Abstract
Applications of near infrared spectroscopy for wine classification and authentication

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Introduction

Wine identification, or classification, mainly in terms of variety and geographical region of origin, has received increasing attention during the past 10 years using multivariate statistical techniques. Recently, the use of multivariate statistical techniques on chemical and sensory data, has gained increasing attention as a means to classify wines from different geographical regions, to describe similar properties, and to discriminate sensory and chemical characteristics. The aim of this work was to investigate the potential of NIR as a rapid and low cost technique to discriminate between commercial wine varieties (e.g. Riesling and Chardonnay, Sauvignon Blanc from different origins) using their spectral properties without depending on chemical composition and sensory characteristics.

Materials and methods

Discrimination models were developed using principal component analysis (PCA), linear discriminant analysis (LDA) and partial least squares – discriminant analysis (PLS-DA) regression. Wine samples (e.g. Riesling, Chardonnay, and Sauvignon Blanc from different origins, Tempranillo) were randomly split into two sets, one used as a calibration set and the remaining samples as a validation set. Each sample in the calibration set was assigned a dummy variable as a reference value. The classification of the wine samples according to geographic or varietal origins was on the basis of the 1.5 cut-off value.

Results and discussion

The score plot (PC1 vs PC2) of Riesling and Chardonnay wines analysed using Vis-NIR is shown in Figure 1.
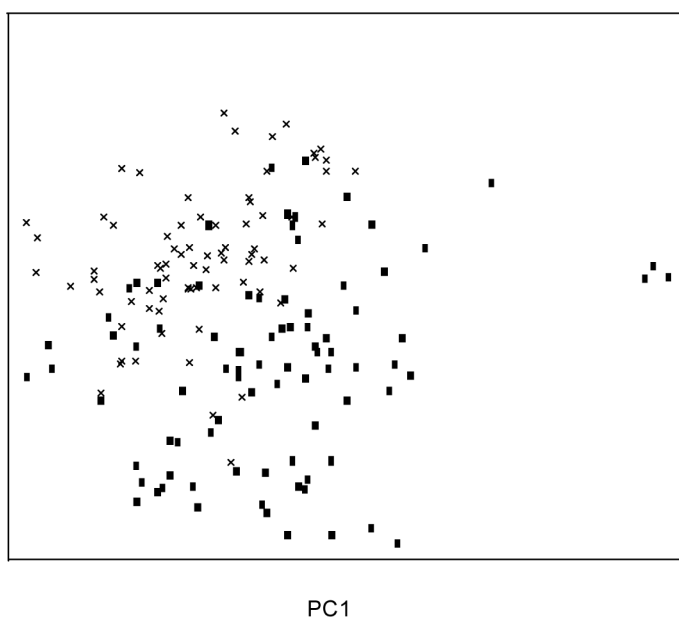
PC1

Figure 1. Score plots for the two first principal components in commercial white wines (x = Riesling; ■ = Chardonnay). Full range (400–2500 nm) and second derivative.

When used to predict the variety of the validation set samples, the PLS discrimination models correctly classified more than 90% of Riesling and up to 80% of Chardonnay wines, respectively. These results showed that NIR using PLS-DA might be a suitable and alternative technology that can be easily implemented by the wine industry to discriminate between Riesling and Chardonnay commercial wine varieties. However, the relatively limited number of samples and varieties involved in the present work suggest caution in extending the potential of such a technique to other wine varieties.