Supplementary material

Figure S1. Tasting sheet (miniaturised from size A4).



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.

