Abstract
In bottle measurements: a possible tool for the wine industry

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Introduction

The aim of this study was to explore the capability of visible (Vis) spectroscopy and short wavelengths in the near infrared (NIR) region for the non-destructive measurement of wine composition.

Materials and methods

Commercial wines produced in Australia sourced from different types of bottles (e.g. colours, diameters, and heights), and of different wine styles and varieties, were analysed. Wine bottles were scanned in the vis-NIR region (400–1100 nm) in a diode array instrument, in transmission-mode. Principal component analysis (PCA) and partial least square (PLS) regression were used to interpret the spectra and develop calibrations for wine composition. Full cross validation (leave-one-out) was used as a validation method.

Results and discussion

This study showed that the assessment of wine composition by vis and short wavelengths in the NIR has some potential for either qualitative analysis (low, medium and high quality) (Table 1), or screening composition during bottling and storage. Although, low accuracy and precision were obtained for the chemical parameters (e.g. ethanol content, and pH) routinely analysed in wine, calibration models for the chemical parameters analysed were considered acceptable for rough screening purposes in terms of the standard errors obtained.

Table 1. Full cross-validation statistics for chemical composition in commercial bottled wines analyses using short NIR wavelengths in transmission (800–1100 nm).

Constituents	*N*	R^2_{cal}	*SECV*	*RPD*	*LV*
Ethanol (% v/v)	96	0.67	0.48	1.8	5
Free SO_2 (mg L^{-1})	53	0.83	4.01	2.2	4
Total SO_2 (mg L^{-1})	111	0.70	28.6	1.7	6
pH	55	0.50	0.15	1.2	3

N: number of samples used to develop the cross validation models; R^2_{cal}: coefficient of correlation in calibration; *SECV*: standard error of cross validation; *RPD*: residual predictive deviation (*RPD* = *SD/SECV*); *LV*: number of latent variables used to develop the PLS calibration models.