COMMERCE

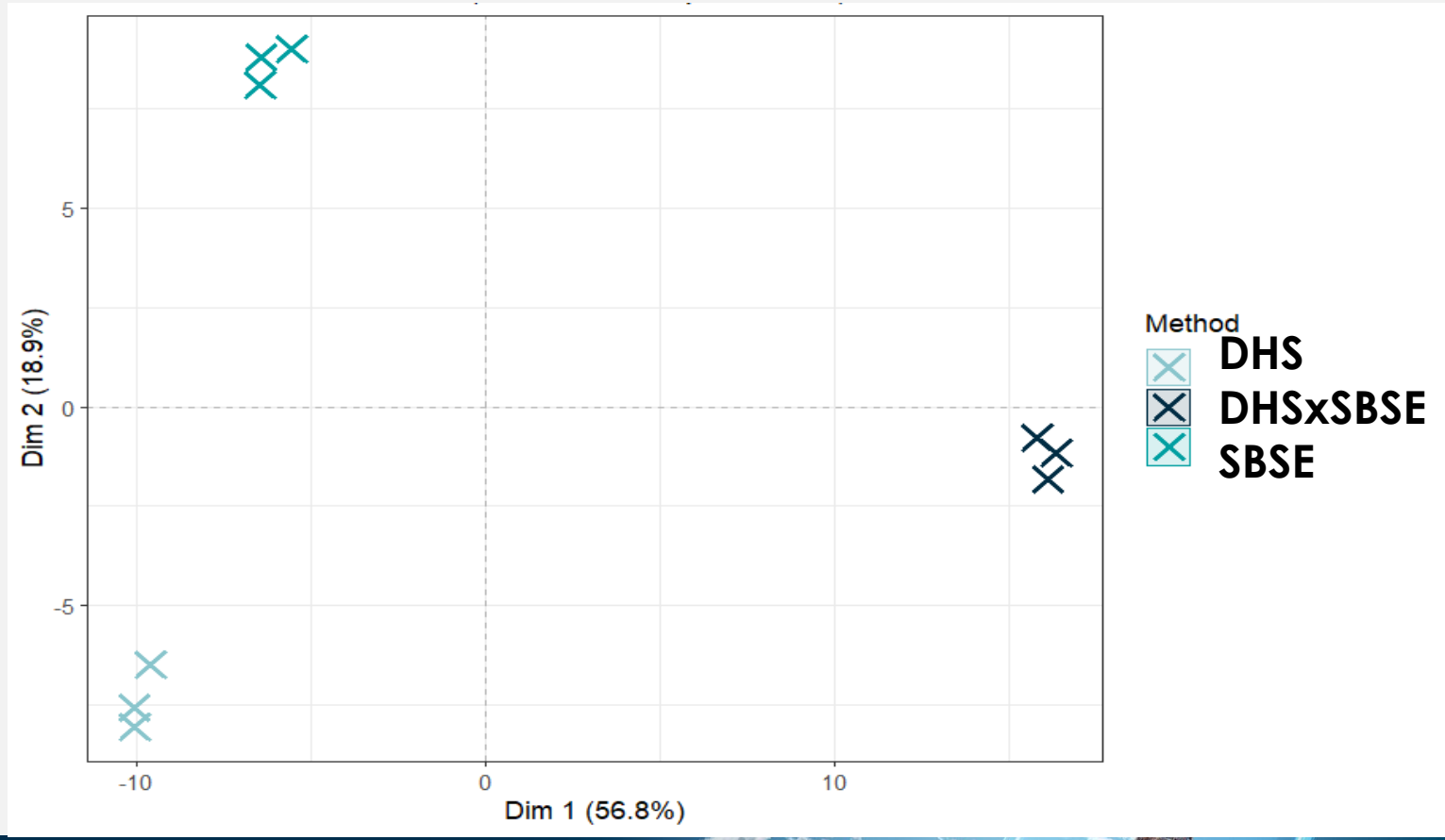
Water Kefir : Method comparison (n=3)

1st Step : Define analytical parameters GC-MS

PCA comparison between DHS, SBSE and DHSxSBSE

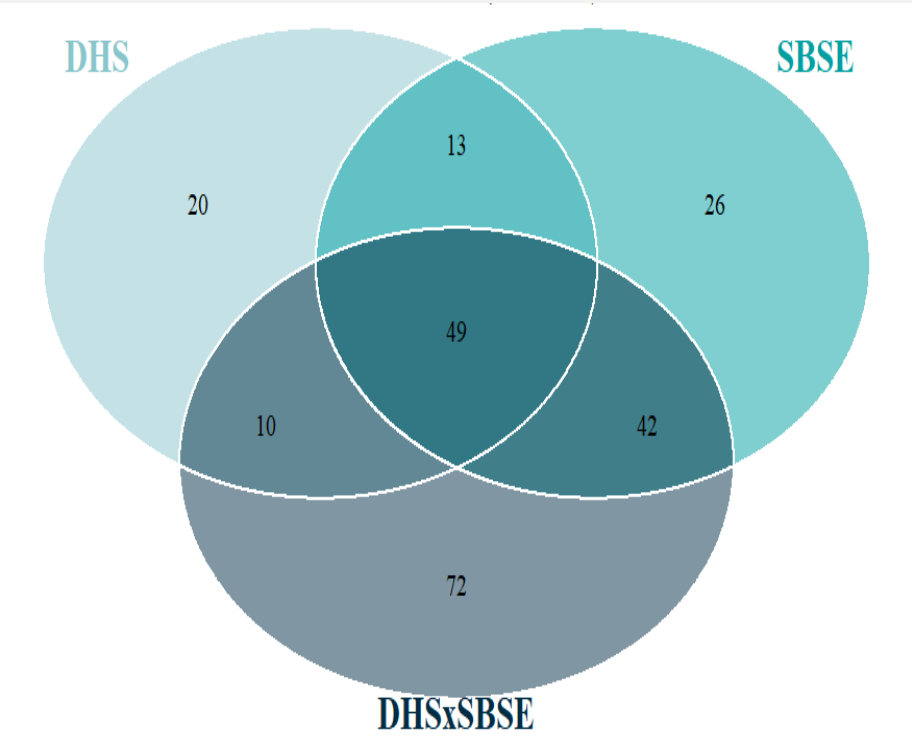
Log + Pareto scaling

Dimension 1 : 56,8%
Dimension 2 : 18,9%

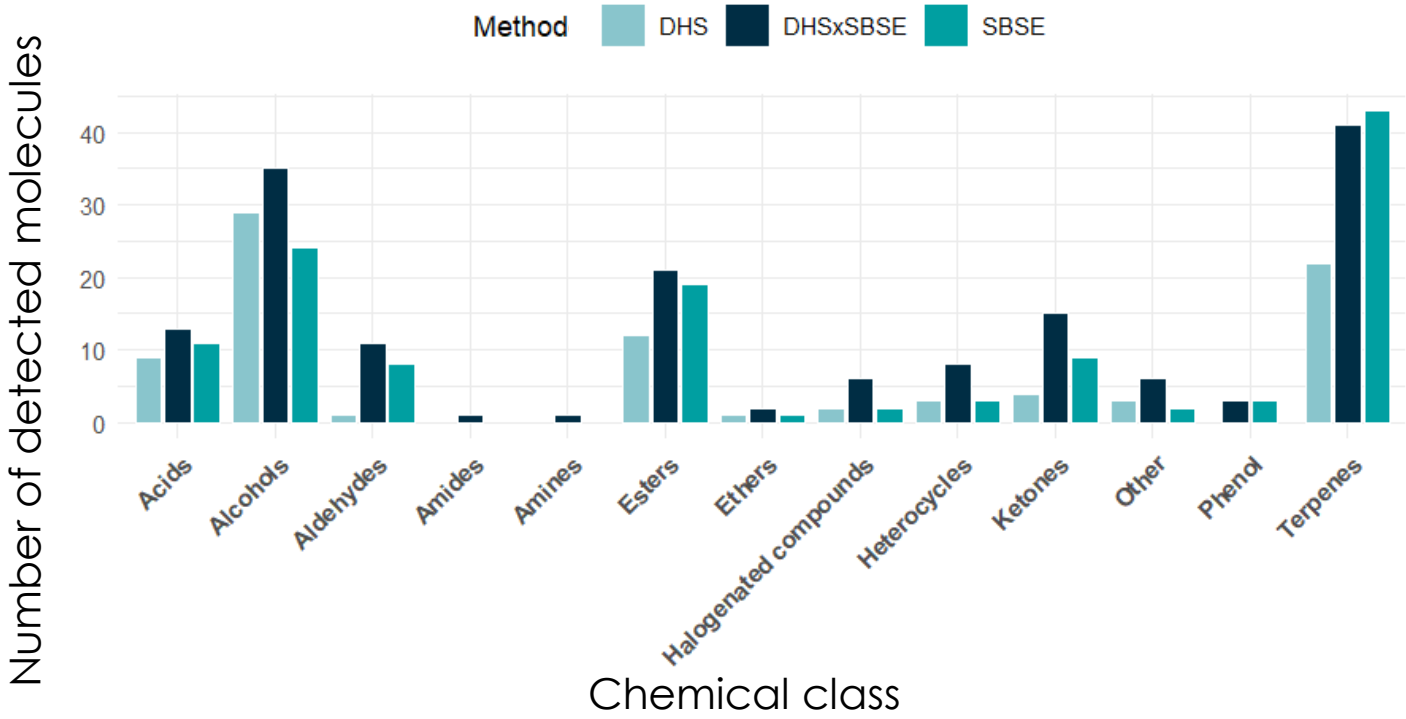


Water Kefir : Method comparison (n=3)

Detected molecules



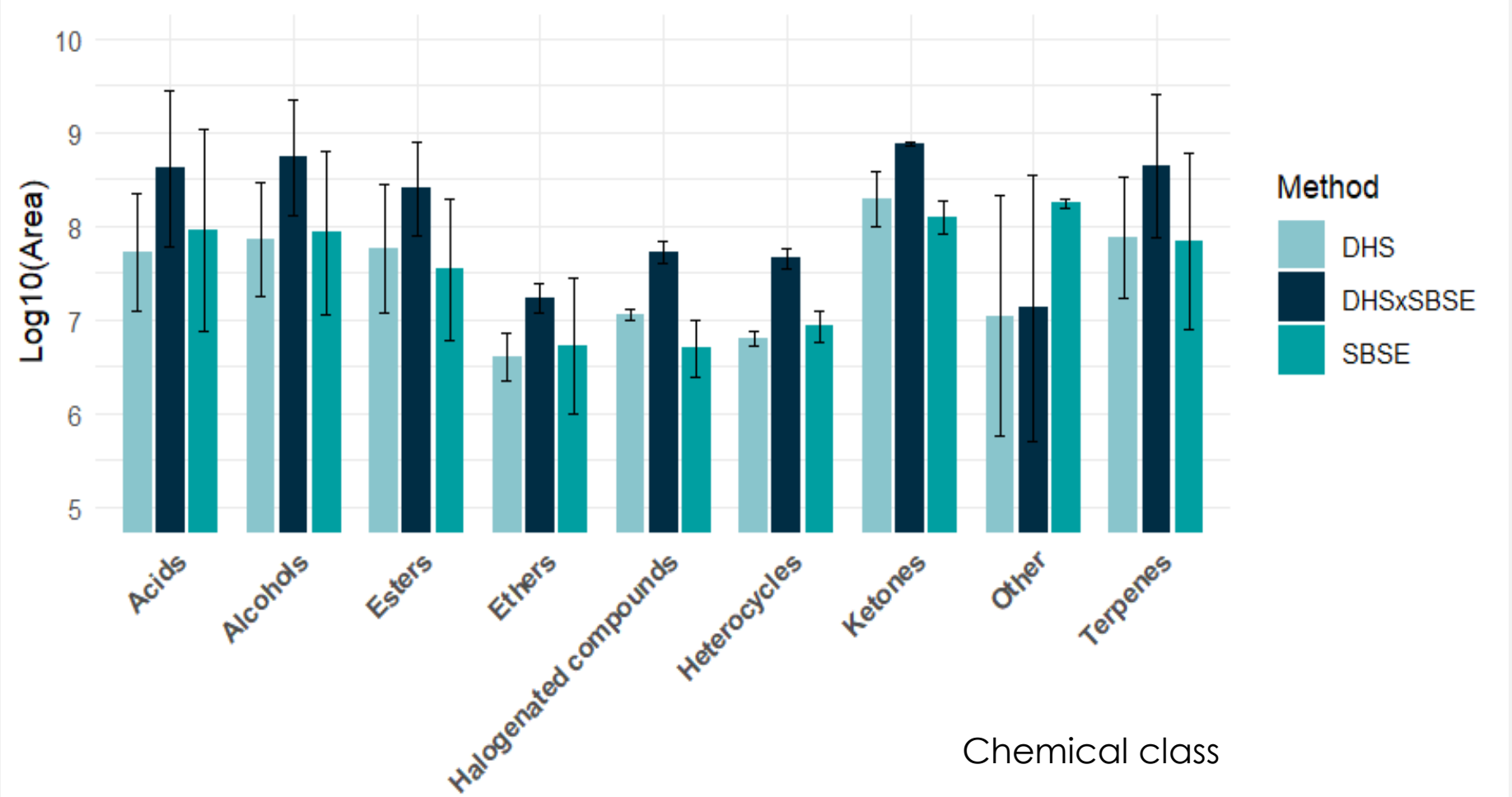
Extraction efficiency by chemical class



DHS = 92 molecules -> 78% found with DHSxSBSE
SBSE = 130 molecules -> 80% found with DHSxSBSE

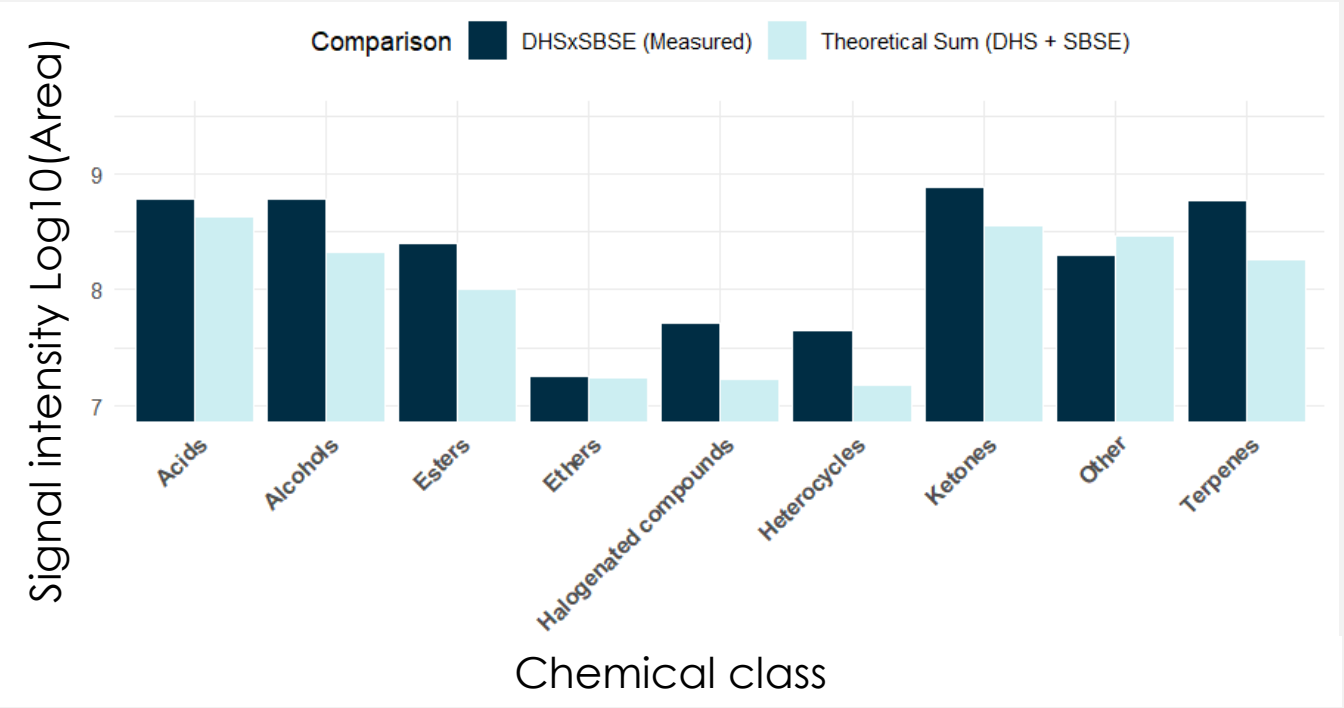
Water Kefir : Method comparison (n=3)

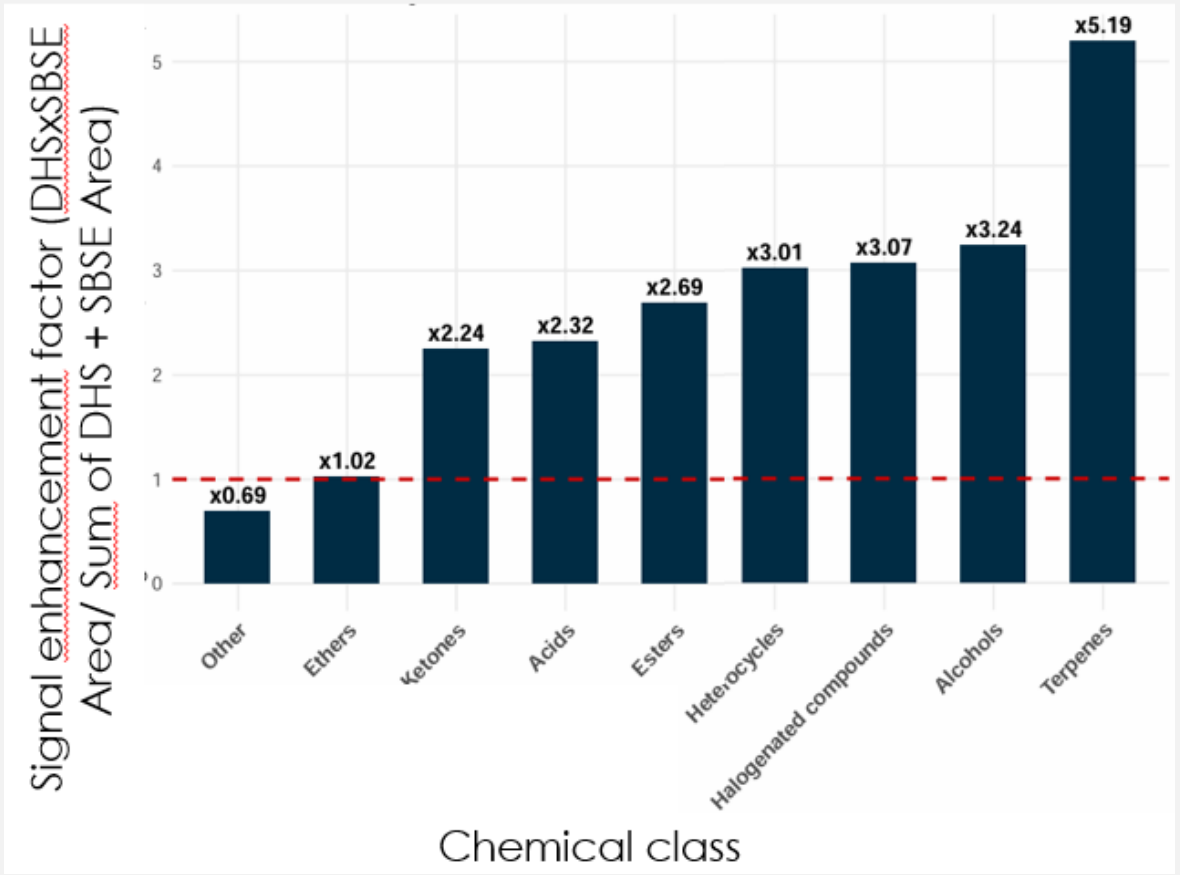
Extract intensities of common molecules by chemical class (Log)



Water Kefir : Method comparison (n=3)

Measured Area DHSxSBSE vs. Calculated Sum (DHS+SBSE)



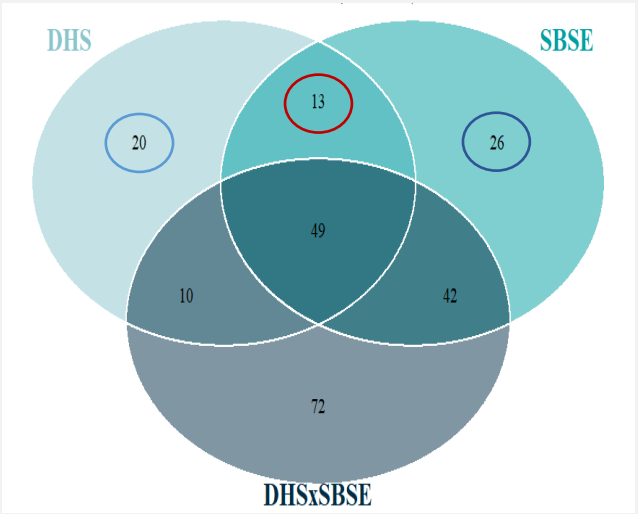


Relative extraction efficiency gain (DHSxSBSE vs. DHS+SBSE)

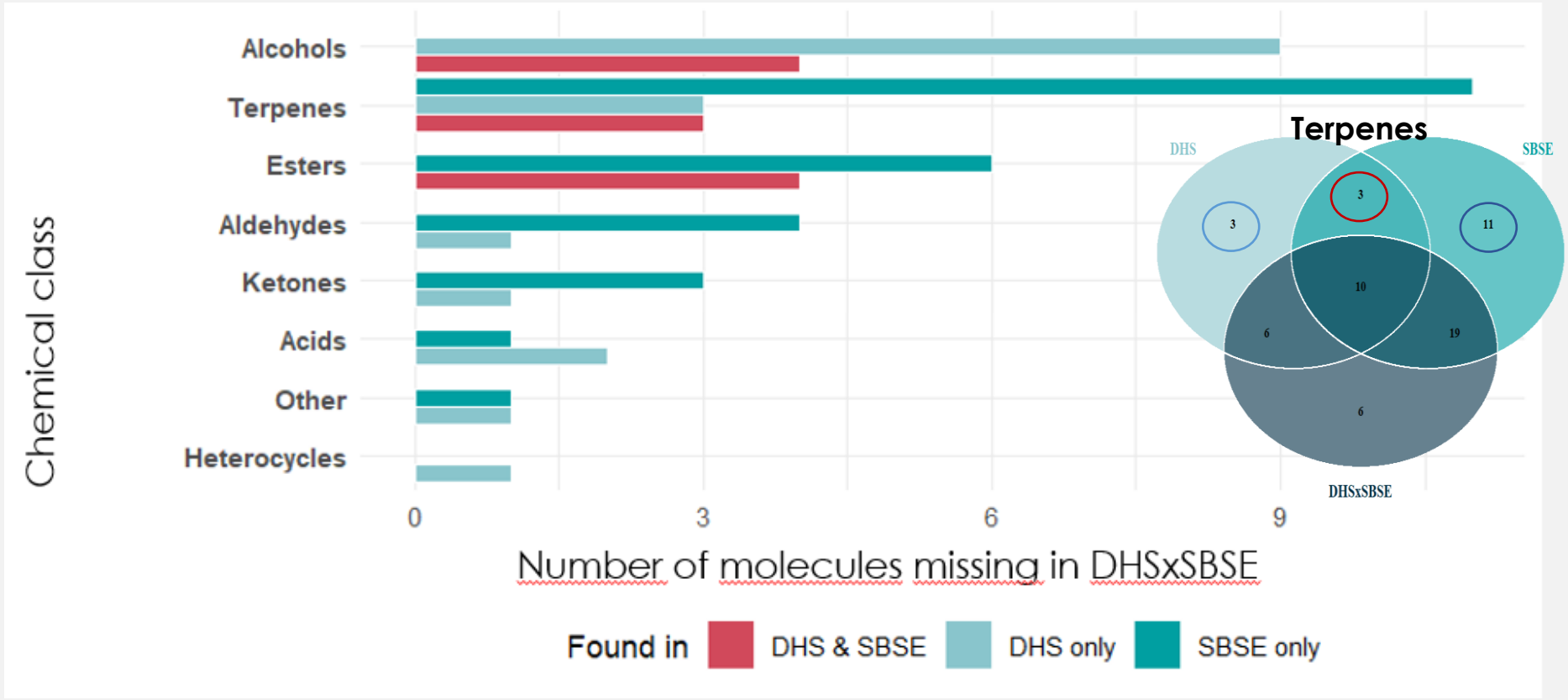
Values > 1 indicate a signal enhancement in the combined method

Water Kefir : Method comparison (n=3)

Detected molecules



59 Compounds missing in DHSxSBSE Method



Water Kefir : Product comparison

Study of 3 **water kefirs from the market** without added flavors.

<u>Water Kefir recipe :</u>

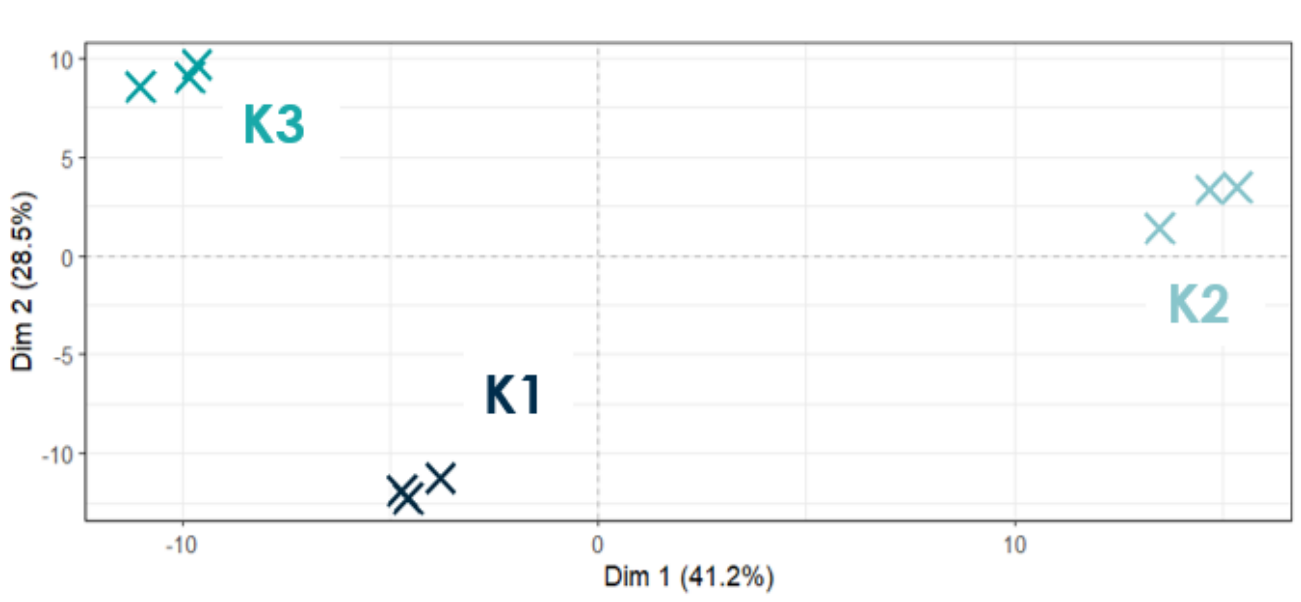
- Kefir grains (ferment)
- Sugar
- Water
- Slice of lemon
- Dried fruit

- Fermentation 24/36h at 20/25°C

Water Kefir : Product comparison (n=3)

2nd Step : VOC analysis by DHSxSBSE

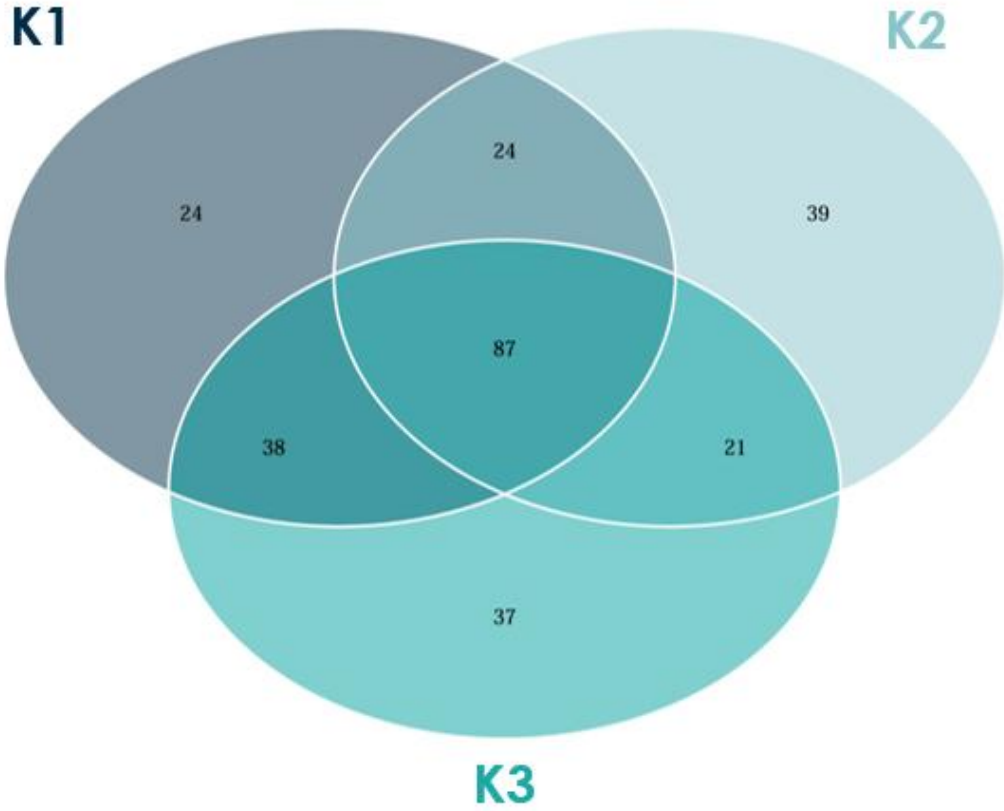
PCA : Water Kefir Comparison



Log + Pareto scaling

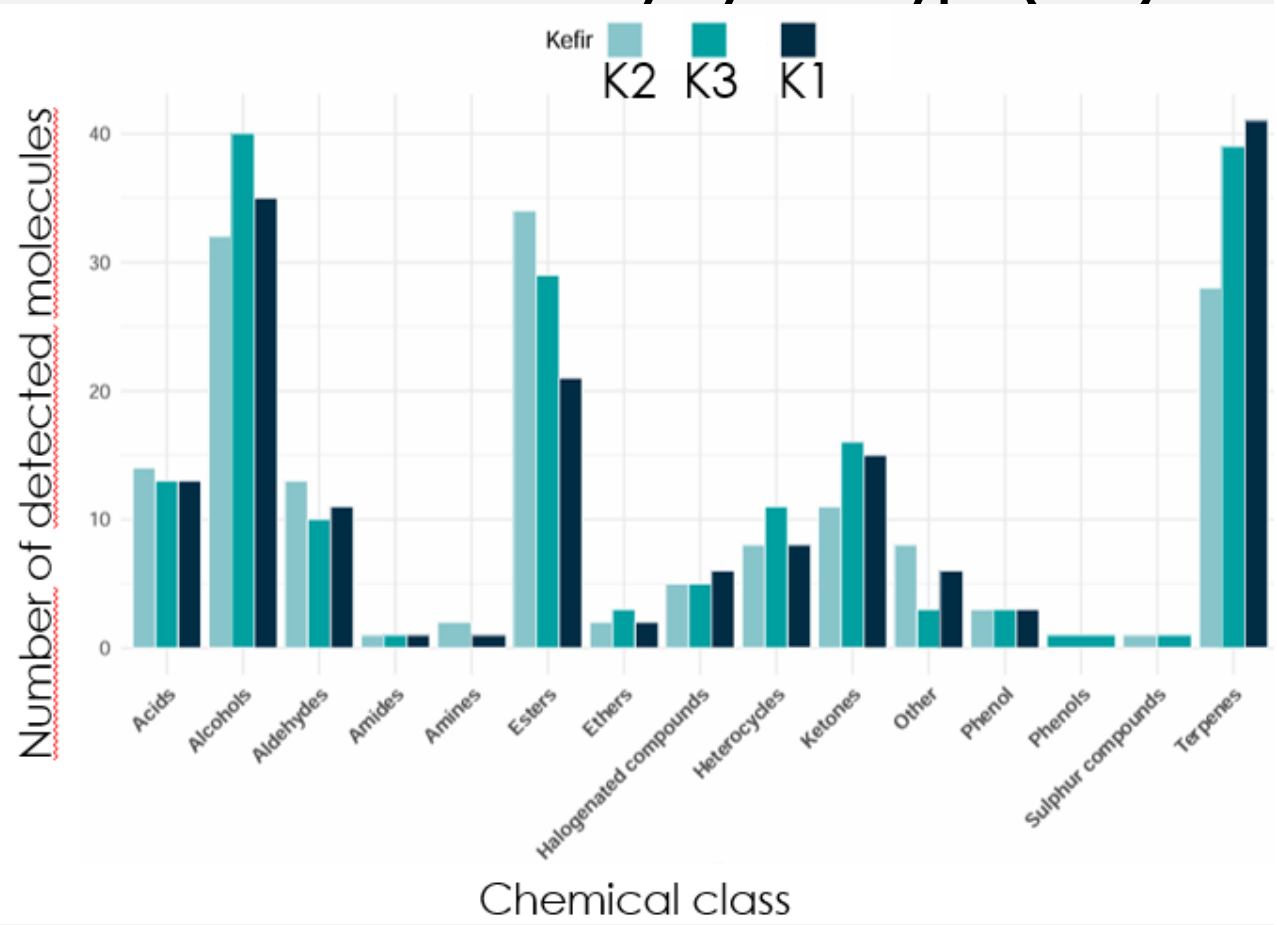
Dimension 1 : 41,2%
Dimension 2 : 28.5%

Detected molecules

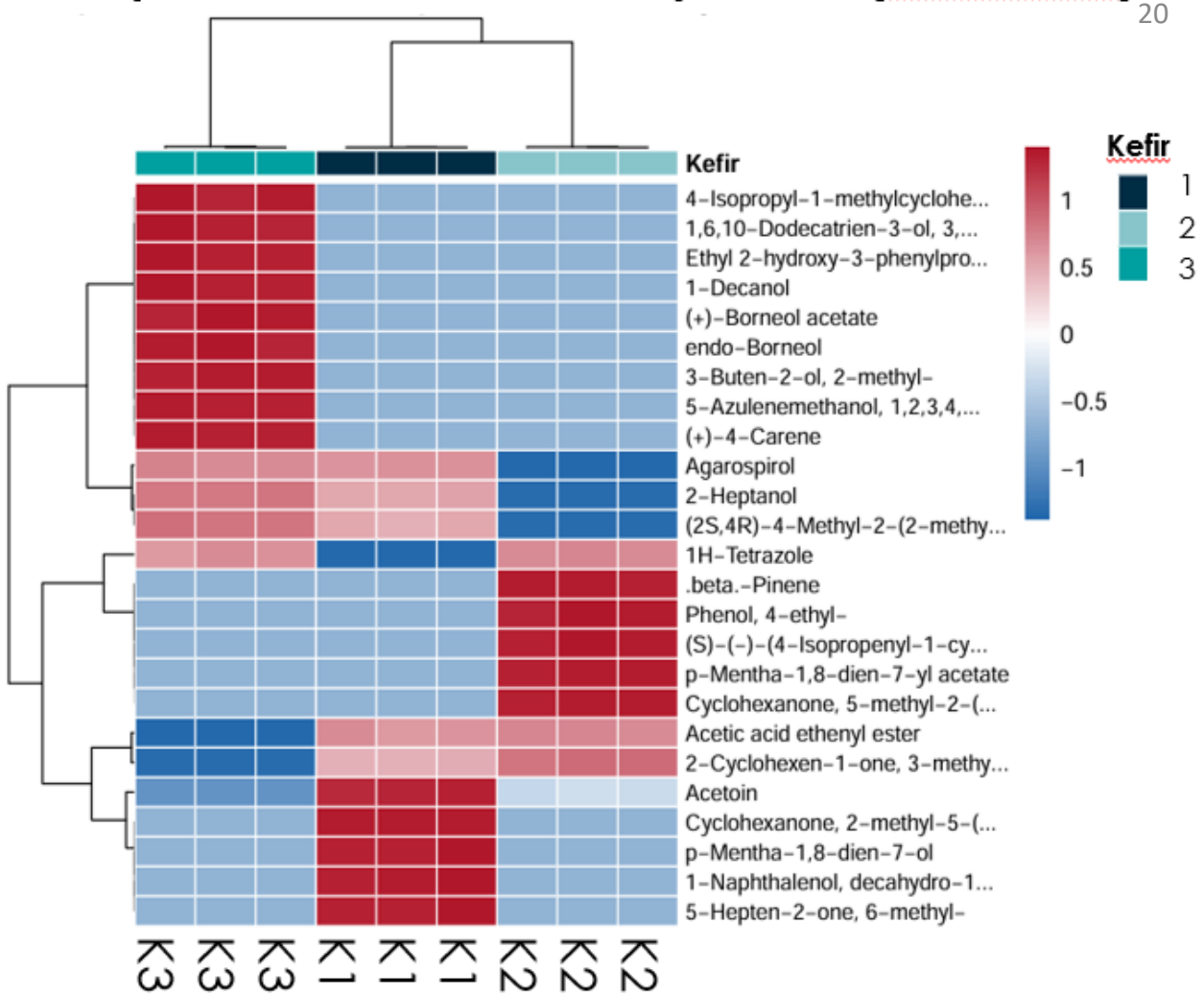


Water Kefir : Product comparison

Chemical diversity by Kefir type (n=3)



Top 25 Discriminant compounds (DHSxSBSE)



Perspectives

3rd Step : Determine correlations between LC and GC results

In progress …

- Study of commercial and homemade milk kefir
- To complete this analytical chemistry approach: DNA analysis of kefir grains ?

Study of other fermented products:

Acknowledgements