OPTIMIZING WINEMAKING WITH CHEMOMETRICS AND SPECTROSCOPIC TECHNIQUES

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Introduction

The vinification process, from the growth of the grape until the bottling, is crucial in winemaking and requires meticulous monitoring to ensure quality and consistency. While large-scale industrial practices dominate, laboratory-scale studies are essential for refining Process Analytical Technologies (PAT) that can be seamlessly integrated into winemaking. Chemometric methods, coupled with spectroscopic techniques, offer a powerful approach for analyzing and interpreting the complex data generated during vinification [1].

Infrared (IR) spectroscopy, known for its rapid, non-destructive analysis and minimal sample preparation, is particularly suited for monitoring various stages of the winemaking process [2]. However, its successful implementation needs a detailed understanding and control of variability sources such as grape cultivar, position, maturity, and specific oenological practices.

Aim of study

Our research focus is to provide an integral framework for setting up lab-scale fermentations and applying spectroscopy to monitor and predict key parameters throughout the vinification process. Our approach emphasizes the importance of chemometric techniques in identifying and quantifying variability sources, ensuring the robustness and reproducibility of spectroscopic data [3]. We also aim at applying different chemometric tools to decompose and interpret complex datasets and identify subtle biochemical reactions that may be masked by dominant reactions [4].

We present the results of variability analysis in vines and alcoholic fermentation using ANOVA-Simultaneous Component Analysis (ASCA), and the use of a new monitoring index for quality control [5].

Materials and methods

Grape must

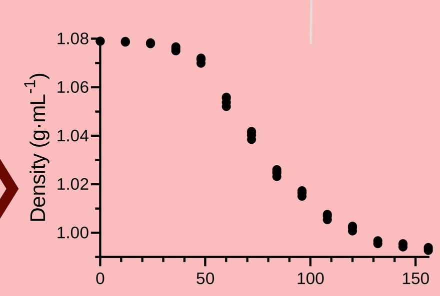
or

Concentrated grape must

Normal Operating Conditions (NOC) and induced deviation

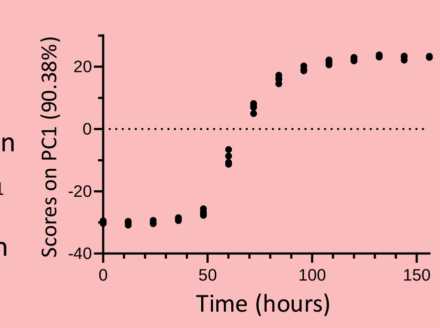
Microfermentations

Densimeter and pH-meter

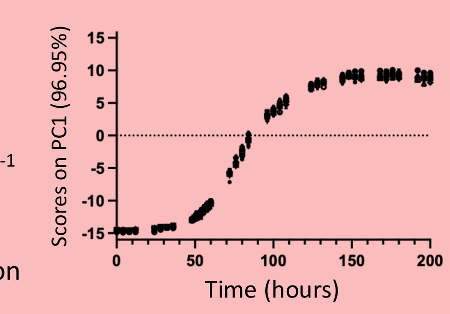


Classical fermentation monitoring

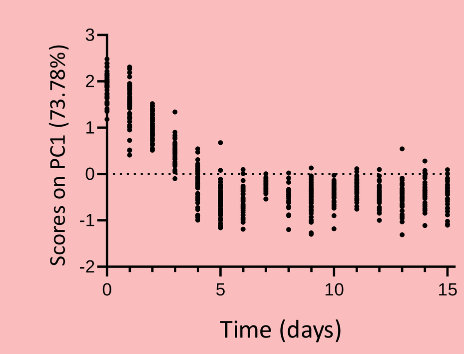
Vaya Raman
Portable
830 nm excitation
350 – 2000 cm⁻¹
1 cm⁻¹ resolution



FTIR ExoScan
Portable
4000 – 850 cm⁻¹
32 scans
8 cm⁻¹ resolution



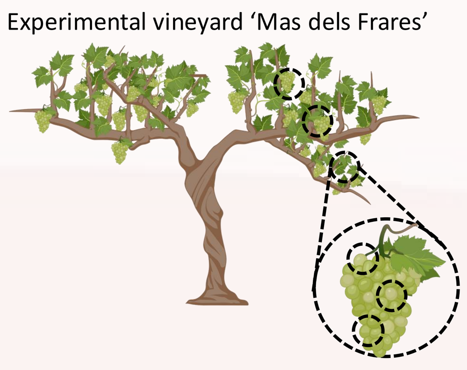
NIR MPA II
12500–4000 cm⁻¹
32 scans
4 cm⁻¹ resolution



Different spectroscopic tecniques were tested to monitor the fermentation and detect deviations of the process

Grape (raw material) variability [3]

Muscat of Alexandria
Experimental vineyard 'Mas dels Frares'



Studied factors:

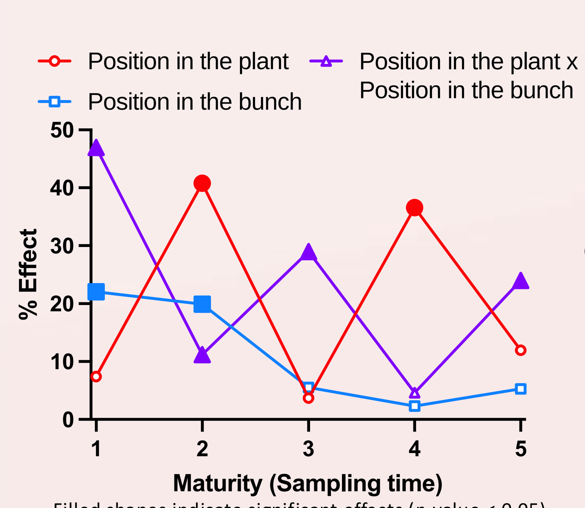
5 Ripening time points
3 bunch-positions in the plant
3 grape-positions in the bunch

Grapes have a great influence on wine characteristics, the effect of position of grapes in the plant is often overlooked.

Factor	% Effect
Maturity (Sampling time)	29.98*
Position in the plant	5.83*
Position in the bunch	2.21*
Maturity x Position in the plant	9.52*
Maturity x Position in the bunch	5.84*
Position in the plant x Position in the bunch	2.14*

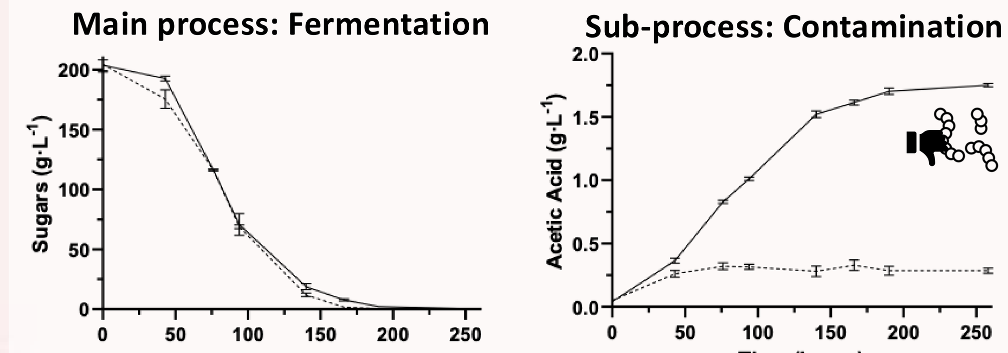
*: significant factor (*p*-value < 0.05)

All the considered factors and interactions are significant, position of grapes has a significant impact on grape composition



When the position is studied over time, its evolution is complex due to the biochemical processes involved in grape ripening

Detection of subtle contamination [4]

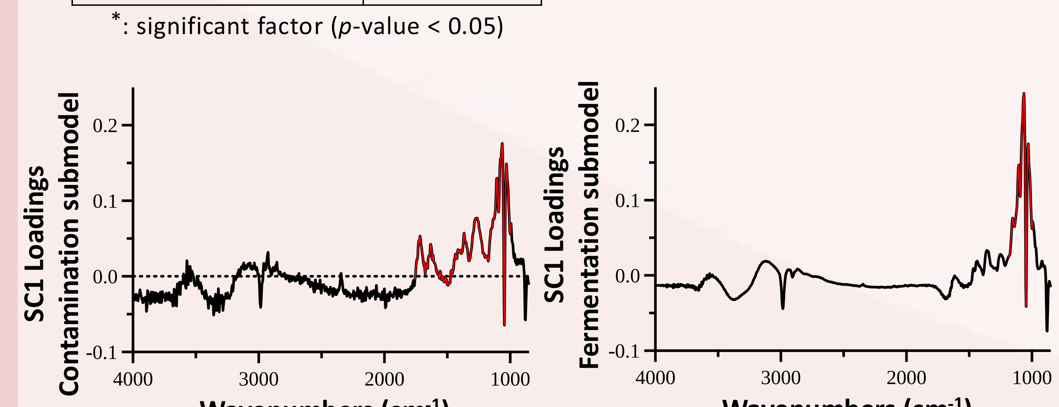


The main process (---) has a greater impact thanthe sub-process (—)

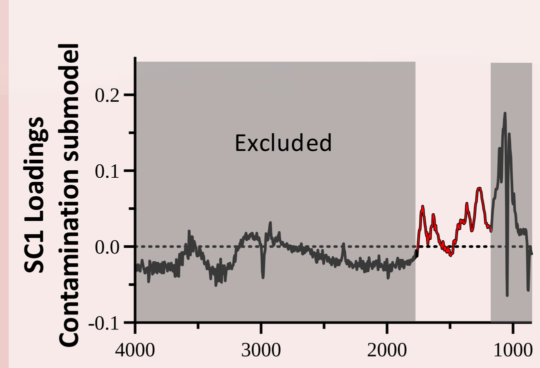
Factor	% Effect
Contamination	0.16*
Fermentation	98.95*
Interaction	0.11

*: significant factor (*p*-value < 0.05)

The effect of the contamination is low taking into consideration the great production of acetic acid.



Both process are caused by microorganism, so the spectroscopic fingerprint of both of them overlap



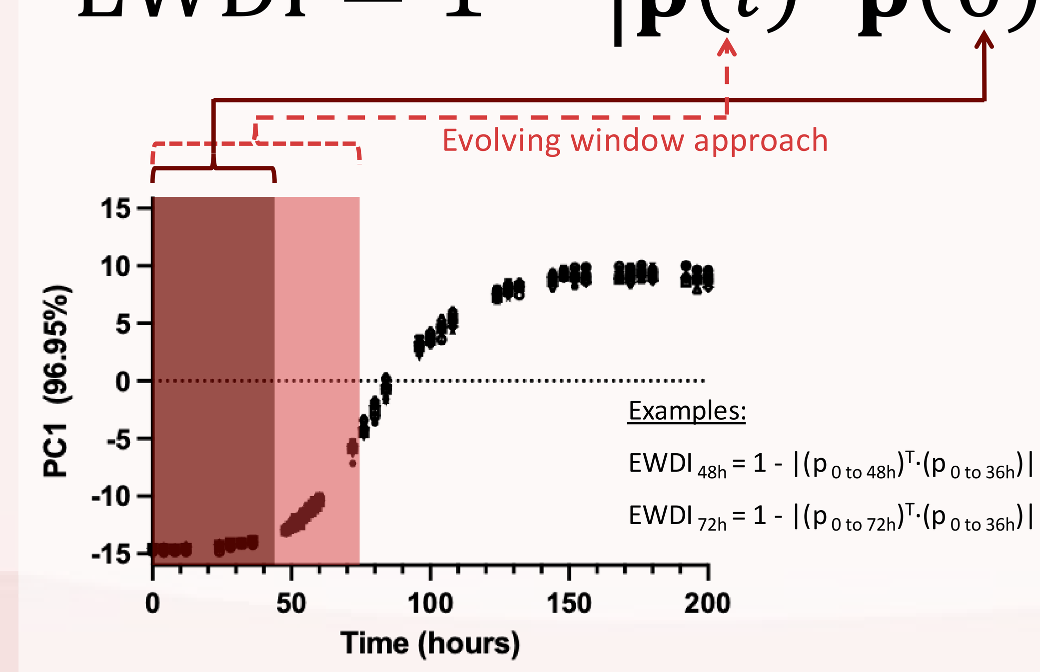
Factor	% Effect
Contamination	0.55*
Fermentation	98.77*
Interaction	0.16*

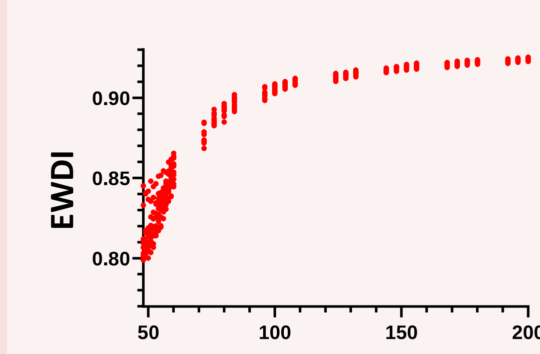
*: significant factor (*p*-value < 0.05)

Focusing on a specific spectroscopic region allows to enhance the contamination factor

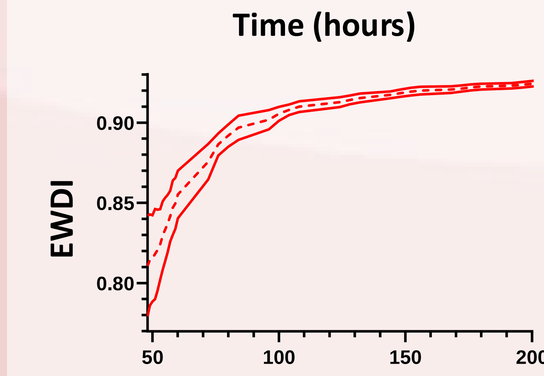
New Index for quality control [5]

$$\mathrm{EWDI} = 1 - \left|\mathbf{p}(i)^{\mathrm{T}}\mathbf{p}(0)\right|$$

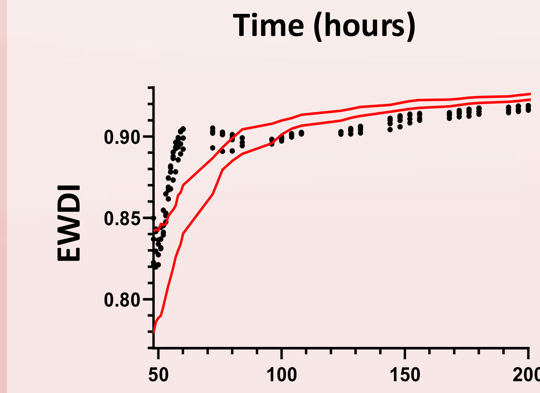




EWDI values are calculated for each NOC fermentation



The control limits (± 2s) are calculated for the different NOC fermentations



Intentionally deviated fermentations are projected

The index can detect deviations at early stages.

Conclusions

» The combination of IR data with ASCA makes it possible to detect the influence of grape global position of the grape on its individual grape ripening. However, the evolution of positional factors throughout ripening is highly intricate.

» The alcoholic fermentation signal in the MIR spectra hides the signal of the bacteria contamination, that needed to be enhance through a targeted selection of spectral regions is necessary.

» The Evolving Window Dissimilarity Index (EWDI) can be used as an MSPC tool, to establish statistical control limits based on fermentations conducted under Normal Operating Conditions.

» IR spectroscopy and chemometrics offer a powerful framework for the winemaking control and monitoring.

References

[1] Schorn-García D, Cavaglia J, Giussani B, Busto O, *et al.* Microchem J. 2021; 166 106215

[2] Cozzolino D. Food Anal Methods. 2022; 15(5) 1390-1396.

[3] Schorn-García D, Giussani B, García-Casa MJ, Rico D, *et al.* Foods. 2023; 12(5) 962.

[4] Schorn-García D, Giussani B, Busto O, Aceña L, *et al.* J Chemom. 2022; e3465.

[5] Schorn-García D, Ezenarro J, Busto O, Aceña L, *et al.* Food Bioprocess Technol. 2023

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