Supplementary material

Immagine che contiene testo, software, Software multimediale, Icona del computer

Descrizione generata automaticamenteFigure S1. Tasting sheet (miniaturised from size A4).

Immagine che contiene software, Software multimediale, Software per la grafica, schermata

Descrizione generata automaticamenteImmagine che contiene software, Software multimediale, schermata, Software per la grafica

Descrizione generata automaticamente



Table S1. Frequency of citation of aroma descriptors of all tasted wines (descriptors used in correspondence analysis are written in bold).

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | AL14 | AL17 | AL19 | AL22 | AR06 | AR10 | AR11 | AR15 | AR17 | PB06 | PB10 | PB12 | PB15 | PB20 | SB13 | SB16 | SB19 | SB21 | Total |
| **Mature Fruit** | 6 | 8 | 7 | 5 | 8 | 11 | 9 | 5 | 10 | 10 | 8 | 10 | 11 | 8 | 4 | 8 | 3 | 1 | 132 |
| **Floral** | 7 | 7 | 8 | 14 | 3 | 3 | 5 | 8 | 5 | 1 | 5 | 10 | 8 | 10 | 7 | 7 | 4 | 12 | 124 |
| **Fresh Fruit** | 7 | 8 | 9 | 17 | 0 | 1 | 4 | 8 | 3 | 1 | 10 | 5 | 8 | 10 | 8 | 4 | 0 | 12 | 115 |
| **Vegetal\_A** | 9 | 9 | 8 | 9 | 2 | 2 | 6 | 4 | 6 | 4 | 5 | 6 | 4 | 8 | 6 | 5 | 7 | 14 | 114 |
| **Spicy** | 5 | 7 | 3 | 4 | 7 | 3 | 4 | 5 | 5 | 5 | 4 | 4 | 3 | 8 | 6 | 5 | 3 | 6 | 87 |
| **Honey** | 0 | 5 | 2 | 4 | 12 | 9 | 3 | 7 | 9 | 10 | 4 | 3 | 4 | 3 | 3 | 2 | 4 | 0 | 84 |
| **Oak** | 8 | 5 | 6 | 3 | 6 | 6 | 9 | 4 | 3 | 3 | 3 | 4 | 2 | 5 | 4 | 2 | 1 | 0 | 74 |
| **Balsamic** | 9 | 5 | 4 | 2 | 9 | 7 | 5 | 5 | 7 | 7 | 0 | 2 | 1 | 1 | 2 | 1 | 3 | 4 | 74 |
| **Dried Fruit** | 1 | 3 | 1 | 2 | 12 | 9 | 5 | 3 | 2 | 6 | 3 | 4 | 3 | 2 | 2 | 4 | 5 | 2 | 69 |
| **Earthy** | 5 | 1 | 2 | 2 | 4 | 2 | 3 | 0 | 3 | 2 | 1 | 1 | 2 | 1 | 2 | 5 | 11 | 4 | 51 |
| Kerosene | 4 | 2 | 6 | 2 | 3 | 2 | 5 | 4 | 3 | 1 | 0 | 2 | 2 | 2 | 1 | 3 | 1 | 3 | 46 |
| WetStone | 3 | 3 | 4 | 2 | 2 | 2 | 5 | 4 | 0 | 2 | 1 | 0 | 0 | 3 | 6 | 4 | 3 | 2 | 46 |
| Straw | 1 | 1 | 3 | 1 | 3 | 2 | 1 | 4 | 1 | 3 | 1 | 2 | 1 | 1 | 3 | 2 | 3 | 2 | 35 |
| Chocolate | 0 | 0 | 0 | 1 | 4 | 3 | 1 | 0 | 2 | 5 | 3 | 1 | 2 | 0 | 1 | 1 | 3 | 0 | 27 |
| Tobacco | 0 | 1 | 0 | 0 | 1 | 1 | 2 | 0 | 1 | 5 | 1 | 1 | 3 | 2 | 1 | 2 | 3 | 0 | 24 |
| Total | 65 | 65 | 63 | 68 | 76 | 63 | 67 | 61 | 60 | 65 | 49 | 55 | 54 | 64 | 56 | 55 | 54 | 62 | 1102 |

Table S2. Frequency of citation of flavour descriptors of all tasted wines (descriptors used in correspondence analysis are written in bold).

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | AL14 | AL17 | AL19 | AL22 | AR06 | AR10 | AR11 | AR15 | AR17 | PB06 | PB10 | PB12 | PB15 | PB20 | SB13 | SB16 | SB19 | SB21 | Total |
| **Acidity** | 16 | 15 | 17 | 18 | 16 | 14 | 20 | 17 | 15 | 8 | 11 | 15 | 11 | 13 | 12 | 10 | 13 | 20 | 261 |
| **Minerality** | 10 | 8 | 15 | 9 | 6 | 6 | 10 | 9 | 8 | 4 | 5 | 8 | 9 | 6 | 9 | 5 | 4 | 8 | 139 |
| **Dryness** | 10 | 8 | 9 | 6 | 8 | 6 | 7 | 8 | 11 | 4 | 7 | 8 | 7 | 6 | 5 | 9 | 9 | 10 | 138 |
| **Saltiness** | 9 | 5 | 8 | 5 | 12 | 6 | 7 | 10 | 9 | 7 | 6 | 3 | 10 | 9 | 9 | 6 | 7 | 9 | 137 |
| **Bitterness** | 7 | 4 | 8 | 5 | 8 | 6 | 7 | 5 | 7 | 7 | 6 | 4 | 3 | 6 | 5 | 9 | 7 | 8 | 112 |
| **Smoothness** | 3 | 9 | 4 | 4 | 5 | 8 | 7 | 8 | 6 | 9 | 8 | 4 | 11 | 7 | 5 | 3 | 3 | 2 | 106 |
| **Sweetness** | 5 | 7 | 3 | 8 | 5 | 6 | 2 | 1 | 2 | 8 | 5 | 12 | 4 | 6 | 3 | 6 | 5 | 4 | 92 |
| **Vegetal\_F** | 7 | 5 | 5 | 4 | 3 | 2 | 4 | 4 | 6 | 2 | 4 | 4 | 6 | 8 | 6 | 3 | 6 | 11 | 90 |
| **Sourness** | 3 | 3 | 4 | 4 | 7 | 2 | 6 | 2 | 4 | 6 | 4 | 3 | 1 | 4 | 4 | 5 | 11 | 5 | 78 |
| Viscosity | 2 | 4 | 2 | 4 | 4 | 4 | 3 | 5 | 4 | 5 | 7 | 2 | 4 | 3 | 2 | 3 | 4 | 3 | 65 |
| Umami | 5 | 3 | 1 | 0 | 6 | 5 | 3 | 3 | 3 | 3 | 4 | 3 | 3 | 2 | 1 | 2 | 3 | 1 | 51 |
| Astringency | 1 | 2 | 4 | 3 | 6 | 3 | 4 | 3 | 2 | 3 | 2 | 2 | 3 | 2 | 2 | 1 | 3 | 2 | 48 |
| Total | 78 | 73 | 80 | 70 | 86 | 68 | 80 | 75 | 77 | 66 | 69 | 68 | 72 | 72 | 63 | 62 | 75 | 83 | 1317 |

Table S3. Frequency of citation of wines clustered according to their sensory descriptors.

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Wines | Freshness | | | | | |  | Austere | | | | | |  | Mellowed | | | | | |  | Acidity |
| Vegetal\_A | Vegetal\_F | Spicy | Sweetness | Floral | FreshFruit |  | Smoothness | Bitterness | Dryness | Saltiness | Minerality | MatureFruit |  | Oak | Balsamic | Honey | DriedFruit | Earthy | Sourness |  | Acidity |
| AL14 | 9 | 7 | 5 | 5 | 7 | 7 |  | 3 | 7 | 10 | 9 | 10 | 6 |  | 8 | 9 | 0 | 1 | 5 | 3 |  | 16 |
| AL19 | 8 | 5 | 3 | 3 | 8 | 9 |  | 4 | 8 | 9 | 8 | 15 | 7 |  | 6 | 4 | 2 | 1 | 2 | 4 |  | 17 |
| AR11 | 6 | 4 | 4 | 2 | 5 | 4 |  | 7 | 7 | 7 | 7 | 10 | 9 |  | 9 | 5 | 3 | 5 | 3 | 6 |  | 20 |
|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| AR15 | 4 | 4 | 5 | 1 | 8 | 8 |  | 8 | 5 | 8 | 10 | 9 | 5 |  | 4 | 5 | 7 | 3 | 0 | 2 |  | 17 |
| AR17 | 6 | 6 | 5 | 2 | 5 | 3 |  | 6 | 7 | 11 | 9 | 8 | 10 |  | 3 | 7 | 9 | 2 | 3 | 4 |  | 15 |
| PB10 | 5 | 4 | 4 | 5 | 5 | 10 |  | 8 | 6 | 7 | 6 | 5 | 8 |  | 3 | 0 | 4 | 3 | 1 | 4 |  | 11 |
| PB15 | 4 | 6 | 3 | 4 | 8 | 8 |  | 11 | 3 | 7 | 10 | 9 | 11 |  | 2 | 1 | 4 | 3 | 2 | 1 |  | 11 |
| PB20 | 8 | 8 | 8 | 6 | 10 | 10 |  | 7 | 6 | 6 | 9 | 6 | 8 |  | 5 | 1 | 3 | 2 | 1 | 4 |  | 13 |
| SB13 | 6 | 6 | 6 | 3 | 7 | 8 |  | 5 | 5 | 5 | 9 | 9 | 4 |  | 4 | 2 | 3 | 2 | 2 | 4 |  | 12 |
| AL17 | 9 | 5 | 7 | 7 | 7 | 8 |  | 9 | 4 | 8 | 5 | 8 | 8 |  | 5 | 5 | 5 | 3 | 1 | 3 |  | 15 |
|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| SB16 | 5 | 3 | 5 | 6 | 7 | 4 |  | 3 | 9 | 9 | 6 | 5 | 8 |  | 2 | 1 | 2 | 4 | 5 | 5 |  | 10 |
| PB12 | 6 | 4 | 4 | 12 | 10 | 5 |  | 4 | 4 | 8 | 3 | 8 | 10 |  | 4 | 2 | 3 | 4 | 1 | 3 |  | 15 |
| AL22 | 9 | 4 | 4 | 8 | 14 | 17 |  | 4 | 5 | 6 | 5 | 9 | 5 |  | 3 | 2 | 4 | 2 | 2 | 4 |  | 18 |
|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| PB06 | 4 | 2 | 5 | 8 | 1 | 1 |  | 9 | 7 | 4 | 7 | 4 | 10 |  | 3 | 7 | 10 | 6 | 2 | 6 |  | 8 |
| AR10 | 2 | 2 | 3 | 6 | 3 | 1 |  | 8 | 6 | 6 | 6 | 6 | 11 |  | 6 | 7 | 9 | 9 | 2 | 2 |  | 14 |
| AR06 | 2 | 3 | 7 | 5 | 3 | 0 |  | 5 | 8 | 8 | 12 | 6 | 8 |  | 6 | 9 | 12 | 12 | 4 | 7 |  | 16 |
|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| SB21 | 14 | 11 | 6 | 4 | 12 | 12 |  | 2 | 8 | 10 | 9 | 8 | 1 |  | 0 | 4 | 0 | 2 | 4 | 5 |  | 20 |

Table S4. Standard wine physical-chemical analysis.

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Wines | Alcoholic strength (% v/v) | Total acidity (g/L) | Volatile acidity (g/L) | Residual sugar  (g/L) | Malic acid (g/L) | Lactic acid (g/L) | pH | Total SO2  (mg/L) | Free SO2  (mg/L) |
| AL14 | 13.5 | 5.7 | 0.25 | 1.1 | 1.9 | Nda | 3.39 | 110 | 5 |
| AL17 | 14.2 | 4.5 | 0.38 | 1.6 | 1.8 | Nd | 3.77 | 116 | 4 |
| AL19 | 13.4 | 6.3 | 0.33 | 1.5 | 1.7 | Nd | 3.42 | 94 | 2 |
| AL22 | 12.5 | 6.7 | 0.30 | 1.4 | 2.5 | Nd | 3.40 | 112 | 6 |
| AR06 | 13.6 | 5.1 | 0.30 | 3.5 | 1.6 | 0.3 | 3.41 | 81 | 18 |
| AR10 | 13.9 | 5.8 | 0.30 | 4.3 | 1.4 | 0.1 | 3.33 | 80 | 7 |
| AR11 | 14.0 | 5.9 | 0.24 | 4.4 | 1.4 | 0.2 | 3.36 | 99 | 17 |
| AR15 | 14.5 | 5.9 | 0.33 | 4.6 | 1.3 | Nd | 3.34 | 62 | 16 |
| AR17 | 13.8 | 6.3 | 0.33 | 1.9 | 1.2 | 0.2 | 3.25 | 123 | 30 |
| PB06 | 11.3 | 6.4 | 0.15 | 8.8 | 1.7 | 0.3 | 3.13 | 56 | 2 |
| PB10 | 13.2 | 6.0 | 0.28 | 10.9 | 1.6 | Nd | 3.25 | 72 | 2 |
| PB12 | 12.8 | 6.0 | 0.23 | 1.8 | 1.2 | Nd | 2.98 | 26 | 2 |
| PB15 | 12.7 | 6.6 | 0.24 | 1.8 | 1.7 | Nd | 3.07 | 54 | 2 |
| PB20 | 11.9 | 5.4 | 0.26 | 2.3 | 1.2 | Nd | 3.12 | 35 | 2 |
| SB13 | 12.2 | 5.7 | 0.33 | 5.8 | 2.2 | Nd | 3.45 | 70 | 3 |
| SB16 | 12.8 | 5.6 | 0.30 | 6.3 | 1.6 | Nd | 3.31 | 91 | 6 |
| SB19 | 12.8 | 6.3 | 0.30 | 6.0 | 1.7 | Nd | 3.14 | 78 | 10 |
| SB21 | 12.6 | 6.1 | 0.33 | 7.4 | 1.0 | 0.1 | 3.06 | 91 | 21 |

a Not detected.

Table S5. Pearson coefficients of correlation among standard physical-chemical analysis.

|  | | Age | | pH | | Ethanol | | Total Acidity | | Volatile Acidity | | Malic Acid | | Lactic Acid | | Sugar | | Total SO2 | | Free SO2 | |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Age |  | — |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| pH |  | 0.004 |  | — |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| Ethanol |  | 0.058 |  | 0.521 | \* | — |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| Total Acidity |  | -0.187 |  | -0.580 | \* | -0.349 |  | — |  |  |  |  |  |  |  |  |  |  |  |  |  |
| Volatile Acidity |  | -0.494 | \* | 0.579 | \* | 0.531 | \* | -0.378 |  | — |  |  |  |  |  |  |  |  |  |  |  |
| Malic Acid |  | -0.055 |  | 0.498 | \* | -0.221 |  | 0.106 |  | 0.050 |  | — |  |  |  |  |  |  |  |  |  |
| Lactic Acid |  | 0.592 | \*\* | -0.065 |  | -0.020 |  | -0.007 |  | -0.343 |  | -0.238 |  | — |  |  |  |  |  |  |  |
| Sugar |  | 0.361 |  | -0.251 |  | -0.289 |  | 0.114 |  | -0.194 |  | -0.129 |  | 0.207 |  | — |  |  |  |  |  |
| Total SO2 |  | -0.275 |  | 0.637 | \*\* | 0.468 |  | -0.091 |  | 0.511 | \* | 0.307 |  | 0.118 |  | -0.200 |  | — |  |  |  |
| Free SO2 |  | -0.074 |  | -0.023 |  | 0.442 |  | 0.035 |  | 0.326 |  | -0.455 |  | 0.514 | \* | -0.014 |  | 0.445 |  | — |  |
| Note: \* p < .05, \*\* p < .01. | | | | | | | | | | | | | | | | | | | | | |
|  | | | | | | | | | | | | | | | | | | | | | |

Table S6. Polyphenolic and Cielab determinations.

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Wines | TPI | HA (mg/L) | Abs420 | L\* | a\* | b\* | C\* | H\* |
| AL14 | 12.3 | 69 | 0.369 | 93.22 | -1.11 | 26.13 | 26.31 | 96.87 |
| AL17 | 11.2 | 70 | 0.187 | 95.66 | -1.04 | 15.68 | 15.76 | 96.63 |
| AL19 | 11.5 | 73 | 0.151 | 97.37 | -0.99 | 11.59 | 11.68 | 96.43 |
| AL22 | 9.9 | 53 | 0.109 | 98.40 | -0.73 | 7.04 | 7.14 | 96.14 |
| AR06 | 11.3 | 42 | 0.381 | 95.20 | -2.01 | 22.58 | 22.63 | 96.95 |
| AR10 | 12.1 | 61 | 0.323 | 95.94 | -1.40 | 16.55 | 16.67 | 96.62 |
| AR11 | 8.3 | 41 | 0.243 | 96.12 | -1.42 | 16.56 | 16.69 | 96.61 |
| AR15 | 9.0 | 65 | 0.143 | 96.31 | -1.48 | 15.80 | 15.86 | 96.52 |
| AR17 | 9.0 | 65 | 0.111 | 96.10 | -1.46 | 16.51 | 16.57 | 96.59 |
| PB06 | 12.8 | 48 | 0.390 | 97.60 | -1.12 | 9.86 | 10.04 | 96.30 |
| PB10 | 10.4 | 58 | 0.258 | 96.96 | -1.39 | 12.05 | 12.17 | 96.44 |
| PB12 | 10.2 | 64 | 0.232 | 97.09 | -1.38 | 12.15 | 12.26 | 96.42 |
| PB15 | 9.9 | 52 | 0.216 | 97.94 | -1.55 | 10.33 | 10.43 | 96.20 |
| PB20 | 10.2 | 46 | 0.214 | 97.83 | -1.26 | 8.28 | 8.34 | 96.03 |
| SB13 | 12.3 | 69 | 0.172 | 96.77 | -1.83 | 16.65 | 16.78 | 96.72 |
| SB16 | 11.0 | 69 | 0.234 | 95.58 | -1.98 | 21.19 | 21.29 | 96.86 |
| SB19 | 11.4 | 73 | 0.166 | 96.63 | -1.60 | 15.39 | 15.52 | 96.56 |
| SB21 | 10.0 | 69 | 0.092 | 97.34 | -1.03 | 8.33 | 8.42 | 96.33 |

TPI, Total polyphenolic index; HA, Hydroxycinnamic Acid; Abs420, Absorbance at 420 nm.

|  | | Age | | TPI | | HA | | A420 | | L\* | | a\* | | b\* | | C\* | | H\* | |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Age |  | — |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| TPI |  | 0.283 |  | — |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| HA |  | -0.395 |  | 0.272 |  | — |  |  |  |  |  |  |  |  |  |  |  |  |  |
| A420 |  | 0.816 | \*\*\* | 0.645 | \*\* | -0.313 |  | — |  |  |  |  |  |  |  |  |  |  |  |
| L\* |  | -0.309 |  | -0.293 |  | -0.311 |  | -0.462 |  | — |  |  |  |  |  |  |  |  |  |
| a\* |  | -0.257 |  | 0.149 |  | 0.260 |  | -0.064 |  | -0.097 |  | — |  |  |  |  |  |  |  |
| b\* |  | 0.381 |  | 0.236 |  | 0.259 |  | 0.467 |  | -0.947 | \*\*\* | 0.129 |  | — |  |  |  |  |  |
| C\* |  | 0.383 |  | 0.239 |  | 0.258 |  | 0.470 | \* | -0.947 | \*\*\* | 0.130 |  | 1.000 | \*\*\* | — |  |  |  |
| H\* |  | 0.416 |  | 0.208 |  | 0.314 |  | 0.376 |  | -0.868 | \*\*\* | 0.142 |  | 0.941 | \*\*\* | 0.941 | \*\*\* | — |  |
| \* p < .05, \*\* p < .01, \*\*\* p < .001 | | | | | | | | | | | | | | | | | | | |
|  | | | | | | | | | | | | | | | | | | | |

Table S7. Pearson coefficients of correlation among spectrophotometric and CIElab colour determinations.

Table S8. Elemental composition of the analysed wines (mg/L).

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Wines | Na | K | Ca | Mg | P | S | Fe | Cu | Zn | Mn | B | Pb | Cr | Ni | Cd |
| AL14 | 13.34 | 754.79 | 81.87 | 67.95 | 154.23 | 197.91 | 1.48 | 0.08 | 0.57 | 1.34 | 2.23 | 0.008 | 0.056 | 0.0009 | 0.000007 |
| AL17 | 14.96 | 667.07 | 72.12 | 68.35 | 121.55 | 231.67 | 0.75 | 0.09 | 0.53 | 1.56 | 1.93 | 0.012 | 0.044 | 0.0011 | 0.000002 |
| AL19 | 11.34 | 464.33 | 53.68 | 54.71 | 119.17 | 172.81 | 0.58 | 0.08 | 0.46 | 1.38 | 1.97 | 0.016 | 0.044 | 0.0009 | 0.000009 |
| AL22 | 8.44 | 436.75 | 49.00 | 53.28 | 104.12 | 128.27 | 0.24 | 0.09 | 0.36 | 1.32 | 1.74 | 0.000 | 0.037 | 0.0011 | 0.000011 |
| AR06 | 55.29 | 605.95 | 67.87 | 96.76 | 113.91 | 209.19 | 0.66 | 0.53 | 0.71 | 1.70 | 3.48 | 0.052 | 0.049 | 0.0199 | 0.000004 |
| AR10 | 35.43 | 527.74 | 46.72 | 81.11 | 138.24 | 138.02 | 0.60 | 0.16 | 0.62 | 1.10 | 3.16 | 0.004 | 0.046 | 0.0008 | 0.000001 |
| AR11 | 33.52 | 393.87 | 30.93 | 49.68 | 109.28 | 81.99 | 0.37 | 0.13 | 0.47 | 0.64 | 2.17 | 0.017 | 0.049 | 0.0009 | 0.000013 |
| AR15 | 37.69 | 471.92 | 66.73 | 91.57 | 147.52 | 176.58 | 0.65 | 0.30 | 0.63 | 1.54 | 2.46 | 0.043 | 0.066 | 0.0008 | 0.000007 |
| AR17 | 26.22 | 500.19 | 32.53 | 41.01 | 111.69 | 101.02 | 0.40 | 0.87 | 0.29 | 0.89 | 2.19 | 0.034 | 0.048 | 0.0007 | 0.000008 |
| PB06 | 17.42 | 751.73 | 49.58 | 67.39 | 199.78 | 190.05 | 0.68 | 0.11 | 0.70 | 1.02 | 4.04 | 0.015 | 0.041 | 0.0014 | 0.000409 |
| PB10 | 14.08 | 625.62 | 46.95 | 70.06 | 216.26 | 174.11 | 0.42 | 0.08 | 0.48 | 0.88 | 3.94 | 0.004 | 0.044 | 0.0015 | 0.000002 |
| PB12 | 15.03 | 708.67 | 53.67 | 70.01 | 237.83 | 223.53 | 0.56 | 0.15 | 0.60 | 0.89 | 3.91 | 0.001 | 0.039 | 0.0013 | 0.000006 |
| PB15 | 13.03 | 627.09 | 54.92 | 73.64 | 234.42 | 177.28 | 0.69 | 0.09 | 0.45 | 0.73 | 3.78 | 0.014 | 0.036 | 0.0013 | 0.000668 |
| PB20 | 13.01 | 658.97 | 53.24 | 69.39 | 208.56 | 216.96 | 0.63 | 0.12 | 0.59 | 0.98 | 3.78 | 0.012 | 0.042 | 0.0010 | 0.000006 |
| SB13 | 28.76 | 841.25 | 71.81 | 70.65 | 156.29 | 218.96 | 0.61 | 0.07 | 0.58 | 0.70 | 4.12 | 0.007 | 0.042 | 0.0007 | 0.000003 |
| SB16 | 61.97 | 1014.58 | 51.45 | 72.27 | 184.37 | 228.71 | 1.00 | 0.08 | 0.61 | 0.53 | 5.37 | 0.021 | 0.049 | 0.0008 | 0.000004 |
| SB19 | 37.54 | 883.18 | 58.00 | 73.26 | 158.46 | 311.71 | 0.66 | 0.18 | 0.49 | 0.62 | 5.72 | 0.002 | 0.045 | 0.0007 | 0.000007 |
| SB21 | 41.20 | 834.30 | 66.86 | 72.77 | 155.06 | 191.83 | 0.82 | 0.08 | 0.52 | 0.65 | 5.07 | 0.012 | 0.053 | 0.0006 | 0.000079 |

Table S9. Concentration of volatile molecules of the analysed wines (mg/L) (value 0 corresponds to non-detected molecules).

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Molecules | AL22 | AL19 | AL17 | AL14 | AR17 | AR15 | AR11 | AR10 | AR06 | PB20 | PB15 | PB12 | PB10 | PB06 | SB21 | SB19 | SB16 | SB13 |
| 3-Methylhexan-2-ol | 0 | 1.01 | 0.79 | 0.58 | 0 | 0 | 0.4 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0.52 | 0.3 | 0 | 0 |
| 2,3-Butane diol | 0.93 | 1.27 | 0 | 0 | 0.56 | 0.58 | 0 | 0 | 0.16 | 0.87 | 0.91 | 0.49 | 0 | 0 | 0 | 0 | 0.4 | 0.5 |
| 4-Methyl-1-pentanol | 0.07 | 0 | 0 | 0 | 0.08 | 0.05 | 0 | 0 | 0.04 | 0.07 | 0.06 | 0.05 | 0.06 | 0.07 | 0 | 0 | 0.05 | 0.05 |
| 2-Hexanol | 0 | 0 | 0 | 0 | 0 | 0 | 0.09 | 0 | 0 | 0 | 0 | 0 | 0.15 | 0 | 0.08 | 0 | 0 | 0 |
| 3-Methylpentanol | 0 | 0.16 | 0.2 | 0.25 | 0.09 | 0.09 | 0.1 | 0 | 0.06 | 0.23 | 0.18 | 0.13 | 0 | 0.11 | 0 | 0.11 | 0.16 | 0.14 |
| Cis-3-esen-1-olo | 0.2 | 0 | 0 | 0 | 0.28 | 0.23 | 0.27 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 1-Hexanol | 2.52 | 2.72 | 2.72 | 2.87 | 4.28 | 3.95 | 3.85 | 3.05 | 2.13 | 1.73 | 1.82 | 1.65 | 2.04 | 1.92 | 0.86 | 0.96 | 1.11 | 1.77 |
| 3-Methyl-2-pentanol | 0.01 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0.02 | 0 | 0 | 0 | 0 |
| Hexadecan-2-ol | 0.01 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0.01 | 0.01 | 0.01 | 0 | 0.01 | 0 | 0 | 0 | 0 | 0 |
| 2,4-dimethylpentan-3-ol | 0 | 0 | 0 | 0 | 0.04 | 0 | 0.03 | 0 | 0 | 0 | 0 | 0 | 0 | 0.03 | 0 | 0 | 0 | 0 |
| Methanol benzene | 0.03 | 0 | 0 | 0 | 1.72 | 0 | 1.09 | 1.04 | 0.11 | 0.11 | 0.07 | 0.1 | 0 | 0 | 0 | 0 | 0.08 | 0 |
| 2-ethylhexanol | 0.03 | 0.05 | 0 | 0 | 0 | 0 | 0.03 | 0 | 0.03 | 0.03 | 0.02 | 0.02 | 0.03 | 0 | 0.05 | 0 | 0.01 | 0.08 |
| 1-octanol | 0 | 0 | 0.17 | 0.33 | 0.08 | 0 | 0.07 | 0 | 0.05 | 0.04 | 0.03 | 0.04 | 0 | 0 | 0 | 0 | 0.08 | 0.04 |
| Ethanol benzene | 36.53 | 27.73 | 25.72 | 23.63 | 34.2 | 24.66 | 29.1 | 22.71 | 46.84 | 36.78 | 27.07 | 24.34 | 21.02 | 19.44 | 39.07 | 36.36 | 35.34 | 25.72 |
| 3-methylbutan-1-olo | 0.79 | 0 | 0 | 0 | 1 | 0.39 | 1 | 0 | 0.72 | 1.01 | 0.67 | 0.47 | 0 | 0 | 0.66 | 0.01 | 0.53 | 1.01 |
| Ethyl butyrate | 0.14 | 0.76 | 1.29 | 1.48 | 0.98 | 0.13 | 1.02 | 1.12 | 0 | 0.48 | 0.07 | 0.06 | 0.75 | 0.66 | 0.48 | 0.38 | 0.34 | 1.1 |
| Lactic acid, ethyl ester | 0 | 1.16 | 1.39 | 1.63 | 0.97 | 1.02 | 0.56 | 0 | 0.53 | 3.68 | 0.36 | 0.37 | 3.94 | 10.36 | 0.74 | 0.48 | 0.35 | 0.98 |
| Ethyl isovalerate | 0.08 | 0 | 0 | 0 | 0 | 0 | 0.29 | 0 | 0 | 0.28 | 0.18 | 0 | 0 | 0.39 | 0 | 0 | 0 | 0 |
| Isoamyl acetate | 9.96 | 0.26 | 0.26 | 0.12 | 3.27 | 0.38 | 0.75 | 0.16 | 0 | 0.96 | 0.3 | 0.09 | 0.15 | 0 | 0.21 | 0.21 | 0.1 | 0.1 |
| Ethyl 3-hydroxybutanoate | 0.04 | 0.04 | 0 | 0 | 0 | 0.03 | 0.03 | 0 | 0 | 0.04 | 0.03 | 0.02 | 0.03 | 0 | 0 | 0 | 0.02 | 0.04 |
| Methyl pentanoate | 0.02 | 0.02 | 0 | 0 | 0.01 | 0.01 | 0 | 0 | 0.01 | 0.01 | 0.01 | 0.01 | 0.01 | 0.01 | 0 | 0 | 0.01 | 0.01 |
| Ethyl hexanoate | 4.78 | 3.55 | 4.54 | 4.34 | 3.18 | 3.39 | 2.69 | 2.53 | 1.44 | 1.76 | 1.48 | 2.06 | 3.15 | 2.87 | 2.08 | 1.87 | 1.72 | 4.04 |
| Ethyl 2-amino-3-methylbutanoate | 0.04 | 0 | 0 | 0 | 0.11 | 0.14 | 0.06 | 0 | 0.07 | 0.05 | 0.06 | 0.07 | 0.07 | 0 | 0.08 | 0 | 0.05 | 0.18 |
| 2-methylpentyl acetate | 0.74 | 0 | 0 | 0 | 0.12 | 1.58 | 0.02 | 0 | 0 | 0 | 0.01 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Ethyl 2-furancarboxylate | 0.04 | 0.2 | 0.29 | 0.12 | 0.09 | 0.29 | 0.07 | 0.12 | 0.07 | 0.1 | 0.09 | 0.06 | 0.16 | 0 | 0.1 | 0.09 | 0.06 | 0.3 |
| Ethyl 2-hydroxy-4-methylvalerate | 0.31 | 0.18 | 0.27 | 0.14 | 0.14 | 0.28 | 0.19 | 0.2 | 0.24 | 0.13 | 0.1 | 0.14 | 0.16 | 0.2 | 0.11 | 0.12 | 0.07 | 0.19 |
| Isopentyl lactate | 0.15 | 0.05 | 0 | 0 | 0.06 | 0 | 0.02 | 0 | 0.03 | 0.14 | 0.08 | 0.07 | 0.12 | 0.5 | 0 | 0 | 0.02 | 0 |
| Diethyl succinate | 4.49 | 20.85 | 26.56 | 31.3 | 20.52 | 24.66 | 37.26 | 43.06 | 24.76 | 28.62 | 42.62 | 44.12 | 41.22 | 42.86 | 28.28 | 29.55 | 36.11 | 26.82 |
| Ethyl octanoate | 2.76 | 1.64 | 1.72 | 1.43 | 1.88 | 1.47 | 1.39 | 1.17 | 0.87 | 1.11 | 0.97 | 1.19 | 1.81 | 1.28 | 0 | 0.86 | 0.93 | 2.23 |
| Benzyl acetate | 0.05 | 0 | 0 | 0 | 0 | 0.16 | 0.07 | 0 | 0.04 | 0.06 | 0.08 | 0.07 | 0.05 | 0 | 0.09 | 0 | 0.04 | 0.03 |
| Diethyl 2-hydroxybutanedioate | 0.93 | 11.52 | 6.8 | 5.5 | 1.84 | 6.47 | 1.73 | 0 | 3.06 | 1.9 | 4.18 | 5.48 | 5.29 | 1.22 | 8.09 | 8.13 | 6.85 | 7.35 |
| Dimethyl, 2-hydroxy-2-mehtylbutane-1,4-dioate | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0.1 | 0.1 | 0 | 0.04 | 0 | 0 | 0 | 0 | 0 |
| Isobutyl succinate | 0.04 | 0 | 0 | 0 | 0 | 0 | 0.03 | 0 | 0 | 0 | 0.06 | 0 | 0.04 | 0.04 | 0 | 0 | 0 | 0.02 |
| Diethyl glutarate | 0.05 | 0.16 | 0.17 | 0.24 | 0.09 | 0.21 | 0.13 | 0.16 | 0.08 | 0.19 | 0.32 | 0.21 | 0.17 | 0.13 | 0.24 | 0 | 0.19 | 0.07 |
| Methyl 2,2-dimethyl-6-oxoheptanoate | 0.03 | 0 | 0 | 0 | 0.05 | 0.04 | 0.05 | 0.05 | 0.09 | 0.05 | 0 | 0.06 | 0.17 | 0.03 | 0 | 0 | 0.08 | 0.03 |
| Ethyl 3-hydroxytridecanoate | 0.21 | 0.18 | 0 | 0 | 0.05 | 0.24 | 0.13 | 0.13 | 0.13 | 0.13 | 0.16 | 0.18 | 0.1 | 0.06 | 0.1 | 0 | 0.2 | 0.25 |
| Diethyl tartrate. | 0.01 | 0.07 | 0 | 0 | 0 | 0.03 | 0.01 | 0.01 | 0 | 0 | 0 | 0.04 | 0.05 | 0.04 | 0 | 0 | 0.07 | 0 |
| Diethyl 2-hydroxyglutarate | 0.16 | 0.6 | 0.42 | 0.65 | 0.55 | 0.58 | 0.34 | 0.57 | 0.33 | 0.53 | 0.65 | 0.65 | 0.5 | 0.43 | 0.46 | 0.67 | 0.31 | 0.48 |
| Ethyl decanoate | 0.14 | 0 | 0 | 0 | 0.14 | 0.07 | 0.04 | 0 | 0 | 0.13 | 0.05 | 0.07 | 0.11 | 0.07 | 0 | 0 | 0.08 | 0.06 |
| Ethyl 3-methylbutylbutanedioate | 0.03 | 0.07 | 0 | 0 | 0.13 | 0.09 | 0.17 | 0.2 | 0.13 | 0.17 | 0.19 | 0.21 | 0.15 | 0.13 | 0.12 | 0 | 0.14 | 0.09 |
| Ethyl 2-hydroxy-3-phenylpropanoate | 0.23 | 0.23 | 0.24 | 0.23 | 0.24 | 0.27 | 0.25 | 0.2 | 0.28 | 0.36 | 0.25 | 0.35 | 0.25 | 0.28 | 0.2 | 0 | 0.16 | 0.22 |
| Ethyl linoleate | 0.06 | 0 | 0.34 | 0 | 0.04 | 0.09 | 0.08 | 0.19 | 0.2 | 0.07 | 0.11 | 0.17 | 0.17 | 0.2 | 0.18 | 0 | 0.22 | 0.31 |
| Ethyl 2-amino-3-phenylpropanoate | 0.04 | 0 | 0 | 0 | 0.13 | 0 | 0.04 | 0 | 0.1 | 0.05 | 0.05 | 0.05 | 0.09 | 0.1 | 0.11 | 0 | 0 | 0.21 |
| Dimethyl benzene-1,3-dicarboxylate | 0.03 | 0 | 0 | 0 | 0.02 | 0.02 | 0.01 | 0 | 0.01 | 0.02 | 0.02 | 0.01 | 0 | 0 | 0 | 0 | 0.02 | 0.03 |
| Triethyl citrate | 0 | 0.07 | 0.1 | 0 | 0 | 0.08 | 0.03 | 0.16 | 0.04 | 0.02 | 0.02 | 0.05 | 0.07 | 0 | 0.13 | 0.04 | 0.33 | 0.44 |
| Methyl 4-hydroxycinnamate | 0 | 0.11 | 0 | 0 | 0.09 | 0 | 0.1 | 0 | 0.08 | 0 | 0 | 0.11 | 0 | 0 | 0 | 0 | 0.11 | 0 |
| Methyl 4-cyanobenzoate | 0.08 | 0 | 0 | 0 | 0 | 0.13 | 0.07 | 0 | 0.01 | 0.07 | 0 | 0.06 | 0 | 0 | 0.73 | 0.86 | 0 | 0 |
| Ethyl coumarate | 0.24 | 0.63 | 0 | 0 | 0.55 | 0 | 0.39 | 0.12 | 0.59 | 0 | 0 | 0.64 | 0 | 0 | 0 | 0.73 | 0.45 | 0 |
| Methyl palmitate | 0.04 | 0.1 | 0 | 0 | 0.11 | 0.1 | 0.05 | 0.08 | 0.08 | 0.08 | 0.056 | 0 | 0.09 | 0 | 0.06 | 0.03 | 0.05 | 0.06 |
| 2,3-dihydroxypropyl hexadecanoate | 0.06 | 0.12 | 0 | 0 | 0 | 0.07 | 0.15 | 0.09 | 0.07 | 0.07 | 0.05 | 0.04 | 0 | 0 | 0.05 | 0 | 0.04 | 0.11 |
| Leucine, ethyl ester | 0.45 | 0.68 | 0.54 | 0.65 | 0.84 | 1.08 | 0.3 | 0.37 | 0.35 | 0.36 | 0.52 | 0.44 | 0.57 | 0 | 0 | 0 | 0.14 | 1.13 |
| Methyl 2,5-dihydroxybenzoate | 0.09 | 0 | 0 | 0 | 0.12 | 0.1 | 0.08 | 0.07 | 0 | 0.01 | 0.01 | 0.01 | 0 | 0 | 0 | 0 | 0.03 | 0 |
| Dimethyl sulphide | 2.22 | 0 | 0 | 0 | 0.14 | 0 | 0.3 | 0 | 0.11 | 0 | 1.86 | 1.92 | 0 | 0 | 0.17 | 0 | 0 | 0.66 |
| Methionol | 0.12 | 0 | 0 | 0 | 0.14 | 0.03 | 0.11 | 0.13 | 0 | 0 | 0.11 | 0.15 | 0 | 0 | 0.16 | 0.1 | 0 | 0.14 |
| Benzaldehyde | 0 | 0 | 0 | 0 | 0.16 | 0.17 | 0.42 | 0 | 0 | 0 | 0 | 0.01 | 0.03 | 0.07 | 0 | 0 | 0.01 | 0 |
| 4-methylbenzaldehyde | 0.31 | 0.23 | 0 | 0 | 0.11 | 0.07 | 0.03 | 0 | 0.07 | 0.01 | 0.08 | 0.11 | 0.11 | 0.23 | 0.14 | 0.11 | 0.05 | 0.13 |
| 2-propenal, 3-(2,6,6-trimethyl-1-cyclohexen-1-yl) | 0.22 | 0.72 | 1.02 | 1.32 | 0.09 | 0.26 | 0.22 | 0.54 | 0.61 | 0.2 | 0.32 | 0.46 | 0.49 | 0.52 | 0.56 | 0.61 | 0.61 | 0.84 |
| L-serine | 0.03 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0.11 | 0.04 | 0.07 | 0.1 | 0.13 | 0 | 0.07 | 0 | 0.08 | 0.14 |
| Iso leucine | 0.13 | 0 | 0 | 0 | 0 | 0.43 | 0.24 | 0 | 0.16 | 0.14 | 0.16 | 0.17 | 0 | 0.25 | 0 | 0 | 0.07 | 0 |
| Cystathionine | 0 | 0.12 | 0 | 0 | 0 | 0.04 | 0.04 | 0 | 0.07 | 0.02 | 0.04 | 0.07 | 0 | 0 | 0 | 0 | 0.09 | 0.1 |
| Tryptophane | 0 | 0.03 | 0 | 0 | 0 | 0 | 0.11 | 0 | 0 | 0 | 0.01 | 0.02 | 0 | 0 | 0 | 0.07 | 0.04 | 0 |
| 3-hydroxy-2-pentanone | 0.04 | 0.05 | 0 | 0 | 0 | 0 | 0 | 0 | 0.03 | 0.04 | 0.03 | 0.02 | 0.04 | 0 | 0 | 0 | 0.03 | 0.04 |
| 3-acetyl-2,4-dimethylpyrrole | 0.02 | 0 | 0 | 0 | 0 | 0.03 | 0.07 | 0 | 0.04 | 0.01 | 0.02 | 0.04 | 0 | 0 | 0 | 0 | 0.03 | 0 |
| 2-tetradecylbenzeneacetic acid. | 0.04 | 0 | 0 | 0 | 0 | 0 | 0.06 | 0 | 0.05 | 0.08 | 0.04 | 0.03 | 0.06 | 0 | 0 | 0 | 0 | 0.07 |
| Campholonic acid | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0.02 | 0 | 0 | 0 | 0 | 0.09 | 0.28 |
| Diethyl-2-hydroxy-2-methylbutanedoic acid | 4.08 | 0 | 0.29 | 0.23 | 0.7 | 0.08 | 0.1 | 0 | 0.06 | 0.25 | 0.09 | 0.13 | 0.16 | 0.25 | 0.13 | 0 | 0.24 | 0 |
| Palmitic acid | 0.02 | 0.03 | 0 | 0 | 0 | 0.03 | 0.25 | 0.03 | 0.02 | 0.03 | 0.02 | 0.01 | 0 | 0 | 0.02 | 0 | 0.01 | 0.04 |
| 3-methylbutanoic acid | 0.15 | 0 | 0 | 0 | 0.31 | 0.37 | 0.31 | 0 | 0.25 | 0 | 0.22 | 0.22 | 0.36 | 0 | 0 | 0.34 | 0.23 | 0.46 |
| Oleanolic acid | 0 | 0.03 | 0 | 0 | 0 | 0.03 | 0.09 | 0 | 0.03 | 0.03 | 0.02 | 0 | 0 | 0 | 0 | 0 | 0.01 | 0.05 |
| Stearic acid | 0.03 | 0.04 | 0 | 0 | 0 | 0.07 | 0.04 | 0 | 0.02 | 0.02 | 0.01 | 0.01 | 0 | 0 | 0.01 | 0 | 0 | 0 |
| Caprinic acid | 2.5 | 1.67 | 1.01 | 0.56 | 0.33 | 0.22 | 0.65 | 0.38 | 0.42 | 0.61 | 0.42 | 0.46 | 0.45 | 0.22 | 0.38 | 0.43 | 0.62 | 0.96 |
| Caprylic acid | 1 | 0.04 | 0.43 | 0 | 0.19 | 0.02 | 0.18 | 0.17 | 0.11 | 0.22 | 0.17 | 0.18 | 0.43 | 0 | 0.28 | 0 | 0.12 | 0.44 |
| 2-methoxy-4-vinylphenol | 0.32 | 0.06 | 0 | 0 | 0 | 0.08 | 0.03 | 0 | 0.02 | 0.02 | 0.02 | 0.03 | 0 | 0 | 0 | 0 | 0.05 | 0.05 |
| Tyrosol | 0.07 | 0.08 | 0 | 0 | 0 | 0 | 0.02 | 0 | 0.08 | 0.01 | 0.04 | 0.08 | 0 | 0.01 | 0.07 | 0 | 0.08 | 0.04 |
| 3,5-dimethylphenol | 0 | 0 | 0 | 0 | 0 | 0 | 0.02 | 0 | 0 | 0 | 0 | 0 | 4.31 | 0 | 0 | 0 | 0.03 | 0 |
| 3,4-dimethylphenol | 9.72 | 6.7 | 7.05 | 6.6 | 6.94 | 7.08 | 4.7 | 4.92 | 5.32 | 4.18 | 5.5 | 4.7 | 0 | 0 | 4 | 4.74 | 4.55 | 6.19 |
| 2,5-dimethylphenol | 0 | 0 | 0 | 0 | 0.1 | 0 | 0.1 | 0 | 0 | 0 | 0 | 0 | 0 | 4.48 | 0 | 0 | 0 | 0 |
| Linalool | 0.06 | 0.12 | 0 | 0 | 0 | 0.08 | 0 | 0 | 0.05 | 0.4 | 0.03 | 0.04 | 0.04 | 0 | 0 | 0 | 0.08 | 0.1 |
| Vitispirane | 0.03 | 0.15 | 0.14 | 0.23 | 0 | 0.03 | 0.06 | 0.17 | 0.17 | 0.01 | 0 | 0.01 | 0 | 0 | 0 | 0 | 0.08 | 0.11 |
| Ascaridole | 0.05 | 0.04 | 0 | 0 | 0.05 | 0 | 0.04 | 0 | 0.06 | 0 | 0 | 0.02 | 0 | 0 | 0 | 0 | 0.02 | 0.03 |
| Curvulol | 0.04 | 0 | 0 | 0 | 0.06 | 0.04 | 0.03 | 0 | 0 | 0.02 | 0.02 | 0.02 | 0.02 | 0 | 0 | 0 | 0.07 | 0.08 |
| 4-nitrophthalimide | 0 | 0 | 0 | 0 | 0 | 0 | 0.01 | 0 | 0 | 0 | 0 | 0 | 0.01 | 0 | 0 | 0 | 0 | 0.02 |
| Gamma-undecalactone | 0.01 | 0 | 0 | 0 | 0 | 0.03 | 0.02 | 0 | 0 | 0.03 | 0.06 | 0 | 0 | 0 | 0 | 0 | 0.07 | 0.21 |
| 2-ethyl-1-[(4-methylphenyl) sulfonyl] azetidin-3-one | 0.17 | 0 | 0 | 0 | 0.17 | 0.09 | 0.04 | 0 | 0.07 | 0.07 | 0.13 | 0.16 | 0 | 0 | 0.06 | 0 | 0.07 | 0.12 |
| 5,7-dimethoxy-2,2-dimethylchromene | 7.52 | 0 | 7.33 | 7.32 | 6.73 | 7.55 | 4.79 | 4.35 | 4.21 | 5.77 | 4.4 | 4.24 | 5.12 | 4.68 | 4.91 | 4.41 | 3.69 | 6.72 |
| 6-chloro-n-ethyl-1,3,5-triazine-2,4-diamine | 0.03 | 0.05 | 0 | 0 | 0.05 | 0.05 | 0.04 | 0 | 0 | 0.04 | 0.03 | 0.04 | 0 | 0 | 0.05 | 0 | 0.03 | 0.09 |
| Dihydroxy vitamin d2 | 0 | 0 | 0 | 0 | 0 | 0.07 | 0.04 | 0 | 0 | 0 | 0.01 | 0 | 0 | 0 | 0.04 | 0 | 0.05 | 0 |
| 1,3,5-cycloheptatriene-1-methanol | 0 | 0 | 0 | 0 | 0 | 0 | 0.07 | 0 | 0 | 0.01 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |

Table S10. Pearson correlation coefficients between wine age and volatile molecules analysed by GC-MS using a polar column.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Chemical families | Volatile moleculesa | Alvarinho | Arinto | Pinot Bianco | Sauvignon Blanc |
| Alcohols | 2,3-Butanediol | -0.760 | -0.764 | -0.886\* | 0.951\* |
|  | 3-Methylpentanol | 0.952\* | -0.464 | -0.731 | 0.804 |
|  | 1-Hexanol | 0.965\* | -0.933\* | 0.554 | 0.931 |
|  | Ethanol benzene | -0.936 | 0.474 | -0.966\*\* | -0.927 |
|  | 3-methylbutan-1-ol | -0.792 | -0.198 | -0.954\* | 0.566 |
| Esters | Ethyl butyrate | 0.970\* | -0.288 | 0.383 | 0.707 |
|  | Ethyl hexanoate | -0.143 | -0.938\* | 0.779 | 0.724 |
|  | Ethyl octanoate | -0.873 | -0.961\*\* | 0.490 | 0.946 |
|  | **Isoamyl acetate** | **-0.800** | **-0.743** | **-0.909\*** | **-0.907** |
|  | **Diethyl succinate** | **0.957\*** | **0.393** | **0.761** | **0.032** |
|  | Diethyl glutarate | 0.971\* | -0.309 | -0.498 | -0.317 |
|  | Ethyl decanoate | -0.792 | -0.912\* | 0.421 | 0.820 |
|  | Methyl 2,2-dimethyl-6-oxoheptanoate | -0.792 | 0.783 | 0.225 | 0.574 |
|  | **Ethyl linoleate** | **0.061** | **0.870** | **0.973\*\*** | **0.671** |
|  | Dimethyl benzene-1,3-dicarboxylate | -0.792 | -0.705 | -0.901\* | 0.968\* |
|  | 2,3-dihydroxypropyl hexadecanoate | -0.621 | 0.500 | -0.935\* | 0.691 |
|  | Methyl 2,5-dihydroxybenzoate | -0.792 | -0.956\* | -0.796 | 0.238 |
| Aldehides | 4-methylbenzaldehide | -0.914 | -0.502 | 0.957\* | -0.242 |
|  | **2-propenal, 3-(2,6,6-trimethyl-1-cyclohexen-1-yl)** | **0.992\*** | **0.884\*** | **0.963\*\*** | **0.884** |
| Ketones | 3-hydroxy-2-pentanone | -0.791 | 0.750 | -0.714 | 0.959\* |
| Acids | Palmitic acid | -0.726 | 0.153 | -0.960\*\* | 0.599 |
|  | Oleanolic acid | -0.198 | 0.236 | -0.905\* | 0.900 |
|  | Caprinic acid | -0.988\* | 0.445 | -0.892\* | 0.970\* |
|  | Stearic acid | -0.768 | -0.148 | -0.941\* | -0.714 |
| Phenols | 3,4-dimethylphenol | -0.811 | -0.778 | -0.734 | 0.887 |
|  | 5,7-dimethoxy-2,2-dimethylchromene | 0.175 | -0.880\* | -0.501 | 0.519 |
| Terpenes | Linalool | -0.621 | 0.053 | -0.823 | 0.951\* |
| Terpenoids | Ascaridole | -0.904 | 0.245 | 0.064 | 0.968\* |
| Tetrahydrofurans | Vitispirane | 0.951\* | 0.904\* | -0.589 | 0.962\* |
| Other | Curvulol | -0.792 | -0.922\* | -0.700 | 0.936 |

a Bold font indicates that molecules were used in Multifactorial Analysis.

\* p < .05, \*\* p < .01.

Figure S2. Projection plan of the set of variables in the Multiple Factorial Analysis, when age perception was used as one of the sets of variables.

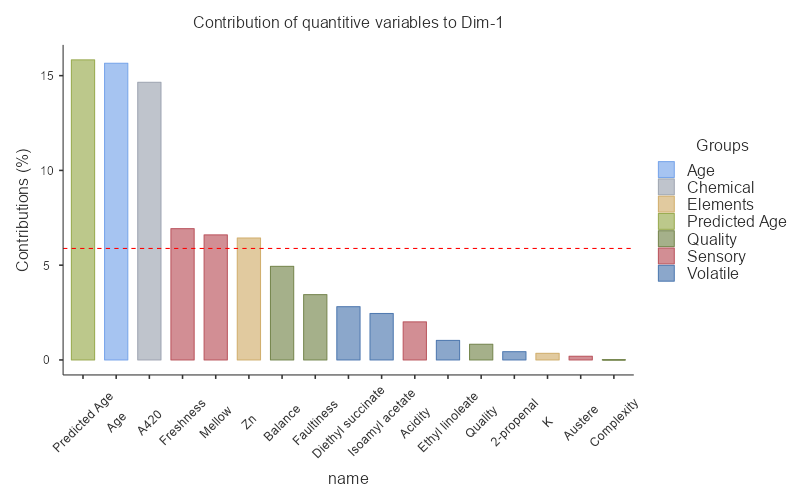


Age perception

Predicted Age

Figure S3. Contribution of quantitative variables to dimensions 1 (a) and 2 (b). The expected average contribution is indicated by a dashed red line.

(a)



(b)

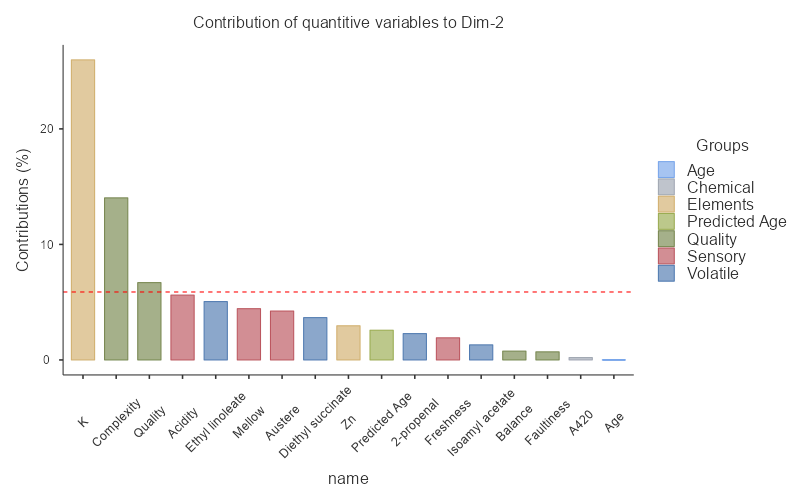


Figure S4. Projection plan of the set of variables in the Multiple Factorial Analysis, when grape was used as one of the sets of variables.

