

Supplementary data for the article:

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Supplementary Material

An insight into quality of Montenegrin *Vranac* red wine

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Supplementary Table 1. Basic parameters of the applied analytes for the analysis of the selected compounds.

| Analyzed compound | Retention time (min) | Molecular formula | ESI | Quantification transition | Cone voltage (V) | Collision energy (eV) |
|-------------------------|----------------------|--|-----|---------------------------|------------------|-----------------------|
| Gallic acid | 4.9 | C ₇ H ₆ O ₅ | - | 169→125 | 30 | 20 |
| Protocatechuic acid | 8.8 | C ₇ H ₆ O ₄ | - | 153→109 | 30 | 20 |
| 4-Hydroxy benzoic acid | 13.4 | C ₇ H ₆ O ₃ | - | 137→93 | 30 | 20 |
| Vanillic acid | 15.7 | C ₈ H ₈ O ₄ | + | 169→93 | 26 | 14 |
| Syringic acid | 17.0 | C ₉ H ₁₀ O ₅ | - | 197→182 | 28 | 14 |
| Ellagic acid | 25.1 | C ₁₄ H ₆ O ₈ | + | 303→89 | 50 | 56 |
| Caffeic acid | 16.9 | C ₉ H ₈ O ₄ | - | 179→135 | 30 | 20 |
| <i>p</i> -Coumaric acid | 23.1 | C ₉ H ₈ O ₃ | + | 165→91 | 22 | 22 |
| Ferulic acid | 24.8 | C ₁₀ H ₁₀ O ₄ | + | 195→145 | 20 | 16 |
| Vanillin | 20.9 | C ₈ H ₈ O ₃ | + | 153→93 | 26 | 16 |
| Siringaldehyde | 22.9 | C ₉ H ₁₀ O ₄ | + | 183→155 | 26 | 10 |
| Catechin | 14.5 | C ₁₅ H ₁₄ O ₆ | + | 291→139 | 26 | 20 |
| Epicatechin | 19.1 | C ₁₅ H ₁₄ O ₆ | + | 291→139 | 26 | 16 |
| Myricetin | 27.6 | C ₁₅ H ₁₀ O ₈ | + | 319→153 | 52 | 38 |
| Quercetin | 29.7 | C ₁₅ H ₁₀ O ₇ | - | 301→151 | 30 | 20 |
| Kaempferol | 31.4 | C ₁₅ H ₁₀ O ₆ | + | 287→153 | 56 | 36 |

Supplementary Table 2. Instrument operating conditions for determination of major elements by ICP-OES.

| | |
|-----------------------------------|--|
| Spectrometer | iCAP 6500 Thermo scientific |
| Nebulizer | Concentric |
| Spray chamber | Cyclonic |
| Radio frequency power (W) | 1150 |
| Principal argon flow rate (L/min) | 12 |
| Auxiliary argon flow rate (L/min) | 0.5 |
| Nebulizer flow rate (L/min) | 0.5 |
| Sample flow rate (ml/min) | 1 |
| Detector | CID86 |
| Selected wavelengths (nm) | Fe (259.9); Na (589.5); Ca (373.6); Mg (279.5); K (766.4) |

Supplementary Table 3. Measured isotopes and instrument operating conditions for determination of trace- and ultra-trace elements by ICP-MS.

| Elements | Measured isotope |
|------------------------|-------------------|
| Al | 27 |
| V | 51 |
| Cr | 53 |
| Mn | 55 |
| Co | 59 |
| Ni | 60 |
| Cu | 65 |
| Zn | 66 |
| As | 75 |
| Se | 82 |
| Ag | 109 |
| Cd | 112 |
| Sb | 121 |
| Ba | 138 |
| Tl | 205 |
| Pb | 208 |
| Rf power (W) | 1548 |
| Gas flows (L/min) | 13.90; 1.09, 0.80 |
| Acquisition time (sec) | 3 × 50 |
| Points per peak | 3 |
| Dwell time (msec) | 10 |
| Detector mode | Pulse |
| Replicates | 3 |

Supplementary Table 4. The contents of major and trace elements determined by ICP-OES or ICP-MS.

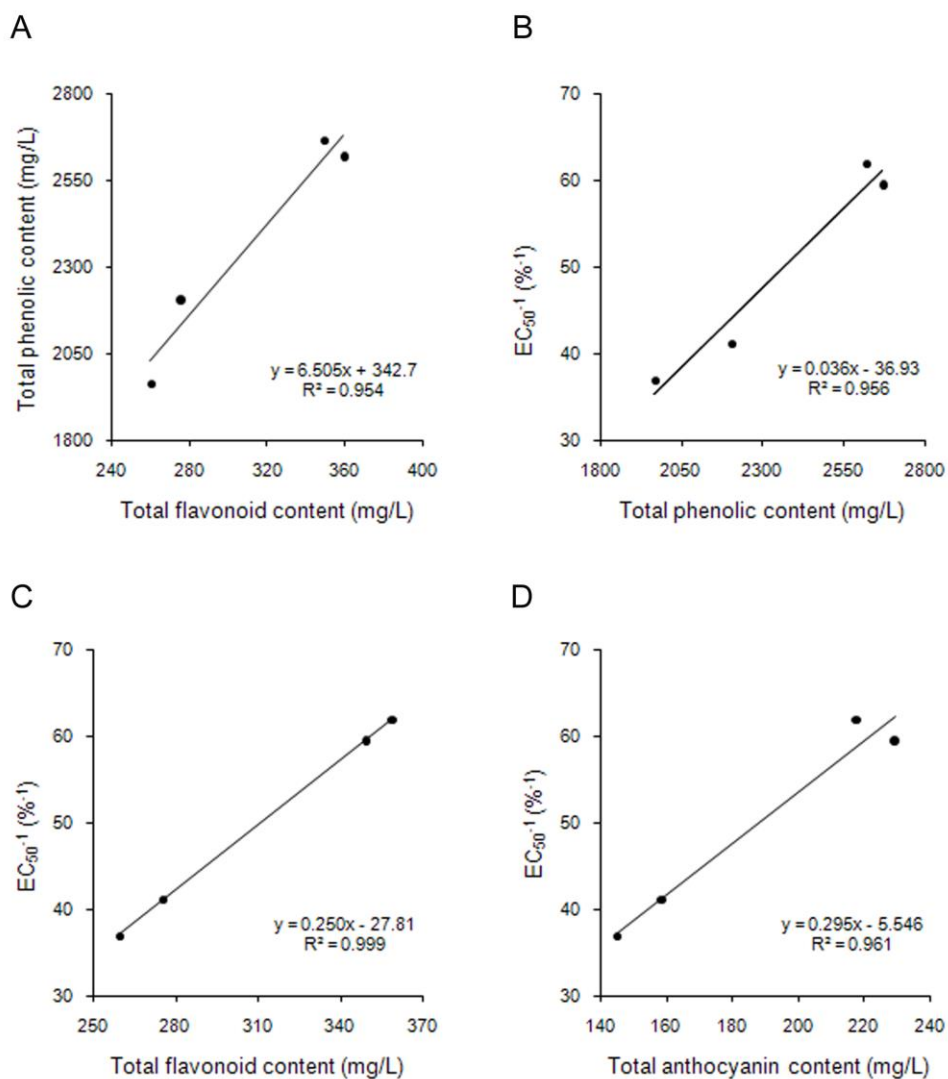
| Sample | MAJOR (mg/L) | | | | TRACE (µg/L) | | | | | |
|---------------|-----------------|------------|------------|------------|-----------------|-------------|-------------|-------------|-------------|-------------|
| | Ca | K | Mg | Na | Al | Fe | Mn | Zn | Cu | |
| BT | 57.1 ± 0.6 | 493 ± 5 | 41.4 ± 0.2 | 9.1 ± 0.3 | 530.6 ± 2.5 | 1041 ± 3 | 440.3 ± 0.4 | 551.7 ± 0.4 | 124.9 ± 1.6 | |
| Vranac | CI | 56.1 ± 0.4 | 523 ± 3 | 40.9 ± 0.2 | 11.4 ± 0.3 | 977.9 ± 1.2 | 1411 ± 3 | 441.5 ± 0.4 | 665.5 ± 0.6 | 543.5 ± 0.5 |
| | CII | 52.7 ± 0.4 | 416 ± 3 | 39.1 ± 0.3 | 9.9 ± 0.3 | 489.8 ± 0.7 | 933 ± 2 | 338.5 ± 0.4 | 473.4 ± 0.1 | 25.0 ± 0.7 |
| | CIII | 54.7 ± 0.3 | 452 ± 1 | 47.4 ± 0.2 | 9.7 ± 0.3 | 546.5 ± 0.5 | 941 ± 2 | 377.9 ± 0.2 | 559.3 ± 0.2 | 61.2 ± 0.4 |
| Maximum value | 57.1 | 523 | 47.4 | 11.4 | 1123.0 | 2346 | 667.1 | 3955.6 | 543.5 | |
| Minimum value | 52.7 | 416 | 39.1 | 9.1 | 328.3 | 933 | 338.5 | 473.4 | 25.0 | |
| Average value | 54.9 | 469 | 43.3 | 10.3 | 716.1 | 1370 | 464.6 | 1004.4 | 206.3 | |

BT bottled wine, CI clone I wine, CII clone II wine, CIII clone III wine. All values are represented as mean ± SD (three replications)

Supplementary Table 5. The content of ultratrace elements determined by ICP-MS.

| Sample | ULTRATRACE | | | | | | | | | | | |
|---------------|-------------|-------------|------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|------------|
| | (µg/L) | | | | | | | | | | | |
| | V | Cr | Ni | Co | As | Se | Cd | Sb | Ba | Tl | Pb | |
| BT | 0.86 ± 0.01 | 29.1 ± 0.2 | 17.6 ± 0.1 | 0.86 ± 0.00 | 0.03 ± 0.02 | 2.55 ± 0.02 | 0.14 ± 0.00 | 4.86 ± 0.03 | 27.6 ± 0.2 | 1.29 ± 0.00 | 17.7 ± 0.1 | |
| Vranac | CI | 1.68 ± 0.01 | 28.1 ± 0.2 | 34.2 ± 0.2 | 1.28 ± 0.00 | 0.50 ± 0.01 | 2.30 ± 0.20 | 0.43 ± 0.01 | 8.36 ± 0.03 | 62.0 ± 0.1 | 0.83 ± 0.01 | 81.1 ± 0.2 |
| | CII | 0.95 ± 0.02 | 36.0 ± 0.2 | 16.8 ± 0.1 | 0.61 ± 0.01 | ND | ND | 0.10 ± 0.00 | 4.88 ± 0.03 | 31.8 ± 0.2 | 1.09 ± 0.01 | 20.8 ± 0.2 |
| | CIII | 0.35 ± 0.01 | 42.3 ± 0.2 | 18.9 ± 0.1 | 0.71 ± 0.01 | 0.12 ± 0.01 | 1.00 ± 0.30 | 0.15 ± 0.01 | 6.12 ± 0.01 | 32.1 ± 0.2 | 1.02 ± 0.01 | 23.7 ± 0.1 |
| Maximum value | 1.68 | 42.3 | 34.2 | 1.28 | 0.12 | 2.55 | 0.43 | 8.36 | 62.0 | 1.29 | 81.1 | |
| Minimum value | 0.35 | 28.1 | 16.8 | 0.61 | ND | ND | 0.10 | 4.86 | 27.6 | 0.83 | 17.7 | |
| Average value | 1.01 | 35.2 | 25.5 | 0.95 | 0.06 | 1.27 | 0.26 | 6.61 | 44.8 | 1.06 | 49.4 | |

ND not detected, BT bottled wine, CI clone I wine, CII clone II wine, CIII clone III wine. All values are represented as mean ± SD (three replications)



Supplementary Figure 1. Correlation diagrams between: A – total phenolic and total flavonoid content ($R^2=0.954$); B – anti-DPPH \cdot activity (expressed as EC_{50}^{-1} value) and total phenolic content ($R^2=0.956$); C – anti-DPPH \cdot activity (expressed as EC_{50}^{-1} value) and total flavonoid content ($R^2=0.999$); D – anti-DPPH \cdot activity (expressed as EC_{50}^{-1} value) and monomeric anthocyanin content ($R^2=0.961$).