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APPLICATION OF NEAR-INFRARED SPECTROSCOPY TO CHARACTERIZE VOLATILE PHENOLS AND SENSORY PROFILE OF AGED WINE SPIRITS

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Volatile phenols are low molecular weight aromatic alcohols, with particular importance in wine spirits aged with wood due to their strong influence on sensory profile. Some of them are responsible for characteristic odor notes of several foods and beverages in wine spirits aged with wood. Currently, the analytical determination of these compounds is mostly carried by time-demanding chromatographic methods. Thus, their identification and/or quantification, especially by a fast, simple and accurate methodology, is of great interest for quality control.

In this study, spectral data acquired by Near-infrared spectroscopic (NIR) technique was used to predict the content of these compounds, in particularly eugenol, guaiacol, 4-methyl-guaiacol, syringol, 4-methyl-syringol and 4-allyl-syringol in samples of aged wine spirits. In addition, the volatile phenols' concentrations were determined by GC-FID (after liquid-liquid extraction) using the same sample set.

The wine spirits were obtained within the Oxyrebrand project (<https://projects.inia.pt/oxyrebrand>, shows a detailed explanation about the experimental design). Briefly, the samples were aged with chestnut or oak wood species, in 250 L wooden barrel and by an alternative technology using 50 L glass demijohns with wood staves and different levels of micro-oxygenation (MOX) in a total of 112 samples.

For the volatile phenols analysis, partial least square regression (PLS-R) models were developed with NIR spectra in the near-IR region of 12500 to 4000 cm^{-1} . In the PLS-R developed method, cross-validation with 50% of the samples was made along with a validation test set with 50% of the remaining samples. Principal component analyses (PCA), using the results obtained with a trained sensory panel and those of IR-Spectra, were made to compare the analytical and the sensory characteristics of the studied wine spirits.

PLS-R models showed good accuracy; R^2 ranged from 0.9732 to 0.9579 for syringol (2-Hydroxy-1,3-dimethoxybenzene) and 4-methylsyringol (2,6-Dimethoxy-4-methylphenol), respectively, with an RPM ranging between 6.11 to 4.88 for the same compounds. Concerning the sensory data, the PCA obtained with the spectral data is quite similar to those obtained with the data collected with the trained sensory panel.

Evidence exists that NIR spectroscopy is suitable as an easy and quick technique for assessing volatile phenols contents of volatile phenols as well as a promising one to access the sensory profile of aged wine spirit. Furthermore, NIR spectroscopy is a potential tool for assessing sensory profiles in aged wine spirits.

Keywords: Volatile phenols; Sensory profile; NIR; Chemometrics; Aged wine spirit