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Combining LC-HRMS and LC-HRMS/MS data to explore a cereal food processed under different conditions

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Context

Characterizing the chemical fingerprint of a processed food is a major challenge to advance **food quality**. New untargeted approaches based on LC-HRMS analysis can unlock the potential to increase our understanding on **how chemical components**, linked to different food quality dimensions, **react and evolve during the manufacturing processes** and thus contribute to food quality design.

Objective

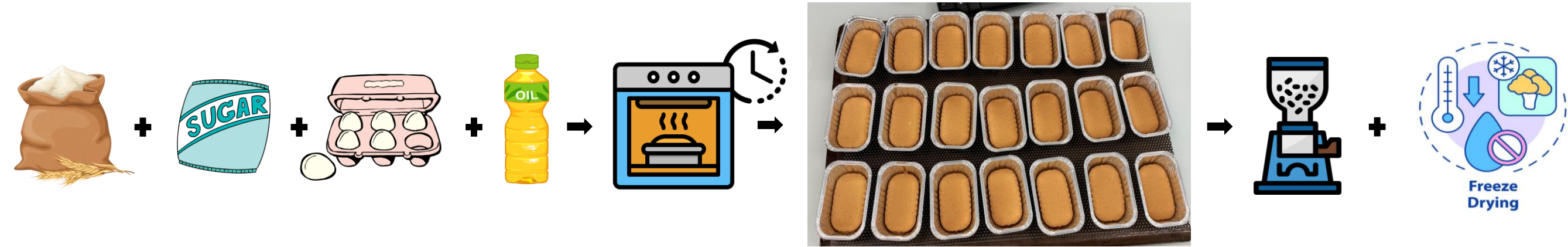
The aim of our project is to develop such new approach on a range of **baked products** prepared under controlled **formulation and processing parameters** to generate a **diversity of chemical profiles**. Our approach is based on a method combining **LC-HRMS and LC-ddA-HRMS/MS** analyses to evaluate at the end whether the use of **molecular networks** can assist us in better understanding the **reactional links** between compounds.

Problematic

First, an LC-HRMS method with a data treatment workflow was developed. To identify the most significant discriminating features, we proceeded with statistical analysis. These features will be chosen for **MS/MS fragmentation** in the LC-ddA-HRMS/MS method applied in second stage. However, **PLS-DA with Anova** and **Volcano plots** produced **different lists of features**. The LC-ddA-HRMS/MS acquisition method will then be applied using each of these lists as **inclusion list**. We will explore whether the choice of LC-HRMS selection method **impacts** on the construction of molecular networks following LC-HRMS/MS.

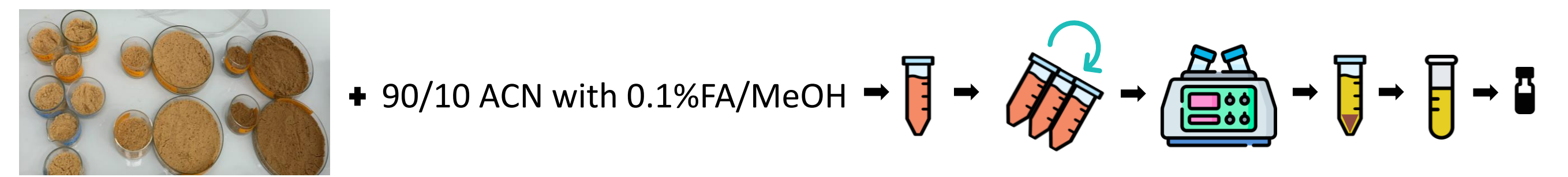
Analytical approach

Sponge cake preparation



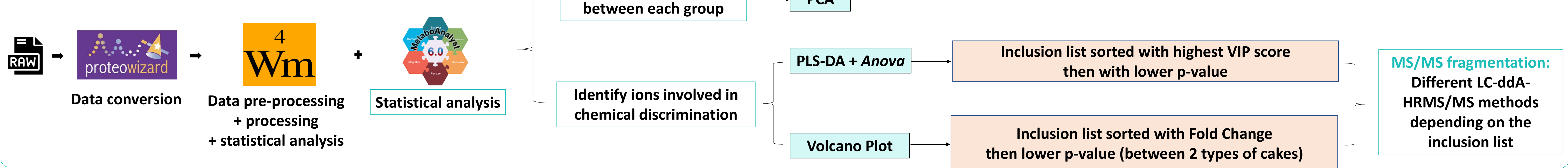
- Wheat sponge cakes were prepared under controlled parameters according to Krause et al. protocol.¹
- Three types of wheat sponge cakes were prepared: **B170_25** (170°C for 25 minutes), **B170_40** (170°C for 40 minutes), and **B200_25** (200°C for 25 minutes).
- Each type of preparation was performed in triplicate to assess the repeatability of the process, e.g., B170_25 **C1**, B170_25 **C2**, and B170_25 **C3**.

Sample extraction and LC-HRMS analysis²



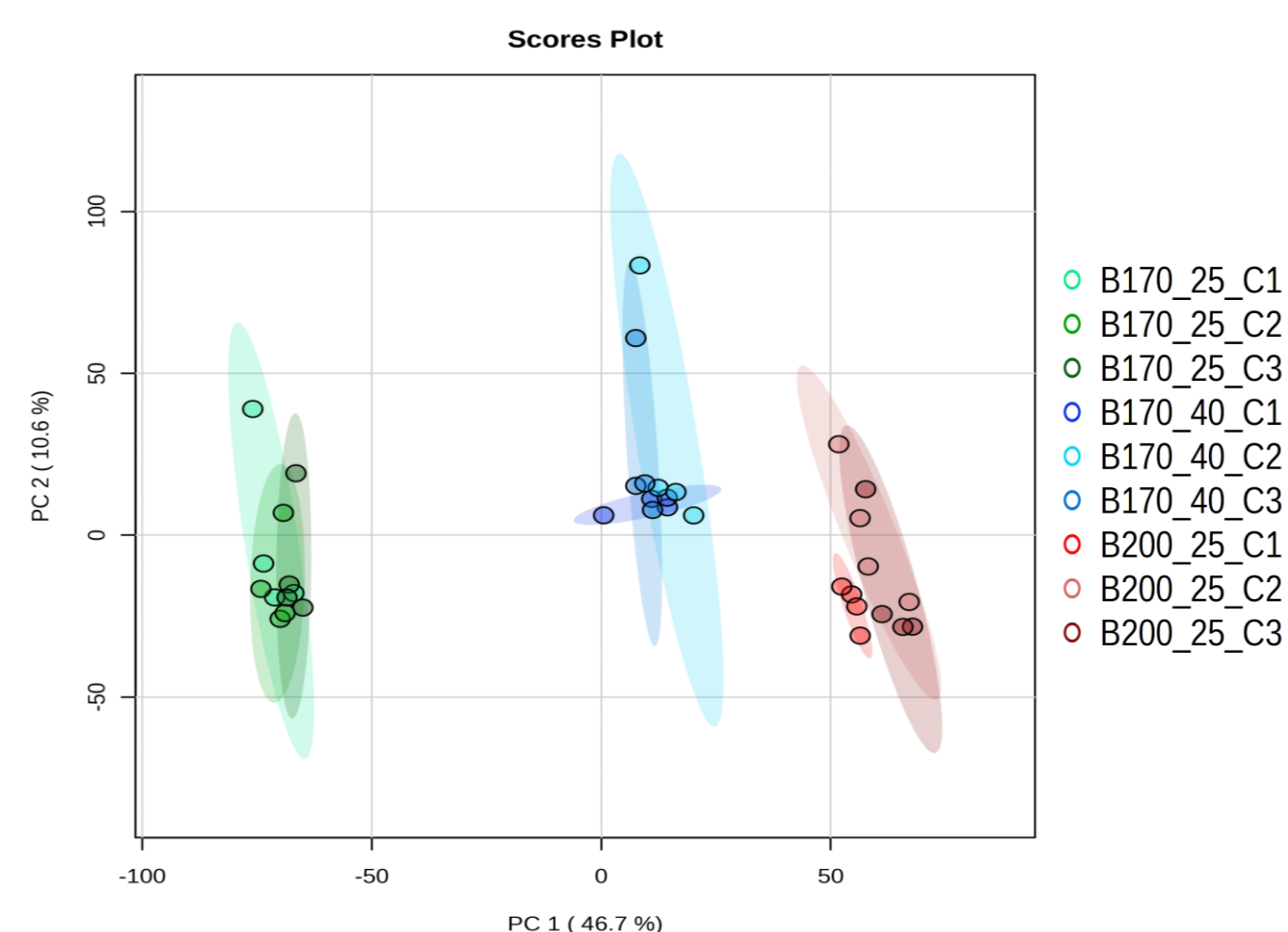
LC-MS System	Waters® Acquity H-Class + Xevo® G2-S Q-ToF	Thermo Scientific UltiMate 3000 + Q-Exactive Orbitrap
Column	ACE C18-PFP (150x2.1 mm ; 2 µm)	
LC conditions	H ₂ O + FA 0.1% (A) / ACN + FA 0.1% (B) / MeOH (C) Flow : 0.4 mL/min , Injection Vol : 10 µL	
Ionisation	ESI +	
MS conditions	<ul style="list-style-type: none"> Resolution: 30,000 FWHM at m/z 200 2 scans/s 	<ul style="list-style-type: none"> Resolution: 70,000 FWHM at m/z 200 AGC target: 10⁶ Maximum IT: 200ms
Run Time	23 minutes	

Data treatment workflow



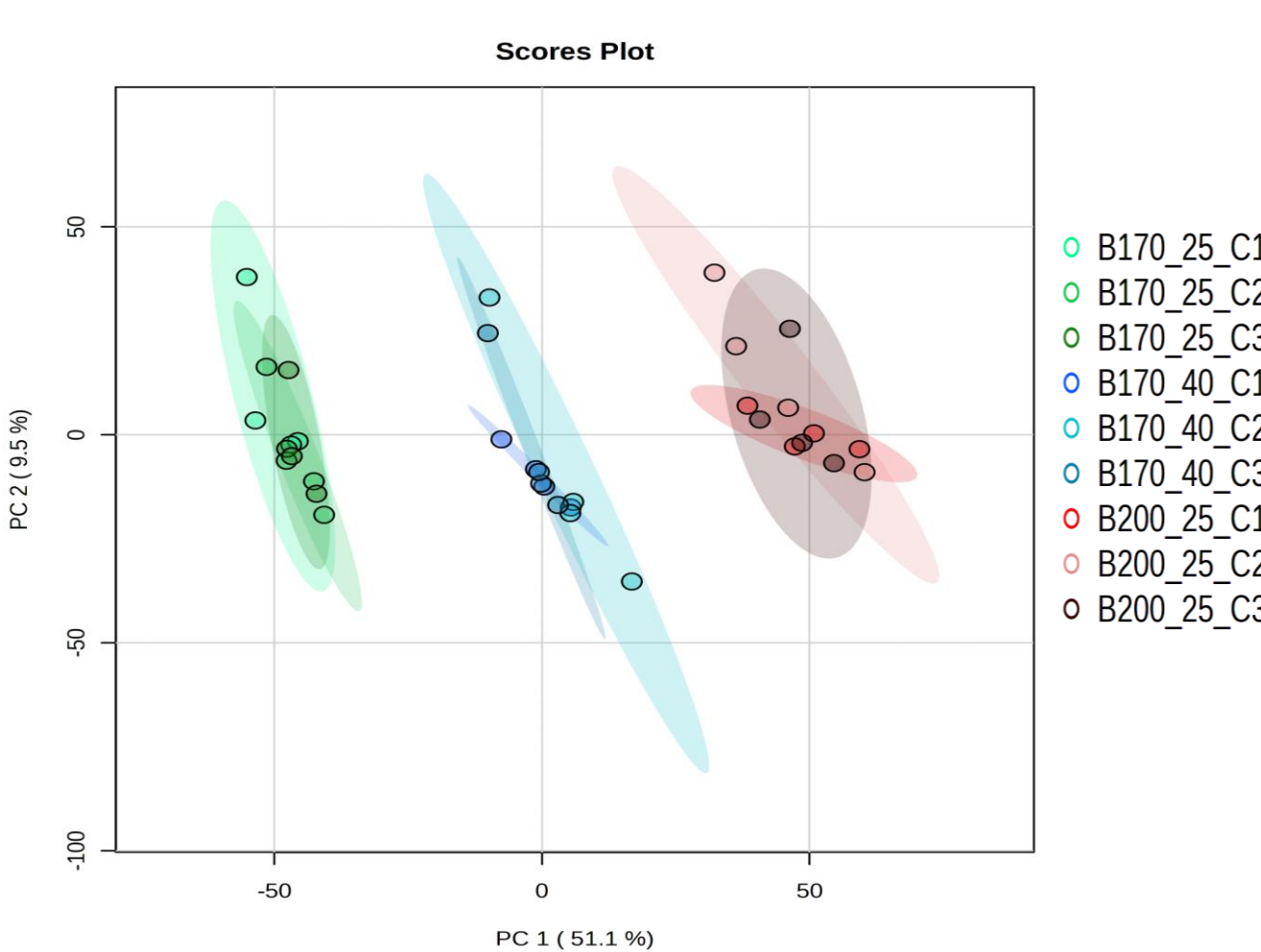
Results and Discussion

PCA test:

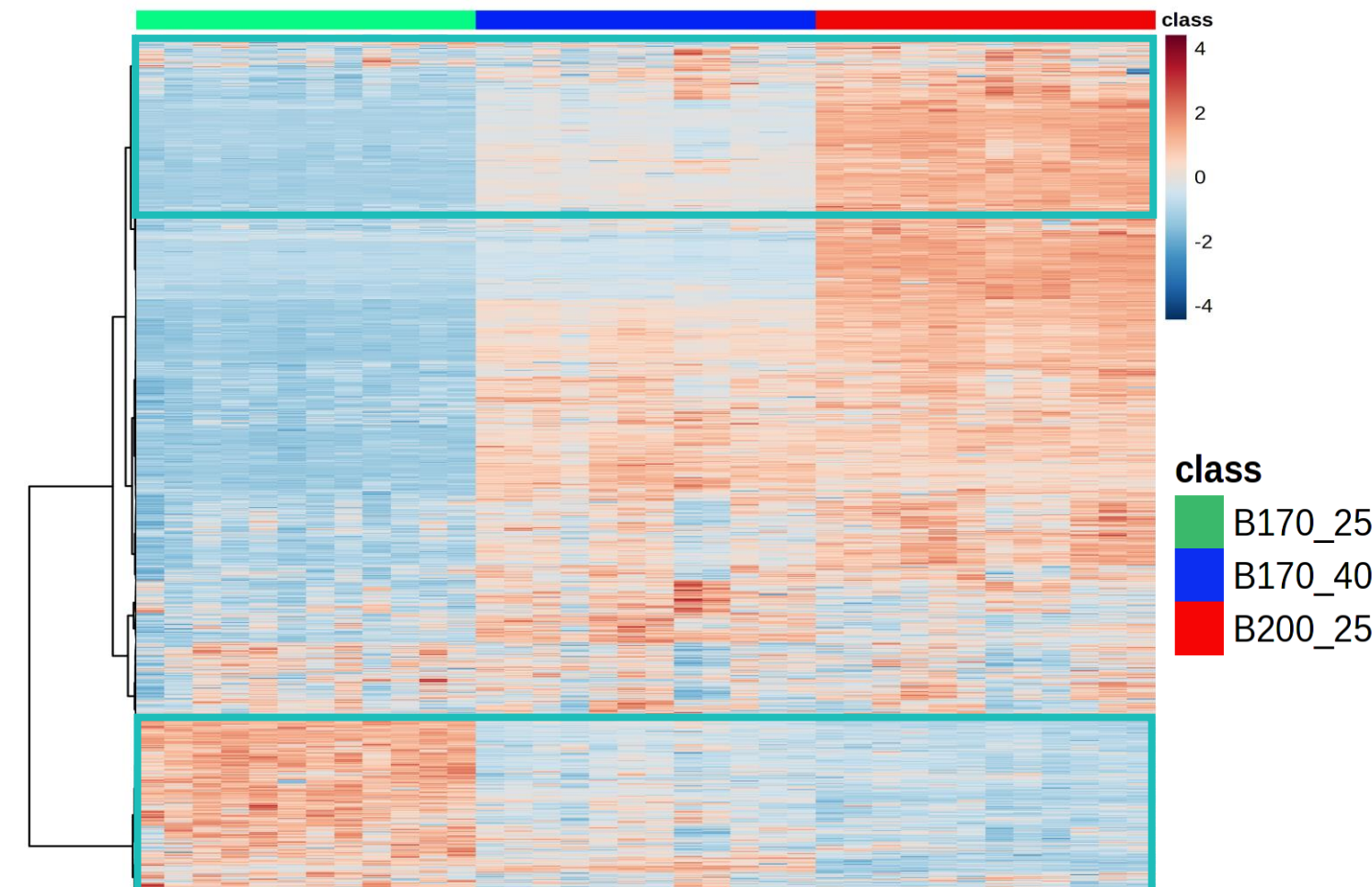


For both instruments (Q-ToF and Q-Orbitrap), PCA results were comparable:

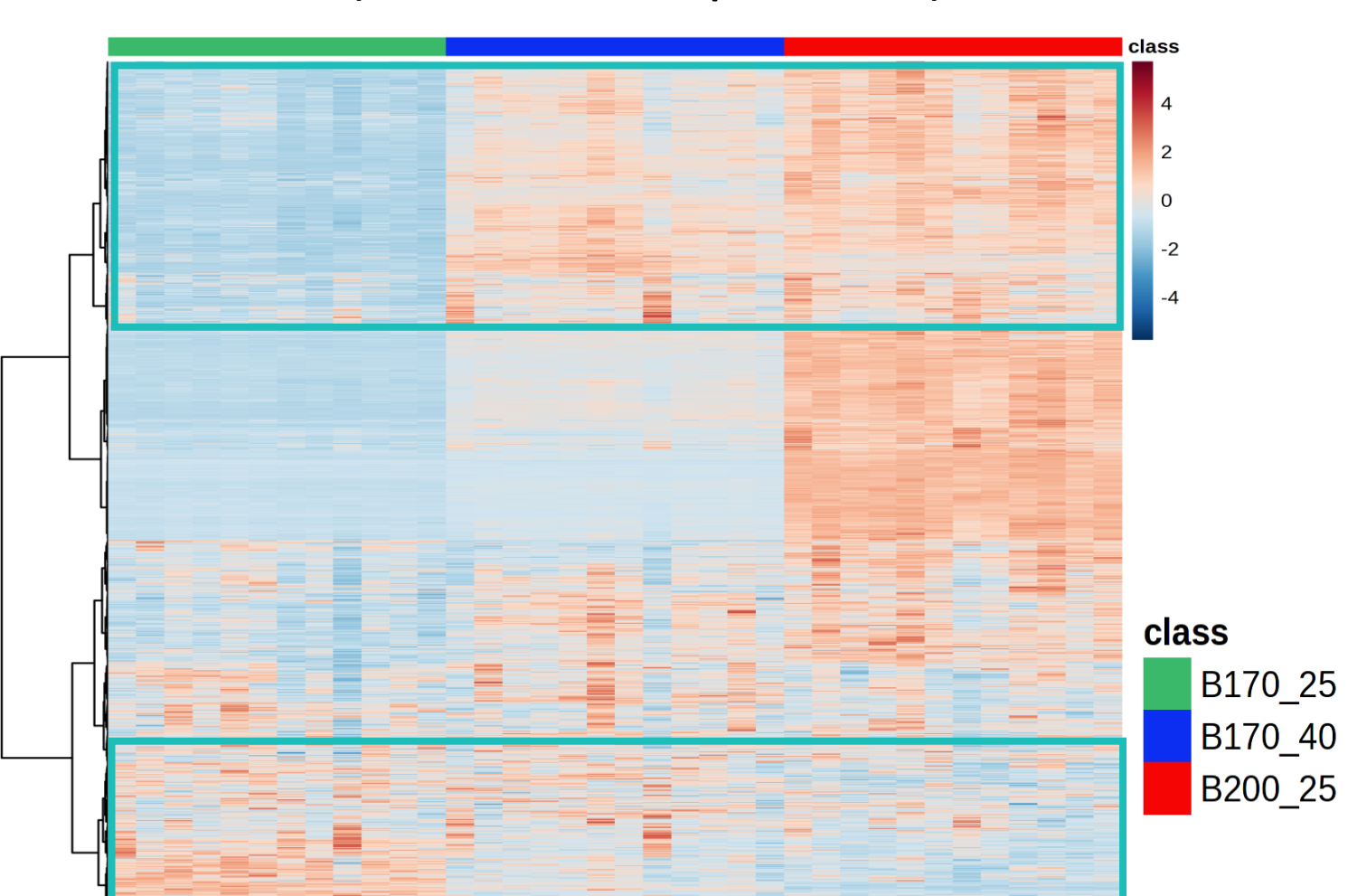
- PCA test successfully discriminated our sponge cakes samples according to their preparation conditions with **PC1** counting respectively for **46.7%** and **51.1%** of the total variability.
- Processing conditions are repeatable. (**C1-C2-C3**) were grouped together.



Raw data

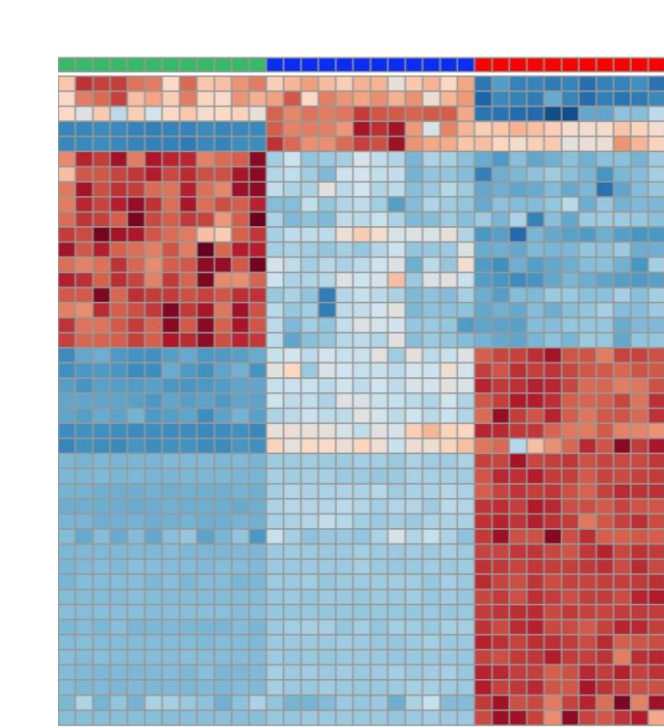


- B170_40** processing condition is intermediate between **B170_25** and **B200_25**.
- At the top, compounds are more intense in **B200_25** than in **B170_25** and **B170_40**, suggesting they may be reaction products with a higher activation energy occurring under high temperature.
- At the bottom, compounds are more intense in **B170_25** than in **B200_25** and **B170_40**, suggesting they may be reaction precursors or intermediates that are degraded with more severe processing conditions (time and temperature).

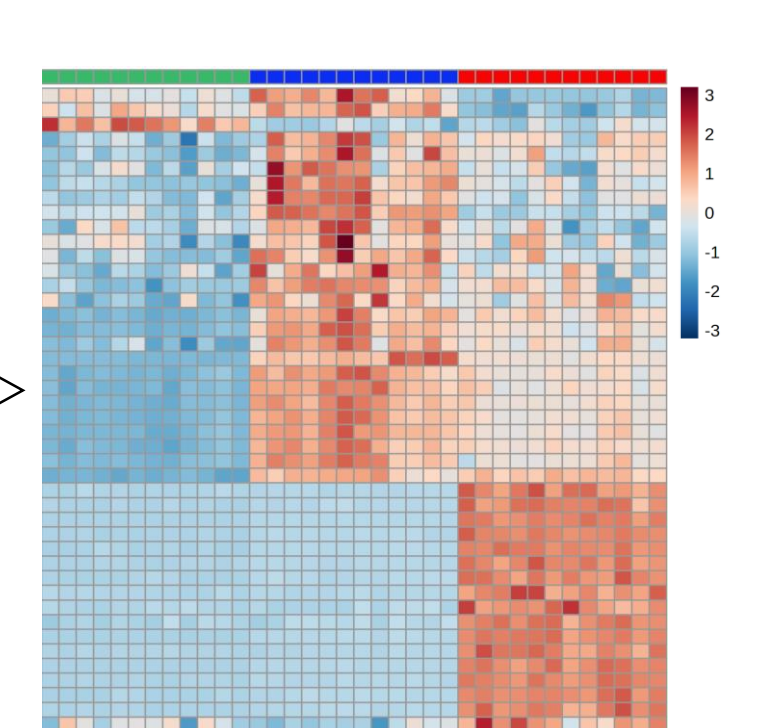


Heatmaps:

Volcano



PLS-DA + Anova



Only 1 feature in common

- Compounds from the 3 types of processing conditions are chosen.
- Compounds presenting higher contrast in intensity specially in **B170_25** and **B200_25** were chosen.

- Compounds from the 3 types of processing conditions are chosen but compounds of **B170_40** are privileged.

Only 6 features in common

Perspectives

LC-ddA-HRMS/MS method along with the data treatment workflow are being optimized to see later if the choice of inclusion list affects the molecular network formed and if the reactional links differ between one inclusion list and the other.



Conclusion

We aim to understand the reactional links of formulated and processed food with this new approach described herein. For the first stage, we were able to distinguish between the different groups of samples, but when we used statistical tests, different results were obtained. We will continue our work by studying if there is an impact of this step on the further stages of the method, especially for the formation of molecular networks.

References

1. Krause et al., Food Chem., 2022, 386, 132653.

2. Delaporte et al., Food Chem., 2019, 98, 510-519