

Spectrofluorometric Analysis for Wine Authentication and Blend Detection

Application Note

A-TEEM™
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Introduction

Wine authentication is crucial in combating fraud within the wine industry, which is valued at hundreds of billions of dollars globally. Various fraudulent activities such as dilution, substitution, and mislabeling necessitate the development of robust authentication and traceability techniques.

Spectrofluorometric analysis, coupled with machine learning modeling, has emerged as a promising approach for authenticating wines based on their molecular fingerprints. This application note details the implementation of spectrofluorometric analysis, specifically absorbance-transmittance and fluorescence excitation-emission matrix (A-TEEM) technique, along with machine learning modeling to trace the molecular fingerprint of wines during the winemaking process and identify the blending percentages of different varietal wines.

Materials and Methods

1. Chemicals and Solvents

High-performance liquid chromatography (HPLC) grade absolute ethanol and analytical grade hydrochloric acid (HCl) were used for sample preparation. High-purity water was obtained from a Milli-Q purification system.

2. Wine Samples

Two sets of wine samples were collected: one set to examine the stage of wine production and another for blending experiments. Monovarietal wines from different regions were collected at various stages of winemaking, including post-primary fermentation, post-malolactic fermentation, and pre-blending. Additionally, commercially produced monovarietal wines were obtained for blending experiments.

3. Analytical Procedures for Basic Chemical Parameters

Basic chemical parameters such as pH, titratable acidity (TA), and alcohol content were measured using standard methods.

4. Sample Preparation and A-TEEM Analysis

Samples were prepared and analyzed using the A-TEEM technique, which involved dilution, centrifugation, and analysis of absorbance spectra and fluorescence excitation-emission matrices (EEMs). Pre-processing of EEM data included normalization and correction for spectral distortion.

Variety	Blending percentage (v/v)							
Shiraz	100	99	95	90	85	60	50	0
Cabernet-Sauvignon or Grenache	0	1	5	10	15	40	50	100

Table 1. Percentages of wine in blends of Shiraz with Cabernet-Sauvignon or Grenache.

5. Statistical Analysis

Statistical analysis included one-way analysis of variance (ANOVA), principal component analysis (PCA), and extreme gradient boosting discriminant analysis (XGBDA) for classification. Regression methods, including partial least squares regression (PLSR) and extreme gradient boosting regression (XGBR), were used for blend proportion modeling.

Results and Discussion

1. Variations According to Stage of Winemaking

Analysis of wine samples at different stages of winemaking revealed variations in basic chemistry and color parameters. PCA of EEM data showed distinct clustering of samples according to origin and winemaking stage, indicating the preservation of molecular fingerprints throughout the production process.

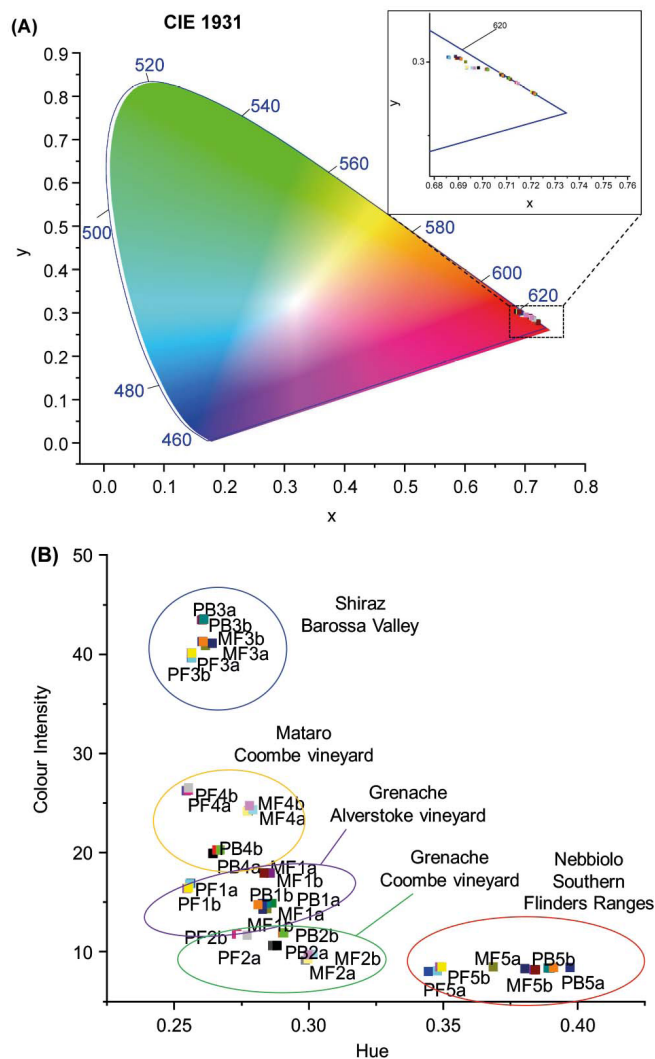


Figure 1. Analysis of colour parameters according to the stage of the winemaking process ($n = 15$, duplicate samples analysed twice) showing (A) CIE 1931 plot (inset shows clustering of samples) and (B) hue vs. colour intensity graph. PF, post-primary fermentation; MF, post-malolactic fermentation; PB, pre-blending. 1, Grenache from Alverstoke vineyard; 2, Grenache from Coombe vineyard; 3, Shiraz from Barossa Valley; 4, Mataro from Coombe vineyard; 5, Nebbiolo from Southern Flinders Ranges.

2. Modelling to Identify Blend Proportions

Regression models were developed to identify blend proportions in wine samples. While PLSR showed good accuracy, XGBR demonstrated superior performance with perfect correlation and minimal error, even at low blend percentages.

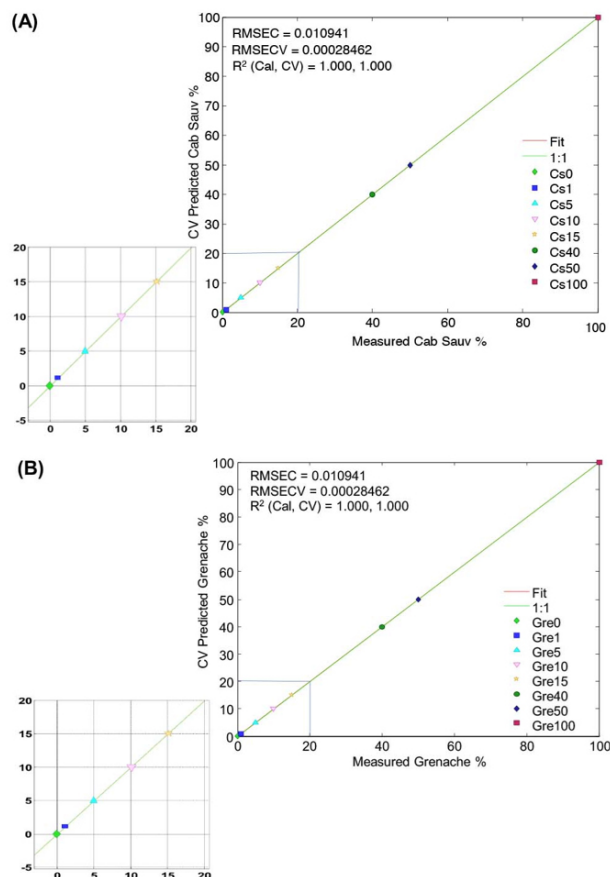


Figure 2. XGB regression of measured vs. CV predicted blending percentages for Shiraz wine containing proportions of (A) Cabernet-Sauvignon or (B) Grenache. Insets show more detail of the sample separation for 0%–15% blends.

Conclusions

The A-TEEM technique coupled with machine learning modeling offers a promising approach for wine authentication and blend detection. By tracing molecular fingerprints throughout the winemaking process and accurately identifying blend proportions, this method could effectively combat wine fraud and ensure product authenticity.

Acknowledgments

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This application note provides a comprehensive overview of the spectrofluorometric analysis method for wine authentication and blend detection, detailing the experimental procedures, results, and implications for the wine industry.

To see the full study, go to:

<https://oeno-one.eu/article/view/4904>

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