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Monitoring fermentation problems in wine production using an ATR-FTIR portable spectrometer and multivariate analysis

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Introduction

Alcoholic fermentation is the biochemical transformation of sugars into ethanol and carbon dioxide by the action of yeast enzymes. Even though it is a well-known process, unexpected deviations can occur that may decrease the final product quality (e.g., development of other microorganisms, such as lactic acid bacteria that are involved in malolactic fermentation (MLF)).

Quality-by-design strategies offer the possibility to early detect deviations and thus 'readjust' the process and minimize rejects[1]. Attenuated Total Reflectance Fourier Transform Infrared spectroscopy (ATR-FTIR) has been previously applied throughout the fermentation process for *on-line* real time monitoring[2].

Aim of the study

At line monitoring of wine fermentations under normal fermentation conditions (NFC) and with lactic acid bacteria contamination, using a portable ATR-FTIR spectrometer and multivariate techniques, to study the fermentation process and detect deviations from NFC due to lactic acid bacteria contamination.

Materials and methods

A total of 6 small-scale alcoholic fermentation experiments were monitored:

64 batches in Normal Fermentation Conditions (NFC).

42 batches intentionally deviated by adding different concentrations of lactic acid bacteria (MLF).

350ml → **1,5ml** → Centrifugation →

Portable FTIR-ATR analysis

3999 – 649 cm^{-1}

(899 variables)

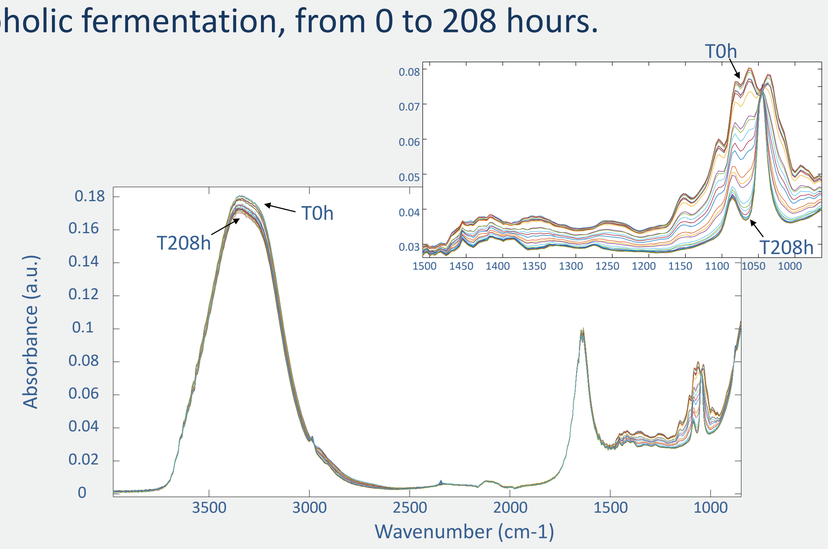
3 replicates

32 scans

8 cm^{-1} resolution

→ Spectral data acquisition →

MIR spectrum variation in time, for a typical white grape must alcoholic fermentation, from 0 to 208 hours.



Relative density, pH and malic acid were also analyzed by standard methods.

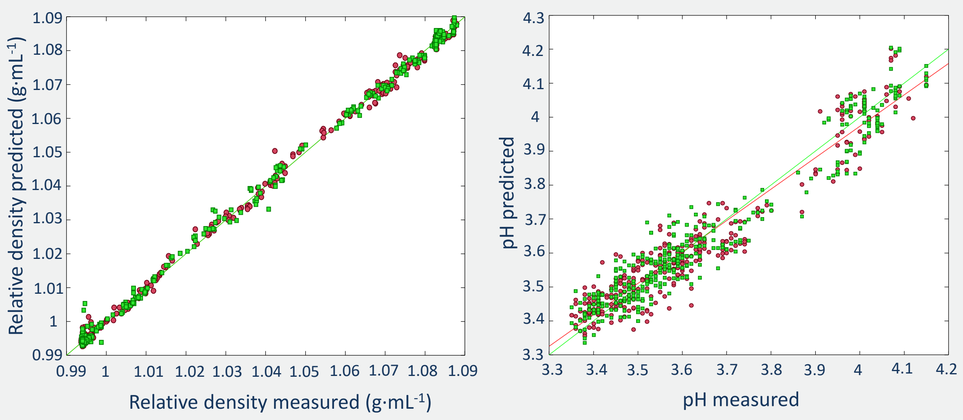
Results and discussion

PREDICTION of the monitored fermentation parameters using PLSR (obtained with the best regions and pre-processing combination).

		Density ($g \cdot mL^{-1}$)	pH	L-malic Acid ($g \cdot mL^{-1}$)	L-Malic Acid* ($g \cdot mL^{-1}$)
Variable range		0.9940-1.0878	3.32–4.15	0.05–2.00	0.05–2.00 $g \cdot L^{-1}$
Pre-processing		Second Order Polynomial through 15 points SNV Mean Center			
Number of Factors		4	6	3	3
Nº Samples		522	352	237	74
Calibration	RMSEC	0.0011	0.06	0.21	0.18
	R^2	0.9990	0.9259	0.9024	0.9212
Cross-validation	RMSECV**	0.0012	0.06	0.22	0.19
	R^2	0.9989	0.9259	0.8968	0.9063
Nº Samples		580	376	267	84
Prediction	R^2	0.9986	0.9345	0.9106	0.9074
	RMSEP	0.0013	0.06	0.21	0.20

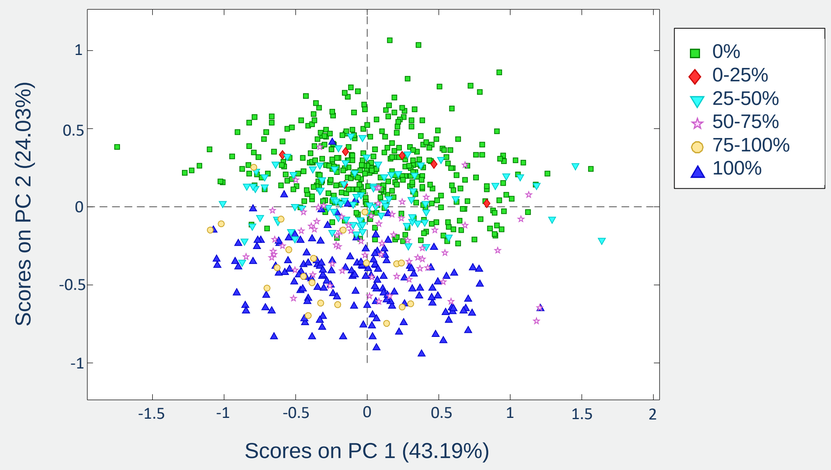
* The model was performed with wine (density < 0.995 $g \cdot L^{-1}$)

**The validation method applied was Random Subsets, 15 data splits, 10? Samples per split.

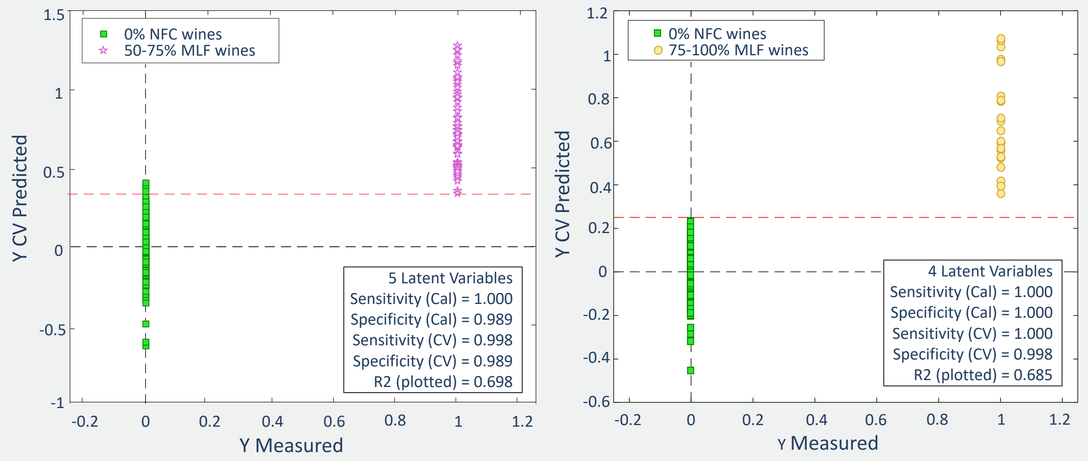


Calibration set (●) Test set (■)

DISTRIBUTION of wine spectra according to the percentage of malolactic fermentation elapsed (% of malic acid consumed by lactic bacteria) using Principal Component Analysis (4 PCs, 81.88% of variability explained).



DISCRIMINATION between NFC wines against MLF deviated wines (50-75% and 75-100% malic acid consumed) using PLS-Discriminant Analysis.



The validation method applied was Random Subsets, 15 data splits, 10? Samples per split.

Conclusions

The prediction of wine fermentation parameters was achieved, demonstrating the possibility to use this portable device to rapidly monitor wine fermentations. The methodology presented shows great potential as a fast and simple at-line analysis tool for early detection of fermentation problems such as lactic acid bacteria contamination: it was possible to discriminate between NFC wines and deviated MLF wines before the end of malolactic fermentation giving the possibility to the winemaker to eventually correct the process and to obtain a good quality product.

Acknowledgements

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