Abstract Grape tannin measurement by near infrared spectroscopy

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Introduction

Tannins are polymeric flavonoid compounds that have a critical role in the final quality of red wines, mainly related with long term colour stability, and astringency, as well as their capacity as antioxidants. For many years several analytical methods have been developed to measure tannin, such as colorimetric techniques, while more recently efforts have focused on the development of rapid and simple methods to be implemented by the wine industry. The search for simple techniques to assess chemical and physical characteristics of grapes has been receiving increasing attention in recent years. Both viticulturists and winemakers have long sought objective measures of grape composition that closely relate to wine quality. However, the lack of simple, fast and reliable methods for the determination of chemical composition of grapes has been one of the main obstacles for the development of rapid quality control methods or techniques in both the industry and commercial trade.

Materials and methods

Samples (n=620) of homogenised red grape berries were analysed using a visible (Vis) and near infrared (NIR) spectrophotometer (400–2500 nm) in reflectance. The spectra and the analytical data were used to develop partial least squares (PLS) calibrations to predict dry matter (DM) content and condensed tannins (CT) concentration.

Results and discussion

Table 1 shows the coefficient of determination for cross validation (R^2_{CV}) and the standard error of cross validation (*SECV*), which were 0.92 and 0.83 % w/w for DM and 0.86 and 0.46 mg/g epicatechin equivalents for CT, respectively.

The standard error of prediction (*SEP*) was 1.34 % w/w for DM and 0.89 mg g⁻¹ epicatechin equivalents for CT, respectively. By implementing a NIR spectroscopy method to measure DM

Items	DM	СТ
n	287	140
$R^2_{\rm CV}$	0.92	0.86
SECV	0.83	0.46
RPD	3.5	3.3
PLS factors	11	13

Table 1. Cross-validation statistics for dry matter (%w/w) and condensed tannins (mg g⁻¹ epicatechin equivalents) in the set of red grape homogenates analysed using visible and NIR reflectance spectroscopy.

DM: dry matter, CT: condensed tannins; *n*: number of samples, R^2_{CV} : coefficient of determination in cross-validation, *SECV*: standard error in cross-validation, *RPD*: residual predictive deviation calculated as *SD/SECV*.

and CT in red grape homogenates, we have developed an approach that is suited to large- scale compositional analysis in commercial wine production facilities, as it enables the analysis of large numbers of samples needed to screen batches of fruit. From an economical point of view the calibration models could be achieved with relatively small data sets. Thus, NIR offers a suitable and efficient tool for the simultaneous measurement of DM and CT in addition to other important parameters in red grape homogenates such as total anthocyanins, total soluble solids, and pH, with minimal sample preparation and low cost.