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Modelling Cabernet-Sauvignon wine sensory traits from spectrofluorometric data

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ABSTRACT

Understanding how wine compositional traits can be related to sensory profiles is an important and ongoing challenge. Enhancing knowledge in this area could assist producers to select practices that deliver wines of the desired style and sensory specifications. This work reports the use of spectrofluorometry in conjunction with chemometrics for prediction, correlation, and classification based on sensory descriptors obtained using a rate-all-that-apply sensory assessment of Cabernet-Sauvignon wines (n = 26). Sensory results were first subjected to agglomerative hierarchical cluster analysis, which separated the wines into five clusters represented by different sensory profiles. The clusters were modelled in conjunction with excitation-emission matrix (EEM) data from fluorescence measurements using extreme gradient boosting discriminant analysis. This machine learning technique was able to classify the wines into the pre-defined sensory clusters with 100 % accuracy. Parallel factor analysis of the EEMs identified four main fluorophore components that were tentatively assigned as catechins, phenolic aldehydes, anthocyanins, and resveratrol (C1, C2, C3, and C4, respectively). Association of these four components with different sensory descriptors was possible through multiple factor analysis, with C1 relating to 'dark fruits' and 'savoury', C2 with 'barnyard', C3 with 'cooked vegetables' and 'vanilla/chocolate', and C4 with 'barnyard' and a lack of C1 descriptors. Partial least squares regression modelling was undertaken with EEM data and sensory results, with a model for perceived astringency being able to predict the panel scores with 68.1 % accuracy. These encouraging outcomes pave the way for further studies that relate sensory traits to fluorescence data and move research closer to the ultimate goal of predicting wine sensory expression from a small number of compositional factors.

KEYWORDS

Rate-all-that-apply, cluster analysis, excitation-emission matrix, partial least squares regression, machine learning, chemometrics

Supplementary data can be downloaded through: https://oeno-one.eu/article/view/4805

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INTRODUCTION

Wine is a luxury product with a highly complex composition that can be affected by the environment in which the grapes are grown as well as techniques applied in the vineyard and winery. The intrinsic complexity of wine has necessitated the development of various techniques to obtain an in-depth understanding of grape and wine metabolites and control points during production that can shape the final product. Relating compositional and technological factors with the sensory expression of a wine, which is a determining factor for the overall consumer experience, remains an ongoing focus of research. Being able to link chemical and sensory information with the practices and techniques that wine endures during production would ultimately equip practitioners with the ability to make more precise decisions for producing targeted wine styles.

Multiple methodologies are available for sensory profiling of wine, but their suitability will depend upon the requirements of the study. Rate-all-that-apply (RATA) is a quantitative sensory methodology that is rapid and effective for wine sensory characterisation (Danner *et al.,* 2018), as shown by its successful use in different studies (Franco-Luesma *et al.,* 2016; Mezei *et al.,* 2021; Nguyen *et al.,* 2020). Similarly to sensory profiling, a range of analytical approaches are available to define wine chemical composition that underpins sensory traits. A common approach has therefore been to combine sensory data with a number of chemical analysis techniques to predict and classify wine sensory characters (Niimi *et al.,* 2018), explore distinctiveness (Geffroy *et al.,* 2016), comprehend the impact of storage and packaging conditions (Hopfer *et al.,* 2013), and understand quality drivers (Gambetta *et al.,* 2016; Hopfer *et al.,* 2015). Many studies rely on analytical methodologies that are time-consuming, expensive, and relatively intricate (e.g., HPLC or GC with mass spectrometry), requiring personnel with specialised skills. There is room, however, for more accessible approaches (usually spectroscopy-based) that can provide chemical information more simply and rapidly. As reviewed by Ranaweera *et al.* (2021a), there are various spectroscopic approaches and each differs in terms of compounds measured, sensitivity, and advantages/disadvantages, among other aspects. The choice of methodology should therefore be defined according to the needs and objectives of the study.

As a spectroscopic technique, spectrofluorometry has often been applied to the analysis of food products because of its time- and cost-effective nature, and its high selectivity and sensitivity (Ranaweera *et al.,* 2021a). It can provide a unique three-dimensional excitation and emission matrix (EEM) that acts as a molecular fingerprint of a sample (Coelho *et al.,* 2015; Ranaweera *et al.,* 2021b). This technique can be a useful tool to authenticate, distinguish and classify different food products through a qualitative investigation of specific fluorescent substances (e.g., phenolic compounds, vitamins, and aromatic amino acids) present at different concentrations depending on the product (Karoui and Blecker, 2011). This methodology is also highly applicable to wine, which contains a myriad of fluorophores. Spectrofluorometry has been applied to wine for authentication and discrimination of samples based on variety, origin, or vintage (Ranaweera *et al.,* 2021b; Ranaweera *et al.,* 2021c; Sádecká and Jakubíková, 2020; Suciu *et al.,* 2019), to analyse oxidative changes and sulfur dioxide addition (Coelho *et al.,* 2015), and to quantitatively assess polyphenol content (Cabrera-Bañegil *et al.,* 2017).

In the quest for a rapid technique that could link wine composition and sensory properties, this study aimed to explore 1) the association between sensory descriptors obtained by RATA and the fluorescence EEM data recorded for Cabernet-Sauvignon wines from the Coonawarra Geographical Indication (GI), and 2) the dominant sensory traits of such regional wines. Specifically, the study tested the applicability of using EEMs with machine learning modelling for sample classification based on sensory profiles, investigated the relationship between the main fluorophores identified by parallel factor analysis (PARAFAC) and sensory descriptors using multiple factor analysis (MFA), and assessed partial least squares (PLS) regression models to predict sensory attributes.

MATERIALS AND METHODS

1. Sample selection

Unreleased vintage 2020 Cabernet-Sauvignon wines were sought from commercial producers using fruit from the Coonawarra GI of South Australia. Most of the wines were monovarietal and had only undergone alcoholic and malolactic fermentation and racking, with minimal oak contact (≤5 months) and limited maturation time.

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In total, 26 Cabernet-Sauvignon wine samples (6 × 750 mL bottles of each wine) were obtained from 8 wineries/vineyards within the GI (Supplementary data, Table S1).

2. Sensory evaluation

Prior to formal evaluation, the wines were tasted by experts as defined by Parr *et al.* (2002) consisting of academics and postgraduate oenology students (n = 6), who evaluated aroma, flavour, taste, and mouthfeel with a free text assessment followed by a discussion of the wines. This informal tasting was used to evaluate whether the sample set was appropriate for a naïve panel to assess (considering that they were not commercially-released wines), to ensure that the samples could be differentiated, and to decide on the sensory attributes that should be included in the formal RATA evaluations.

Naïve wine consumers (n = 60; 27 females and 33 males from 18 to 77 years of age) were recruited based on being 18 years of age or older and having consumed red wine at least once a month. Evaluations were conducted in a purpose-built sensory laboratory at the University of Adelaide's Waite Campus, in individual booths equipped with a computer, under white fluorescent lighting, and at room temperature (22–23 °C). Samples (20 mL) were served at room temperature in clear stemmed ISO wine glasses coded with a random four-digit number and covered by a petri dish.

Due to the number of samples and to avoid palate fatigue, assessments were divided into three sessions: 9 samples in the first, 9 samples in the second, and 8 samples in the last session. The samples were randomly presented monadically for each subject within a session and the same panel was used for all three sessions. RATA methodology was used to characterise samples by rating the intensity only of the attributes that applied from a list of 53 comprising aroma, flavour, taste, and mouthfeel descriptors (Supplementary data, Table S2) on a 7-point scale (from "extremely low" to "extremely high"). Between samples, the panellists were forced to have a 1-min break and could cleanse their palate with deionised water and unsalted crackers. A 5-min break was enforced at the mid-point of the tasting (between samples 4 and 5). Data were collected with RedJade software (2016, Redwood City, USA). Informed consent was obtained from panellists and this study was approved by the Human Research Ethics Committee of the University of Adelaide (approval number: H-2019-031).

3. Chemicals

HPLC grade absolute ethanol and analytical grade 37 % hydrochloric acid (HCl) were purchased from Chem-Supply (Port Adelaide, SA, Australia). High purity water was obtained from a Milli-Q purification system (Millipore, North Ryde, NSW, Australia).

4. Spectrofluorometric analysis

After sensory analysis, the remainder of each wine was subsampled into a 4 mL centrifuge tube that was completely filled and stored in a refrigerator at 4 °C until measurements were performed. After warming to room temperature, samples were centrifuged at 9300 × *g* for 10 min and diluted with 50 % aqueous ethanol that had been adjusted with HCl to pH 2 and vacuum filtered (0.45 µm PTFE membrane). The samples were diluted 150-fold (Ranaweera *et al.,* 2021c), and analysed in a Hellma type 1FL (1 cm path length) Macro Fluorescence cuvette (Sigma-Aldrich, Castle Hill, NSW, Australia). Samples were prepared in duplicate and two measurements of each sample were undertaken with a Horiba Scientific Aqualog® spectrophotometer (version 4.2, Quark Photonics, Adelaide, SA, Australia). The excitation wavelength ranged from 240 to 700 nm with an increment of 5 nm under medium gain and 0.2 s integration time and the emission wavelength ranged from 242 to 824 nm with an increment of 4.66 nm. Data acquisition was controlled with Origin software (version 8.6, OriginLab® Corporation, Massachusetts, USA) and EEMs were normalised using water Raman scattering units and corrected for the inner filter effects, solvent background, dark detector signals, and Rayleigh masking (Gilmore *et al.,* 2017).

5. Basic analytical measurements of pH, TA, ethanol, and SO_2

Sample pH and titratable acidity (TA) were obtained with a T50 auto-titrator (Mettler Toledo, Melbourne, VIC, Australia). Ethanol was measured in triplicate by HPLC analysis (Li *et al.,* 2017) of undiluted samples that were centrifuged at 9300 × *g* for 10 min. Separation was performed with an Aminex HPX-87H column (300 mm × 7.8 mm, BioRad, Hercules, California, USA) thermostatted at 60 °C using 2.5 mM H_2SO_4 as mobile phase with a flow rate of 0.5 $mLmin^{-1}$. Peaks were detected with a refractive index detector (RID-10A, Shimadzu, Kyoto, Japan) and quantified by comparison with standards prepared in model wine using ChemStation for

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LC 3D Systems software (Agilent Technologies, Santa Clara, CA, USA). Free and total SO_2 concentrations were determined in duplicate using the method described by Iland *et al.* (2004).

6. Statistical analysis

The raw sensory data were firstly analysed through two-way analysis of variance (ANOVA) with panellists as a random factor and samples as a fixed factor to identify significantly different attributes between the samples. Attributes that presented a p-value ≤ 0.1 were selected for agglomerative hierarchical cluster (AHC) analysis of all samples with an automatic entropy truncation and Euclidean distance using Ward's method or unweighted pair-group average (UPGMA). With a superior cophenetic correlation (0.676 for UPGMA *versus* 0.511 for Ward's method), UPGMA was chosen and truncation configured with a minimum of five classes. Correlation principal component analysis (PCA) was performed to identify sensory profiles that arose for different clusters based on the AHC analysis.

EEM data were unfolded using unfold multiway (mode 1) in Solo software (version 8.7.1, Eigenvector Research, Inc., Manson, WA, USA). For classification according to the clusters defined by AHC analysis, extreme gradient boosting discriminant analysis (XGBDA) was conducted (Ranaweera *et al.,* 2021c) using pre-processing with mean centring, PLS compression to yield a maximum of 25 latent variables (LVs), and decluttering with generalised least squares weighting at 0.2 for calibration and cross-validation (k = 10, Venetian blinds procedure). Confusion matrix score probabilities were used to assess the model effectiveness. PARAFAC was performed with a non-negativity constraint in all modes imposed and the model was validated by split-half analysis (Murphy *et al.,* 2013).

Loadings for the components determined by PARAFAC were analysed in conjunction with the sensory data (significantly different attributes, $\alpha = 0.1$) through MFA. Separately, a calibration model was created with PLS1 regression of sensory scores for perceived wine astringency and the EEM data to predict astringency ratings. The model was optimised through assessment of LVs, root mean square error of calibration (RMSEC), root mean square error of cross-validation (RMSECV, Venetian blinds with 10 splits), and root mean square error of prediction (RMSEP).

ANOVA, PCA, AHC, and MFA were performed with XLSTAT (version 2019.4.1, Addinsoft, New York, USA). XGBDA, PARAFAC, and PLS regression analysis were conducted with Solo software (version 8.7.1).

RESULTS AND DISCUSSION

Unreleased Cabernet-Sauvignon wines sought for the study went through minimal post-fermentation processes (e.g., fining, maturation, blending) and were bottled at early stages of production so that the impact of the Coonawarra GI could be assessed with minimal influence of downstream winemaking operations. Basic analytical measurements were within the normal range for red wines at such a stage of production. The total and free SO_2 content ranged from 0.4 to 70.8 mgL^{-1} and 0.4 to 33.4 mgL^{-1}, respectively, TA ranged from 5.6 to 7.5 gL^{-1}, pH values ranged from 3.40 to 3.87, and ethanol concentration ranged from 12.9 % to 15.3 % (Supplementary data, Table S1).

1. RATA sensory profiling and clustering of wines

Of the 53 sensory attributes rated by panellists using RATA methodology, 20 were significantly different ($\alpha = 0.1$) according to ANOVA and comprised 8 aromas, 8 flavours, 3 tastes, and 1 mouthfeel attribute (Supplementary data, Table S3). The means of the 20 descriptors were analysed through a correlation PCA (Figure 1) following the AHC analysis (Supplementary data, Figure S1). The first factor (F1) in Figure 1A accounted for 30.6 % of the data variance and the second factor (F2) explained a further 19.6 %. Cluster 1 (shown in red, 7 wines) appeared on the right side of F1 and spread across both segments of F2, with 5 samples in the upper half and 2 in the lower half. Cluster 2 (green, 14 samples) mostly presented near the origin, with 11 samples on the left and 3 samples on the right of F1, and a more or less even spread across F2. Cluster 3 (cyan, 2 samples) was found on the left side of F1 and upper half of F2, and Cluster 4 (pink, 1 sample) was separated from the rest in the bottom right portion of the plot. Squared cosine values for samples in Cluster 5 (data not shown) indicated a higher representation on F3, in the lower half as seen in Figure 1B.

In terms of the sensory descriptors, 'barnyard' flavour and aroma, and bitterness and astringency were plotted on the right side of F1 and lower part of F2; 'minty', 'cooked vegetables', 'dark fruits', 'tobacco', and 'earthy' aromas and flavours, 'oaky' and 'savoury' aromas, and acidity were plotted

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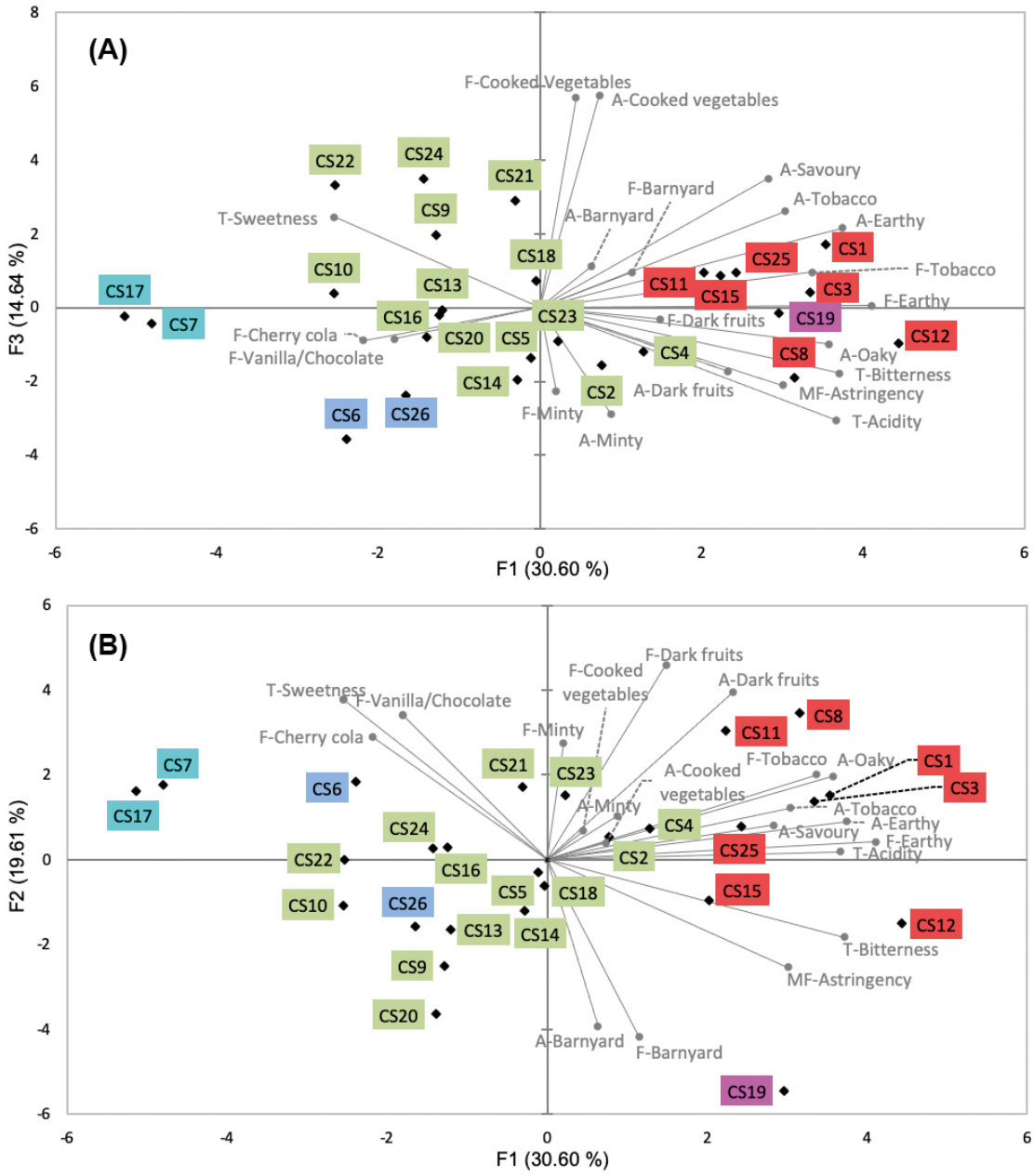


FIGURE 1. Principal component analysis biplots of Cabernet-Sauvignon wines (n = 26) using significantly different (α = 0.1) RATA attributes, showing (A) F1 *versus* F2 and (B) F1 *versus* F3.

Colour coding represents the clusters resulting from the agglomerative hierarchical cluster analysis (Supplementary data, Figure S1), with samples in the same cluster bearing the same colour. Cluster 1, red; Cluster 2, green; Cluster 3, cyan; Cluster 4, pink; Cluster 5, blue. A-, aroma; F-, flavour; MF-, mouthfeel; T-, taste.

on the right side of F1 and upper half of F2; and 'vanilla/chocolate' and 'cherry cola' flavours, and sweetness were plotted on the left side of F1 and upper half of F2 (Figure 1A). The aroma and flavour of 'cooked vegetables' were better represented in the upper half of F3 (Figure 1B).

The clusters defined by AHC analysis (Supplementary data, Figure S1) could be explained through different sensory profiles as shown in Figure 1. Cluster 1 was characterised by savoury characters including 'earthy' and 'tobacco', along with 'oaky' and 'dark fruits' aromas, and higher acidity, whereas Cluster 2 on the opposite side was generally characterised by a lack of those characters. Considering that these were young wines, the results might indicate the presence of some oak contact during fermentation for most samples in Cluster 1 as opposed to no oak contact for samples in Cluster 2 (Crump *et al.,* 2015).

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Cluster 3 was associated with higher sweetness and 'cherry cola' flavour and low bitterness and astringency. Cluster 4 was characterised by 'barnyard' aroma and flavour, relatively low 'vanilla/chocolate' and 'cherry cola' flavours, a higher bitter taste and astringent mouthfeel, and a lack of sweetness. Cluster 5 was especially related to 'cherry cola' and 'vanilla/chocolate' flavours (Figure 1B), as opposed to the savoury profile found for Cluster 1 (Figure 1A). Sensory profiles have similarly been used in the past for regional classification of Australian Cabernet-Sauvignon wines (Souza Gonzaga *et al.,* 2019; Souza Gonzaga *et al.,* 2020) and Australian Shiraz and Chardonnay wines (Kustos *et al.,* 2020). Those studies with commercial wines reported that some distinctive sensory traits can be more important and more associated with a specific wine-producing region, with the current work on unreleased wines also indicating the existence of perceived differences within a GI according to Figure 1.

The main differences reported previously for Cabernet-Sauvignon wines were the duality between 'green' and 'fruity' related characters and between 'oak' related traits and 'eucalyptus' or 'minty' attributes (Heymann and Noble, 1987; Souza Gonzaga *et al.,* 2020). In the present study, the contrast was between 'barnyard', astringency and bitterness attributes, and 'cherry cola', 'vanilla/chocolate', and sweetness. Oak-related and savoury attributes and the 'minty' trait were found in the same quadrant, not in direct contrast, and the same was evident for fruity and vegetal characters (Figure 1A). Considering the samples were dominated by or exclusively produced from Cabernet-Sauvignon (Supplementary data, Table S1) and were all from the same GI, albeit from different vineyards and wineries, the disparity in the sensory profiles of the present work might be associated with differences in the winemaking processes, as seen previously by Kustos *et al.* (2020) with Australian Chardonnay and Shiraz wines. Additionally, the wines in the present study had a minimal influence of oak (i.e., less than 5 months) or other maturation treatments compared to commercially released red wines, which might have allowed sensory traits that could be attributed to aspects of terroir (e.g., soil, topography, and vineyard management practices) to be more perceivable, such as the 'minty' and fruity attributes.

Some samples in Cluster 2 indicated that 'minty' flavour was an important characteristic, although in general not much difference was seen between the samples (Figure 1A). A 'minty' character has been reported previously for Coonawarra Cabernet-Sauvignon wines, which might indicate this as a dominant trait for the Coonawarra region (Robinson *et al.,* 2011; Souza Gonzaga *et al.,* 2019; Souza Gonzaga *et al.,* 2020). Characters described as 'minty' and 'eucalyptus' in Cabernet-Sauvignon wines have been associated with the presence of eucalyptol (i.e., 1,8-cineole) and hydroxycitronellol, and although 'eucalyptus' aroma and flavour were not statistically significant ($\alpha = 0.1$) in the present work (Supplementary data, Table S3), studies have shown that they might be interchangeable and indistinguishable by a sensory panel (Capone *et al.,* 2012; Robinson *et al.,* 2011; Souza Gonzaga *et al.,* 2020). The current study did not explore the presence of volatile compounds so the link between 'minty' and 'eucalyptus' from both sensory and chemical viewpoints is open for further examination. Among the possibilities, the occurrence of 1,8-cineole in wine has been related to the presence of *Eucalyptus* trees within the vineyard environment (Capone *et al.,* 2012), whereas some studies report the presence of 'minty' traits associated with an aged profile of Bordeaux red wines specifically under the influence of the proportion of Cabernet-Sauvignon in the blend (Picard *et al.,* 2015; Picard *et al.,* 2016b). Mint aroma in that case has been associated with the presence of piperitone (Picard *et al.,* 2016a). Considering that the present study examined young Cabernet-Sauvignon wines, it seemed unlikely that piperitone or other limonene-derived compounds (Picard *et al.,* 2017) were responsible for the presence of the 'minty' attribute, although further investigation is required to clarify the role of various monoterpenoids in the perception of mint-related characters.

2. Classification of sensory clusters based on spectrofluorometric analysis

To examine whether sensory information could be classified using spectrofluorometric data, the results from AHC (Supplementary data, Figure S1) were modelled in conjunction with the EEMs of the wine samples through machine learning with the XGBDA algorithm. Various algorithms and machine learning tools exist for wine classification based on EEM data, such as soft independent modelling of class analogy and support vector machine, but XGBDA performs well when analysing a complex heterogeneous matrix with uneven class distribution (Babajide Mustapha and Saeed, 2016). The analysis was undertaken

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after PLS compression, used to improve the stability of the model by making it less disposed to overfitting. The class CV prediction demonstrated in Figure 2 shows each cluster (denoted using different symbols and colours) that was predefined by AHC. The model attempted to predict the class (cluster) to which each sample belonged, based on the relationship of the sensory profiles and EEM data. Figure 2 and the confusion matrix obtained from cross-validation (data not shown) highlighted that all clusters were 100 % correctly classified with a discrete segregation between the classes in the cross-validated model. This result indicated that the underlying composition of the wines encompassed in the fluorescence fingerprints might be driving the sensory differences of the clusters determined from RATA evaluation.

Classification methods using fluorescence spectroscopy have been previously applied for wine varietal, vintage and origin authentication (Ranaweera *et al.,* 2021b; Ranaweera *et al.,* 2021c; Sádecká and Jakubíková, 2020; Suciu *et al.,* 2019), which tends to yield similar or even better performance compared to other spectroscopic methods like UV-vis, near-infrared, mid-infrared, synchronous fluorescence, or Raman (Mandrile *et al.,* 2016; Riovanto *et al.,* 2011; Tan *et al.,* 2016). Ultimately, studies involving spectrofluorometry and chemometrics have demonstrated the approach as a valid tool for authenticating wine, and along with the present work, highlight the extent to which this type of data can be used to understand important traits related to wine chemical and sensory properties.

3. Using PARAFAC to identify main fluorophoric compounds

Attempting to shed light on the relationship between fluorescence data and sensory properties, PARAFAC was performed on the EEM data to identify the main fluorophores present in the samples. The percentage of core consistency of the data can be applied in combination with split-half analysis to assess the model suitability, especially with high complexity matrices such as wine (Airado-Rodríguez *et al.,* 2011; Murphy *et al.,* 2013). The split-half analysis compares the similarity between each half of

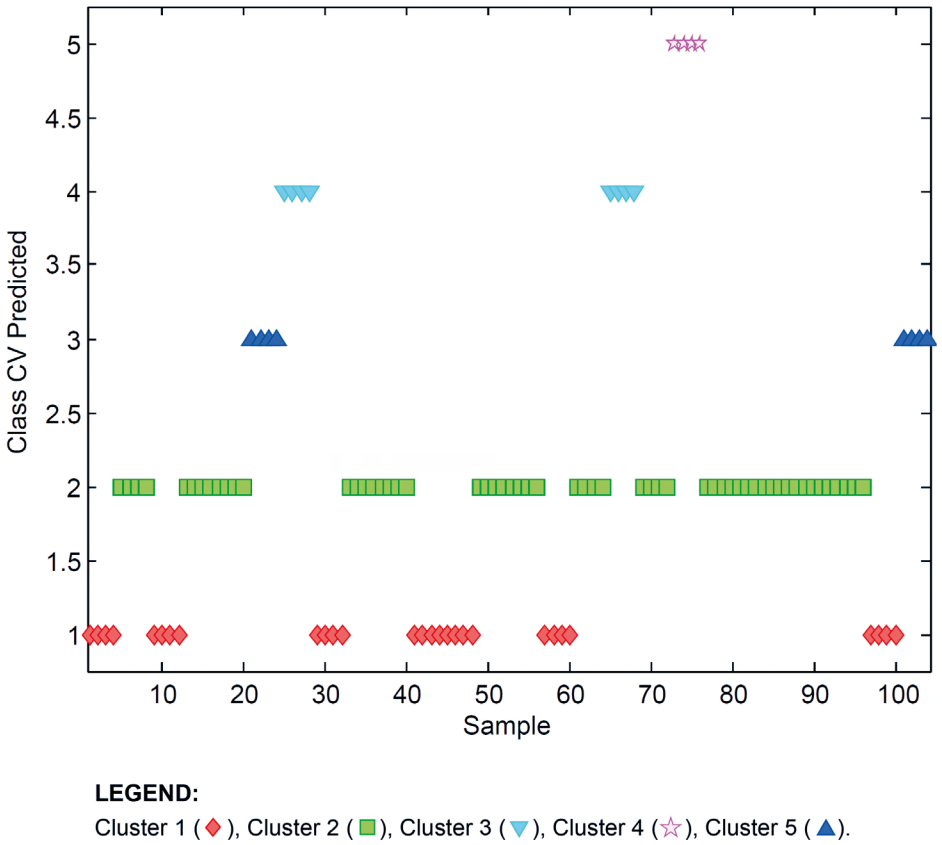


FIGURE 2. Class CV predicted for classification of RATA clusters arising from AHC based on XGBDA modelling for the set of Cabernet-Sauvignon wines (n = 26).

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the data set, and like with core consistency, a higher percentage is desirable when deciding on the number of components for the model (Murphy *et al.,* 2013). Using all samples in the first PARAFAC model generated a core consistency of less than 0 % and a split-half result of less than 19 %. Investigating further, analysis of residuals of the samples showed that three (CS2, CS7 and CS26) of the 26 wines were outliers and presented equally high residuals for the four determinations (i.e., duplicate readings of duplicate samples) compared to the other samples. Based on the available data, no possible reason was identified that could explain the three samples as outliers. Although sample CS7 was the only sample produced with 100 % uninoculated alcoholic and malolactic fermentation, which might indicate a possible factor, that was not the case for the other two outlier samples. Nonetheless, PARAFAC modelling was performed again without the outlier samples, this time yielding a core consistency of 61 % and split half analysis of 93.7 % for the four main fluorescent components (Figure 3).

From PARAFAC it was possible to identify the maximum intensities (λ_{ex} and λ_{em}) for the four components as demonstrated in Figure 3, and therefore to tentatively assign chemical compound classes that are naturally present in wine (Airado-Rodríguez *et al.,* 2011; Airado-Rodríguez *et al.,* 2009). Such spectral data can typically be related to fluorophoric compounds such as vitamins (Christensen *et al.,* 2006) and especially phenolic compounds (Schueuermann *et al.,* 2018). For PARAFAC component 1, maximum intensities of λ_{ex} = 275 nm and λ_{em} = 310 nm were tentatively

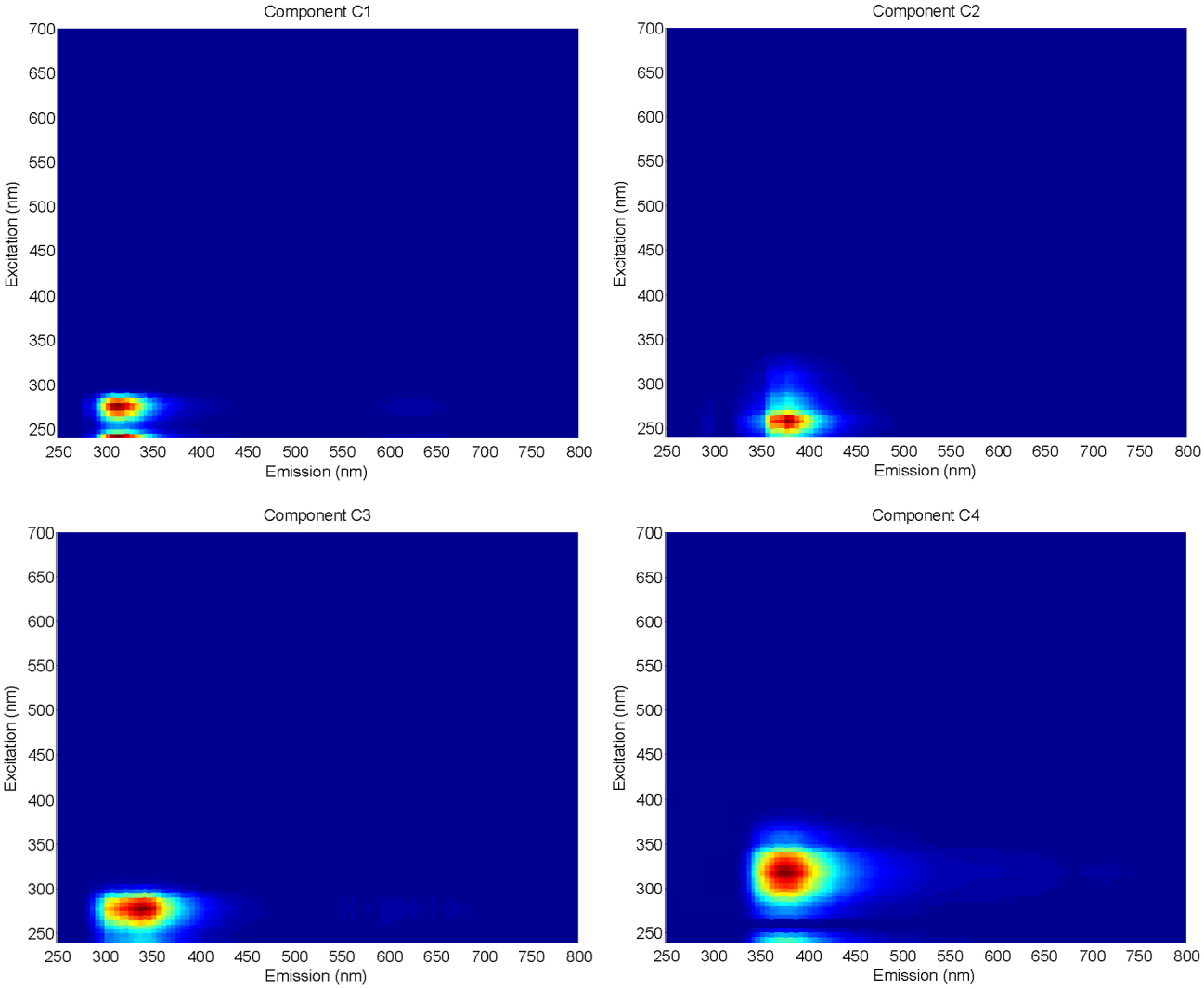


FIGURE 3. Contour plots for excitation and emission wavelengths identified from the PARAFAC model, indicating the four main fluorescent components (i.e., C1, C2, C3, C4) present in the sample set.

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identified as compounds associated with catechin (including tannin). Component 2 peak intensities were λ_{ex} = 255 nm and λ_{em} = 375 nm and can be proposed to result from phenolic aldehyde related compounds. Component 3 peak intensities were λ_{ex} = 270 nm and λ_{em} = 335 nm and were considered to be associated with anthocyanins. Finally, component 4 peak intensities were λ_{ex} = 315 nm and λ_{em} = 375 nm and tentatively assigned to stilbenoids such as *trans*-resveratrol.

Ranaweera *et al.* (2021c) and Airado-Rodríguez *et al.* (2009) proposed similar assignments for PARAFAC model components in red wine, which are reasonable considering the main compounds (i.e., catechins, anthocyanins, and other phenolics) expected to be abundant in red wine. It is noteworthy that compound classes assigned from the PARAFAC modelling (i.e., phenolics) were not necessarily driving the sensory characters themselves, but could act as indirect markers that indicated compositional aspects of the wines that were not essentially measured by fluorescence. For example, different gene copies responsible for the biosynthesis of important wine compounds such as anthocyanins in grape berry can belong to multicopy families, having an expression profile coinciding with other specific flavonoids that may impact wine sensory profile by correlation rather than causation (Kuhn *et al.,* 2013). In contrast, there could be a direct relationship with compounds associated with aspects such as the taste and mouthfeel of the wine, as explained in more detail in the next section.

4. Relation between PARAFAC components and RATA results according to MFA

Considering the compound classes tentatively identified by PARAFAC modelling of EEM data can impact wine sensory profile (either directly or by implying an indirect correlation), the relative loadings of the four classes were analysed in conjunction with RATA results through MFA. Means of the significantly different (α = 0.1) descriptors and means of the four compound class loadings from 23 wines (excluding CS2, CS7 and CS26) were used for the analysis (Figure 4). MFA yielded an RV coefficient of 0.232 between both sets of data, an RV coefficient of 0.751 between PARAFAC data and the MFA model, and an RV coefficient of 0.816 between the RATA data and the MFA model.

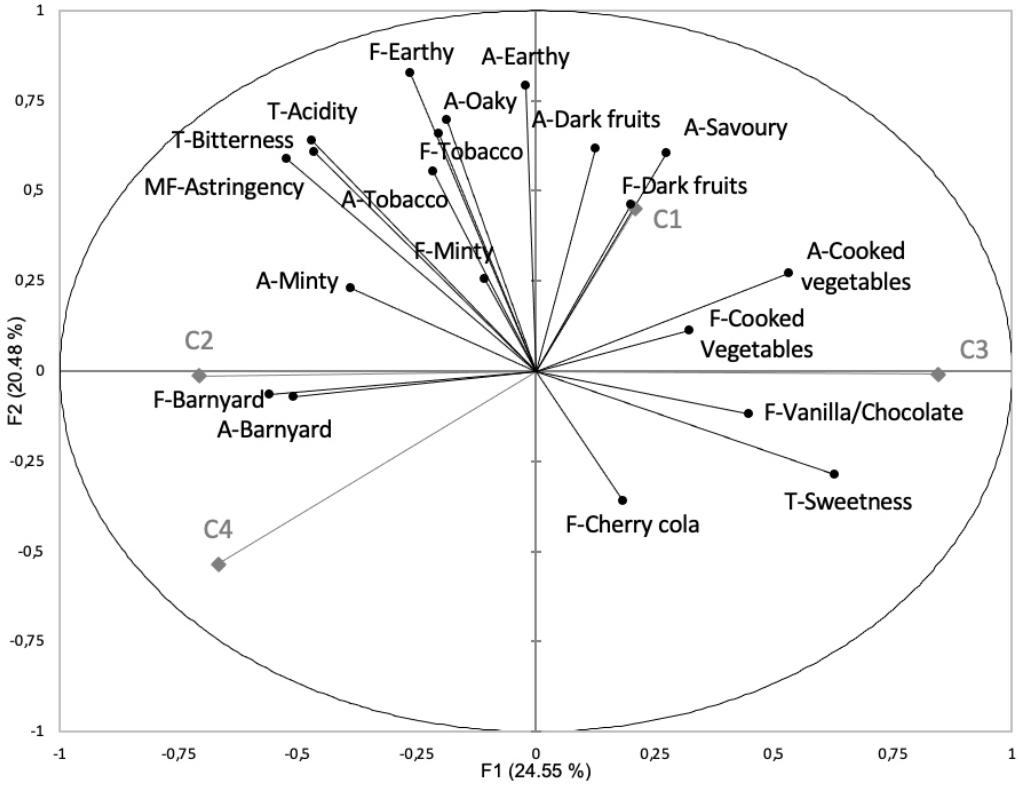


FIGURE 4. Multiple factor analysis biplot of the four components from PARAFAC (in grey, ◆) using significantly different (α = 0.1) descriptors from RATA evaluation (in black, ●) for 23 Cabernet-Sauvignon wine samples (excluding CS2, CS7 and CS26).

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The MFA biplot explained 45 % of the variance in the data, with 24.6 % represented by F1 and 20.5 % by F2. PARAFAC C1 was plotted on the right side of F1 and the upper portion of F2, C2 and C3 were explained entirely along F1, with C3 on the right side and C2 on the left side, and C4 was plotted on the left side of F1 and lower part of F2, more or less opposite to C1 (Figure 4).

Catechin monomers associated with C1 are usually extracted from grape skin and seed and can increase the bitter taste of wine (Fischer and Noble, 1994) whereas polymers of catechin (e.g., tannins), extracted from the same sources, are related with astringency (Waterhouse *et al.,* 2016a). Figure 4 shows C1 was associated with 'dark fruits' and 'cooked vegetables' aromas and flavours and 'savoury' aroma, which is likely to be an indirect relationship as mentioned in the previous section. Analysing the RV coefficients, the correlation between bitterness and C1 was not significant ($p = 0.313$), thus indicating that there might not be an association. In contrast, the correlation between astringency and C1 was significant ($p = 0.006$) and had an RV coefficient of 0.315, demonstrating a moderate association. This implied that polymers had a greater influence on the expression of C1 than monomers, which would be reasonable given their relative concentrations in red wine.

Phenolic aldehydes assigned to C2 can be influenced by the origin of wood (usually oak) incorporated either during fermentation or maturation and can vary in concentration depending on ageing time — such compounds can be responsible for some oak-related aroma traits (e.g., vanillin) in wine (del Alamo Sanza *et al.,* 2004). Other oak compounds (e.g., volatile phenols, hydrolysable tannins) that may influence sensory traits would undoubtedly be extracted as well. C2 was related to 'barnyard' aroma and flavour and 'minty' aroma. Anthocyanins assigned to C3 are pigments present in red grape skins that are important to the colour of red wine (He *et al.,* 2012). Anthocyanins might also be responsible for an increase in the 'fullness' of a wine (Vidal *et al.,* 2004), as well as perceived astringency and bitterness (Ferrero-del-Teso *et al.,* 2020; Paissoni *et al.,* 2018). Additionally, as explained in the section dealing with PARAFAC, genes involved in the biosynthesis of anthocyanins in grapes are expressed through pathways that coincide with the biosynthesis of other flavonoids and volatile compounds (Czemmel *et al.,* 2012; Kuhn *et al.,* 2013). This could explain why anthocyanins could act as markers for compounds that impart aroma or flavour (Ristic *et al.,* 2010) but lack a fluorophore themselves. From the MFA, C3 was linked to 'cooked vegetables' aroma and flavour, 'vanilla/chocolate' flavour, and sweetness. Lastly, stilbenoids assigned to C4 are compounds that can be found in grape berry skins and are extracted into wine during fermentation (Waterhouse *et al.,* 2016b). Stilbenoids, especially *trans*-resveratrol, are responsible for the antioxidant characteristics of red wine and its association with the prevention of age-related diseases in consumers (Pawlus *et al.,* 2012). According to Gaudette and Pickering (2011), *trans*-resveratrol seems to have minimal impact on the sensory qualities of wine (when spiked at less than 200 mgL^{-1}). Figure 4 shows that C4 was associated with 'barnyard' aroma and flavour, which is likely to be another example of an indirect relationship between the fluorophoric component and the sensory data.

It is worth noting that the associations between sensory traits and tentative compound types found through PARAFAC do not allow for strict conclusions. It is possible, considering the complexity of what is being modelled, that some relationships may arise due to chance, and more in-depth research is necessary to better understand and explain the proposed relationships.

5. Regression model for astringency prediction

Considering that most of the compounds detected by spectrofluorometric analysis can directly affect basic mouthfeel and taste attributes in wine, PLS regression was performed with the two mouthfeel and three taste attributes described by the sensory evaluation of the 26 wines. Astringency was the only attribute that could be well modelled from the EEM data without overfitting, based on the model parameters. An optimal model was generated with eight LVs, giving RMSEC = 0.085, RMSECV = 0.132, RMSEP = 0.222, R^2 calibration = 0.936, R^2 cross-validation = 0.848, and R^2 prediction = 0.681. The model was thus able to explain 84.8 % of the variance in the samples and able to predict the results with 68.1 % accuracy (Figure 5). Furthermore, the low value for RMSECV indicated that the error associated with the prediction of astringency was around 2 % in relation to the sensory scale used (7-point), demonstrating that the model appeared to be suitable. This outcome showed that spectrofluorometric data had reasonable capabilities for predicting a perceived mouthfeel attribute rating for this data set, which was

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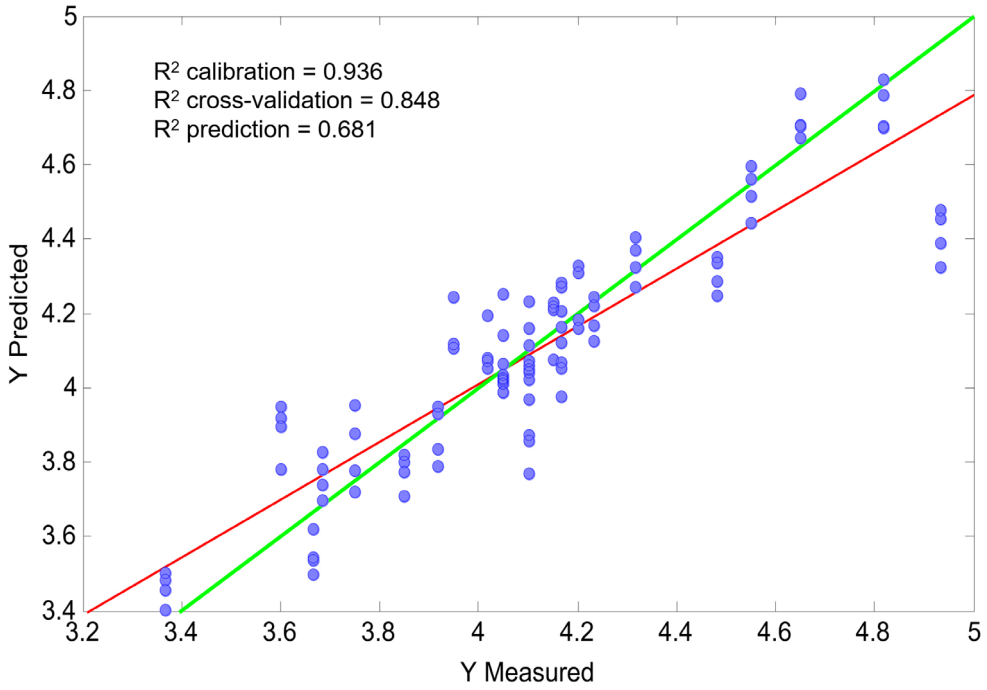


FIGURE 5. Correlation between the predicted and measured ratings for perceived astringency according to partial least squares regression modelling for Cabernet-Sauvignon wines (n = 26).
The green line shows the 1:1 correlation and the red line is the model fit.

encouraging given the simplicity of the approach and the complexity of what was being modelled.

The chemical composition of Cabernet-Sauvignon wines has also previously been used for sensory profile prediction, with regression models described by Niimi *et al.* (2018) explaining between 44.2 % and 69.1 % of the variance in the sample set, and 56.5 % for astringent mouthfeel. In that work, the model for predicting perceived astringency score involved anthocyanin concentration and colour measures, both of which can be determined using the A-TEEM approach and used in combination with a multi-block analysis (Ranaweera *et al.,* 2021c) to add information beyond that encompassed in the EEM data alone. Notably, the present study is the first known attempt to correlate and predict wine sensory profiles from EEM readings, and although the outcomes are positive, further work with additional samples will be necessary to improve and extend the modelling. Furthermore, different spectroscopic methods have been validated before for determining phenolic compound concentrations in a way that is less time consuming and more cost-effective than other options, and such approaches could become a valuable tool for assisting winemakers in monitoring and controlling phenolic composition (Cozzolino *et al.,* 2008; Cozzolino *et al.,* 2004; Dambergs *et al.,* 2012; Janik *et al.,* 2007; Ranaweera *et al.,* 2021c). Fluorescence spectroscopy in particular can quantify compounds that are present in the sample at a lower concentration than other spectroscopic methods (Gilmore and Chen, 2020), thus providing an attractive option for additional development in future.

CONCLUSIONS

This study aimed to explore the association between sensory traits and spectrofluorometric data of unreleased, commercially produced 2020 Coonawarra Cabernet-Sauvignon wines. It combined cluster analysis of sensory profiles obtained using RATA with fluorescence data by using a machine learning algorithm, and examined the prediction of sensory ratings from fluorophoric compounds via regression modelling. Thus, five distinctive clusters arose that could be well explained by the sensory results of the RATA evaluation. Cluster 1 wines were characterised by savoury-related characters, Cluster 2 by 'minty' traits and a lack of the savoury-related attributes, Cluster 3 by 'cherry cola' flavour and low bitterness and astringency, Cluster 4 by higher sweetness and 'barnyard' aroma and flavour, and Cluster 5 by 'vanilla/chocolate' flavour.

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Additionally, the EEM data analysed through XGBDA were able to predict with 100 % accuracy the clusters that arose from the sensory profiling, demonstrating that there might be a good association between the EEMs and sensory ratings (whether direct or indirect). After excluding three outlier samples, PARAFAC analysis showed that four main fluorophores could be segregated to explain the data set, with compound classes tentatively associated with the intensity readings being catechins (C1), phenolic aldehydes (C2), anthocyanins (C3) and stilbenoids (C4). MFA was used to identify associations between the PARAFAC components and the sensory ratings, revealing that C1 was associated with 'dark fruits' and 'savoury' characters, C2 was associated with 'barnyard', C3 was related to 'cooked vegetables' and 'vanilla/chocolate', and C4 was related with 'barnyard' but more characterised by the lack of attributes associated with C1. However, the nature of any relationship between the proposed compound classes and perceived sensory attributes requires further study. PLS regression resulted in a suitable model that was able to predict perceived astringency score with 68.1 % accuracy, although no suitable model was found for the other sensory attributes. Overall, the correlation of sensory profiles with spectrofluorometric data was quite an optimistic feat, yet the results from this study were promising. This work may inspire further research that is designed to better understand the chemical drivers of sensory traits and the most influential factors throughout wine production using a rapid technique like spectrofluorometry, perhaps with the inclusion of a small selection of compositional variables.

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