Rapid and environmentally friendly wine analysis using Vis/NIR Spectroscopy and Support Vector Machine regression

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Visible and Near Infrared (Vis/NIR) spectroscopy has been investigated extensively during the last decade to measure quality parameters in wine. This technique has the advantages of being fast, non-destructive, requires no sample preparation and is chemical reagent-free, leading to no generation of residues. However, calibration models developed for the determination of some quality parameters in wine can exhibits non-linearities, leading to poor predictive performances when linear regression techniques are used. Therefore, a regression method that is able to work with non-linearities is an interesting alternative to improve the robustness and the predictive performance of the calibration models. The aim of this study was to calibrate and validate models that can be used to determine quality parameters in red wine using Vis/NIR spectroscopy and the Least Squares Support Vector Machine (LS-SVM) regression.

A total of 72 experimental 'Syrah' red wines produced in the São Francisco River Valley, Brazil, were used in this study. Wine samples were kept at 33ºC and subjected to transflectance analysis using a benchtop spectrometer (XDS, FOSS NIRSystems, MD, USA) in the spectral range from 400 to 2500 nm. Four separate measurements were carried out on each sample and the four spectra were averaged to provide a mean spectrum. Standard Normal Variate (SNV) was used as spectral preprocessing and the samples were divided into calibration and validation sets using the SPXY (Sample set Partitioning based on joint **x**–*y* distances) algorithm. Multivariate calibration models were developed using LS-SVM regression. Predictive performance of the models was evaluated using the coefficient of determination in the external validation step (R^2_v) and the root mean square error of prediction (RMSEP). Reference analyses were accomplished for the determination of pH, total acidity (TA), volatile acidity (VA), total monomeric anthocyanins (TMA), total phenolic compounds (TPC), color intensity (CI), tonality (TO), total polyphenolic index (TPI), dry extract (DE) and alcohol content (AC).

The predictive performance of the models are shown as follows in terms of R^2_v and RMSEP, respectively. pH: 0.80 and 0.08 (range: 3.25-3.86); TA: 0.73 and 7.68 mEq L^{-1} (range: 65.96-142.92 mEq L^{-1}); VA: 0.71 and 0.82 mEq L^{-1} (range: 3.87-14.33 mEq L^{-1}); TMA: 0.67 and 20.5 mg L^{-1} (range: 77.2-265.9 mg L^{-1}); TPC: 0.72 and 212 mg L^{-1} (range: 1,233-2,835 mg L^{-1}); CI: 0.95 and 0.78 (range: 7.07-21.97); TO: 0.87 and 0.03 (range: 0.26-0.79); TPI: 0.90 and 3.19 (range: 38.9-87.0); DE: 0.67 and 3.33 g L^{-1} (range: 15.50-43.85 g L^{-1}); and AC: 0.99 and 0.22% (range: 5.92-17.81% v/v). The models obtained were able to predict with acceptable accuracy the wine quality parameters evaluated in this study. The results show that the Vis/NIR spectroscopy associated with LS-SVM has potential to provide rapid and accurate wine analysis without generation of dangerous residues.

Acknowledgements

The authors would like to acknowledge the EMBRAPA, CNPq, INCTAA, FACEPE and NUQAAPE for financial support and Miolo Wine Group for providing the grapes used to produce the wine.

Novelty

Brazilian red wine physico-chemical profile was determined by visible/near infrared (Vis/NIR) spectroscopy for the first time. The technique is fast, non-destructive, requires no sample preparation, is chemical reagent-free, and does not generate dangerous residues. Some parameters evaluated in 'Syrah' red wines exhibited a non-linear behavior. The use of Vis/NIR spectroscopy associated with Least Squares Support Vector Machine regression is a promising alternative to be used in wine quality control.