



Raman spectroscopy as a rapid tool for monitoring lactic acid concentration during wine malolactic fermentation directly in the winery

Anna Lisa Gilioli ^{a,b}, Alessio Sacco ^{b,*}, Andrea Mario Giovannozzi ^b, Simone Giacosa ^c, Antonella Bosso ^d, Loretta Panero ^d, Silvia Raffaella Barera ^d, Stefano Messina ^d, Marco Lagori ^{c,d}, Silvia Motta ^d, Massimo Guaita ^d, Ettore Vittone ^a, Andrea Mario Rossi ^b

^a Physics Department, University of Turin, Via P. Giuria 1, 10125 Turin, Italy

^b Istituto Nazionale di Ricerca Metrologica (INRiM), Strada delle Cacce 91, 10135 Turin, Italy

^c Department of Agricultural, Forest and Food Sciences Department, University of Turin, Corso Enotria 2/C, 12051 Alba, Italy

^d Consiglio per la ricerca in agricoltura e l'analisi dell'economia agraria (CREA), Via Pietro Micca 35, 14100 Asti, Italy

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ABSTRACT

Lactic acid is mainly produced during the process of malolactic fermentation and evolution of its concentration is associated with the wine stabilization process and the quality of the final product. The quantitative analysis of lactic acid is carried out offline in the laboratory using various analytical techniques, the most used being high performance liquid chromatography (HPLC). Because of this, there is a clear demand in the winemaking community for analytical tools that allow real-time, fast and inexpensive quantification of lactic acid. An approach using Raman spectroscopy has positioned itself as a feasible alternative in this regard. The primary goal of this work is therefore to monitor the concentration of lactic acid (which changes rapidly during the malolactic fermentation process) in the analysed samples, specifically, Nebbiolo wine samples for making the Barolo wine. The collected Raman spectra using a portable Raman apparatus are processed using an algorithm that applies Partial Least Squares (PLS) regression to determine the lactic acid concentration for each sample. It proves to be a precise and reliable method that leads to the determination of a predictive model characterised by $R^2 = 0.76$ (on the validation set), $R^2_{\text{test}} = 0.94$ (on the test set) and RMSE of the lactic acid concentration predicted by the model of 0.22 g/l (on the validation set) and 0.11 g/l (on the test set) respectively. This approach produces results comparable to those obtained via HPLC. Moreover, unlike the latter, it allows rapid and easy monitoring of the lactic acid concentration during fermentation directly in the winery.

Glossary

BT	back-thinned
CCD	charge-coupled device
CV	cross validation
DSS	decision supporting system
HCAs	hydroxycinnamic acids
HPLC	high performance liquid chromatography
LV	latent variable
MIR	mid-infrared
ML	machine learning
MSC	multiplicative scatter correction
MSE	mean square error
MST	mean total sum

NIR	near-infrared
ODR	orthogonal distance regression
PCR	principal component regression
PLS	partial least square
RMSE	root mean square error

Introduction

Lactic acid is a useful indicator for monitoring fermentation processes, and its concentration is closely related to the flavor and texture of the final product [1]. It is mainly produced during malolactic fermentation, an oenological process (lasting from a few weeks to months) in which lactic acid bacteria convert malic acid, with a sour taste, into lactic acid and carbon dioxide, with a softer flavor. This transformation

* Corresponding author.

E-mail address: a.sacco@inrim.it (A. Sacco).

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