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Classification of Wine Grape Based on Different Phytosanitary Status by Using Visible/Near Infrared Spectroscopy

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The grape selection at the consignment is crucial for big cooperative companies with thousands of members, and therefore grapes may have different quality characteristics and health status. The quantification of diseases on wine grapes is commonly performed by a visual evaluation of the infection symptoms in grape bunches. Based on grapes quality, wineries often enforce a price penalty downgrading the grapes value imposing a severe reduction of vine growers' income. The application of optical techniques could minimize contentious between members and winery and could improve the standardization of the grape quality and therefore of the wine.
The aim of this work was to investigate the applicability of vis/NIR spectroscopy for a rapid assessment of phytosanitary status of grape bunches directly at the check point at the grape consignment. This preliminary experimental step was conducted in lab-scale condition using a vis/NIR device built specially for analysis of non-homogeneous product in the spectral range 400-1650 nm. Spectral measurements were carried out on healthy (1235 samples) and diseased bunches (1324) from white and red grapes for a total of 2559 spectra.
Quantitative (Partial Least Squares – Discriminant Analysis, PLS-DA) analyses were applied on grape spectra in order to test the performance of vis/NIR spectroscopy to classify healthy and infected bunches. The results obtained from PLS-DA models, in cross-validation, gave positive predictive values of classification between 89.8 % and 91.1 %.
Results demonstrated that vis/NIR spectroscopy is capable to provide useful information about wine grape phytosanitary status. However, further studies and real scale measurements are needed to determine the best operating conditions for a future engineering phases to perform the measurements directly at the consignment check point station.

1. Introduction

The grape selection at the check point station entering the winery is an important phase to obtain a qualitatively good product. Especially for big companies, such as cooperatives with a high number of partners, the vineyards spread over large spaces can lead to differences in term of grapes features also inside the same variety, showing possible different qualities and healthy status.
Disease quantification on grapes is nowadays performed by a visual estimation of the infection symptoms in bunches and calculating the healthy degree of the sample (Hill et al. 2014 and 2013). Depending on quality level and phytosanitary status, wineries downgrade the grapes enforcing price penalties imposing a reduction of vine growers' income. This subjective method is liable, as expected, to errors and therefore an objective and possibly cost-effective and useful quantification method is needed.
The development of a timely method to evaluate grape quality and relative phytosanitary status could absolve wineries experts from subjective downgrade decisions and optimize the selection phase for a better management of the vinifications. For this purpose, could be used some optical non-destructive technologies usable at the check point station. The application of optical techniques could minimize problems between

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members and winery inspectors and could improve the standardization of the grape quality and therefore of the wine.

Optical techniques as visible near infrared (vis/NIR) and near infrared NIR (NIRs) spectroscopy, image, and multi/hyperspectral analyses are applied for quality evaluation in the food sector, thanks to several advantages (non-destructive techniques, rapid, accurate) (Giovenzana et al., 2015). Moreover, these techniques allow the complete analysis of the lots at a reasonably affordable cost (Guidetti et al., 2012).

Regarding the application of optical techniques for the analysis of quality and phytosanitary status of wine grape some studies can be found in literature. NIR spectroscopy was used as a non-destructive technique for the assessment of changes in quality properties of wine grapes during ripening and at harvest (González-Caballero et al., 2010). NIR was applied in the field to measure quality parameters of wine grape and to define the best harvesting time (Giovenzana et al., 2014; Guidetti et al., 2010; Kemps et al., 2010), to control crucial parameters during the withering process (Beghi et al., 2015), and to measure the mould contamination degree at winery arrival determining the payment amount (Gishen et al., 2005).

The botrytis bunch rot was evaluated in white wine grapes by Hill et al. (2014) comparing four quantification methods: digital image analysis, near-infrared (1260-1370 nm) and mid-infrared (8760-9520 nm) spectroscopy, and quantitative real-time polymerase chain reaction. Image analysis was applied to quantify the proportion of the area of individual bunches affected by Botrytis cinerea, while near-infrared and mid-infrared spectroscopy were performed on homogenised berry samples to estimate botrytis bunch rot.

Oberti et al. (2014) used multispectral imaging on grapevine leaf samples exhibiting symptoms at different levels in a view of an automatic detection of powdery mildew on grapevine leaves.

Rustioni et al. (2014) investigated changes in the optical properties (450-750 nm) of white-berried grapes with the objective of monitoring spectra evolution related to browning symptoms appearance, to identify chemical features related to sunburning predisposition.

NIR spectroscopy is also used on grapevine leaves to reach information regarding vigour levels and for an early detection of vine diseases (Hall et al. 2002), or for the monitoring of water stress (De Bei et al. 2011).

The aim of this preliminary work is to apply visible/near infrared spectroscopy for a rapid evaluation of grape phytosanitary status in a view of a grape classification directly at the check point station entering the winery. The experimentation was conducted using grape bunches naturally infected by the most common grape diseases.

2. Materials and Methods

2.1 Sampling

Spectral acquisitions were performed during the grape harvest period on bunches deriving from different white grapes varieties and red grapes (Vitis vinifera L.). Grape bunches were collected directly from the consignment wagons at the check point station entering a winery.

Spectral acquisitions were performed without any sample preparation in the winery laboratory (lab-scale conditions), soon after bunches classification. The laboratory scale measurement setup was necessary in this first step of the research to simulate in controlled environmental conditions a future operative use feasible in real scale use directly at the check point station. The laboratory setup was studied to be easily transferable to the operative scale. Measurements were performed on healthy and diseased bunches for a total of 2559 analyzed samples as detailed in Table 1.

Table 1: Sampling details.

Samples type	Phytosanitary status of grape		
	Healthy	Infected	Total samples
White grape	589	595	1184
Red grape	646	729	1375
Total grape	1235	1324	2559
Total grape (%)	48	52	100

2.2 Disease assessment

Prior to spectral acquisition, each bunch was evaluated from a pathological point of view for the identification of infection. For each grape bunch, disease severity was estimated visually (by a plant pathologist and by an oenologist from the winery) as the proportion of berries showing disease symptoms when viewed from one side of the bunch, using a standard area diagram (Hill et al. 2010).

2.3 Spectral acquisitions

Spectral acquisitions were performed by using a vis/NIR device (Corona Process, Zeiss, Germany) suitable to operate in process conditions for non-contact analysis of non-homogeneous product (device features: dimension 40 x 30 x 30 cm, weight about 15 kg). Measurements were performed in reflectance mode in the vis/NIR spectral range (400-1650 nm, spectral resolution 2.0 nm) at a variable autofocused distance between sensor and sample ranged 80 - 600 mm. This device is therefore particularly suited for application during the grape selection process at the consignment.
As a function of the classification results, it could be envisaged a use of the system by the winery operators to define product acceptability thresholds and an objective indicator useful for a better management of grapes during the consignment phase.
Considering the operative conditions, spectra were acquired in reflectance mode: the sample surface was illuminated by the halogen lamp with a 6 cm spotlight. Each spectral sample was an average of three acquisitions in three different spots of the bunch. Each acquisition represents an average of ten reflectance spectra. The measurements were performed at a distance of about 30 cm between sensor and sample (Figure 1), simulating the real distance between sensor and samples in a future real scale application.

Figure 1: Particular of the illumination spotlight during vis/NIR measurements on a white grape bunch (left) and on a red grape sample (right).

2.4 Data analysis

Spectra were used to calibrate classification models using statistical tools for multivariate analysis. The chemometric analyses of vis/NIR spectra were performed using the Unscrambler 9.8 software package (CAMO ASA, Oslo, Norway). Vis/NIR spectra were pre-processed using moving average smoothing (10 point-wide window) to improve the signal-to-noise ratio for a reduction of the effects caused by the physiological high variability of samples. Prior to model calibration, a Principal Component Analysis (PCA) was applied on smoothed spectra for explorative purposes and for a qualitative initial evaluation of the spectral dataset (Beebe et al., 1998). PCA was used to highlight the optical differences of the spectra acquired on healthy samples and on diseased samples (data not shown).
The partial least square discriminant analysis (PLS-DA) method was applied for the classification analysis using the grape bunches spectra.

The objective of the PLS-DA application is to find models that allow the maximum separation among classes of objects (Wold et al., 2001). PLS-DA accomplishes a rotation of the projection to latent variables focusing on class separation. A matrix of artificial (dummy) variables, assuming a discrete numerical value (zero or one), was used as Y data.
The Y dummy matrix is constructed to ensure that the value of the objects belonging to the class corresponds to one, and the value of all other objects corresponds to zero (Liu, et al., 2008; Musumarra et al., 2005). In this work, PLS-DA was used to distinguish the healthy from the diseased samples. All the classification rules were evaluated using a cross-validation leave-more-out procedure using five cancellation groups (Casale et al., 2008) and the PLS-DA cut-off value for samples discrimination was fixed at 0.5.

3. Results and discussion

Regarding the white grape, spectra shows important absorbance in the 550-680 nm range, around the chlorophyll absorption peak at 670 nm, and throughout the NIR region (700-1650 nm). As expected, a peak in the band centered around 540 nm associated with green samples' reflectance peak can be noticed. Regarding the red grape, the observed changes in the visible region between 500 and 700 nm are mainly due to changes in the amount of pigment linked to the ripening progress. This behaviour leads to a decrease in reflectance in the visible band associated with the anthocyanin absorption peak of red grapes centered around 540 nm (Tamura and Yamagami 1994).
A reflectance peak is shown around 760 nm in the NIR region (700-1650 nm). Moreover, a peak at 970 nm can be noticed (absorption peak relative to the second overtone of the water O–H bond in the near infrared region). This in-depth peak at 970 nm is characteristic of the vis/NIR measurements on products very rich in water, like fruits (Nicolaï et al. 2007). The peaks around 1180 nm and 1400 nm have an analogous origin and they arise also from typical water absorption (León et al. 2005).

3.1 Results of the PLS-DA analysis

The spectral data were used for the elaboration of PLS-DA classification models in order to classify the samples as healthy or diseased.
Table 2 shows the results deriving from the different considered samples datasets, resulting in different classification models: a model considering the white grapes, a model considering the red ones, and a model combining all the analysed bunches. For each PLS-DA model, the percentage of correctly classified samples (positive predictive value, PPV) was reported. For all the analysed models, considering the single white or red cultivar and considering a single classification model for both the white and red cultivars, the PPV (in validation) ranged from 89.8% for the red grape group to 91.1% for the white grape dataset.
The model elaborated considering all the available bunches achieved a classification PPV of about 90% in validation.
Porep et al. (2015) studied the use of an on-line vis/NIR spectrometer for rapid grape rot indicators assessment upon receival at wineries: in this study the authors obtained prediction R^2 equal to 0.70, 0.78, 0.57 and RPD equal to 1.3, 1.1, 1.2 for glycerol, gluconic acid and acetic acid estimation, respectively.
A study for the prediction of botrytis bunch rot in white wine grapes was carried out by Hill et al. (2013), obtaining also in this case encouraging results; the calibrated PLS model showed the highest predictive performance in the NIR spectral region, with a RPD of 2.2.

Table 2: Statistics and accuracy of the PLS-DA classification models calculated for different sample sets (white and red samples, total grape bunches).

Samples type	N° of samples	Calibration		Cross-validation	
		R^2_{cal}	PPV_{cal} (%)	R^2_{cval}	PPV_{cval} (%)
White grape	1184	0.67	91.6	0.66	91.1
Red grape	1375	0.62	90.0	0.61	89.8
Total bunches	2559	0.63	90.2	0.62	89.9

4. Conclusions

In this preliminary work was investigated the possibility to perform classification using vis/NIR spectroscopy for the rapid grape infection assessment. Results were encouraging and more investigation and tests are desirable for a future real scale application. In particular, further studies are needed to determine the best operating conditions and the engineering phases to perform the measurements directly at the consignment

check point station, and considering that the tested optical device can be easily positioned in an operative context. Moreover, important factors for a success of this application are the identification of the diseases typology and the fast quantification of the infection level. For this purpose, also quantitative predictive models need to be calibrated.

Different possible solutions for a future real scale use and an overall automation of the selection process can be highlighted. The optical system could be positioned on a conveyor belt between the grape reception area and the grape discharge hopper. In this case the grape is discharged from the wagon on the belt to be conveyed under the optical analysis system, and then from here discharged in the destination hopper. Applying this solution, the measurement of the whole mass of grapes (transported in a thin layer on the tape) could be performed, resulting in a less approximate assessment of the infection degree of the total grape amount.

In conclusion, automation is envisaged as a significant contribution to addressing issues such as relieving humans from conducting tedious, intensive, fatiguing operations, while extending working time and production timeliness, allowing on-line control and automation of sorting and classification, and objectifying the evaluation of quality and phytosanitary status of products.

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