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MULTIVARIATE CHARACTERIZATION OF ITALIAN MONOVARIETAL RED WINES USING FTIR SPECTROSCOPY

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The assessment of wine authenticity is of great importance for consumers, producers and regulatory agencies to guarantee the geographical origin of wines and grape variety as well. Since mid-infrared (MIR) spectroscopy with chemometrics represent a suitable tool to ascertain the wine composition, including features associated with the polyphenolic compounds, the aim of this study was to generate MIR spectra of red wines to be exploited for classification of red wines based on the relationship between grape variety and wine composition. Several multivariate data analyses were used, including Principal Component Analysis (PCA), Discriminant Analysis (DA), Support Vector Machine (SVM), and Soft Intelligent Modelling of Class Analogy (SIMCA).

The aim of this study was to investigate the application of MIR spectroscopy (from 4000 to 700 cm-1) combined with multivariate analysis to provide a rapid screening tool for discriminating among different red monovarietal Italian wine varieties.

A total of 110 monovarietal red wines vintage 2016 were collected directly from the companies across different regions of Italy, including the following eleven grape varieties: Sangiovese, Nebbiolo, Aglianico, Nerello Mascalese, Primitivo, Raboso, Cannonau, Teroldego, Sagrantino, Montepulciano and Corvina.

PCA showed five wavelengths that mainly contributed to the PC1, including much-closed peak at 1043 cm^{-1} that correspond to the C–O stretch absorption bands that are important regions for glycerol, whereas the ethanol peaks at about 1085 cm^{-1}. The band at 877 cm^{-1} would be related to C-C stretching vibration of organic molecules, whereas the asymmetric stretching for C–O in aromatic –OH group of polyphenols within the spectral regions from 1050 to 1165 cm^{-1}. In particular, the (1175) - 1100 - 1060 cm^{-1} vibrational bands are combination bands involving C–O stretching and O-H deformation of phenolic rings. The 1166-1168 cm^{-1} peaks are attributable to in-plane bending deformations of C-H and C–O groups of polyphenols, respectively, which polymerization may cause a slight peak shift due to the formation of H-bridges.

The best results were obtained with the SVM that achieved an overall correct classification up to 72.2% for test set, and 44.4% for the validation set of wines, respectively. The Sangiovese wines (n=19) were splitted in two sub-groups (Sang-Romagna n=12; Sang-Tuscany n=7) considering the indeterminacy of its origins, disputed between Romagna and Tuscany. Although the classification of three grape varieties was problematic (i.e. Nerello Mascalese, Raboso and Primitivo), the remaining wines were almost correctly assigned to their actual classes.

In conclusion, MIR spectroscopy coupled with chemometrics represents an interesting approach for the classification of monovarietal red wines, which is important in quality control and authenticity monitoring.

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