Abstract
Measurement of volatile compounds in wine by near infrared spectroscopy

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Introduction

Volatile chemical compounds responsible for the aroma of wine are derived from a number of different biochemical and chemical pathways. These chemical compounds are formed during grape berry metabolism, crushing and fermentation processes (i.e. yeast and malolactic) and also from the ageing and storage of wine. Not surprisingly, there are a large number of chemical classes of compounds found in wine that are present at varying concentrations (ng L^{-1} to mg L^{-1}), exhibiting different potencies, and having a broad range of volatilities and boiling points. The aim of this work was to investigate the potential use of near infrared (NIR) spectroscopy combined with chemometrics as a rapid and low cost technique to measure volatile compounds in Riesling wines.

Materials and methods

Samples of commercial Riesling wine were analysed using an NIR instrument in transmittance (400–2500 nm). Volatile compounds were determined by gas chromatography (GC) coupled with selected ion monitoring (SIM). Correlations between the NIR and GC data were developed using partial least squares (PLS) regression, using full cross-validation (leave-one-out).

Table 1. Cross validation statistics for volatile compounds measured in Riesling wine by NIRS. (Unit: µg L^{-1}).

Constituents	*N*	R^2	*SECV*	*RPD*	PLS terms
Esters	160	0.74	313.6	1.8	12
Monoterpenes	171	0.90	20.9	3.1	9
Short chain fatty acids	130	0.80	1658	1.3	12

N: number of samples in calibration; R^2: coefficient of determination in cross validation; *SECV*: standard error in cross validation; *RPD*: ratio of standard deviation of reference data in validation set to *SECV*

Results and discussion

Coefficients of determination in cross validation (R^2) and the standard error of cross validation (*SECV*) were 0.74 (*SECV*: 313.6 µg L^{-1}) for esters, 0.90 (*SECV*: 20.9 µg L^{-1}) for monoterpenes and 0.80 (*SECV*: 1658 µg L^{-1}) for acids, respectively. This study has shown that some of the volatile chemical compounds present in wine can be estimated by NIR spectroscopy. Further development with larger data sets will be required to verify the predictive ability of the NIR calibration models.