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Describing Australian emerging red grape varietal wines by sensory profiles and volatile chemical composition

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ABSTRACT

Adapting to climate change is crucial for Australian viticulture, with a shift towards drought-tolerant grape varieties being a potential strategy. This study explored the sensory and volatile profiles of three emerging red grape varieties – Montepulciano, Nero d'Avola, and Touriga Nacional – grown in Australia, comparing them to traditional varieties (Cabernet-Sauvignon, Grenache, and Shiraz). Thirty-six trained tasters used Rate-All-That-Apply (RATA) to assess 35 wines, and GC-MS analysis determined the volatile composition of the wines. Seventeen out of 35 targeted volatiles were revealed odour-active across all varieties. However, linalool, associated with floral notes, was odour-active only in Touriga Nacional. Conversely, 1,8-cineole was found in emerging varieties and Cabernet-Sauvignon, but not in Shiraz and Grenache. Canonical Variance Analysis (CVA) identified key volatile compounds characterising each variety. Touriga Nacional wines were most distinct, denoted by linalool and α-terpineol. Shiraz and Montepulciano shared similar volatile profiles, both distinguished by β-damascenone and 2-phenylethyl acetate. Cabernet-Sauvignon and Grenache were characterised by 2-phenylethanol, while Nero d'Avola showed overlap with this group while additionally featuring 1,8-cineole. Sensory and volatile profiles suggest potential similarities between Shiraz – Montepulciano and Grenache – Nero d'Avola wines, whereas Touriga Nacional generated more diverse red wine styles encompassing wines similar to mainstream varieties. Collectively, these findings highlight the potential of emerging varieties to complement traditional Australian red wines as sustainable warm climate options, with some varieties showing closer stylistic similarities to mainstream styles than others.

KEYWORDS: Rate-All-That-Apply, gas chromatography-mass spectrometry, Nero d'Avola, Montepulciano, Touriga Nacional, drought-tolerance, alternative varieties

INTRODUCTION

Australia is defined as a new world wine country and the fifth largest wine producer and exporter globally (OIV, 2023). With over 1.43 million tonnes of grapes crushed during the 2024 vintage and nearly 1 billion litres of wine produced, the wine industry contributes over $45 billion every year to the Australian economy (Wine Australia, 2024a). Australia's wine sector consists of 65 geographical indications and an estimated total vineyard area of 146,000 ha, with ancient and diverse soils and climates, offering a wide range of wine styles, from everyday table wines to fine and iconic wines. Despite this diversity, 70 % of Australia's wine grape production occurs in three hot to very hot inland regions (Jones *et al.*, 2010), including the Riverland (32 %), Murray Darling-Swan Hill (19 %), and Riverina (19 %) (Remenyi *et al.*, 2019; Wine Australia, 2022). Climate is a critical factor for all agricultural businesses, determining whether a crop is suitable for a given region, significantly influencing yield and quality and underpinning economic sustainability. In wine grape production, climate is the most critical aspect in ripening fruit to achieve optimum characteristics to produce a desired wine style (Rouxinol *et al.*, 2023). Like other wine-producing countries, Australian wine regions face increasing pressure from climate change which threatens to deplete natural resources, such as water, and significantly impact the quality of table wine grapes in the near future (Mosedale *et al.,* 2016; van Leeuwen & Darriet, 2016).

To date, traditional or noble French grape varieties dominate Australia's grape plantings, including Shiraz, Cabernet-Sauvignon, Merlot, and Pinot noir for red varieties, and Chardonnay, Sauvignon blanc, Pinot gris, and Semillon for white varieties, which originate from cooler European climates. Other white varieties with currently significant plantings grown in Australia, such as Muscat Gordo Blanco and Colombard, originate from warmer Mediterranean regions (Wine Australia, 2024b). Aside from the uniformity and lack of diversity this scenario presents, the varieties, which originate from cooler European climates, may struggle to maintain quality under the increasingly warmer conditions expected in Australia (Jones *et al.*, 2012).

To lessen the effects of climate change on grape growing in Australia, it is necessary to adapt to projected climate scenarios by increasing the use of drought-tolerant varieties better suited to these conditions. As irrigation water becomes scarcer and more costly, understanding the drought-tolerance of different cultivars becomes critical for sustainable vineyard management (Medrano *et al.*, 2018). Improved knowledge of these differences can help growers choose less water-demanding plant material and thus support more sustainable production (Gambetta *et al.*, 2020). In parallel, demand for sustainable products continues to grow (Elhoushy *et al.*, 2020; Flores, 2018; Flint *et al.*, 2009) and wines made from less water-demanding grape varieties may therefore respond both to climate pressures and to evolving market expectations. In practical terms, this means that any move towards better adapted, drought-tolerant red grape varieties must be informed by how their wine styles compare, in sensory and volatile terms, with the principal Australian red varieties that currently dominate production and consumption and that the consumer market is familiar with.

Previous studies showed strong potential for wines made from emerging red varieties in the Australian wine consumer market. Montepulciano, Nero d'Avola and Touriga Nacional (Long *et al.,* 2023; Mezei *et al.*, 2021), all originate from hot Mediterranean regions with similar climatic conditions to many of Australia's warm wine regions (Gladstones, 1992) and demonstrated similarities in aroma and flavour to Shiraz, Grenache, and Cabernet-Sauvignon, respectively. These varieties represent the most planted and consumed red varieties in Australia and have a solid history of consumer acceptance. It should be noted that whilst Cabernet-Sauvignon and Shiraz dominate in terms of current production volumes, Grenache has a long-established history in Australia, particularly for fortified wines and blends, and is experiencing renewed interest as a premium single-varietal and blended Rhône-style table wine.

Numerous studies on the sensory and chemical profiles of wines made from the emerging varieties mentioned above can be found in the scientific literature (Ascrizzi *et al.*, 2022; Baiano *et al.*, 2016; De Pinho *et al.*, 2007; Petronilho *et al.*, 2021; Sagratini *et al.*, 2012; Slaghenaufi *et al.,* 2022; Symington *et al.*, 2011; Verzera *et al.*, 2016). However, these studies were performed on wines made with grapes grown in continental Europe. To our knowledge, there is scant sensory and volatile chemistry research of wines made from these varieties when grown in Australia (Long *et al.*, 2023; Mezei *et al.*, 2021). These Australian studies revealed that the emerging varietal wines Montepulciano and Nero d'Avola shared some sensorial similarities with Shiraz and Grenache wines, respectively. Moreover, they showed the consumer acceptance of these alternative varietal wines, accentuating their local market potential.

This investigation aimed to (i) generate sensory and volatile chemical profiles of three emerging red grape varietal wines made with Australian grown fruit: Montepulciano, Nero d'Avola, and Touriga Nacional; and (ii) to compare these profiles with those of three principal Australian red varieties (Cabernet-Sauvignon, Shiraz, Grenache), which serve as benchmark styles in the domestic market. The traditional varieties used as benchmarks (Cabernet-Sauvignon, Grenache, and Shiraz) were chosen based on the facts that they constitute the most produced, consumed and researched red wines/varieties in Australia.

The knowledge obtained from this study may give wine producers greater confidence in adopting emerging red grape varieties to produce a range of wine styles that could meet the flavour preferences of both Australian and international markets, while potentially fostering a more sustainable wine industry. Adopting drought-tolerant varieties better suited to the Australian climate can help prevent yield loss, lower production costs, and ultimately increase profit margins and overall income.

MATERIALS AND METHODS

1. Wine samples

Thirty-five commercially available Australian single varietal, red wines were selected for this study. These included 27 potentially drought-tolerant, emerging varietal wines (9 Montepulciano, 10 Nero d'Avola, and 8 Touriga Nacional), plus 3 Cabernet-Sauvignon, 2 Grenache, and 3 Shiraz wines, with the latter three being used as benchmark wines (Table S1).

The emerging varietal red wines were sourced from producers that were commercially available at the time and represented multiple Australian geographical indications and vintages (Table S1), to reflect the current diversity of production contexts for each variety. Although the sample sizes for benchmark varieties (n = 2–3) are smaller than for emerging varieties (n = 8–10), the former were screened by 8 wine experts with five years or more wine industry experience to confirm they were typical of Australian Grenache, Shiraz, and Cabernet-Sauvignon wines and served as stylistic comparators rather than as a separate experimental group. This asymmetry is justified by our methodological approach: (i) sensory profiling via RATA with a large trained panel (n = 36) is inherently robust to limited wine sample sizes, as the statistical power derives from the panel size and number of sensory attributes assessed, and (ii) multivariate analyses (PCA, clustering) operate on individual wine observations (n = 35 total), providing sufficient data points for robust patterns despite unequal varietal representation.

2. Sensory profiling and preliminary liking

This study was approved by the Human Research Ethics Committee of the University of Adelaide, Approval Number: H-2021-131. A panel of trained tasters (n = 36; age range: 18–65+ years; 56 % male, 44 % female) were recruited to undertake Rate-All-That-Apply (RATA) sensory analysis of wine samples following the published method (Danner *et al.*, 2018). The panel consisted of staff members and postgraduate oenology students from the School of Agriculture, Food and Wine at The University of Adelaide, all previously trained in wine sensory evaluation and RATA. The panellists attended three sessions where they evaluated the 35 samples, 12 in the first and second sessions, and 11 samples in the third session. These sensory sessions were held in the sensory laboratory in individual, computerised booths, equipped with fluorescent lighting at a constant temperature of 21 °C. Thirty millilitres of each sample was presented in 215 ml clear XL5 wine glasses labelled with 4-digit codes, with a 1-minute break between samples. All tasters had an enforced 10-minute break between samples 6 and 7, with free access to plain crackers and water, to cleanse the palate and avoid fatigue.

To obtain preliminary liking data, the trained panellists were first asked to rate their liking of the samples on a 9-point hedonic scale (1 = dislike extremely, 5 = neither liked nor disliked, and 9 = liked extremely). This was followed by rating the intensity of each applicable sensory attribute (choice from n = 67, details in Table S2) perceived in the wines (*i.e.,* only those that apply to a given sample) using a 7-point scale (1 = extremely low, 4 = moderate, and 7 = extremely high). The sensory data were collected using RedJade software (2016, Redwood City, USA).

3. Oenological parameters

Basic chemical composition measures such as pH and Titratable Acidity (TA, as tartaric acid, g/L) were measured using a pH-meter (CyberScan pH 1100, Thermo Fisher, USA) according to the methods stated in Iland *et al.* (2004). TA was determined by titration to pH 8.2. Volatile acidity (as acetic acid, g/L), residual sugar and SO_2 measurements (free and total) were obtained through ChemWell 2910 autoanalyzer (Awareness Technology, United States) using D-glucose and D-fructose, acetic acid and free and total sulphur dioxide kits from Vintessential Laboratories (Orange, Australia). AntonPaar Alcolyzer Wine ME and DMA 4500M alcolyzer (North Ryde, NSW, Australia) was utilised to obtain the ethanol content (% *v/v*) of the wines (Table S3).

4. Volatile composition analysis

Major volatile compounds in all 35 wine samples, including higher alcohols, fatty acids, ethyl esters, acetates, and terpenes, were analysed. Wines were subsampled at the same time as sensory evaluation and were prepared for GC-MS analysis in duplicate using the same instruments and following the published method of Wang *et al.* (2016). The samples were stored in a cold room (4 °C) before analysis. Briefly, volatile compounds were analysed by headspace solid-phase microextraction gas chromatography-mass spectrometry (HS-SPME-GC-MS). Wine samples (0.5 mL) were diluted with Milli-Q water (4.5 mL) and spiked with an internal standard mixture in 20 mL amber headspace vials containing sodium chloride (2 g). Vials were equilibrated at 50 °C with agitation, and volatiles were extracted for 30 min using a 50/30 µm DVB/CAR/PDMS SPME fibre. Chromatographic separation was carried out on a gas chromatograph equipped with a DBWAXetr capillary column (60 m × 0.25 mm × 0.25 µm). The oven temperature programme was 40 °C for 1 min, then increased to 135 °C at 2 °C/min, 212 °C at 5 °C/min, and 250 °C at 15 °C/min, and held for 10 min. Ultra-high purity helium was used as carrier gas at a constant flow of 2.0 mL/min. The GC was coupled to a single quadrupole mass spectrometer operated in electron impact mode at 70 eV, with an ion source temperature of 230 °C and quadrupole at 150 °C, acquiring data in full-scan mode over *m/z* 29–300. Volatile compounds were identified by comparison of mass spectra and retention indices with those of authentic standards and library spectra, and quantified using calibration curves constructed with standards in model wine and the internal standard method.

5. Statistical analyses

All statistical analyses for this evaluation were performed using XLSTAT (Sensory pack, 2021.2, Addinsoft SARL,

France). The sensory profiling data (RATA data) were subjected to a two-way analysis of variance (ANOVA) with participants as a random factor and wine samples as a fixed factor effect ($\alpha = 0.1$). Preliminary liking results and volatile chemical compounds were analysed by one-way ANOVA followed by Fisher's LSD post hoc test ($\alpha = 0.05$). For these analyses, we relied on the robustness of ANOVA to moderate departures from normality and homogeneity of variance, given the use of individual wines ($n = 35$) as observations and the primary role of multivariate methods (PCA, AHC) for pattern detection.

Significantly different RATA attributes, preliminary liking, and volatile compounds were further analysed by principal component analysis (PCA, correlation), with the significant volatile chemical compounds and preliminary liking dataset as supplementary variables.

Canonical variates analysis (CVA, *i.e.*, discriminant analysis function in XLSTAT) and agglomerative hierarchical cluster (AHC) analysis (using Ward's method and Euclidean distance with automatic truncation) were performed on the chemical volatile compounds data to inspect varietal correlation patterns.

RESULTS AND DISCUSSION

1. Oenological parameters

Oenological parameters (pH, titratable acidity, volatile acidity, residual sugar, free and total SO_2, and ethanol content) for all 35 wine samples are provided in Table S3, to provide chemical profiles of the wines and confirm they were dry, not faulty from volatile acidity and the measures fell within expected and legal ranges for commercially produced Australian dry red table wines.

2. Sensory and volatile profiling plus preliminary liking of red wine varieties

Quantitative analysis of major volatile compounds was obtained through GC-MS on the studied 35 wine samples. Thirty-five volatile compounds comprising acetates (4), ethyl esters (11), higher alcohols (9), fatty acids (7), terpenes (3), and C_{13}-norisoprenoids (1) were quantified. Of the 35 compounds analysed, 34 showed statistically significant differences between wine samples according to one-way ANOVA ($p < 0.05$), with the exception of 1-propanol. The minimum, maximum, median, and mean concentrations of the volatile compounds detected in wines of emerging varietals, including Montepulciano (Table S4), Nero d'Avola (Table S5), and Touriga Nacional (Table S6), and their benchmarks, including Cabernet-Sauvignon (Table S7), Grenache (Table S8), and Shiraz (Table S9), are illustrated in the Supplementary Data.

The mean odour active value (OAV) for each volatile compound was calculated by dividing the mean concentration of a compound in a wine by its odour detection threshold (Waterhouse *et al.*, 2024) which was used to evaluate the potential contribution of volatile compounds to the overall perceived aroma. Generally, a compound is likely to contribute directly to a specific aroma when the OAV is higher than 1, which is regarded as odour active (Gambetta *et al.*, 2014). Although, this is an oversimplified way of estimating contributions of aroma compounds to wine sensory attributes due to potential matrix effects, such as masking, and synergistic effects (Waterhouse *et al.*, 2024).

Based on existing research, no studies have examined the volatile compounds in single-varietal table wines made from Montepulciano, Nero d'Avola, and Touriga Nacional grapes cultivated in Australia.

Out of the 35 volatile compounds quantified in this study, the concentrations of ethyl acetate, 3-methylbutyl acetate, ethyl 2-methylbutanoate, ethyl 3-methylbutanoate, ethyl hexanoate, ethyl lactate, ethyl octanoate, 1-propanol, 1-butanol, 3-methyl-1-butanol, 1-octanol, 2-phenylethanol, acetic acid, 3-methylbutanoic acid, hexanoic acid, octanoic acid, and β-damascenone were determined higher than their odour detection thresholds in all samples, implying a potential direct impact on wine sensory attributes. Ethyl esters are known to be responsible for the very important fruity aromas in red wines, as well as β-damascenone (Ferreira *et al.*, 2021).

Other compounds, including 1,8-cineole and isobutanol were found above their odour detection thresholds in most samples except for Grenache and Shiraz wines; and linalool was higher in most of the Touriga Nacional wines only. The remaining compounds were often found below their odour detection thresholds in both emerging and traditional varieties.

The concentrations of 3-methylbutyl acetate ranged from 2,343 to 5,098 µg/L in emerging varieties, with 2,630–5,098 µg/L in Montepulciano (Table S4), 2,540–2,590 µg/L in Nero d'Avola (Table S5), and 2,434–4,813 µg/L in Touriga Nacional (Table S6). Comparatively, 3-methylbutyl acetate was reported to be between 2,316 and 4,429 µg/L in traditional varieties, with 2,712–3,093 µg/L in Cabernet-Sauvignon (Table S7), 2,316–4,429 µg/L in Shiraz (Table S8), and 3,036–3,775 µg/L in Grenache (Table S9). This compound was found at suprathreshold concentration in all emerging and traditional varieties (OAV ranged from 99 to 110). 3-Methylbutyl acetate is a key ester contributing to fruity aromas in young red wines and has been previously reported at significant concentrations in Cabernet-Sauvignon wines. In a comparative analysis of traditional Bordeaux and other red wines, including Shiraz, the concentration of 3-methylbutyl acetate was found to be 196 and 187 µg/L, respectively (Garbay *et al.*, 2024). The lower levels of this compound reported in the wines of the Garbay *et al.* (2024) study relative to the current findings could be due to their wines being more aged upon volatile chemical analyses. Previous research examining isoamyl acetate (3-methylbutyl acetate) levels in these emerging varieties has reported concentrations of 560–660 µg/L in Montepulciano wines (Canonico *et al.*, 2025) and up to 383.54 µg/L in Montepulciano wines from Abruzzo and Marches (Stój *et al.*, 2017), 131–134 µg/L (first harvest) and 75–85 µg/L (second harvest) in Nero d'Avola

wines (Verzera *et al.*, 2016), with limited quantitative data available for Touriga Nacional wines, where comprehensive volatile profiling has focused primarily on varietal terpenic compounds rather than fermentation-derived acetate esters (Dinis *et al.*, 2024). These substantially lower concentrations reported in previous studies (75–660 µg/L) compared to the current study (2,343–5,098 µg/L) may reflect differences in winemaking practices, including yeast strain selection (Plata *et al.*, 2003; Eder *et al.*, 2018), fermentation temperature, and nitrogen management (Godillot *et al.*, 2023, Godillot *et al.*, 2022), grape maturity at harvest (Verzera *et al.*, 2016) and vintage-related effects (Dinis *et al.*, 2024).

Linalool was reported to contribute to the flowery/lychee-like aroma in Gewurztraminer wines (Ong & Acree, 1999) and only had suprathreshold concentrations in all Touriga Nacional samples in our study (OAV = 1 to 4, Table S6), except for TOU7 (7.9 µg/L, OAV = 0). This might explain the floral aroma present in wines of this variety, which agreed with previous studies (De Pinho *et al.*, 2007; Petronilho *et al.*, 2021; Symington *et al.*, 2011).

1,8-Cineole was detected as odour active in all the emerging varieties (Montepulciano OAV = 6, Table S4; Nero d'Avola OAV = 21, Table S5; Touriga Nacional OAV = 6, Table S6) as well as in Cabernet-Sauvignon (OAV = 5, Table S7), but not in Shiraz and Grenache. 1,8-Cineole, a compound commonly reported in Australian Cabernet-Sauvignon wines, responsible for the eucalyptus-like aroma (Capone *et al.*, 2011), was also found in the headspace of crushed and destemmed Tuscan Montepulciano grapes at a relative abundance greater than 1 %, contributing to the overall volatile profile (Ascrizzi *et al.*, 2022). Discrepancies about the origins of this compound can be found in the relevant literature, as some studies attributed the presence of 1,8-cineole in wines to exogenous contamination, such as eucalyptus trees and an invasive weed, *Artemisia verlotiorum* (Poitou *et al.*, 2017), whereas others related it to varietal origins (Fariña *et al.*, 2005). Therefore, it is unclear whether the presence of this compound in Australian grown Nero d'Avola and Touriga Nacional wines can be due to the proximity of these vines to eucalyptus trees (Capone *et al.*, 2012), or due to varietal characteristics, as only one study reporting 1,8-cineole in the Touriga Nacional wines was found in the literature (Gomes da Silva, 2012).

The same 35 commercial Australian red wines were evaluated by a RATA panel (n = 36), using a rapid, cost-effective, descriptive sensory profiling technique to assess and define their sensory characteristics (Danner *et al.*, 2018). Out of a possible 67 attributes, 46 were identified as statistically significant ($p < 0.1$) by the panel (Table S2). Table S2 reports the *p*-values for each RATA attribute by wine; varietal-level interpretation of these univariate differences is then provided in the main text and in the PCA biplot (Figure 1A).

Principal component analysis (PCA) was performed on the statistically significantly different sensory attributes ($p < 0.1$), using the hedonic scores and volatile concentrations as supplementary data, with PC1, PC2, and PC3 accounting for 31.62 %, 12.37 %, and 11.80 % of the total variance, respectively. PCA is shown in two separate plots for clarity (Figures 1A and 1B), corresponding to the two biplots with distribution of the wine samples and loadings of sensory attributes (Figure 1A) and chemical volatile compounds (Figure 1B).

PC1 separated samples according to primary and secondary aroma/flavour, with samples having more secondary aroma/flavour to the right side of the biplots (Figure 1) and other samples having more primary aroma/flavour to the left side of the biplots (Figure 1). Specifically, wine samples of CABS2, TOUR1, TOUR7, SHZ1, MON8, and NERO10 were located to the right side of the biplot and were perceived with higher intensity aromas of leather, earthy, meaty/salami, and tobacco, and flavours of dried fruits, tobacco, savoury, and mouthfeel, alcohol, and astringency (Figure 1A). These sensory attributes were close to volatile compounds, including ethyl 2-methylbutanoate, ethyl 3-methylbutanoate, ethyl 2-methylpropanoate, isobutanoic acid, 3-methyl-1-butanol, 3-methylbutanoic acid, β-damascenone, 1-butanol, ethyl acetate, ethyl lactate, acetic acid, α-terpineol, diethyl succinate, and ethyl propanoate (Figure 1B).

Wine samples, such as MON3, NERO (1, 3, 4, 5, 6, 8, and 9), GREN (1 and 2), TOUR (5 and 8), were situated to the left side of the biplots, where higher intensity of floral, confectionery, and red fruit aroma in those wines were perceived (Figure 1A). These sensory attributes were close to volatile compounds, including 2-ethyl-1-hexanol, isobutanol, benzyl alcohol, 2-phenylethyl acetate, 1-octanol, linalool, 3-methylbutyl acetate, decanoic acid, ethyl hexanoate, hexyl acetate, and ethyl butanoate (Figure 1B). This aligns with a previous study that found positive correlations between flower sensory notes and linalool and ripe fruit characters with decanoic acid (Vilanova *et al.*, 2010). However, it is important to note that the concentrations of linalool and decanoic acid in the current study were close to their respective odour detection thresholds (Tables S4–S9). Preliminary liking, only shown on the left-hand side of Figure 1B as a supplementary variable, was positively associated with linalool, α-terpineol, hexyl acetate, benzyl alcohol, 1-butanol, and 1-hexanol, volatile compounds possessing fruity, floral, and sweet, aromas which supports the floral and confectionery sensory attributes observed to positively correlate with liking.

It should be noted that PC1 was separating samples with primary and secondary aromas and flavours such as confectionery, floral and red fruits (left-hand side) from those wines with aged/tertiary characters, presumably derived from oak contact/bottle maturation, such as leather, meaty/salami, tobacco on the right-hand side of the plot. After reviewing the compounds in the PCA plot, the left-hand side encompassed the volatiles mentioned above with odours mostly in line with those described by the sensory panel, such as ethyl esters like ethyl hexanoate and ethyl butanoate; both with fruity and strawberry aromas (Forney *et al.*, 2000; Francis, 2013), and acetates like hexyl acetate and 2-phenylethyl acetate (Carlin *et al.*, 2019;



FIGURE 1. Principal component analysis biplots of distribution of wine samples and loadings of significant (A) RATA attributes ($p < 0.1$) and (B) volatile compounds ($p < 0.05$) on PC 1 & 2. Wine samples are black in colour, sensory attributes are in red, and volatile chemical data are in blue. The letters A, F, and MF in front of an attribute in (A) refers to an aroma note, flavour note, or mouthfeel note, respectively. More details of sensory attributes can be found in Table S1. Sample abbreviations: MON, Montepulciano. NERO, Nero d'Avola. TOUR, Touriga Nacional. CABS, Cabernet-Sauvignon. SHZ, Shiraz. GREN, Grenache.

Siebert *et al.*, 2005), associated with fruity/floral aromas in wines, as well as benzyl alcohol (floral/fruity/sweet) and linalool (flowery/lychee) (Francis, 2013; Nan *et al.*, 2021). However, the volatile compounds identified on the right side of the diagram only reflect the primary and secondary sensory attributes of the samples, primarily originating from grapes and fermentation processes, including alcohols, ethyl esters, along with three fatty acids, an acetate (ethyl acetate), and an isoprenoid (α-terpineol), amongst others. Oak and age derived volatiles were not measured in the current research, but could account for the sensory characteristics observed in this section of the plot.

The second principal component PC2 (12.37 %), distinguished wine samples of NERO2 and CABS (1, 2, and 3) in the top half of the biplot perceived as possessing aromas and flavours of mint, dried herbs, eucalypt, vegetal, and green; and volatile compounds such as 1,8-cineole, ethyl 2-phenylacetate, and 2-phenylethanol. Wine samples of TOUR6 and SHZ3 that were positioned in the lower half of the biplots were associated with more pronounced jammy, sweet oak, chocolate, and caramel/butterscotch notes (Figure 1A), and were close to volatile compounds such as butanoic acid, ethyl octanoate, hexanoic acid, 1-hexanol, octanoic acid, and ethyl decanoate (Figure 1B). The bottom part of the plot also displayed volatiles in accordance with the sensory attributes, such as ethyl octanoate, known for its ripe fruit/woody odour, as well as hexanoic and octanoic acids, responsible for cheesy/fatty and butter/almond aromas, respectively (Francis, 2013).

Regarding the wine samples in the left upper quadrant (Figure 1A), wines such as MON3, GREN2, TOUR9, NERO3, NERO4, and NERO9 were perceived as having aromas of blue flowers and red fruits. Our results showed similarities with previous findings (Long *et al.*, 2023; Mezei *et al.*, 2021) as both studies described Grenache and Nero d'Avola wines as having aromas and flavours of floral and red fruits. CABS3 and NERO2 were characterised as minty, which is in line with the findings presented by Gonzaga *et al.* (2019) and Robinson *et al.* (2011), where the attribute minty is considered a key characteristic of Australian Cabernet-Sauvignon.

In the right upper quadrant, CABS1 and MON5 were perceived as having characteristics of green, herbaceous eucalypt/mint, vegetable, and dried herbs. TOUR3, MON6, MON1, MON9, CABS2, and TOUR7, displayed attributes of cooked vegetables, savoury, tobacco with an astringent mouthfeel and alcohol heat.

In the lower-left quadrant, TOUR5, TOUR8, GREN1, NERO1, NERO5, NERO6, NERO8, and MON10 wines were perceived as having aromas and flavours of confectionery, floral and flavours of red fruits.

In the lower right quadrant, TOUR4, TOUR6, and SHZ3 were found where the most predominant attributes which described these wines were; aromas and flavours of caramel/butterscotch, sweet oak and chocolate, all attributes most likely derived from oak maturation, although no oak volatiles were analysed in this study to validate this statement. Lastly, wines including MON8, NERO10, SHZ2, TOUR1, NERO7, MON2, MON4, and SHZ1 were characterised as having attributes such as earthy, leathery, oaky, meaty/salami, dark, fruits, dried fruits with a bitter taste, fuller body, and long aftertaste/length, again, most of these attributes (except for dark fruits) are related to oak/age maturation and winemaking techniques, rather than to varietal characteristics (Kustos *et al.*, 2020).

The third principal component PC3 (11.80 %, Figure S1) separated wines from the upper half (TOUR1, TOUR4, TOUR5, TOUR6, TOUR8, MON3, MON4, MON5, MON6, MON8, NERO2, NERO4, NERO8, NERO9, CABS1, CABS2, CABS3, and SHZ3), with attributes such as mint, eucalypt, dark fruits, and blue flowers with high astringency and volatile compounds like 2-phenylethyl acetate, linalool, hexyl acetate and β-damascenone. This differed from wines in the lower half (NERO1, NERO3, NERO5, NERO6, NERO7, NERO10, TOUR3, TOUR7, TOUR9, MON1, MON2, MON9, GREN1, GREN2, SHZ1, and SHZ2) with aromas of caramel/butterscotch, vegetal, earthy, and meaty/salami, and flavours of meaty/salami and caramel/butterscotch and volatiles such as 2-ethyl-1-hexanol, benzyl alcohol and 1-octanol.

In addition to performing a RATA on the 35 wines, the panellists were also asked to provide a hedonic response to each wine. The mean hedonic value was situated in the bottom left-hand side of the PCA biplot (Figure 1B) along with the sensory attributes of floral, blue flowers, confectionery, and red fruits. In terms of volatile compounds, benzyl alcohol, 2-phenylethyl acetate, 1-octanol, linalool, ethyl decanoate, octanoic acid, decanoic acid, ethyl hexanoate, hexyl acetate, ethyl butanoate, hexanoic acid, ethyl octanoate, and 3-methyl butyl acetate were also found in the same quadrant. Our results agreed with previous studies that Australian red wine drinkers preferred red wines with sensory characteristics of fruity/floral, red fruits, and confectionery (Bastian *et al.*, 2010; Copper *et al.*, 2019; Kustos *et al.*, 2020; Lattey *et al.*, 2010; Long *et al.*, 2023; Mezei *et al.*, 2021; Nguyen *et al.*, 2020). TOU8, the most liked wine (mean hedonic score of 6.47) was perceived as floral, confectionery and having aromas and flavours of red fruits, which was in agreement with previous studies that found floral attributes in Touriga Nacional wines (De Pinho *et al.*, 2007; Long *et al.*, 2023; Symington *et al.*, 2011).This could potentially be explained by the fact that linalool, described as flower and lavender (Campo *et al.*, 2021), was more abundant in TOUR8 (62 µg/L, OAV = 4) than the rest of the wines (2 to 21 µg/L, OAV = 0). Moreover, Ristic *et al.* (2019) found that berry-like odours were liked most by consumers from Australia, UK, and US, followed by the attributes of vanilla, chocolate, citrus, and honey. Furthermore, it reiterated the efficacy of the RATA method utilised to describe sensorially intricate products like wine (Danner *et al.*, 2018).

3. Varietal characteristics based on volatile profiles

CVA was performed using the 34 out of 35 significantly different volatile compounds ($p < 0.05$, Figures 2A and 2B) (except for 1-propanol), to explore which specific volatile compounds might characterise each variety and to identify potential chemical similarities between the wines of the three emerging and mainstream varieties. Given that CVA is a supervised technique designed to maximise varietal group separation, we focused the interpretation on the key volatile compounds driving the observed groupings (Figure 2B), integrating these findings with the sensory patterns revealed by PCA (Figure 1A). Touriga Nacional wines formed the most distinctive group, separated from the other varieties. Shiraz and Montepulciano wines were situated adjacent to each other, suggesting shared volatile profiles. Similarly, Cabernet-Sauvignon and Grenache grouped together, with Nero d'Avola positioned in proximity to this latter group. These results complement the sensory patterns observed from the PCA findings by indicating which specific volatile compounds are most strongly associated with each varietal grouping.

Examination of the compounds associated with Touriga Nacional in Figure 2B revealed that linalool and α-terpineol were the most distinctive volatiles characterising this variety, along with decanoic acid.

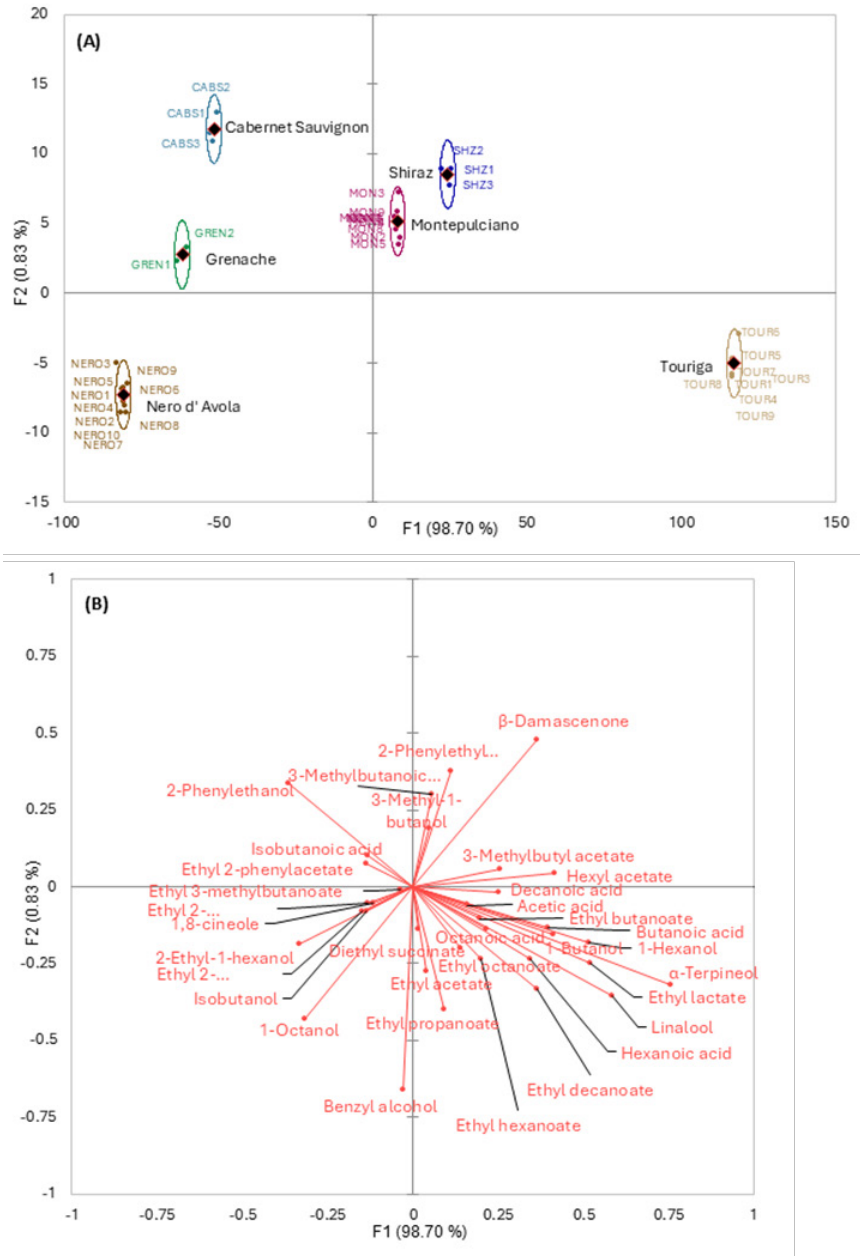


FIGURE 2. Canonical Variates Analysis (CVA) based on 34 significant volatile compounds ($p < 0.05$) showing (A) varietal groupings and (B) loadings of key volatile compounds distinguishing varieties. Wine abbreviations: MON, Montepulciano. NERO, Nero d'Avola. TOUR, Touriga Nacional. CABS, Cabernet-Sauvignon. SHZ, Shiraz. GREN, Grenache. More details for sample codes and geographical indication can be found in Table S1.

According to the literature, there are no studies investigating the volatile composition of Touriga Nacional single varietal table wines, made with fruit grown in Australia. The only studies found on this topic are from continental Europe. These results were consistent with previous studies where Touriga Nacional wines were described as having a floral, bergamot-like aroma that were attributed to volatile compounds of linalool, α-terpineol, and linalyl acetate alone or combined (De Pinho *et al.*, 2007; Petronilho *et al.*, 2021; Symington *et al.*, 2011). Based on the results of the sensory profiling (Figure 1A), wines like TOUR9, TOUR5 and TOUR8 were perceived as having aromas/flavours of blue flowers (TOUR9) and floral (TOUR5 and TOUR8) which could be attributed to the presence of compounds such as linalool and α-terpineol, previously discussed.

Shiraz and Montepulciano wines were characterised primarily by β-damascenone and 2-phenylethyl acetate (Figure 2B), suggesting a shared volatile basis for potential sensory similarities.

Montepulciano wines recorded high levels of β-damascenone, a compound known for its fruity/flowery, apple/baked apple scent (Kotseridis & Baumes, 2000), in a study performed on Italian red wines (Slaghenaufi *et al.*, 2022). Baiano *et al.* (2016) also found this compound to be one of the most representative volatile compounds in Montepulciano wines aged with or without oak chips. Similarly, our results showed the presence of β-damascenone in Montepulciano wines at suprathreshold concentration (OAV mean = 87, concentrations ranged from 3.93 to 5 µg /L). Sagratini *et al.* (2012) identified 3-methyl-1-butanol as the most prominent alcohol in Montepulciano wines from Abruzzo, noting its nail polish-like aroma this compound was also specifically analysed and confirmed as significant in the present investigation.

In contrast to Montepulciano, a multitude of studies describing the volatile composition of Australian Shiraz wines can be found in the literature (Antalick *et al.*, 2015; Mayr *et al.*, 2014; Parker *et al.*, 2007; Pearson *et al.*, 2021). Similar to our results, Kustos *et al.* (2020) reported that compounds like β-damascenone, 2-phenylethyl acetate, and hexyl acetate were found in all the Shiraz samples across the sub-regions investigated. Hranilovic *et al.* (2018) noted that 3-methyl-1-butanol was present (at different concentrations) in all Shiraz wines irrespective of the yeast strain chosen for the fermentation of the samples. In addition, Wang *et al.* (2022) reported compounds like β-damascenone, 2-phenylethyl acetate, 3-methylbutanoic acid, 3-methyl-1-butanol, 3-methylbutyl acetate, and hexyl acetate present in Australian Shiraz wines.

Cabernet-Sauvignon and Grenache wines were characterised primarily by 2-phenylethanol, while Nero d'Avola was positioned in close proximity to this group, sharing 2-phenylethanol but additionally distinguished by 1,8-cineole and ethyl 3-methylbutanoate (Figure 2B). The volatile similarities identified through CVA were further supported by sensory assessment. As discussed in the PCA analysis (Figure 1A), wines such as MON3, GREN2, TOUR9, NERO3, NERO4, and NERO9 were perceived as having aromas of blue flowers and red fruits, consistent with the previous findings of Long *et al.* (2023) and Mezei *et al.* (2021), where Grenache and Nero d'Avola wines shared sensory attributes of floral and red fruits. These sensory similarities align with the volatile groupings observed in the CVA, where Nero d'Avola clustered in proximity to Grenache based on shared compounds including 2-phenylethanol, which contributes to floral notes (Segurel *et al.*, 2009).

Both Cabernet-Sauvignon (Capone *et al.*, 2020; Cordente *et al.*, 2018; Kalua & Boss, 2009; Tao *et al.*, 2008) and Grenache (Ferreira *et al.*, 2002; Garde-Cerdán *et al.*, 2013; López *et al.*, 1999; Sabon *et al.*, 2002; Segurel *et al.*, 2009) have been well researched, and several studies describing the volatile composition of these varieties can be found in the scientific literature.

Akin to our findings, Armstrong *et al.* (2021) reported the presence of ethyl 2-phenylacetate in all the Australian Cabernet-Sauvignon wines vinified with different levels of grape maturity heterogeneity as well as in the controls. The authors found that wines made with high grape maturity heterogeneity (meaning vinified with different levels of grape ripeness) recorded twice as much ethyl 2-phenylacetate concentration than the control samples. In a study investigating the terroir impact on wine aroma composition, Jiang *et al.* (2013) recorded 2-phenylethanol as one of the seven most influential volatile compounds quantified in Cabernet-Sauvignon wines from the Shacheng area of the Hebei region in China. This compound was also reported by Segurel *et al.* (2009) in synthetic model wines from Grenache grapes, enriched with glycoconjugates, from the Rhône Valley. Using GC-Olfactometry, Segurel *et al.* (2009) identified 2-phenylethanol as the compound driving the floral notes in synthetic wines enriched with glycosidic precursors from Rhône Valley Grenache and Syrah wines. Garde-Cerdán *et al.* (2013) also reported the presence of 2-phenylethanol in Grenache wines treated with pulse electric field technique, a non-thermal technology used to enhance the volatile composition of food products.

A European study conducted by Verzera *et al.* (2016) on Nero d'Avola wines, showed that ethyl esters such as ethyl 2-methylbutanoate and ethyl 3-methylbutanoate along with β-damascenone might be responsible for the red fruit attributes in the Sicilian wines analysed. Our results are consistent with these findings, as most of the Nero d'Avola wines examined in this investigation presented similar sensory attributes such as floral and red fruits (Figure 1A), as well as chemical composition, in regard to ethyl 2-methylbutanoate and ethyl 3-methylbutanoate, as seen in Figure 2B. Although no studies have reported on the volatile composition of Nero d'Avola wines made with Australian grown grapes.

Taken together, the volatile patterns highlighted by CVA are consistent with the sensory similarities and differences identified in the PCA (Figure 1), reinforcing that Montepulciano and Nero d'Avola align most closely with Shiraz and Grenache, respectively, while Touriga Nacional retains a more distinctive floral profile.

As the first study to characterise the sensory and volatile profiles of Australian-grown Montepulciano, Nero d'Avola and Touriga Nacional wines, these results provide an initial indication of how these emerging warm-climate varieties express their chemical and sensory characteristics across different Australian regions and their potential to develop distinctive regional styles alongside established benchmark varieties.

4. Modelling relationships between chemical measures and sensory properties

To relate the different varietal wines to each other, we wanted to determine whether the emerging variety wines are close in chemical composition to the mainstream variety wines. As such, an agglomerative hierarchical clustering (AHC) analysis was performed on the volatile chemical data and 4 clusters were obtained as shown in Figure 3. For clarity of presentation, Figures 4 and 5 show the cluster centroids identified by AHC in the PCA space to summarise the average position of wines within each cluster, rather than plotting all individual wines again, as the full distribution of samples is already presented in the PCA of all wines (Figure 1).

Cluster 1 (C1) encompasses 3 Cabernet-Sauvignon samples (CABS1, CABS2, and CABS3), 2 Shiraz wines (SHZ1 and SHZ2), one Montepulciano (MON3), and one Nero d'Avola (NERO2). Cluster 2 (C2) includes 2 Grenache wines (GREN1 and GREN2), one Montepulciano (MON6), 4 Nero d'Avola wines (NERO4, NERO5, NERO6, and NERO9), and 4 Touriga samples (TOUR1, TOUR3, TOUR5, and TOUR9). Cluster 3 consists of 5 Montepulciano samples (MON1, MON4, MON8, MON9, and MON10), 2 Nero d'Avola (NERO1 and NERO8), a Shiraz (SHZ3), and 3 Touriga wines (TOUR4, TOUR6, and TOUR8). Finally, Cluster 4 (C4) is composed of 2 Montepulciano (MON2 and MON5), 3 Nero d'Avola (NERO3, NERO7, and NERO10), and a single example of Touriga (TOUR7). Based on the clusters identified by AHC, PCA analysis (covariance) was executed on the volatile data only (Figure 4), in order to identify the main compounds driving the clusters described above. With a total of 87.62 % of the variance of the data explained within the first 2 principal components, PC1 accounted for 72.06 % and PC2 15.56 % (Figure 4).

Cluster 1 was characterised mainly by 3-methylbutanoic acid (Figure 4), a volatile compound described as having a cheesy, sweaty rancid aroma (Fang & Qian, 2005; Rocha *et al.*, 2004). Cluster 2 by benzyl alcohol (Figure 4), described as floral, fruity, and sweet (Fang & Qian, 2005; Rocha *et al.*, 2004; Welke *et al.*, 2022). Cluster 3 by ethyl hexanoate, ethyl propanoate, ethyl butanoate, ethyl octanoate and decanoic acid (Figure 4). Most of these compounds are responsible for the fruity aromas in wine, whereas ethyl octanoate and decanoic acid are described as having ripe fruit and woody odours (Fang & Qian, 2005; Rocha *et al.*, 2004; Welke *et al.*, 2022). Cluster 4 does not appear to be driven by any volatiles in particular (Figure 4), as it exhibited generally moderate levels across nearly all the compounds examined.

In a similar manner, PCA was performed on the statistically significant sensory data (Figure 5) to identify the main attributes driving the clusters detected by AHC. With a total of 79.24 % of the total of the variance explained across the first 2 PCs, PC1 accounted for 52.78 % and PC2 for 26.46 %.

Cluster 1 was characterised by higher ratings of mint, herbaceous and eucalypt, as well as more complex descriptors such as oak, leather, meaty/salami, and savoury. These complex sensory attributes, savoury in particular, could be related to the presence of 3-methylbutanoic acid mentioned above (OAV 19-33, Tables S4 to S9 for all varieties), as this compound is usually related to cheesy/sweaty odour (Mayr *et al.*, 2014). Cluster 2 encompassed wines with aromas and flavours of red fruits, confectionery, floral and sweet taste, which might relate to the presence of benzyl alcohol, whose odour (floral, fruity, sweet) matched the attributes described in the literature (Fang & Qian, 2005; Rocha *et al.*, 2004; Welke *et al.*, 2022), although benzyl alcohol was found at subthreshold concentrations (OAV = 0, Tables S4 to S10). Considering that this cluster encompasses both Grenache and 4 Nero d'Avola wines (GREN1 and GREN2, and NERO4, NERO5, NERO6, and NERO9) along with one Montepulciano (MON6) and 4 Touriga Nacional wines (TOUR1, TOUR3, TOUR5, and TOUR9) (Figure 3), these results supported the findings presented by Mezei *et al.* (2021) and Long *et al.* (2023), where Nero d'Avola wines were described as having aromas and flavours of floral, red fruits, confectionery, and sweet taste. Once again, Nero d'Avola wines were proven to have similar sensory and volatile profiles to Grenache wines from Australia.

Cluster 3 (Figure 5) was composed of wines with aromas and flavours of dark fruits, blue flowers, sweet oak that matched the odours of the compounds found in this cluster (ethyl hexanoate, ethyl propanoate, ethyl butanoate, ethyl octanoate, and decanoic acid) and mouthfeel aspects like fuller body, higher astringency, and alcohol. When looking at the wine samples, 5 of the 9 Montepulciano wines (MON1, MON4, MON8 MON9, and MON10), 2 Nero d'Avola (NERO1 and NERO8), a Shiraz wine (SHZ3), and 3 Touriga Nacional samples (TOUR4, TOUR6, and TOUR8) were located in this cluster, which were characterised with more intense/rich dark fruit and sweet oak attributes. Again, these results support the previous findings reported by Mezei *et al.* (2021) and Long *et al.* (2023), where Montepulciano and Shiraz wines were proven to be similar (by expert and consumer panels) in aroma and flavour, and now, in volatile profiles as well. In contrast, Touriga wines were evenly spread both on the PCA and AHC results, as these samples were found in all quadrants of the PCA (Figure 1A) and in all AHC clusters (Figure 5).

Lastly, Cluster 4 (MON2, MON5, NERO3, NERO7, NERO10, and TOUR7) (Figure 5) was characterised by mainly flavours of dried fruits and aromas of cooked vegetables, though no volatile compounds were concise enough to justify this cluster. A potential explanation to this cluster could be the fact that some of these sensory attributes may be related to low molecular weight sulfur compounds such as dimethylsulfide, dimethyl disulfide etc. (Smith *et al.*, 2015), which were not targeted in this investigation.

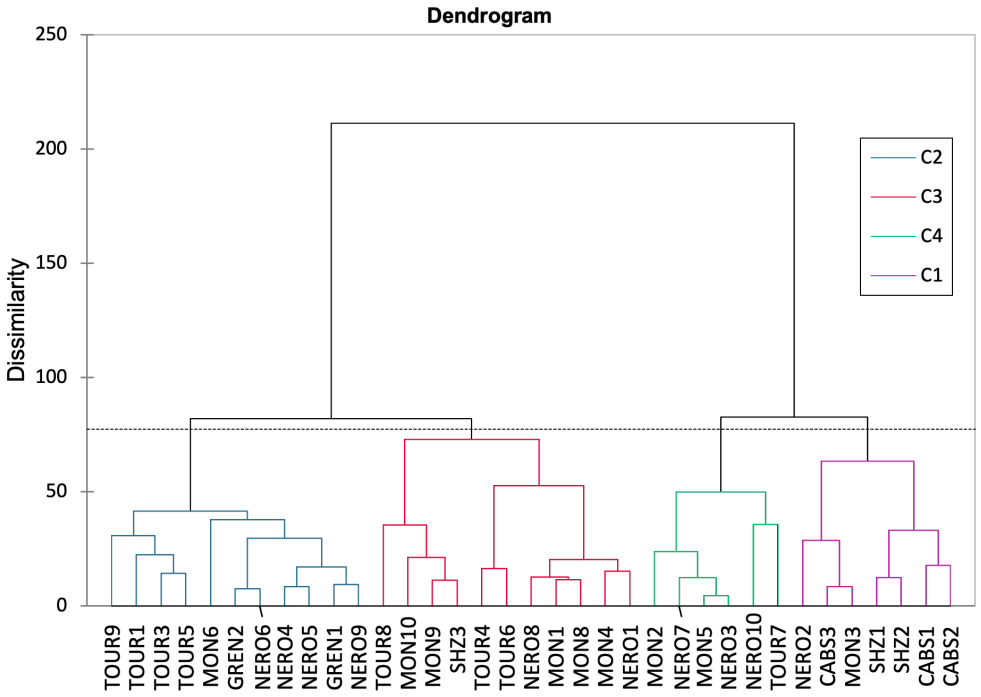


FIGURE 3. Agglomerative hierarchical clustering dendrogram on the volatile composition of the 35 wines. Cluster 1 (C1) is shown in purple, Cluster 2 (C2) in blue, Cluster 3 (C3) in red and Cluster 4 (C4) in green. Wine abbreviations: MON – Montepulciano, NERO – Nero d'Avola, TOUR – Touriga Nacional, CABS – Cabernet-Sauvignon, SHZ – Shiraz and GREN – Grenache. More details for sample codes and geographical indication can be found in Table S1.

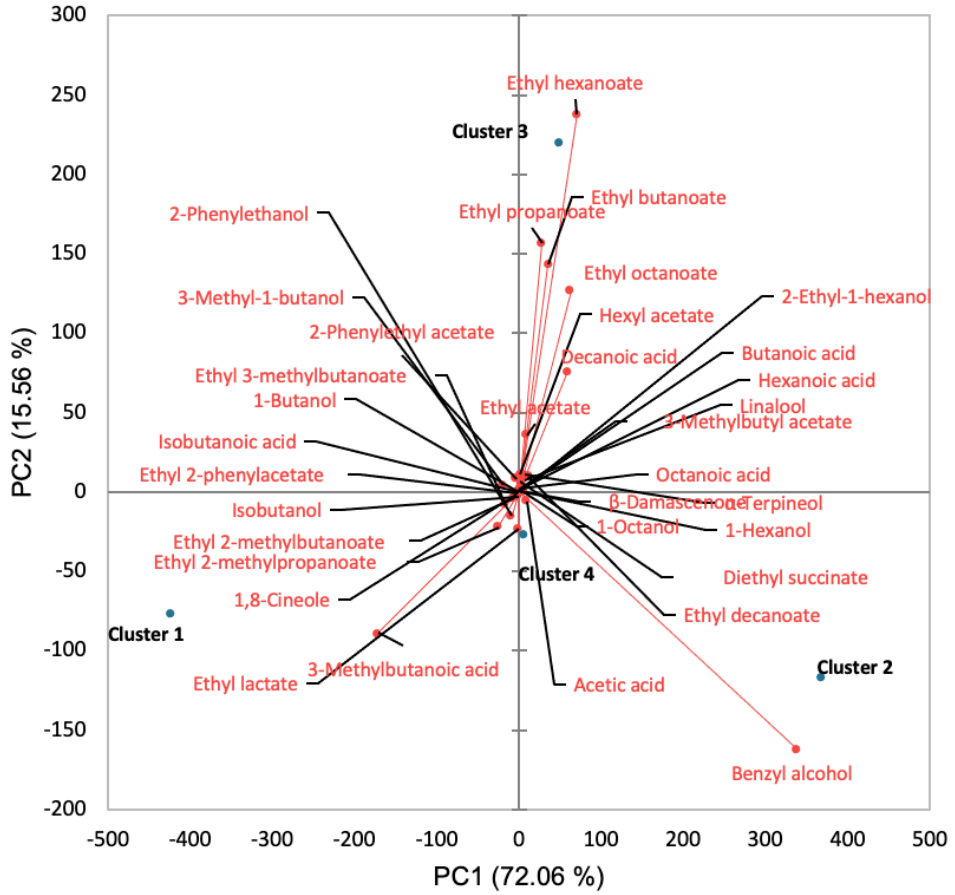


FIGURE 4. Principal component analysis biplot showing the distribution of agglomerative hierarchical clusters (blue dots) and the loadings of significant volatile compounds (red lines, $p < 0.05$) on the first two PCs.

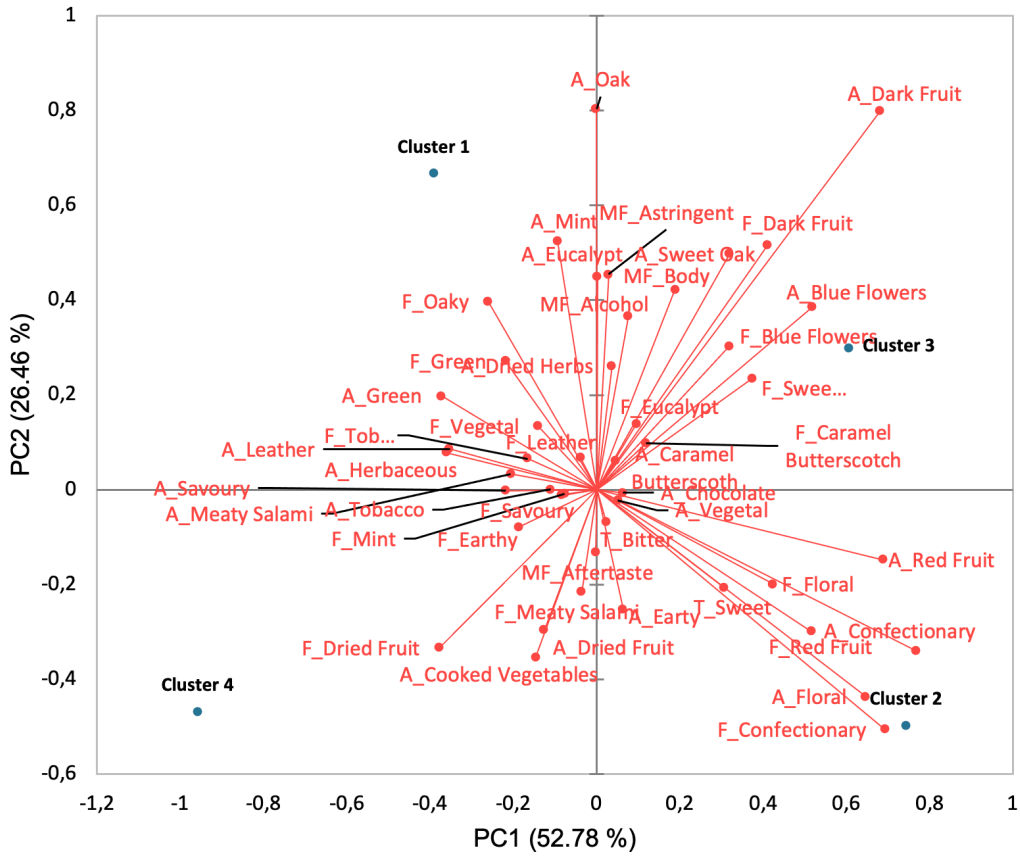


FIGURE 5. Principal component biplot of significant sensory attributes (red lines, $p \leq 0.1$) in combination with the agglomerative hierarchical clustering results (blue dots).

CONCLUSION

According to the results of the RATA sensory study and major volatile compounds analysis by GC-MS, Nero d'Avola wines were characterised by red fruit, confectionery, and floral sensory notes and key volatile compounds including 2-phenylethanol and 1,8-cineole. Montepulciano wines showed intense/rich dark fruit and sweet oak attributes as well as cooked vegetables, savoury, tobacco with an astringent mouthfeel and alcohol heat characteristics. This variety was characterised by β-damascenone and 2-phenylethyl acetate as key volatiles. Commercial Australian Nero d'Avola wines assessed in this investigation presented similar sensory attributes and chemical volatile profiles to Grenache wines, both corroborated by sensory assessment (expert and trained RATA panels) and chemical analyses (GC-MS). Similarly, Shiraz and Montepulciano samples showed similarities in sensory flavour and aromas, as well as in volatile composition. In contrast, Touriga Nacional wines displayed distinctive volatile profiles characterised by floral attributes (particularly linalool and α-terpineol), which differentiated them from the other wines. The considerable within-variety sensory profile variation observed in Touriga Nacional wines – likely attributable to clonal diversity and/or winemaking practices – suggests this variety has the ability to produce a range of wine styles that are directly comparable to numerous wine styles made from the traditional Australian reds explored in this study.

This study characterised the wine sensory and volatile profiles of three emerging drought-tolerant red wine grape varieties grown in Australia (Nero d'Avola, Montepulciano, and Touriga Nacional). Montepulciano and Nero d'Avola exhibited sensory and chemical similarities to Shiraz and Grenache wines, respectively, indicating potential market acceptance among consumers familiar with these established styles. Touriga Nacional, characterised by distinctive floral attributes and one of the highest hedonic scores in the study (TOUR8, mean score 6.47), represented an offering that may appeal to consumers seeking novel wine varieties that are not too dissimilar to wines they would be familiar with in the Australian market. Together, these emerging varieties could contribute to a more diversified and sustainable Australian wine portfolio, with some functioning as stylistic alternatives to mainstream varieties and others expanding the available range of wine styles.

To gain a true understanding of the sensory properties of these emerging red varieties, wine samples vinified under standardised methods should be employed to avoid confounding factors such as differences in oak treatments, yeast selection, malolactic fermentation, etc.

Whilst the main volatile compounds were identified in the samples selected for both emerging and traditional varieties (used as benchmarks), the method utilised only encompassed a selected group of compounds not able to cover the vast complexity of wine volatile composition. Oak related

compounds such as oak lactones, guaiacol, eugenol, vanillin, etc., as well as grape derived methoxypyrazines and low molecular sulfur compounds should be measured in future research to extend the knowledge on these red wine varietals.

Future work evaluating wines of a specific variety made from numerous sites within a region would allow a more rigorous assessment of site-typicity and the relative contributions of variety and terroir to these emerging cultivars.

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