

Supplementary data for the article:

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## **Supplementary Material**

### **An insight into quality of Montenegrin *Vranac* red wine**

**N. Đorđević<sup>a</sup>, M. Novaković<sup>b</sup>, B. Pejin<sup>c,\*</sup>, M. Živković<sup>b</sup>, A. Savić<sup>c</sup>, J. Mutić<sup>d</sup>,  
V. Tešević<sup>d</sup>**

**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 <sub>7</sub> H <sub>6</sub> O <sub>5</sub>	-	169→125	30	20
Protocatechuic acid	8.8	C <sub>7</sub> H <sub>6</sub> O <sub>4</sub>	-	153→109	30	20
4-Hydroxy benzoic acid	13.4	C <sub>7</sub> H <sub>6</sub> O <sub>3</sub>	-	137→93	30	20
Vanillic acid	15.7	C <sub>8</sub> H <sub>8</sub> O <sub>4</sub>	+	169→93	26	14
Syringic acid	17.0	C <sub>9</sub> H <sub>10</sub> O <sub>5</sub>	-	197→182	28	14
Ellagic acid	25.1	C <sub>14</sub> H <sub>6</sub> O <sub>8</sub>	+	303→89	50	56
Caffeic acid	16.9	C <sub>9</sub> H <sub>8</sub> O <sub>4</sub>	-	179→135	30	20
<i>p</i> -Coumaric acid	23.1	C <sub>9</sub> H <sub>8</sub> O <sub>3</sub>	+	165→91	22	22
Ferulic acid	24.8	C <sub>10</sub> H <sub>10</sub> O <sub>4</sub>	+	195→145	20	16
Vanillin	20.9	C <sub>8</sub> H <sub>8</sub> O <sub>3</sub>	+	153→93	26	16
Siringaldehyde	22.9	C <sub>9</sub> H <sub>10</sub> O <sub>4</sub>	+	183→155	26	10
Catechin	14.5	C <sub>15</sub> H <sub>14</sub> O <sub>6</sub>	+	291→139	26	20
Epicatechin	19.1	C <sub>15</sub> H <sub>14</sub> O <sub>6</sub>	+	291→139	26	16
Myricetin	27.6	C <sub>15</sub> H <sub>10</sub> O <sub>8</sub>	+	319→153	52	38
Quercetin	29.7	C <sub>15</sub> H <sub>10</sub> O <sub>7</sub>	-	301→151	30	20
Kaempferol	31.4	C <sub>15</sub> H <sub>10</sub> O <sub>6</sub>	+	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.

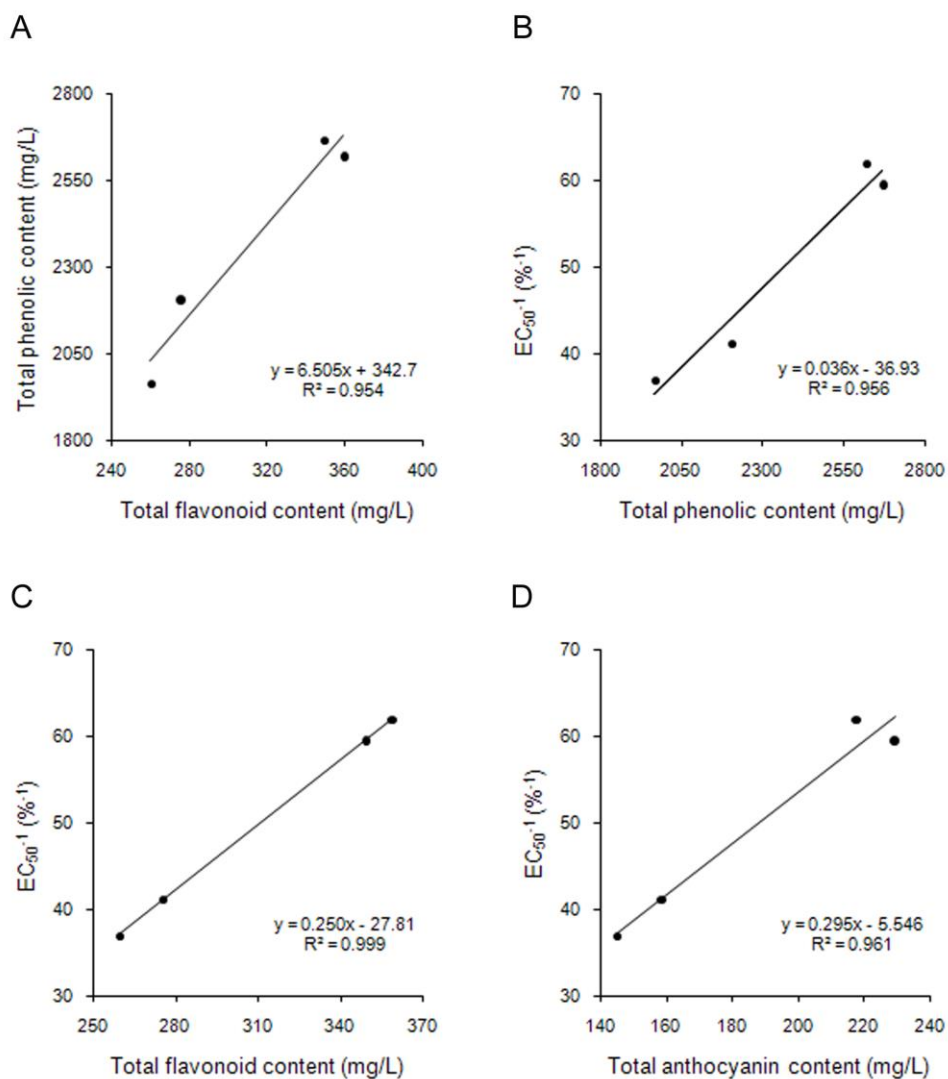
Sample	MAJOR (mg/L)				TRACE (µg/L)					
	Ca	K	Mg	Na	Al	Fe	Mn	Zn	Cu	
BT	57.1 ± 0.6	493 ± 5	41.4 ± 0.2	9.1 ± 0.3	530.6 ± 2.5	1041 ± 3	440.3 ± 0.4	551.7 ± 0.4	124.9 ± 1.6	
Vranac	CI	56.1 ± 0.4	523 ± 3	40.9 ± 0.2	11.4 ± 0.3	977.9 ± 1.2	1411 ± 3	441.5 ± 0.4	665.5 ± 0.6	543.5 ± 0.5
	CII	52.7 ± 0.4	416 ± 3	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 ( $R^2=0.961$ ).