Data Article

Data on changes in red wine phenolic compounds, headspace aroma compounds and sensory profile after treatment of red wines with activated carbons with different physicochemical characteristics

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A B S T R A C T

Data in this article presents the changes on phenolic compounds, headspace aroma composition and sensory profile of a red wine spiked with 4-ethylphenol and 4-ethylguaiacol and treated with seven activated carbons with different physicochemical characteristics, namely surface area, micropore volume and mesopore volume ("Reduction of 4-ethylphenol and 4-ethylguaiacol in red wine by activated carbons with different physicochemical characteristics: impact on wine quality" Filipe-Ribeiro et al. (2017) [1]). Data on the physicochemical characteristics of the activated carbons are shown. Statistical data on the sensory expert panel consistency by General Procrustes Analysis is shown. Statistical data is also shown, which correlates the changes in chemical composition of red wines with the physicochemical characteristics of activated carbons used.

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### Value of the data

- Data from this research highlights the effect of the physicochemical characteristics of activated carbons on the phenolic, headspace aroma and sensory profile of wines spiked with 4-ethylphenol and 4-ethylguaiacol.
- We analysed the phenolic profile by RP-HPLC and the aroma compounds by HS-SPME-GC/MS in red wines treated with activated carbons presenting different physicochemical characteristics and the results were analysed by principal component analysis for highlighting relations between chemical composition of red wines and physicochemical characteristics of activated carbons.
- Activated carbons removal efficiency of red wine ethylphenols was related to their surface area and micropore volume.
- High surface area of mesopores and total pore volume were important for the anthocyanin removal and decrease in colour intensity.
- This data could serve as a benchmark for other researchers, evidencing the influence of activated carbons treatment on the individual phenolic, chromatic and aroma compounds and sensory profile of red wine.

### 1. Data

The data reported includes information about the adsorption isotherms of activated carbons (ACs) (Fig. 1), metal composition of activated carbons (Table 1) and surface group chemistry of activated carbons (Fig. 2 and Table 2). Also the sensory profile of wines (Fig. 3a) and consistency of the sensory panel scores were analysed by General Procrustes Analysis (GPA) (Fig. 3b and Table 3) and the scaling factor of each expert were determined (Table 4). The headspace aroma profile of red wines before and...
Fig. 1. Adsorption isotherms (N₂, –196 °C) of activated carbons; → adsorption; ← desorption.
after treatment with activated carbons were determined (Table 5) and the reduction of total aroma compounds and reduction of each class of chemical compounds were calculated (Fig. 4). The head-space aroma compounds decrease and structural characteristics of each aroma compound were correlated (Table 6 and Fig. 5). The phenolic composition (total phenols, flavonoid phenols, non-flavonoid phenols, total anthocyanins) and colour properties (colour intensity, hue and chromatic characteristics) of treated and untreated wines were determined (Table 7). The phenolic profile of wines were determined by RP-HPLC that included the phenolic acids and flavonoids (Table 8) and monomeric anthocyanins (Table 9). The relation between aroma abundance and the activated carbons physicochemical characteristics were analysed by principal component analysis (Fig. 6a) and between the phenolic compounds content and activated carbons physicochemical characteristics (Fig. 6b).

2. Experimental design, materials and methods

2.1. Wine sample

A red wine from Douro Valley (vintage 2013) was used in this work, their main characteristics were follows: alcohol content 13.4% (v/v), specific gravity (20 °C) 0.9921 g/mL, titratable acidity 5.1 g/L expressed as tartaric acid, pH 3.84, volatile acidity 0.50 g/L expressed as acetic acid.

2.2. Analysis of conventional oenological parameters

Alcohol, specific gravity, pH, titratable acidity and volatile acidity were analysed using a FTIR Bacchus Micro (Microderm, France).

Table 1
Metal composition of activated carbons ashes.

| Samples | Calcium (mg/g) | Iron (mg/g) | Magnesium (mg/g) | Potassium (mg/g) | Sodium (mg/g) | Copper (µg/g) | Aluminium (µg/g) |
|---------|----------------|-------------|------------------|------------------|---------------|---------------|-----------------|
| C1      | 1.64 ± 0.11b   | 0.21 ± 0.01c | 1.64 ± 0.09d    | 1.22 ± 0.06b    | 152 ± 0.07e   | n.d.          | n.d.            |
| C2      | 4.78 ± 0.09e   | 1.68 ± 0.01f | 3.12 ± 0.03e    | 0.82 ± 0.04e    | 1.03 ± 0.08d  | n.d.          | n.d.            |
| C3      | 6.02 ± 0.22f   | 0.04 ± 0.01a | 1.06 ± 0.01a    | 0.72 ± 0.05a    | 0.96 ± 0.01f  | 0.66 ± 0.66b  | n.d.            |
| C4      | 0.92 ± 0.08a   | 0.60 ± 0.02e | 1.44 ± 0.05f    | 4.96 ± 0.13e    | 0.56 ± 0.05e  | 0.70 ± 0.70bc | n.d.            |
| C5      | 2.94 ± 0.04c   | 0.12 ± 0.01b | 1.25 ± 0.01b    | 3.89 ± 0.18d    | 0.51 ± 0.04e  | 0.77 ± 0.77c  | n.d.            |
| C6      | 4.08 ± 0.05d   | 0.28 ± 0.03d | 1.77 ± 0.01d    | 1.92 ± 0.08e    | 0.79 ± 0.07b  | 0.76 ± 0.76c  | 85797 ± 8.46    |
| C7      | 5.26 ± 0.16c   | 1.28 ± 0.01ab| 1.18 ± 0.02ab   | 0.58 ± 0.011    | 0.70 ± 0.03ab | n.d.          | n.d.            |

Values are presented as mean ± standard deviation. Means within a column followed by the same letter are not significantly different ANOVA and Tuckey post-hoc test (p < 0.05); n.d. – not detected.
### Table 2
Assignment of FTIR bands of activated carbons main functional groups [2–4].

| Wavenumber (cm⁻¹) | Vibration Assignment | Functional Group                  |
|-------------------|----------------------|-----------------------------------|
| ~ 1731            | C=O stretching       | Carboxylic acids and carboxylic anhydrides and lactones |
| ~ 1637            | C=O stretching       | Quinone and keto-enol groups      |
| ~ 1590            | C=C stretching       | Aromatic                          |
| ~ 1466            | O-H bend             | Carboxyl-carbonate structures     |
| ~ 1122            | C-O stretching       | Ethers                            |
| ~ 1054            | C-O(H) stretching    | Phenolic groups                   |
| ~ 649             | C-C stretching       |                                   |

**Fig. 3.**
a) Sensory profile of volatile phenols free (T0) and volatile phenols spiked (TF) red wines and wines treated with the seven ACs (C1–C7); Consensus configuration for red wines treated with ACs with different physicochemical properties for removing 4-Ethylphenol and 4-Ethylguaiacol and sensory attributes; b) projection of wine samples and clouds for the first two dimensions and c) projection of sensory attributes on the first and second dimensions of Generalised Procrustes Analysis [5].
2.3. Experimental design

The addition of 4-ethylphenol and 4-ethylguaiacol was carried out on the red wine sample at the highest concentrations found in literature, 1500 $\mu$g/L for 4-ethylphenol and 300 $\mu$g/L for 4-ethylguaiacol (4-EP1500 and 4-EG300) [18] and were also prepared at medium level of contamination with 750 $\mu$g/L of 4-ethylphenol and 150 $\mu$g/L of 4-ethylguaiacol (4-EP750 and 4-EG150). Seven solid commercial activated carbons, characterized by [1], were used: C1 (powder), C2 (powder), C3 (powder), C4 (powder), C5 (powder), C6 (granulated) and C7 (powder). The activated carbons were next added at 100 (g/ hl) maximum dosage authorized [19] to the wine placed in 250 mL graduated cylinders. After 6 days the wines were removed from graduated cylinders and then were centrifuged at 10,956 $g$, 10 min at 20 °C in order to be analysed. All the assays and analyses were performed in duplicate.

2.4. Colour and total anthocyanins

Colour intensity and hue was determined by measuring absorbance at 420 nm, 520 nm and 620 nm (1 mm cell) according to [20]. The content of total anthocyanins was determined according to [21].

2.5. Chromatic characterization

The chromatic characteristics of wines calculated using the CIELab method according to [20]. The colour difference was calculated using the following equation: $\Delta E^*=[(\Delta L^*)^2+(\Delta a^*)^2+(\Delta b^*)^2]^{1/2}$. 

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**Table 3**

| Source                                | DF | SS    | MS  | F   | P       |
|---------------------------------------|----|-------|-----|-----|---------|
| Residuals after scaling               | 160| 41.48 | 0.259|     | <0.0001 |
| Scaling                               | 5  | 10.06 | 2.012| 7.759|         |
| Residuals after rotation              | 165| 51.54 | 0.312|     |         |
| Rotation                              | 275| 82.76 | 0.301| 1.161| 0.150   |
| Residuals after translation           | 440| 134.31| 0.305|     |         |
| Translation                           | 55 | 147.59| 2.683| 10.349| <0.0001 |
| Corrected total                       | 495| 281.900| 0.570|     |         |

DF = Degrees of freedom.

**Table 4**

Scaling factors of experts for each configuration after GPA [5] of the sensory aromatic, taste and tactile/textural attributes data of volatile phenols free (T0) and volatile phenols spiked (TF) red wine and after treatment with different activated carbons (C1 to C7).

| Object   | Factor |
|----------|--------|
| Expert 1 | 0.8448 |
| Expert 2 | 0.7695 |
| Expert 3 | 0.9335 |
| Expert 4 | 1.0430 |
| Expert 5 | 1.2248 |
| Expert 6 | 1.8165 |
| Compounds                      | ID | RI calculated | MW (g/mol) | Odour descriptor | ODT (mg/L) | T0       | TF       | C1       | C2       | C3       | C4       | C5       | C6       | C7       |
|-------------------------------|----|---------------|------------|-----------------|-------------|----------|----------|----------|----------|----------|----------|----------|----------|----------|
| Ethyl acetate                 | ... | 728           | 715        | 88.11           |             |          |          |          |          |          |          |          |          |          |
| 2-Methylpropan-1-ol           | ... | 1118.5        | 1114       | 74.12           |             |          |          |          |          |          |          |          |          |          |
| 3-Methylbutan-1-ol acetate    | std | 1200          | 1126       | 130.18          |             |          |          |          |          |          |          |          |          |          |
| 3-Methylbutan-1-ol acetate    | std | 1223.3        | 1223       | 88.15           |             |          |          |          |          |          |          |          |          |          |
| Ethyl hexanoate               | std | 1235.1        | 1238       | 144.21          |             |          |          |          |          |          |          |          |          |          |
| Ethyl octanoate               | std | 1436.2        | 1436       | 172.27          |             |          |          |          |          |          |          |          |          |          |
| Ethyl decanoate               | std | 1638.1        | 1640       | 200.32          |             |          |          |          |          |          |          |          |          |          |
| Diethyl succinate             | std | 1682          | 1698       | 174.19          |             |          |          |          |          |          |          |          |          |          |
| Phenylethyl acetate           | std | 1809.9        | 1833       | 164.2           |             |          |          |          |          |          |          |          |          |          |
| Hexanoic acid                 | std | 1841.7        | 1857       | 116.16          |             |          |          |          |          |          |          |          |          |          |
| 2-Phenylethanol               | std | 1912.7        | 1911       | 122.16          |             |          |          |          |          |          |          |          |          |          |
| 4-Ethylguaiacol               | std | 1987          | 1989       | 152.18          |             |          |          |          |          |          |          |          |          |          |
| Octanoic acid                 | std | 2031.6        | 2030       | 144.21          |             |          |          |          |          |          |          |          |          |          |
| 4-Ethylphenol                 | std | 2084          | 2142       | 122.16          |             |          |          |          |          |          |          |          |          |          |
| Decanoic acid                 | ... | 2143          | 2196       | 172.27          |             |          |          |          |          |          |          |          |          |          |
| Dodecanoic acid               | std | 2254          | 2156       | 200.32          |             |          |          |          |          |          |          |          |          |          |

Results expressed in absolute area (area*10^5). Values are presented as mean ± standard deviation; $ ID – Identification; std – Standard; * RI (retention index) from: [6–8]. MW (molecular weight). ODT (olfactory detection threshold). Odour descriptor from: [9–11]. Means within a column followed by the same letter are not significantly different ANOVA and Tuckey post-hoc test (p < 0.05). n.d., not detected; volatile phenols free (T0) and volatile phenols spiked (TF) red wines and wines treated with seven activated carbons, C1 to C7.
2.6. Quantification of non-flavonoids, flavonoids and total phenols

The phenolic content of the wines was quantified using the absorbance at 280 nm before and after precipitation of the flavonoid phenols, through reaction with formaldehyde, according to [22]. The results were expressed as gallic acid equivalents by means of calibration curves with standard gallic acid. The total phenolic content was also determined by a spectrophotometric method, using a UV–vis spectrophotometer according to [23].
Fig. 5. Correlation between fractions of headspace aroma average content of wines treated with activated carbons with a) molecular weight of aroma compounds; b) Log P of aroma compounds; c) polarizability of aroma compounds; d) McGowan characteristic volume.
Table 7
Total phenols, flavonoid phenols, non-flavonoid phenols, total anthocyanins and chromatic properties of red wines spiked with volatile phenols (TF) and after treatment with activated carbons with different physicochemical characteristics (C1–C7).

| Samples | Total phenols (mg/L gallic acid) | Flavonoid phenols (mg/L gallic acid) | Non-flavonoid phenols (mg/L gallic acid) | Total anthocyanins (mg/L) | Colour intensity A.U. | Hue | L* | a* | b* | ΔE* |
|---------|----------------------------------|--------------------------------------|------------------------------------------|--------------------------|-----------------------|-----|-----|-----|-----|------|
| TF      | 2023 ± 2d                        | 1623 ± 14c                          | 416 ± 23c                                | 354 ± 5.6c               | 9.5 ± 0.23d           | 0.71 ± 0.01a | 11.9 ± 0.5a | 42.47 ± 0.66a | 38.53 ± 0.18a | -    |
| C1      | 1808 ± 0h                        | 1493 ± 14a                          | 315 ± 7c                                 | 337 ± 3.7h               | 9.0 ± 0.15c           | 0.72 ± 0.02a | 12.3 ± 0.0a  | 42.83 ± 0.09a | 38.88 ± 0.18a | 0.74 ± 0.53a |
| C2      | 1870 ± 7c                        | 1510 ± 24b                          | 360 ± 16b                                | 324 ± 11.8b              | 8.8 ± 0.23c           | 0.70 ± 0.01a | 12.6 ± 0.0a  | 43.18 ± 0.14a | 38.67 ± 0.23a | 1.10 ± 0.94b |
| C3      | 1745 ± 19a                       | 1413 ± 33a                          | 332 ± 14a                                | 281 ± 0.0a               | 7.3 ± 0.08a           | 0.73 ± 0.00a | 16.6 ± 0.3a  | 47.33 ± 0.35d | 38.78 ± 0.04a | 6.78 ± 1.25d |
| C4      | 1858 ± 9g                        | 1537 ± 09h                          | 322 ± 00a                                | 346 ± 10.5c              | 9.4 ± 0.36d           | 0.68 ± 0.02a | 11.7 ± 0.5a  | 42.16 ± 0.71a | 38.48 ± 0.70a | 0.49 ± 0.07a |
| C5      | 1817 ± 7c                        | 1505 ± 07h                          | 312 ± 14a                                | 310 ± 14.2a              | 8.3 ± 0.02b,c         | 0.70 ± 0.01a | 13.9 ± 0.2b  | 44.62 ± 0.31b | 38.93 ± 0.30a | 3.02 ± 1.22c |
| C6      | 1825 ± 14c                       | 1487 ± 19a                          | 338 ± 05a                                | 311 ± 2.5a               | 8.1 ± 0.18b           | 0.71 ± 0.01a | 14.7 ± 0.1b  | 45.59 ± 0.08a | 39.51 ± 0.16a | 4.32 ± 0.91c |
| C7      | 1767 ± 16a                       | 1448 ± 16a                          | 318 ± 00a                                | 288 ± 4.9a               | 7.3 ± 0.11a           | 0.73 ± 0.00a | 16.4 ± 0.2c  | 47.24 ± 0.24d | 39.16 ± 0.04a | 6.51 ± 0.67d |

Values are presented as mean ± standard deviation; Means within a column followed by the same letter are not significantly different ANOVA and Tuckey post-hoc test ($p < 0.05$). L* - lightness, a* - redness, b* - yellowness, $\Delta E^*$ - colour difference. The values corresponding to $\Delta E^*$ were obtained taking as a reference the untreated wine (TF). A.U. – absorbance units, wines treated with seven activated carbons, C1 to C7.
| Samples | Gallic acid | Catechin | trans-Caftaric acid | GRP | Coutaric acid | Caffeic acid | Coumaric acid | Ferulic acid | Caffeic acid ethyl ester | Coumaric acid ethyl ester |
|---------|------------|----------|---------------------|-----|---------------|--------------|---------------|--------------|--------------------------|---------------------------|
| TF      | 9.92 ± 1.03a | 13.33 ± 0.94a | 31.70 ± 0.27b | 0.11 ± 0.00a | 12.14 ± 0.04a | 3.17 ± 0.19a | 3.96 ± 1.56b | 0.79 ± 0.06b | 1.06 ± 0.25b | 2.89 ± 0.03d |
| C1      | 5.69 ± 0.25a | 7.49 ± 3.72b | 27.91 ± 0.87b | 0.20 ± 0.06a | 9.72 ± 0.07a | 0.66 ± 0.09a | 0.62 ± 0.13a | 0.12 ± 0.01a | 0.10 ± 0.01a | 2.28 ± 0.01a |
| C2      | 6.28 ± 2.30a | 13.85 ± 0.05a | 29.95 ± 0.70a | 0.14 ± 0.04a | 11.22 ± 1.11b,c | 1.71 ± 0.10b | 1.23 ± 0.09a | 0.12 ± 0.01a | 0.16 ± 0.04a | 1.90 ± 0.07c |
| C3      | 6.28 ± 2.30a | 12.29 ± 0.05a | 29.64 ± 0.13a | 0.25 ± 0.11a | 10.79 ± 0.13b | 1.11 ± 0.09a | 0.84 ± 0.06a | 0.05 ± 0.01a | 0.03 ± 0.02a | 0.93 ± 0.01a |
| C4      | 6.28 ± 2.30a | 12.24 ± 0.21a | 29.68 ± 0.21a | 0.30 ± 0.05a | 10.56 ± 0.10b | 1.00 ± 0.01a | 0.46 ± 0.49a | 0.06 ± 0.01a | 0.09 ± 0.05a | 2.60 ± 0.02d |
| C5      | 6.28 ± 2.31a | 11.88 ± 0.21a | 29.64 ± 0.40a | 0.37 ± 0.25a | 10.51 ± 0.09b | 0.84 ± 0.05a | 0.27 ± 0.13a | 0.79 ± 0.04b | 0.03 ± 0.01a | 1.50 ± 0.07b |
| C6      | 6.28 ± 2.31a | 13.09 ± 0.08a | 30.83 ± 0.49a | 0.48 ± 0.14a | 10.98 ± 0.10b | 0.93 ± 0.02a | 0.10 ± 0.01a | 0.73 ± 0.07b | 0.09 ± 0.05a | 1.45 ± 0.01b |
| C7      | 6.28 ± 2.31a | 11.76 ± 0.10a | 29.67 ± 0.18a | 0.06 ± 0.09a | 10.23 ± 0.69b | 0.75 ± 0.14a | 0.07 ± 0.02a | 0.67 ± 0.06b | 0.02 ± 0.00a | 1.29 ± 0.42b |

Values are presented as mean ± standard deviation; Means within a column followed by the same letter are not significantly different ANOVA and Tuckey post-hoc test (p < 0.05). GRP - 2-S-glutathionyl caftaric acid.
### Table 9
Monomeric anthocyanin composition (mg/L) of red wines spiked with volatile phenols (TF) and after treatment with activated carbons with different physicochemical characteristics (C1–C7).

| Samples | Del-3-Glc | Cya-3-Glc | Pet-3-Glc | Peo-3-Glc | Mal-3-Glc | Del-3-AcGlc | Cya-3-AcGlc | Pet-3-AcGlc | Peo-3-AcGlc | Mal-3-AcGlc | Del-3-CoGlc | Cya-3-CoGlc | Pet-3-CoGlc | Peo-3-CoGlc | Mal-3-CoGlc |
|---------|-----------|-----------|-----------|-----------|-----------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|
| TF      | 1.00 ± 0.21a | 5.94 ± 0.07b | 10.64 ± 0.11c | 11.51 ± 0.11d | 59.28 ± 0.79e | 2.67 ± 0.35f | n.d.         | 0.11 ± 0.01g | 7.51 ± 0.15h | n.d.         | 0.06 ± 0.04i | n.d.         | 0.71 ± 0.06j | 9.02 ± 0.08k |
| C1      | 0.83 ± 0.14a | 5.23 ± 0.33ab | 9.15 ± 0.29d | 9.22 ± 0.58e | 52.48 ± 0.02b | 2.14 ± 0.08b | n.d.         | n.d.        | n.d.        | 6.64 ± 0.03b | n.d.         | n.d.         | n.d.         | 7.18 ± 0.29c |
| C2      | 0.95 ± 0.07a | 5.53 ± 0.90b | 8.95 ± 0.25c | 9.20 ± 0.74d | 51.16 ± 0.84e | 1.85 ± 0.06b | n.d.         | n.d.        | n.d.        | 6.08 ± 0.28b | n.d.         | n.d.         | n.d.         | 5.86 ± 0.48b |
| C3      | 0.97 ± 0.05a | 4.32 ± 0.31ab | 7.67 ± 0.05a | 8.65 ± 0.18b | 43.99 ± 0.30a | 0.97 ± 0.12a | n.d.         | n.d.        | n.d.        | 4.32 ± 0.18a | n.d.         | n.d.         | n.d.         | 2.48 ± 0.16c |
| C4      | 0.97 ± 0.14a | 5.57 ± 0.44b | 9.43 ± 0.20d | 9.75 ± 0.89e | 55.39 ± 2.49g | 2.14 ± 0.11b | n.d.         | n.d.        | n.d.        | 7.83 ± 0.91d | n.d.         | n.d.         | n.d.         | 8.77 ± 1.27c |
| C5      | 0.65 ± 0.07a | 4.47 ± 0.01h | 8.12 ± 0.09b | 7.97 ± 0.70b | 49.00 ± 0.99b | 1.43 ± 0.04b | n.d.         | n.d.        | n.d.        | 5.53 ± 0.27a | n.d.         | n.d.         | n.d.         | 4.16 ± 0.06c |
| C6      | 0.61 ± 0.08a | 4.22 ± 0.19b | 7.73 ± 0.32a | 8.27 ± 0.04c | 48.31 ± 0.19d | 1.00 ± 0.44c | n.d.         | n.d.        | n.d.        | 5.71 ± 0.39a | n.d.         | n.d.         | n.d.         | 4.04 ± 0.19c |
| C7      | 0.92 ± 0.15a | 3.68 ± 0.23a | 7.04 ± 0.43a | 7.44 ± 1.42d | 43.57 ± 1.21g | 0.91 ± 0.10a | n.d.         | n.d.        | n.d.        | 4.18 ± 0.24a | n.d.         | n.d.         | n.d.         | 2.64 ± 0.08c |

Values are presented as mean ± standard deviation; Del-3-Glc-Delphinidin-3-glucoside, Cya-3-Glc-Cyanidin-3-glucoside, Pet-3-Glc-Petunidin-3-glucoside, Peo-3-Glc-Peonidin-3-glucoside, Mal-3-Glc-Malvidin-3-glucoside, Del-3-AcGlc-Delphinidin-3-acetylglucoside, Cya-3-AcGlc-Cyanidin-3-acetylglucoside, Pet-3-AcGlc-Petunidin-3-acetylglucoside, Peo-3-AcGlc-Peonidin-3-acetylglucoside, Mal-3-AcGlc-Malvidin-3-acetylglucoside, Del-3-CoGlc-Delphinidin-3-coumaroylglucoside, Cya-3-CoGlc-Cyanidin-3-coumaroylglucoside, Pet-3-CoGlc-Petunidin-3-coumaroylglucoside, Peo-3-CoGlc-Peonidin-3-coumaroylglucoside, Mal-3-CoGlc-Malvidin-3-coumaroylglucoside. Means within a column followed by the same letter are not significantly different ANOVA and Tuckey post-hoc test (p<0.05).
2.7. High performance liquid chromatography (HPLC) analysis of anthocyanins and phenolic acids

Analyses were carried out with an Ultimate 3000 HPLC equipped with a PDA-100 photodiode array detector and an Ultimate 3000 pump according to [24]. Quantification was performed with calibration curves with standards caffeic acid, coumaric acid, ferulic acid, gallic acid and catechin. The results of trans-caftaric acid, 2-S-glutathionylcaftaric acid (GRP) and caffeic acid ethyl ester were expressed as caffeic acid equivalents by means of calibration curves with standard caffeic acid. On the other hand, coutaric acid, coutaric acid isomer and coumaric acid ethyl ester were expressed as coumaric acid equivalents by means of calibration curves with standard coumaric acid. A calibration curve of malvidin-3-glucoside, cyanidin-3-glucoside and peonidin-3-glucoside were used for quantification of anthocyanins. Using the coefficient of molar absorptivity ($\epsilon$) and by extrapolation, it was possible to obtain the slopes for delphinidin-3-glucoside, petunidin-3-glucoside, and malvidin-3-coumaroylglicoside and perform the quantification. The results of delphinidin-3-acetylglucoside, petunidin-3-acetylglucoside, peonidin-3-acetylglucoside, cyanidin-3-acetylglucoside and cyanidin-3-coumaroylglicoside were expressed as respective glucoside equivalents.
2.8. Determination of 4-EP and 4-EG by liquid-liquid extraction and GC–MS analysis

The extractions were carried out following and adapting the methodology described by [25].

2.9. Headspace wine aroma composition by solid phase microextraction (HS-SPME)

For the determination of the headspace aroma composition of red wines a validated method, confirmed in our laboratory was used [6].

2.10. Sensory evaluation

Sensory analysis was performed by a panel composed by six experts [26]. Fifteen attributes were selected: visual (limpidity, hue, colour intensity and oxidised), aroma (fruity, floral, vegetable character, phenolic and oxidised aroma) and taste and tactile/textural descriptors (taste–bitterness, acidity, tactile/textural–astringency, body, balance and persistence) using an adapted tasting sheet based on that recommended by the OIV [27]. The attributes were quantified using a five-point intensity scale [28]. Scales were anchored with the terms “low intensity” for score one and “high intensity” for score five, and panellists only scored integer values. All evaluations were conducted from 10:00 to 12:00 p.m. in an individual booth [29], using the recommended glassware according to [29]. A wine volume of 50 mL was used in order to be possible for the tasters to taste twice 25 mL of wine [30] and presented in random order [26].

2.11. Statistical treatment

Statistically significant differences between means were determined by analysis of variance (ANOVA) followed by Tukey honestly significant difference (HSD, 5% level) post-hoc test for the physicochemical data and a post-hoc Duncan test for sensory data. A principal component analyses was also performed to analyse the data and to study the relations between physicochemical ACs characteristics and wine volatile phenols removal and on phenolic and aromatic wine composition. These analyses were performed using Statistica 7 Software (StatSoft, Tulsa, OK U.S.A.). Generalised Procrustes Analysis [5] (GPA, XLSTAT-MX) of the sensory data was performed using XLSTAT (Addinsoft, Anglesey, UK). Multiple Factor Analysis (MFA, XLSTAT-RIB) of the sensory and chemical data were performed using XLSTAT (Addinsoft, Anglesey, UK).

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Transparency document. Supplementary material

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