# SUPPLEMENTARY DATA

**Table S1.** Australian red wines from emerging and mainstream varieties utilised for Rate-All-That-Apply, chemical analyses and consumer hedonic trials with corresponding average liking scores.

| Code | Vintage | Variety | GI[a] | Hedonic mean[b] |
|---|---|---|---|---|
| TOUR8 | 2020 | Touriga Nacional | Riverland | 6.47 a |
| TOUR6 | 2018 | Touriga Nacional | Langhorne Creek | 6.45 ab |
| NERO1 | 2018 | Nero d'Avola | Barossa | 6.39 abc |
| TOUR1 | 2019 | Touriga Nacional | Barossa | 6.36 abcd |
| GREN1 | 2020 | Grenache | McLaren Vale | 6.28 abcde |
| TOUR9 | 2020 | Touriga Nacional | Adelaide Plains | 6.25 abcdef |
| MON4 | 2019 | Montepulciano | McLaren Vale | 6.22 abcdef |
| TOUR5 | 2019 | Touriga Nacional | McLaren Vale | 6.20 abcdefg |
| NERO8 | 2020 | Nero d'Avola | Barossa | 6.17 abcdefgh |
| NERO4 | 2020 | Nero d'Avola | McLaren Vale | 6.14 abcdefghi |
| NERO9 | 2020 | Nero d'Avola | Riverland | 6.08 abcdefghij |
| NERO5 | 2020 | Nero d'Avola | McLaren Vale | 6.06 abcdefghij |
| NERO3 | 2019 | Nero d'Avola | Adelaide Hills | 5.97 abcdefghijk |
| MON10 | 2020 | Montepulciano | Riverland | 5.95 abcdefghijk |
| MON1 | 2018 | Montepulciano | Barossa | 5.89 abcdefghijk |
| NERO2 | 2018 | Nero d'Avola | Adelaide Hills | 5.89 abcdefghijk |
| CABS3 | 2018 | Cabernet-Sauvignon | Clare Valley | 5.86 abcdefghijkl |
| GREN2 | 2020 | Grenache | McLaren Vale | 5.81 abcdefghijkl |
| NERO7 | 2018 | Nero d'Avola | McLaren Vale | 5.75 bcdefghijkl |
| MON5 | 2018 | Montepulciano | McLaren Vale | 5.72 cdefghijkl |
| MON6 | 2019 | Montepulciano | Barossa | 5.70 cdefghijkl |
| MON3 | 2018 | Montepulciano | Limestone Coast | 5.67 defghijkl |

| | | | | |
|---|---|---|---|---|
| CABS2 | 2018 | Cabernet-Sauvignon | Coonawarra | 5.67 defghijkl |
| SHZ3 | 2019 | Shiraz | Barossa | 5.64 efghijkl |
| SHZ1 | 2017 | Shiraz | Clare Valley | 5.61 efghijkl |
| NERO6 | 2019 | Nero d'Avola | McLaren Vale | 5.56 fghijklm |
| MON8 | 2019 | Montepulciano | Barossa | 5.50 ghijklm |
| CAB1 | 2019 | Cabernet-Sauvignon | Margaret River | 5.47 hijklm |
| SHZ2 | 2019 | Shiraz | Barossa | 5.45 ijklm |
| NERO10 | 2017 | Nero d'Avola | McLaren Vale | 5.42 jklm |
| TOUR4 | 2018 | Touriga Nacional | Langhorne Creek | 5.39 jklm |
| MON9 | 2020 | Montepulciano | McLaren Vale | 5.28 klm |
| TOUR3 | 2017 | Touriga Nacional | Barossa | 5.28 klm |
| TOUR7 | 2017 | Touriga Nacional | Riverland | 5.17 lm |
| MON2 | 2018 | Montepulciano | Barossa | 4.89 m |

[a] *GI, Geographical Indication.*

[b] *Wines sharing a letter in the hedonic response column are not significantly different (Fisher's LSD $p < 0.05$).*

**Table S2.** Sensory descriptors for aroma, flavour, taste, and mouthfeel evaluated by RATA.

| Attribute[a] | Description | Mean | Minimum | Maximum | SD | *p*-value |
|---|---|---|---|---|---|---|
| **A_Dark fruit** | Blackberry, Mulberry, Plum, Dark cherry, Forrest fruits | 3.60 | 2.17 | 4.78 | 0.63 | <0.0001 |
| **A_Red fruit** | Strawberry, Raspberry, Red cherry, Boysenberry | 2.45 | 1.22 | 3.81 | 0.66 | <0.0001 |
| **A_Dried fruit** | Prunes, Raisins, Fig | 1.60 | 0.94 | 2.44 | 0.33 | 0.014 |
| **A_Confectionery** | Lollies, candy | 1.46 | 0.78 | 2.89 | 0.48 | <0.0001 |
| A_Jammy | Preserved or cooked fruit | 1.80 | 1.28 | 2.61 | 0.33 | 0.121 |
| A_Marmalade | Marmalade | 0.57 | 0.22 | 1.08 | 0.18 | 0.407 |
| **A_Floral** | Rose, Hibiscus | 1.24 | 0.58 | 2.67 | 0.47 | <0.0001 |
| **A_Blue flowers** | Violet, Lavender | 0.97 | 0.36 | 1.92 | 0.38 | <0.0001 |
| A_Spices | Anise, Clove, Cinnamon, Liquorice, Nutmeg | 1.64 | 0.97 | 2.11 | 0.27 | 0.352 |
| **A_Green** | Green pepper, Capsicum, Green bean | 0.78 | 0.33 | 1.44 | 0.30 | 0.000 |
| **A_Herbaceous** | Stemmy, Stalky, Tomato leaf | 1.09 | 0.56 | 1.58 | 0.29 | 0.049 |
| **A_Vegetal** | Cut grass, Hay | 0.63 | 0.17 | 1.11 | 0.23 | 0.027 |
| **A_Dried herbs** | Thyme, Oregano | 0.87 | 0.19 | 1.56 | 0.26 | 0.059 |
| **A_Mint** | Spearmint, Peppermint | 0.75 | 0.33 | 1.53 | 0.26 | 0.013 |
| **A_Eucalypt** | Eucalypt leaves | 0.60 | 0.11 | 1.25 | 0.25 | 0.017 |
| A_Pepper | Black or White pepper | 0.80 | 0.44 | 1.11 | 0.18 | 0.774 |
| **A_Savoury** | Broth, Stock | 1.12 | 0.53 | 2.00 | 0.37 | <0.0001 |
| **A_Meaty/Salami** | Meaty, Soy sauce, Black olive, Salami | 0.73 | 0.22 | 1.39 | 0.32 | <0.0001 |
| A_Nutty | Nutty | 0.54 | 0.22 | 0.92 | 0.16 | 0.556 |
| A_Tea | Black tea leaves | 0.58 | 0.22 | 0.97 | 0.17 | 0.556 |
| **A_Cooked vegetables** | Cooked corn/cabbage, Reductive, Sulfide | 0.76 | 0.31 | 1.67 | 0.34 | <0.0001 |
| A_Barnyard | Horsey | 0.42 | 0.06 | 0.72 | 0.16 | 0.438 |
| **A_Earthy** | Mushroom, Truffle, Forest floor | 1.27 | 0.42 | 1.81 | 0.35 | 0.001 |
| **A_Tobacco** | Smoky, Cigar | 0.84 | 0.25 | 1.47 | 0.30 | 0.001 |
| **A_Leather** | Leather | 0.82 | 0.31 | 1.58 | 0.34 | <0.0001 |
| **A_Chocolate** | Chocolate | 0.75 | 0.39 | 1.28 | 0.24 | 0.020 |

| | | | | | | |
|---|---|---|---|---|---|---|
| **A_Caramel/Butterscotch** | Butterscotch | 0.85 | 0.28 | 1.58 | 0.30 | 0.000 |
| **A_Sweet oak** | Vanilla | 1.59 | 0.92 | 2.83 | 0.41 | <0.0001 |
| **A_Oaky** | Woody, Pencil shavings, Toast, Cedar, Coconut | 2.00 | 0.92 | 3.31 | 0.57 | <0.0001 |
| A_Liquorice | Liquorice | 1.47 | 0.92 | 1.97 | 0.28 | 0.233 |
| **F_Dark fruit** | As per aroma | 3.73 | 2.17 | 4.64 | 0.63 | <0.0001 |
| **F_Red fruit** | As per aroma | 2.49 | 1.50 | 3.78 | 0.65 | <0.0001 |
| **F_Dried fruit** | As per aroma | 1.64 | 0.89 | 2.56 | 0.40 | <0.0001 |
| **F_Confectionery** | As per aroma | 1.38 | 0.50 | 2.50 | 0.47 | <0.0001 |
| F_Jammy | As per aroma | 1.80 | 1.14 | 2.47 | 0.31 | 0.190 |
| F_Marmalade | As per aroma | 0.60 | 0.19 | 0.97 | 0.17 | 0.567 |
| **F_Floral** | As per aroma | 0.98 | 0.42 | 1.83 | 0.36 | <0.0001 |
| **F_Blue flowers** | As per aroma | 0.72 | 0.22 | 1.81 | 0.31 | <0.0001 |
| F_Spices | As per aroma | 1.80 | 1.28 | 2.28 | 0.26 | 0.451 |
| **F_Green** | As per aroma | 0.74 | 0.36 | 1.39 | 0.27 | 0.004 |
| F_Herbaceous | As per aroma | 0.98 | 0.64 | 1.50 | 0.21 | 0.792 |
| **F_Vegetal** | As per aroma | 0.53 | 0.22 | 1.08 | 0.21 | 0.009 |
| F_Dried herbs | As per aroma | 0.72 | 0.39 | 1.19 | 0.21 | 0.190 |
| **F_Mint** | As per aroma | 0.58 | 0.19 | 1.31 | 0.24 | 0.003 |
| **F_Eucalypt** | As per aroma | 0.42 | 0.11 | 0.89 | 0.20 | 0.008 |
| F_Pepper | As per aroma | 1.06 | 0.50 | 1.69 | 0.26 | 0.117 |
| **F_Savoury** | As per aroma | 1.09 | 0.42 | 1.75 | 0.34 | 0.000 |
| **F_Meaty/Salami** | As per aroma | 0.66 | 0.19 | 1.33 | 0.24 | 0.018 |
| F_Nutty | As per aroma | 0.52 | 0.25 | 0.86 | 0.13 | 0.915 |
| F_Tea | As per aroma | 0.64 | 0.25 | 1.00 | 0.19 | 0.451 |
| **F_Cooked vegetables** | As per aroma | 0.55 | 0.28 | 1.00 | 0.18 | 0.058 |
| F_Barnyard | As per aroma | 0.31 | 0.11 | 0.67 | 0.13 | 0.22 |
| **F_Earthy** | As per aroma | 1.17 | 0.53 | 2.03 | 0.36 | 0.000 |
| **F_Tobacco** | As per aroma | 0.84 | 0.14 | 1.47 | 0.31 | 0.000 |
| **F_Leather** | As per aroma | 0.77 | 0.19 | 1.58 | 0.33 | <0.0001 |
| F_Chocolate | As per aroma | 0.78 | 0.31 | 1.28 | 0.22 | 0.149 |
| **F_Caramel/Butterscotch** | As per aroma | 0.68 | 0.31 | 1.31 | 0.24 | 0.008 |
| **F_Sweet oak** | As per aroma | 1.63 | 0.83 | 2.94 | 0.38 | 0.000 |
| **F_Oaky** | As per aroma | 2.18 | 1.17 | 3.42 | 0.50 | <0.0001 |
| F_Liquorice | As per aroma | 1.48 | 0.78 | 1.86 | 0.25 | 0.529 |
| **T_Bitter** | | 2.50 | 2.03 | 3.08 | 0.25 | <0.0001 |

| | | | | | |
|---|---|---|---|---|---|
| T_Acidity | 4.06 | 3.61 | 4.31 | 0.18 | 0.149 |
| **T_Sweet** | 2.58 | 2.14 | 3.17 | 0.28 | <0.0001 |
| **MF_Body** | 4.02 | 3.31 | 4.53 | 0.34 | <0.0001 |
| **MF_Astringent** | 4.27 | 3.58 | 5.33 | 0.34 | <0.0001 |
| **MF_Alcohol** | 4.20 | 3.39 | 4.58 | 0.27 | <0.0001 |
| **MF_Aftertaste** | 4.47 | 3.75 | 5.06 | 0.26 | <0.0001 |

*[a] Significant attributes are shown in bold. (Fisher's LSD p < 0.1). Acronyms meaning are as follows:*

*A = Aroma, F = Flavour, T = Taste, MF = Mouthfeel, and SD, standard deviation.*

*[b] SD, standard deviation.*

**Table S3.** Basic chemical composition of the 35 wine samples.

| Wine sample | pH[b] | TA[ab] (g/L) | RS[ab] (g/L) | VA[ab] (g/L) | % ABV[ab] | Free $SO_2$[b] (mg/L) | Total $SO_2$[b] (mg/L) |
|---|---|---|---|---|---|---|---|
| **MON1** | 3.4 | 5.4 | 0.5 | 0.5 | 14.1 | 5.3 | 54.6 |
| **MON2** | 3.5 | 4.7 | 0.6 | 0.6 | 14.6 | 0.0 | 45.2 |
| **MON3** | 3.4 | 4.6 | 0.5 | 0.4 | 12.2 | 0.0 | 16.6 |
| **MON4** | 3.4 | 5.2 | 0.4 | 0.5 | 14.2 | 4.6 | 30.0 |
| **MON5** | 3.4 | 4.9 | 0.5 | 0.5 | 14.2 | 0.0 | 53.2 |
| **MON6** | 3.2 | 5.4 | 0.4 | 0.4 | 14.0 | 0.0 | 39.5 |
| **MON8** | 3.5 | 5.1 | 0.4 | 0.5 | 14.9 | 1.7 | 80.5 |
| **MON9** | 3.7 | 4.9 | 0.5 | 0.4 | 14.1 | 12.9 | 57.2 |
| **MON10** | 3.6 | 5.3 | 0.5 | 0.5 | 15.3 | 14.1 | 55.7 |
| **NERO1** | 3.3 | 5.5 | 0.8 | 0.5 | 13.7 | 8.0 | 38.8 |
| **NERO2** | 3.4 | 5.7 | 0.6 | 0.5 | 14.2 | 7.7 | 60.8 |
| **NERO3** | 3.2 | 5.8 | 0.4 | 0.6 | 14.4 | 11.7 | 42.7 |
| **NERO4** | 3.6 | 5.4 | 0.4 | 0.4 | 14.0 | 2.8 | 38.2 |
| **NERO5** | 3.6 | 4.9 | 0.4 | 0.3 | 14.0 | 19.3 | 45.2 |
| **NERO6** | 3.4 | 6.1 | 0.7 | 0.5 | 14.7 | 12.0 | 64.8 |
| **NERO7** | 3.5 | 5.4 | 0.7 | 0.5 | 13.9 | 1.0 | 37.6 |
| **NERO8** | 3.3 | 7.0 | 0.2 | 0.6 | 13.8 | 5.5 | 50.2 |
| **NERO9** | 3.6 | 5.7 | 0.9 | 0.1 | 15.4 | 14.2 | 46.7 |
| **NERO10** | 3.5 | 5.9 | 1.2 | 0.6 | 14.3 | 13.5 | 111.3 |
| **TOUR1** | 3.5 | 5.7 | 0.8 | 0.6 | 14.9 | 1.7 | 86.2 |
| **TOUR3** | 4.1 | 5.1 | 0.0 | 0.5 | 14.5 | 0.0 | 79.9 |
| **TOUR4** | 4.0 | 4.7 | 0.6 | 0.5 | 15.3 | 0.0 | 48.1 |
| **TOUR5** | 3.6 | 5.6 | 0.4 | 0.4 | 13.8 | 0.0 | 36.7 |
| **TOUR6** | 3.5 | 5.6 | 0.8 | 0.6 | 15.8 | 2.7 | 88.2 |
| **TOUR7** | 3.4 | 6.9 | 1.0 | 0.6 | 16.1 | 0.0 | 11.7 |
| **TOUR8** | 3.6 | 5.1 | 0.4 | 0.4 | 15.0 | 6.5 | 84.2 |
| **TOUR9** | 3.4 | 6.4 | 0.1 | 0.6 | 13.8 | 12.2 | 134.3 |
| **SHZ1** | 3.5 | 5.3 | 0.7 | 0.4 | 14.0 | 1.9 | 25.3. |
| **SHZ2** | 3.7 | 5.3 | 0.5 | 0.4 | 14.6 | 11.7 | 48.9 |
| **SHZ3** | 3.6 | 5.3 | 3.3 | 0.4 | 14.6 | 10.5 | 79.8 |
| **CABS1** | 3.5 | 5.7 | 0.2 | 0.3 | 14.2 | 9.7 | 95.2 |
| **CABS2** | 3.6 | 5.4 | 0.5 | 0.6 | 14.0 | 0.7 | 71.6 |
| **CABS3** | 3.4 | 5.6 | 1.0 | 0.4 | 14.0 | 11.4 | 51.2 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| **GREN1** | 3.5 | 5.1 | 2.0 | 0.4 | 15.1 | 5.4 | 32.4 |
| **GREN2** | 3.5 | 5.1 | 0.2 | 0.5 | 14.3 | 5.9 | 35.5 |

*[a] TA, titratable acidity. RS, residual sugar. VA, volatile acidity expressed as acetic acid. % ABV, alcohol by volume.*

*[b] Values are single measurements.*

**Table S4.** Concentrations (µg/L) of volatile compounds quantified in Montepulciano wines (n = 9).

| Volatile compounds | Min[a] | Max[a] | Median | Mean | OAV[a] Mean | SD[b] |
|---|---|---|---|---|---|---|
| Ethyl acetate | 104,195 | 204,230 | 157,295 | 162,048 | 10.80 | 27,078 |
| 3-Methylbutyl acetate | 2,630 | 5,098 | 2,996 | 3,289 | 110 | 770 |
| Hexyl acetate | 5.6 | 30 | 7.4 | 11.6 | 0.02 | 7.7 |
| 2-Phenylethyl acetate | 81.1 | 126 | 97.3 | 101 | 0.4 | 12.6 |
| Ethyl propanoate | 202 | 503 | 310 | 328 | 0.2 | 91.6 |
| Ethyl 2-methylpropanoate | 207 | 689 | 289 | 339 | 0.1 | 138 |
| Ethyl butanoate | 186 | 415 | 299 | 295 | 0.5 | 71.1 |
| Ethyl 2-methylbutanoate | 10.8 | 78.5 | 37.4 | 39.3 | 39.3 | 21.0 |
| Ethyl 3-methylbutanoate | 22.0 | 141 | 83.1 | 73.6 | 24.5 | 34.9 |
| Ethyl hexanoate | 176 | 613 | 383 | 380 | 27.1 | 122 |
| Ethyl lactate | 68,230 | 132,178 | 98,450 | 97,421 | 6.7 | 15,883 |
| Ethyl octanoate | 166 | 781 | 579 | 574 | 28.7 | 134 |
| Ethyl decanoate | 12.5 | 60.1 | 35.7 | 38.6 | 0.2 | 14.1 |
| Ethyl 2-phenylacetate | 0.9 | 5.9 | 3.2 | 3.1 | <0.01 | 1.5 |
| Diethyl succinate | 11,457 | 44,961 | 25,363 | 25,451 | 0.02 | 8,768 |
| 1-Propanol | 21,577 | 952,961 | 38,525 | 82,506 | 165 | 200,144 |
| Isobutanol | 30,694 | 59,727 | 39,982 | 40,647 | 1.0 | 7,855 |
| 1-butanol | 752 | 1,449 | 1,189 | 1,136 | 7.1 | 191 |
| 3-Methyl-1-butanol | 32,818 | 262,962 | 176,445 | 181,440 | 6.1 | 47,517 |
| 2-Ethyl-1-hexanol | 3.6 | 16.4 | 7.2 | 8.0 | 0.0 | 3.4 |
| 1-Octanol | 7.7 | 36.4 | 19.2 | 20.2 | 28.9 | 7.0 |
| Benzyl alcohol | 242 | 949 | 566 | 581 | 0.01 | 231 |
| 2-Phenylethanol | 25,828 | 61,714 | 40,643 | 42,600 | 3.0 | 11,475 |
| 1-Hexanol | 788 | 2,383 | 1,433 | 1,475 | 0.2 | 454 |
| Acetic acid | 119,616 | 580,096 | 186,639 | 201,070 | 10 | 91,537 |
| Isobutanoic acid | 308 | 3,445 | 1,302 | 1,491 | 0.01 | 660 |
| Butanoic acid | 573 | 1,528 | 1,127 | 1,096 | 0.1 | 274 |
| 3-Methylbutanoic acid | 503 | 1,151 | 702 | 743 | 22 | 199 |
| Hexanoic acid | 2,527 | 3,886 | 3,125 | 3,146 | 7.5 | 435 |
| Octanoic acid | 5,020 | 10,029 | 7,344 | 7,432 | 15 | 1,447 |
| Decanoic acid | 483 | 1023 | 680 | 707 | 0.7 | 157 |

| | | | | | | |
|---|---|---|---|---|---|---|
| 1,8-Cineole | 6.9 | 8.3 | 7.3 | 7.4 | 6.8 | 0.6 |
| Linalool | 2.4 | 9.7 | 4.7 | 5.0 | 0.3 | 2.1 |
| α-Terpineol | 15 | 54 | 22 | 25 | 0.10 | 10 |
| β-Damascenone | 3.9 | 5.0 | 4.3 | 4.4 | 87.2 | 0.3 |

[a] *Min, minimum concentration. Max, maximum concentration. OAV mean, odour active value of mean concentration, calculated by dividing the mean concentration by its odour detection threshold (ODT) obtained from Guth (1997) and Wang* et al. *(2016).*

[b] *SD, standard deviation for all samples (n = 9).*

**Table S5.** Concentrations (µg/L) of volatile compounds quantified in Nero d'Avola wines (n = 10).

| Volatile compounds | Min[a] | Max[a] | Median | Mean | OAV[a] Mean | SD[b] |
|---|---|---|---|---|---|---|
| Ethyl acetate | 87,331 | 252,409 | 159,227 | 154,812 | 10.3 | 42,930 |
| 3-Methylbutyl acetate | 2,540 | 3,490 | 2,860 | 2,972 | 99.1 | 260 |
| Hexyl acetate | 5.8 | 13.8 | 9.3 | 9.7 | 0.0 | 2.7 |
| 2-Phenylethyl acetate | 81.3 | 127 | 93.3 | 95.9 | 0.4 | 12.8 |
| Ethyl propanoate | 165 | 569 | 341 | 349 | 0.2 | 108 |
| Ethyl 2-methylpropanoate | 206 | 512 | 334 | 341 | 0.1 | 87.9 |
| Ethyl butanoate | 160 | 363 | 236 | 249 | 0.4 | 45.1 |
| Ethyl 2-methylbutanoate | 11.0 | 74.7 | 38.7 | 41.2 | 41.2 | 18.0 |
| Ethyl 3-methylbutanoate | 38.7 | 130 | 73.1 | 79.2 | 26.4 | 29.5 |
| Ethyl hexanoate | 159 | 580 | 321 | 332 | 23.8 | 98.8 |
| Ethyl lactate | 77,493 | 182,063 | 100,535 | 110,731 | 7.6 | 26,457 |
| Ethyl octanoate | 369 | 827 | 544 | 559 | 27.9 | 117 |
| Ethyl decanoate | 21.0 | 57.3 | 42.9 | 40.4 | 0.2 | 12.2 |
| Ethyl 2-phenylacetate | 2.2 | 7.6 | 3.3 | 3.9 | 0.0 | 1.6 |
| Diethyl succinate | 15,839 | 48,627 | 21,955 | 26,082 | 0.0 | 9,640 |
| 1-Propanol | 22,409 | 66,944 | 33,416 | 37,049 | 74.1 | 12,503 |
| Isobutanol | 34,336 | 59,287 | 42,043 | 43,818 | 1.1 | 6,544 |
| 1-butanol | 995 | 1,665 | 1,118 | 1,176 | 7.4 | 170 |
| 3-Methyl-1-butanol | 167,520 | 222,665 | 189,391 | 191,820 | 6.4 | 16,804 |
| 2-Ethyl-1-hexanol | 4.3 | 25.4 | 9.7 | 10.6 | 0.0 | 5.7 |
| 1-Octanol | 17.9 | 45.0 | 24.3 | 27.7 | 39.6 | 8.7 |
| Benzyl alcohol | 675 | 2,182 | 1,075 | 1,288 | 0.0 | 493 |
| 2-Phenylethanol | 25,079 | 65,225 | 48,448 | 47,279 | 3.4 | 10,002 |
| 1-Hexanol | 798 | 2,480 | 1,585 | 1,642 | 0.2 | 393 |
| Acetic acid | 116,787 | 335,147 | 188,203 | 1964,96 | 9.8 | 53,217 |
| Isobutanoic acid | 1,260 | 2,059 | 1,622 | 1,649 | 0.0 | 207 |
| Butanoic acid | 741 | 1,412 | 949 | 1,012 | 0.1 | 197 |
| 3-Methylbutanoic acid | 619 | 1,175 | 757 | 777 | 23.3 | 143 |
| Hexanoic acid | 2,034 | 4,237 | 2,898 | 3,015 | 7.2 | 578 |
| Octanoic acid | 3,079 | 10,726 | 6,138 | 6,478 | 13.0 | 1,969 |
| Decanoic acid | 509 | 810 | 683 | 676 | 0.7 | 92.0 |
| 1,8-Cineole | 23.0 | 24.0 | 23.5 | 23.5 | 21.4 | 0.5 |
| Linalool | 2.1 | 21.1 | 7.6 | 9.0 | 0.5 | 6.0 |

| | | | | | | |
|---|---|---|---|---|---|---|
| α-Terpineol | 13.7 | 25.9 | 19.0 | 19.1 | 0.1 | 3.0 |
| β-Damascenone | 3.5 | 4.0 | 3.8 | 3.8 | 75.3 | 0.1 |

[a] *Min, minimum concentration. Max, maximum concentration. OAV mean, odour active value of mean concentration, calculated by dividing the mean concentration by its odour detection threshold (ODT) obtained from Guth (1997) and Wang et al. (2016).*

[b] *SD, standard deviation for all samples (n = 10).*

**Table S6.** Concentrations (µg/L) of volatile compounds quantified in Touriga Nacional wines (n = 10).

| Volatile compounds | Min[a] | Max[a] | Median | Mean | OAV[a] Mean | SD[b] |
|---|---|---|---|---|---|---|
| Ethyl acetate | 36,465 | 212,796 | 147,273 | 146,945 | 9.8 | 46,630 |
| 3-Methylbutyl acetate | 2,434 | 4,813 | 3,082 | 3,273 | 109 | 735 |
| Hexyl acetate | 6.5 | 34.7 | 14.0 | 17.8 | 0.0 | 9.9 |
| 2-Phenylethyl acetate | 72.3 | 138 | 106 | 99.5 | 0.4 | 20.3 |
| Ethyl propanoate | 38.0 | 660 | 364 | 347 | 0.2 | 166 |
| Ethyl 2-methylpropanoate | 137 | 484 | 258 | 276 | 0.1 | 97.8 |
| Ethyl butanoate | 98.2 | 387 | 288 | 264 | 0.4 | 82.1 |
| Ethyl 2-methylbutanoate | 3.6 | 78.8 | 24.4 | 28.4 | 28.4 | 21.9 |
| Ethyl 3-methylbutanoate | 26.1 | 165 | 57.2 | 66.9 | 22.3 | 40.8 |
| Ethyl hexanoate | 46.6 | 545 | 382 | 352 | 25.1 | 153 |
| Ethyl lactate | 98,064 | 282,703 | 139,159 | 158,460 | 10.9 | 50,629 |
| Ethyl octanoate | 506 | 838 | 550 | 573 | 28.7 | 81.8 |
| Ethyl decanoate | 25.0 | 80.5 | 52.2 | 50.1 | 0.3 | 15.0 |
| Ethyl 2-phenylacetate | 1.9 | 7.5 | 2.8 | 3.4 | 0.0 | 1.7 |
| Diethyl succinate | 7,516 | 40,641 | 22,820 | 24,105 | 0.0 | 10,178 |
| 1-Propanol | 29,543 | 51,407 | 44,328 | 42,835 | 85.7 | 6,226 |
| Isobutanol | 30,954 | 48,952 | 40,607 | 40,740 | 1.0 | 5,094 |
| 1-butanol | 1,113 | 2,006 | 1,331 | 1,393 | 8.7 | 248 |
| 3-Methyl-1-butanol | 141,153 | 250,415 | 195,166 | 194,387 | 6.5 | 31,900 |
| 2-Ethyl-1-hexanol | 3.2 | 9.1 | 5.9 | 6.0 | 0.0 | 1.7 |
| 1-Octanol | 10.1 | 29.4 | 24.3 | 21.8 | 31.2 | 5.4 |
| Benzyl alcohol | 792 | 2,253 | 992 | 1,279 | 0.0 | 484 |
| 2-Phenylethanol | 24,229 | 47,534 | 34,095 | 35,942 | 2.6 | 7,748 |
| 1-Hexanol | 1,711 | 3,539 | 2,440 | 2,426 | 0.3 | 629 |
| Acetic acid | 160,943 | 272,034 | 209,047 | 214,299 | 10.7 | 34,206 |
| Isobutanoic acid | 1,036 | 2,007 | 1,448 | 1,449 | 0.0 | 261 |
| Butanoic acid | 878 | 1,505 | 1,140 | 1,144 | 0.1 | 178 |
| 3-Methylbutanoic acid | 511 | 1,056 | 772 | 786 | 23.6 | 158 |
| Hexanoic acid | 2,641 | 4,351 | 3,181 | 3,299 | 7.9 | 484 |
| Octanoic acid | 4,665 | 9,633 | 7,040 | 6,960 | 13.9 | 1,279 |
| Decanoic acid | 534 | 949 | 748 | 725 | 0.7 | 103 |
| 1,8-Cineole | 6.2 | 6.6 | 6.4 | 6.4 | 5.8 | 0.2 |
| Linalool | 7.5 | 63.7 | 26.8 | 30.9 | 2.1 | 17.7 |

| | | | | | | |
|---|---|---|---|---|---|---|
| α-Terpineol | 29.7 | 70.8 | 46.4 | 46.9 | 0.2 | 10.7 |
| β-Damascenone | 3.6 | 4.6 | 4.2 | 4.1 | 82.0 | 0.3 |

[a] *Min, minimum concentration. Max, maximum concentration. OAV mean, odour active value of mean concentration, calculated by dividing the mean concentration by its odour detection threshold (ODT) obtained from Guth (1997) and Wang et al. (2016).*

[b] *SD, standard deviation for all samples (n = 10).*

**Table S7.** Concentrations (µg/L) of volatile compounds quantified in Cabernet-Sauvignon wines (n = 3).

| Volatile compounds | Min [a] | Max [a] | Median | Mean | OAV [a] Mean | SD [b] |
|---|---|---|---|---|---|---|
| Ethyl acetate | 58,878 | 156,199 | 109,219 | 111,775 | 7.5 | 32,071 |
| 3-Methylbutyl acetate | 2,712 | 3,093 | 2,980 | 2,923 | 97.5 | 157 |
| Hexyl acetate | 6.4 | 12.0 | 8.8 | 8.9 | 0.0 | 2.2 |
| 2-Phenylethyl acetate | 89.9 | 134 | 123 | 120 | 0.5 | 14.3 |
| Ethyl propanoate | 104 | 298 | 243 | 230 | 0.1 | 59.6 |
| Ethyl 2-methylpropanoate | 209 | 436 | 305 | 310 | 0.1 | 66.9 |
| Ethyl butanoate | 143 | 215 | 194 | 183 | 0.3 | 25.9 |
| Ethyl 2-methylbutanoate | 18.7 | 54.4 | 31.5 | 33.0 | 33.0 | 10.7 |
| Ethyl 3-methylbutanoate | 37.8 | 107 | 81.7 | 78.5 | 26.2 | 20.6 |
| Ethyl hexanoate | 120 | 282 | 200 | 192 | 13.7 | 52.0 |
| Ethyl lactate | 64,143 | 118,690 | 113,701 | 106,645 | 7.3 | 19,204 |
| Ethyl octanoate | 299 | 467 | 414 | 401 | 20.1 | 52.4 |
| Ethyl decanoate | 25.0 | 51.3 | 26.6 | 30.8 | 0.2 | 9.3 |
| Ethyl 2-phenylacetate | 2.5 | 9.9 | 6.3 | 6.5 | 0.0 | 2.6 |
| Diethyl succinate | 8,473 | 35,116 | 17,151 | 19,833 | 0.0 | 10,896 |
| 1-Propanol | 21,278 | 30,799 | 27,560 | 27,061 | 54.1 | 3,154 |
| Isobutanol | 28,925 | 56,485 | 45,320 | 44,512 | 1.1 | 9,304 |
| 1-butanol | 854 | 1,324 | 1,128 | 1,125 | 7.0 | 161 |
| 3-Methyl-1-butanol | 138,427 | 292,779 | 231,670 | 233,804 | 7.8 | 50,745 |
| 2-Ethyl-1-hexanol | 2.8 | 16.1 | 4.0 | 7.7 | 0.0 | 5.7 |
| 1-Octanol | 10.8 | 20.5 | 19.1 | 17.7 | 25.3 | 3.4 |
| Benzyl alcohol | 355 | 571 | 527 | 507 | 0.0 | 74.4 |
| 2-Phenylethanol | 35,048 | 91,413 | 77,010 | 72,750 | 5.2 | 18,960 |
| 1-Hexanol | 925 | 2,139 | 1,660 | 1,679 | 0.2 | 407 |
| Acetic acid | 128,785 | 232,768 | 166,167 | 177,011 | 8.9 | 42,226 |
| Isobutanoic acid | 979 | 2,686 | 2,015 | 1,994 | 0.0 | 586 |
| Butanoic acid | 549 | 850 | 765 | 730 | 0.1 | 116 |
| 3-Methylbutanoic acid | 523 | 1,356 | 1,131 | 1,063 | 31.8 | 267 |
| Hexanoic acid | 1,923 | 2,841 | 2,457 | 2,432 | 5.8 | 300 |
| Octanoic acid | 2,494 | 5,671 | 4,057 | 4,099 | 8.2 | 1,032 |
| Decanoic acid | 529 | 786 | 587 | 613 | 0.6 | 86.7 |
| 1,8-Cineole | 4.5 | 7.9 | 6.2 | 6.2 | 5.6 | 1.7 |
| Linalool | 2.6 | 5.6 | 5.1 | 4.6 | 0.3 | 1.1 |

| | | | | | | |
|---|---|---|---|---|---|---|
| α-Terpineol | 11.6 | 16.7 | 14.7 | 14.8 | 0.1 | 1.7 |
| β-Damascenone | 3.8 | 4.3 | 4.2 | 4.1 | 82.7 | 0.2 |

*[a] Min, minimum concentration. Max, maximum concentration. OAV mean, odour active value of mean concentration, calculated by dividing the mean concentration by its odour detection threshold (ODT) obtained from Guth (1997) and Wang et al. (2016).*

*[b] SD, standard deviation for all samples (n = 3).*

## Table S8. Concentrations (µg/L) of volatile compounds quantified in Shiraz wines (n = 3).

| Volatile compounds | Min[a] | Max[a] | Median | Mean | OAV[a] Mean | SD[b] |
|---|---|---|---|---|---|---|
| Ethyl acetate | 12,129 | 158,927 | 136,914 | 103,038 | 6.9 | 63,815 |
| 3-Methylbutyl acetate | 2,316 | 4,429 | 3,248 | 3,285 | 110 | 786 |
| Hexyl acetate | 4.1 | 39.8 | 27.0 | 24.2 | 0.0 | 14.0 |
| 2-Phenylethyl acetate | 89.4 | 152 | 118 | 117 | 0.5 | 22.6 |
| Ethyl propanoate | 269 | 403 | 300 | 318 | 0.1 | 50.6 |
| Ethyl 2-methylpropanoate | 140 | 414 | 248 | 256 | 0.1 | 84.5 |
| Ethyl butanoate | 68.7 | 356 | 239 | 217 | 0.4 | 110 |
| Ethyl 2-methylbutanoate | 2.3 | 69.3 | 19.8 | 23.9 | 23.9 | 22.4 |
| Ethyl 3-methylbutanoate | 51.1 | 144 | 59.2 | 76.3 | 25.4 | 32.9 |
| Ethyl hexanoate | 287 | 413 | 338 | 344 | 16.4 | 45.6 |
| Ethyl lactate | 90,718 | 238,661 | 119,601 | 139,417 | 9.6 | 55,035 |
| Ethyl octanoate | 483 | 618 | 552 | 551 | 27.5 | 58.4 |
| Ethyl decanoate | 16.4 | 44.5 | 35.3 | 31.3 | 0.2 | 11.3 |
| Ethyl 2-phenylacetate | 1.7 | 4.6 | 2.4 | 2.8 | 0.0 | 1.0 |
| Diethyl succinate | 8,314 | 36,571 | 17,572 | 20,824 | 0.0 | 11,540 |
| 1-Propanol | 26,552 | 34,931 | 30,504 | 30,617 | 61.2 | 2,664 |
| Isobutanol | 33,788 | 43,880 | 38,659 | 38,597 | 1.0 | 3,605 |
| 1-butanol | 1,142 | 1,635 | 1,362 | 1,377 | 8.6 | 176 |
| 3-Methyl-1-butanol | 186,276 | 255,295 | 2167,66 | 215,205 | 7.2 | 23,493 |
| 2-Ethyl-1-hexanol | 2.6 | 7.4 | 3.6 | 4.2 | 0.0 | 1.6 |
| 1-Octanol | 8.5 | 20.2 | 17.3 | 15.2 | 21.7 | 4.4 |
| Benzyl alcohol | 339 | 532 | 471 | 446 | 0.0 | 77.2 |
| 2-Phenylethanol | 33,410 | 59,855 | 48,340 | 46,869 | 3.4 | 10,428 |
| 1-Hexanol | 2,037 | 2,243 | 2,219 | 2,173 | 0.3 | 83.1 |
| Acetic acid | 146,726 | 279,691 | 194,955 | 206,789 | 10.3 | 52,200 |
| Isobutanoic acid | 839 | 2,672 | 1,598 | 1,644 | 0.0 | 681 |
| Butanoic acid | 850 | 1,551 | 1,186 | 1,188 | 0.1 | 251 |
| 3-Methylbutanoic acid | 722 | 1,925 | 950 | 1,127 | 33.8 | 433 |
| Hexanoic acid | 2,743 | 3,522 | 2,946 | 3,044 | 7.3 | 284 |
| Octanoic acid | 5,250 | 7,363 | 6,037 | 6,274 | 12.6 | 748 |
| Decanoic acid | 623 | 871 | 734 | 740 | 0.7 | 92.2 |

| | | | | | | |
|---|---|---|---|---|---|---|
| 1,8-Cineole | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| Linalool | 4.2 | 13.0 | 8.7 | 8.6 | 0.6 | 2.9 |
| α-Terpineol | 16.0 | 18.2 | 16.3 | 16.6 | 0.1 | 0.7 |
| β-Damascenone | 3.6 | 4.4 | 4.0 | 4.0 | 79.6 | 0.3 |

[a] *Min, minimum concentration. Max, maximum concentration. OAV mean, odour active value of mean concentration, calculated by dividing the mean concentration by its odour detection threshold (ODT) obtained from Guth (1997) and Wang et al. (2016).*

[b] *SD, standard deviation for all samples (n = 3).*

**Table S9.** Concentrations (µg/L) of volatile compounds quantified in Grenache wines (n = 2).

| Volatile compounds | Min[a] | Max[a] | Median | Mean | OAV[a] Mean | SD[b] |
|---|---|---|---|---|---|---|
| Ethyl acetate | 69,837 | 152,487 | 128,932 | 117,392 | 7.8 | 29,305 |
| 3-Methylbutyl acetate | 3,036 | 3,775 | 3,130 | 3,288 | 110 | 292 |
| Hexyl acetate | 11.5 | 47.2 | 12.2 | 23.4 | 0.0 | 16.3 |
| 2-Phenylethyl acetate | 90.0 | 113 | 95.2 | 99.1 | 0.4 | 8.7 |
| Ethyl propanoate | 172 | 533 | 279 | 291 | 0.1 | 118 |
| Ethyl 2-methylpropanoate | 127 | 259 | 203 | 201 | 0.0 | 52.7 |
| Ethyl butanoate | 205 | 383 | 246 | 266 | 0.4 | 55.9 |
| Ethyl 2-methylbutanoate | 7.0 | 34.2 | 17.2 | 17.3 | 17.3 | 8.8 |
| Ethyl 3-methylbutanoate | 14.9 | 47.3 | 35.0 | 32.3 | 10.8 | 13.1 |
| Ethyl hexanoate | 249 | 390 | 306 | 309 | 22.1 | 44.4 |
| Ethyl lactate | 48,482 | 88,724 | 81,487 | 72,233 | 5.0 | 16,885 |
| Ethyl octanoate | 450 | 661 | 569 | 559 | 27.9 | 80.7 |
| Ethyl decanoate | 37.0 | 51.3 | 45.7 | 45.5 | 0.2 | 4.7 |
| Ethyl 2-phenylacetate | 1.3 | 2.3 | 1.7 | 1.8 | 0.0 | 0.4 |
| Diethyl succinate | 2,262 | 26,875 | 13,549 | 14,057 | 0.0 | 9,791 |
| 1-Propanol | 31,324 | 51,044 | 34,520 | 38,176 | 76.4 | 7,476 |
| Isobutanol | 34,265 | 39,660 | 37,041 | 36,942 | 0.9 | 1,775 |
| 1-butanol | 947 | 1,283 | 1,207 | 1,144 | 7.2 | 127 |
| 3-Methyl-1-butanol | 164,305 | 183,065 | 176,522 | 174,928 | 5.8 | 6,281 |
| 2-Ethyl-1-hexanol | 2.5 | 17.7 | 8.0 | 9.3 | 0.0 | 6.1 |
| 1-Octanol | 18.1 | 43.8 | 27.8 | 29.9 | 42.7 | 9.8 |
| Benzyl alcohol | 459 | 1,514 | 684 | 883 | 0.0 | 438 |
| 2-Phenylethanol | 36,035 | 48,230 | 39,773 | 41,112 | 2.9 | 4,622 |
| 1-Hexanol | 1,399 | 2,450 | 2,158 | 2,003 | 0.3 | 414 |
| Acetic acid | 126,200 | 236,669 | 142,247 | 166,469 | 8.3 | 45,517 |

| | | | | | | |
|---|---|---|---|---|---|---|
| Isobutanoic acid | 1,087 | 1,374 | 1,227 | 1,239 | 0.0 | 95.3 |
| Butanoic acid | 818 | 950 | 880 | 887 | 0.1 | 46.5 |
| 3-Methylbutanoic acid | 569 | 794 | 617 | 656 | 19.6 | 86.3 |
| Hexanoic acid | 2,671 | 3,064 | 2,985 | 2,926 | 7.0 | 141 |
| Octanoic acid | 6,471 | 7,634 | 7,032 | 7,081 | 14.2 | 450 |
| Decanoic acid | 649 | 854 | 783 | 769 | 0.8 | 75.5 |
| 1,8-Cineole | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| Linalool | 7.8 | 15.6 | 11.6 | 11.5 | 0.8 | 2.8 |
| α-Terpineol | 14.6 | 25.3 | 20.9 | 20.3 | 0.1 | 4.3 |
| β-Damascenone | 3.9 | 4.9 | 4.0 | 4.3 | 85.6 | 0.4 |

[a] *Min, minimum concentration. Max, maximum concentration. OAV mean, odour active value of mean concentration, calculated by dividing the mean concentration by its odour detection threshold (ODT) obtained from Guth (1997) and Wang et al. (2016).*

[b] *SD, standard deviation for all samples (n = 2).*

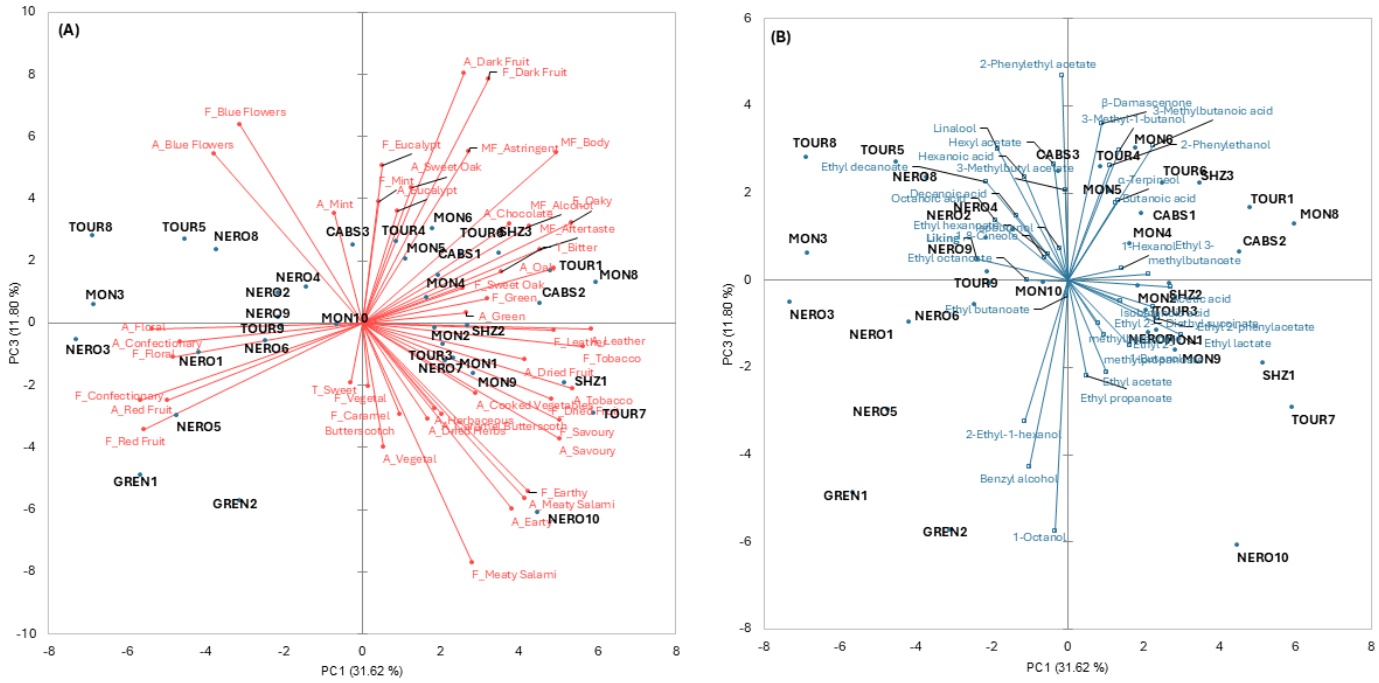



**Figure S1.** Principal component analysis biplots of distribution of wine samples and loadings of significant (A) RATA attributes ($p < 0.1$) and (B) volatile compounds ($p < 0.05$) on PC1 and PC3.

*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, and mouthfeel note, respectively. More details of sensory description notes can be found in Table S2. Sample 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.*