

Development of multivariate models to monitor and control grape quality and wine production

Daniel Schorn-García^a, Barbara Giussani^b, Ricard Boqué^c, Olga Busto^a, Laura Aceña^a, Montserrat Mestres^a

^aiSens Group. Dpt. of Analytical Chemistry and Organic Chemistry. Universitat Rovira i Virgili, Campus Sescelades, 43007 Tarragona, Spain

^bDipartimento di Scienza e Alta Tecnologia, Università degli Studi dell'Insubria, 22100 Como, Italy

^cChemometrics, Qualimetrics and Nanosensors Group. Dpt. of Analytical Chemistry and Organic Chemistry. Universitat Rovira i Virgili, Campus Sescelades, 43007 Tarragona, Spain

e-mail: isens@urv.cat www.isens.urv.cat



UNIVERSITAT ROVIRA I VIRGILI



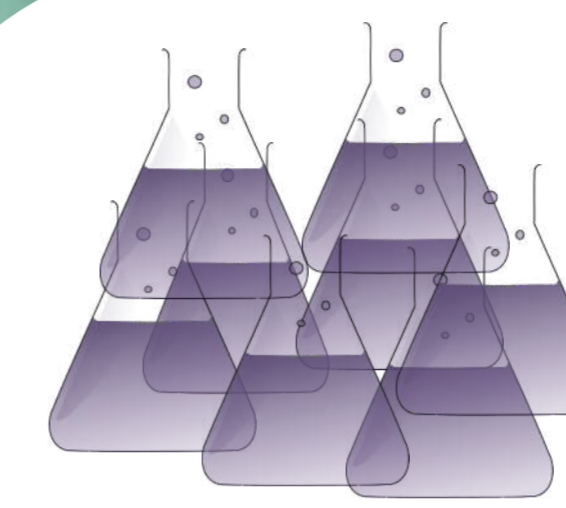
Introduction

Spanish agricultural sector has a great economic impact due to the quality of its production, both in raw fruits and in later processed products. A well-known example are grapes and wine. However, increasing production in vineyards in recent years harms agricultural sector as wineries could not assume it, which cause low prices in origin.

Taking into account grape quality, there could be different solutions: best grapes can be directly consumed, while grapes with lower quality can be derived to juices or pre-prepared convenience food products with added value. In order to classify and derive the products, prior physicochemical analysis would be needed.

Modern fast techniques allow obtaining a huge amount of data more quickly, more greenly and with less sample pretreatment, without destroying the sample, and directly from the vineyard.

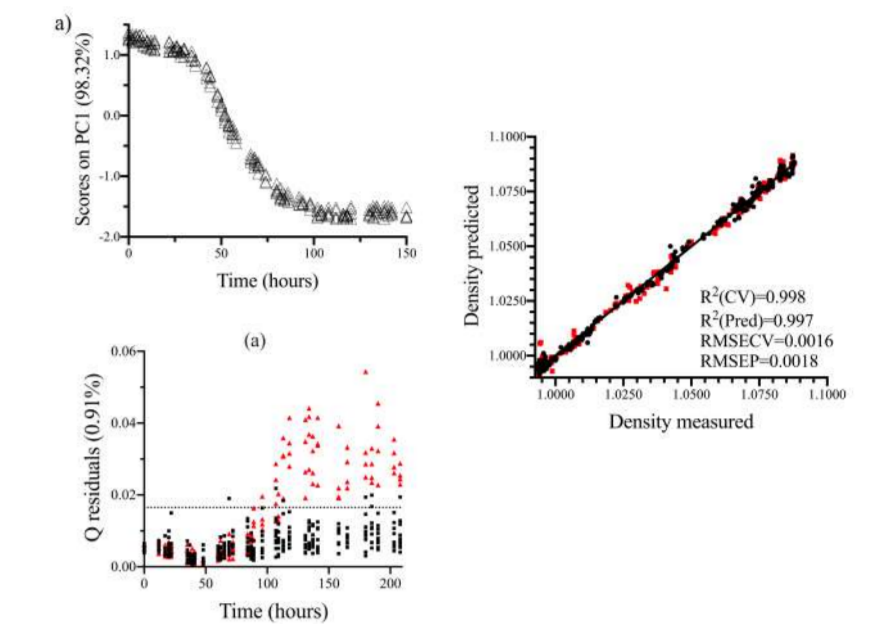
Previous work*



Alcoholic fermentation



Portable MIR



Analytical measures optimization

The alcoholic fermentation was analyzed using a portable MIR. The process was monitored at micro-scale in order to obtain a greater number of samples. The optimization achieved a complete monitoring of the process, which obtain the same profile of the density measured typically used in wineries. Moreover, sluggish fermentations (fermentations which slow their fermentation rates) and lactic acid bacteria contaminations were detected in early stages. Finally, typical oenological parameters were also predicted along the fermentation.

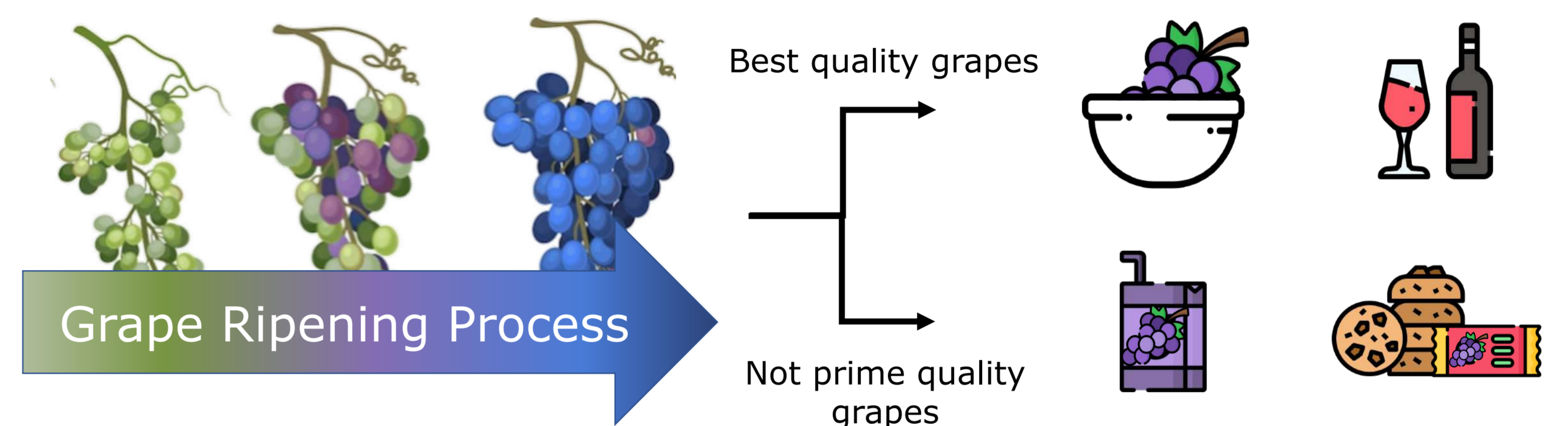


Process Control
 Early detection of deviations
 Parameters prediction

Objectives

The main goals are to predict the physicochemical parameters of the final wine along the entire grape ripening process. And to establish a classification model that sorts grapes, according to their quality, to the different products. These objectives would be achieved using chemometric tools.

Process

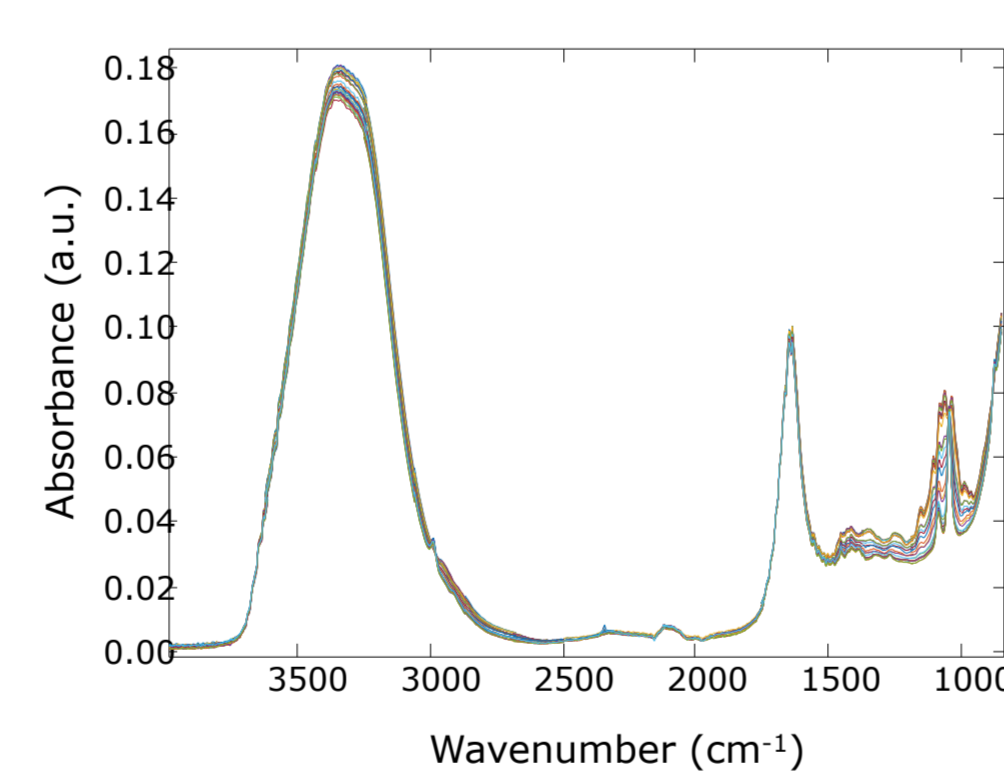


Methodology

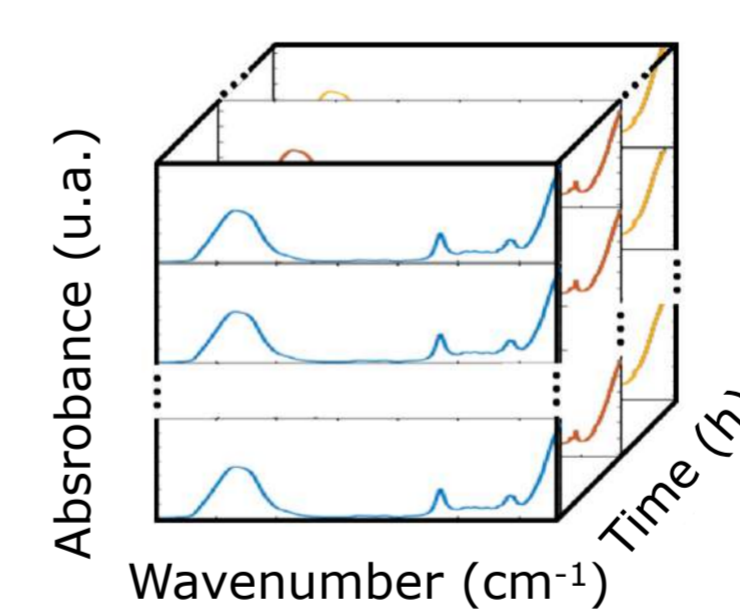
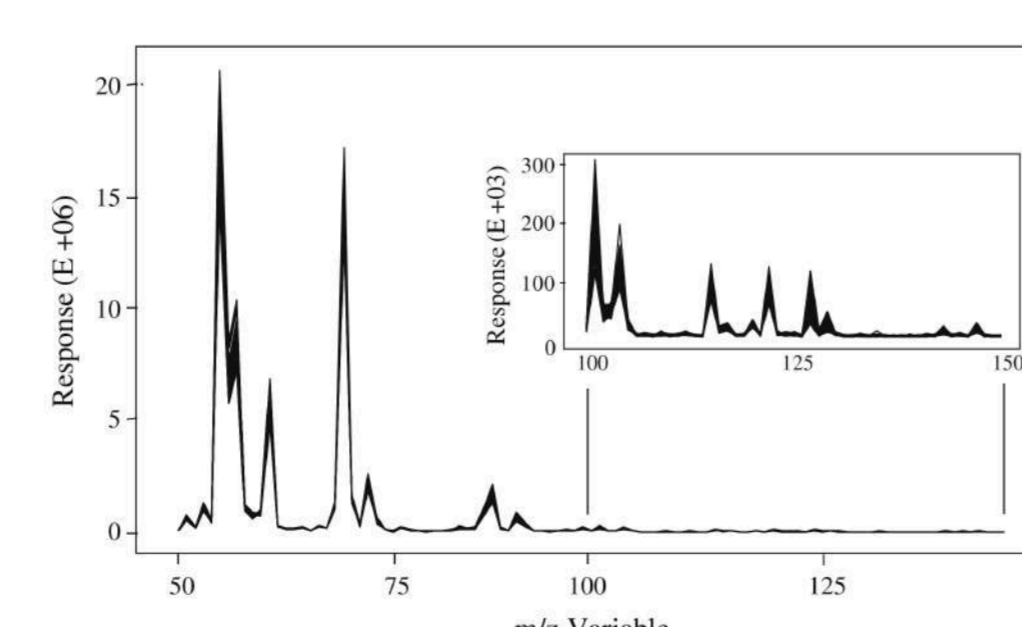
Portable MIR



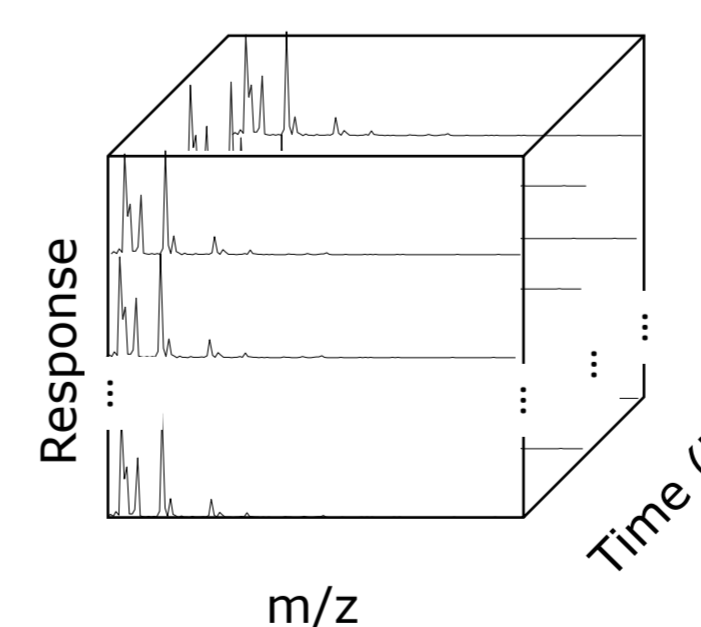
Grape or grape must ATR or DRIFT as sampling devices



Bidimensional examples of the analytical response



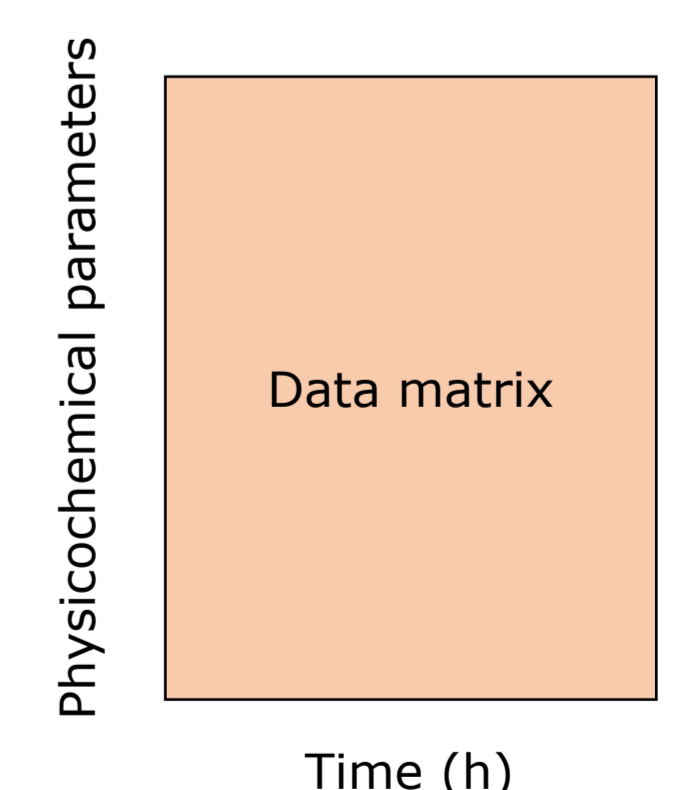
Data is contained in a three-dimensional matrix as it is measured during ripening



Combination of one or both fast analytical techniques matrices with physicochemical data



Physicochemical analysis



Physicochemical parameters & Classification to final products

Chemometrics approaches to unravel the information contained in the large data matrices

HS-MS (electronic nose)



Analysis of the whole volatile fraction without chromatographic separation

Acknowledgments

The authors thank the Spanish Ministry of Science and Technology for the project AGL2015-70106-R and PID2019-104269RR-C33 (AEI/FEDER, EU) and the Catalan Research Council (AGAUR) for the FI-SDUR Grant 2020 FISDU 00221.



Fondo Europeo de Desarrollo Regional

*Bibliography

Cavaglia, J. et al., 2019. Early detection of undesirable deviations in must fermentation using a portable FTIR-ATR instrument and multivariate analysis. *Journal Of Chemometrics*, 33(8).

Cavaglia, J. et al., 2020. ATR-MIR spectroscopy and multivariate analysis in alcoholic fermentation monitoring and lactic acid bacteria spoilage detection. *Food Control*, 109.

Cavaglia, J. et al., 2020. Monitoring wine fermentation deviations using an ATR-MIR spectrometer and MSPC charts. *Chemometrics and Intelligent Laboratory Systems*, 201.