Supplementary material for the article:

Radovanovic, A.; Jovancicevic, B.; Arsic, B.; Radovanovic, B.; Bukarica, L. G. Application of Non-Supervised Pattern Recognition Techniques to Classify Cabernet Sauvignon Wines from the Balkan Region Based on Individual Phenolic Compounds. *Journal of Food Composition and Analysis* **2016**, *49*, 42–48. https://doi.org/10.1016/j.jfca.2016.04.001

Original research article

Application of non-supervised pattern recognition techniques to classify Cabernet Sauvignon wines from the Balkan region based on individual phenolic compounds

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Supplementary Tables and Figures

Table S1

Contents of total phenols, hydroxycinnamoyl tartaric acids esters of wine acids and flavonols (mg L^{-1}), as well as values of the present alcohol (%) and pH in chosen samples of Cabernet Savignon wines

Wines	Alcohol (%)	pH value	Total phenols	Hydroxycinnamoyl tartaric acids	Total flavonols
CS1	12.0	3.55	1285±1	220±0	116±1
CS2	12.5	3.28	1551±0	286±0	126±0
CS3	12.5	3.45	1409±2	261±1	152±1
CS4a	13.0	3.41	1760±1	289±1	155±0
CS4b	12.0	3.40	1968±1	353±1	209±1
CS5a	11.5	3.54	1434±1	211±1	114±1
CS5b	11.7	3.46	1785±0	313±0	176±1
CS6a	12.5	3.45	1642±0	278±0	176±0
CS6b	11.5	3.44	1744±0	312±1	171±0
CS7	12.5	3.54	1193±1	209±1	121±1
CS8	11.5	3.55	997±1	200±1	110±1
CS9a	11.5	3.21	1555±0	250±1	132±1
CS9b	11.5	3.25	1631±0	269±0	138±0
CS10	12.5	3.63	1770±0	260±0	129±0
CS11	13.0	3.65	1517±0	281±±0	123±0
CS12	14.0	3.67	1585±1	266±1	151±1

Data are means±SD, n=3

Table S2

The contents of hydroxybenzoic and hydroxycinnamic acids in Cabernet Sauvignon wines from the Balkan region, determined at 280 and 320 nm

Wine	Gallic	Vanillic	Syringic	Ellagic	*trans*-Caftaric	*trans*-Coutaric	Caffeic	Chloro-genic	*p*-Coum-aric	Ferulic	∑Hydroxy-benzoic acids	∑Hydroxycinnamic acids
CS1	32±1	3±0	2±0	5±0	18±1	2±1	5±1	3±1	8±1	0±0	42±0	36±0
CS2	76±0	1±0	4±0	6±0	15±0	8±0	3±0	2±1	3±0	3±0	88±0	34±0
CS3	32±1	2±0	2±1	6±0	18±1	2±1	7±1	4±1	4±1	3±1	42±0	37±1
CS4a	75±1	2±0	5±0	12±0	27±1	4±1	1 ±1	0±0	0±1	0±0	94±0	33±0
CS4b	70±0	2±0	8±0	16±0	25±0	2±0	1±0	1±0	2±0	3±1	96±0	34±0
CS5a	57±1	n.d.[a]	n.d.	5±1	20±0	9±0	9±0	1±1	6±0	1±0	57±1	45±1
CS5b	64±1	1±0	11±0	5±1	22±1	7±0	5±1	2±1	6±0	0±1	62±0	43±1
CS6a	64±1	2±0	8±1	n.d.	21±0	2±0	6±1	2±0	4±1	2±1	74±0	37±0
CS6b	67±0	1±	11±0	n.d.	16±1	9±0	7±1	3±0	4±1	0±1	78±0	39±0
CS7	45±1	3±1	1±0	4±0.88	15±0	7±1	2±1	n.d.	1±0	1±0	45±0	26±1
CS8	23±1	0±1	1±0	4±0	5±0	2±1	2±1	1±0	1±1	1±1	20±1	12±1
CS9a	102±1	1±0	5±0	5±1	23±1	4±1	4±1	2±0	3±0	1±1	102±1	36±0
CS9b	111±0	4±1	11±1	14±1	22±0	4±0	4±1	1±0	5±0	1±0	140±0	37±0
CS10	112±0	1±1	8±1	5±1	10±0	8±0	4±0	1±0	3±0	5±1	127±1	24±0
CS11	96±1	1±0	2±0	5±0	19±1	1±1	8±1	n.d.	8±1	3±1	104±1	38±0
CS12	69±1	1±1	1±0	4±1	21±0	10±0	5±0	n.d.	3±1	1±1	74±0	40±1

Data are means ± SD, mg L^{-1}, n=3
[a] n.d. = not detected

Table S3

The content of flavan-3-ols (at 275/322 nm), the content of flavonols and flavons (at 360 nm), the content of naringinin (at 280 nm) and total flavonoids in Cabernet Sauvignon wines from the Balkan region

Wine	Catechin	Procyanidin B2	Epicatechin	Epigallo-catechin- gl	Quercetin-3-gl	Rutin	Myricetin	Quercetin	Kaempherol	Luteolin	Apigenin	Naringin	Σ Flavonoids
CS1	29±0	8 ±1	15±1	3±0	5±1	7±0	2±0	4±1	1±1	n.d. [a]	0±0	1±0	76±0
CS2	31±0	9±0	10±0	8±0	3±0	4±0	1±0	4±0	1±0	n.d.	1±0	1±0	61±0
CS3	29±0	19±1	16±1	5±0	12±1	5±0	5±0	4±0	8±1	3±0	1±1	1±0	103±0
CS4a	20±1	11±1	15±1	10±0	2±1	5±0	n.d.	6±1	1±1	n.d.	n.d.	2±0	94±0
CS4b	50±0	20±0	11±0	17±1	11±0	10±0	4±0	3±0	4±0	1±0	n.d.	4±0	134±0
CS5a	24±0	14±1	20±0	4±0	5±1	3±0	n.d.	5±1	n.d.	n.d.	0±0	1±1	74±0
CS5b	36±1	16±1	22±1	8±0	5±1	3±0	n.d.	3±1	1±0	n.d.	1±0	1±1	94±91
CS6a	19±1	19±1	11±1	4±1	4±0	3±0	1±0	3±1	0±0	n.d.	1±0	1±1	66±0
CS6b	29±0	12±0	11±0	4±1	4±1	5±1	1±0	4±1	2±1	n.d.	0±1	1±1	74±0
CS7	36±0	24±1	24±1	8±0	2±1	3±0	2±0	5±1	1±1	n.d.	0±1	1±1	106±0
CS8	15±0	12±1	13±0	10±0	7±1	4±0	1±0	4±1	3±1	0±1	0±0	1±1	69±1
CS9a	28±0	16±1	26±1	5±1	8±1	5±0	n.d.	3±1	2±1	n.d.	2±0	6±1	103±0
CS9b	35±0	26±1	24±1	10±0	8±0	6±0	n.d.	3±0	1±0	n.d.	n.d.	6±1	118±0
CS10	39±0	18±0	19±0	3±1	11±0	3±0	3±0	5±0	2±0	3±0	3±0	1±0	109±0
CS11	28±0	10±1	8±1	5±0	3±0	3±0	1±0	3±0	1±1	n.d.	n.d.	1±0	64±0
CS12	56±0	46±0	39±0	3±0	3±1	6±0	2±0	3±1	5±1	1±0	1±0	1±0	167±1

Data are means ± SD, mg L^{-1}, n=3
[a] n.d. = not detected

Table S4

The content of monomeric anthocyanins in the form of glycosides, 3-acetylglycosides, 3-*p*-cumaroylglycosides and vitisin A and malvidin-vinylglucoside in Cabernet Sauvignon wines on 520 nm

Wine	Dp-3gl	Cy-3-gl	Pt-3gl	Pn-3-gl	Mv-3-gl	Dp-3-acet-gl	Cy-3-acet-gl	Pt-3-acet-gl	Pn-3-acet-gl	Mv-3-acet-gl	Vitisin A	Pt-3-*p*-cum-gl	Pn-3-*p*-cum-gl	Mv-3-*p*-cum-gl	Mv-vin-ylphenol-gl
CS1	25±0	n.d. [a]	33±1	11±1	248±1	12±1	7±1	9±1	5±1	56±1	n.d.	6±1	6±1	6±1	n.d.
CS2	11±0	8±0	10±0	9±1	37±0	11±0	9±1	9±1	9±1	97±1	19±1	16±1	28±0	56±1	25±1
CS3	18±1	7±0	34±2	36±2	249±2	17±2	7±1	9±1	11±1	46±2	n.d.	17±1	15±2	38±1	n.d.
CS4a	24±0	6±0	23±0	9±1	115±1	27±1	19±1	17±0	17±1	30±0	17±0	30±1	57±1	44±1	49.2±0
CS4b	90±0	15±1	81±0	59±0	625±1	61±1	55±1	21±1	28±1	202±1	30±0	54±1	35±0	76±0	31±1
CS5a	11±1	n.d.	15±0	11±0	103±1	6±1	n.d.	7±0	n.d.	32±1	10±0	8±1	n.d.	13±1	n.d.
CS5b	11±0	n.d.	12±0	8±1	104±0	n.d.	n.d.	n.d.	n.d.	37±1	n.d.	n.d.	n.d.	13±1	4±1
CS6a	n.d.	n.d.	n.d.	n.d.	21±1	n.d.	n.d.	n.d.	n.d.	n.d.	15±0	n.d.	n.d.	6±1	n.d.
CS6b	n.d.	n.d.	n.d.	n.d.	11±0	n.d.	n.d.	n.d.	n.d.	n.d.	9±1	n.d.	n.d.	7±0	n.d.
CS7	19±2	n.d.	22±1	20±1	267±1	7±1	n.d.	11±0	18±1	83±1	13±0	8±1	n.d.	12±1	8±0
CS8	7±1	n.d.	13±1	5±0	169±1	17±0		8±1	9±1	87±1	11±0	n.d.	n.d.	10±1	n.d.
CS9a	10±1	n.d.	30±1	30±0	187±1	24±1	n.d.	9±1	8±1	49±1	10±0	11±1	13±1	23±1	4±1
CS9b	11±1	n.d.	16±1	17±1	122±1	14±1	n.d.	5±1	5±1	27±2	n.d.	n.d.	n.d.	22±1	n.d.
CS10	n.d.	n.d.	n.d.	n.d.	33±1	n.d.	n.d.	n.d.	n.d.	11±1	13±1	n.d.	n.d.	6±1	3±0
CS11	n.d.	n.d.	n.d.	n.d.	11±0	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	7±1	3±0
CS12	21±0	n.d.	28±1	22±0	301±0	18±1	9±1	9±1	7±1	97±0	8±1	19±0	10±0	40±0	5±0

Data are means ± SD, mg L^{-1}, n=3
[a] n.d. = not detected

Table S5

Results of Grubb's test

Compounds	Samples connected to outliers	Grubb's test for outliers Two-tailed test
Total phenols	-	α=0.05, n=16, G(critical value)=2.587
Esters of wine acid	-	α=0.05, n=16, G(critical value)=2.587
Hydroxycinnamic acids	-	α=0.05, n=16, G(critical value)=2.587
Hydroxybenzoic acids	CS4a, CS4b, CS9b	α=0.05, n=13, G(critical value)=2.462
Flavan-3-ols	CS1, CS4b, CS6a, CS10, CS12	α=0.05, n=11, G(critical value)=2.355
Flavonols	CS1, CS2, CS3, CS4a, CS4b, CS5a, CS5b, CS7, CS9a, CS9b, CS11, CS12	α=0.05, n=4, G(critical value)=1.481
Luteolin and apigenin	CS1, CS2, CS3, CS4a, CS5a, CS5b, CS6a, CS6b, CS7, CS9a, CS9b, CS11, CS12	α=0.05, n=4, G(critical value)=1.481
Main monomeric anthocyanins in the form of glycosides	CS1, CS5a, CS5b, CS6a, CS6b, CS7, CS8, CS9a, CS9b, CS10, CS11, CS12	α=0.05, n=4, G(critical value)=1.481
Monomeric anthocyanins in the form of 3-acetyl glycosides	CS4a, CS4b, CS5b, CS6a, CS6b, CS10, CS11	α=0.05, n=9, G(critical value)=2.215
Anthocyanins in the form of 3-*p*-cumaroyl glycosides and malvidin-vinylglucoside	CS1, CS3, CS5a, CS5b, CS6a, CS6b, CS7, CS8, CS9b, CS10, CS11	α=0.05, n=5, G(critical value)=1.715

a)

b)

c)

d)
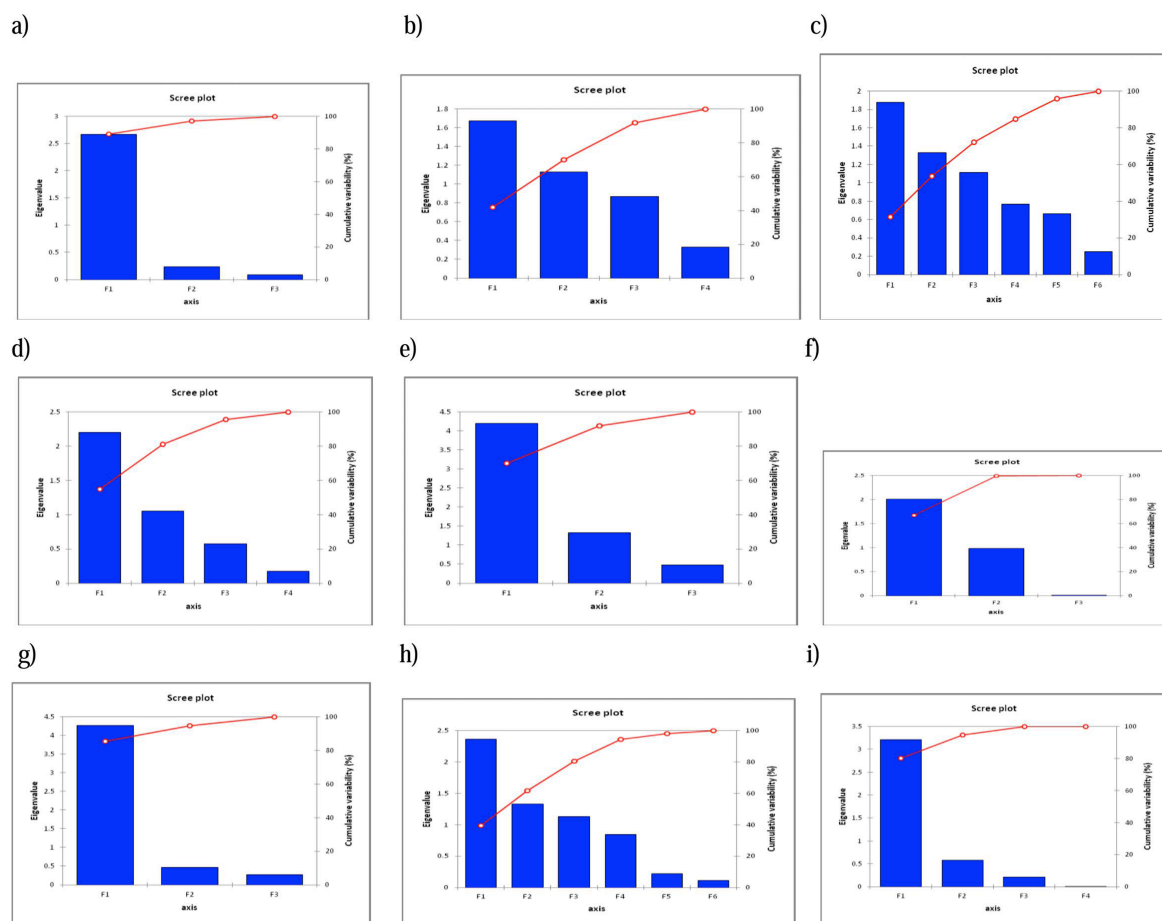

e)

f)

g)

h)

i)

Fig. S1. Scree plots of Eigen values of the principal components in PCA

a) the contents of total phenols, esters of wine acid and flavonols
b) the contents of hydroxybenzoic acids
c) the contents of hydroxycinnamic acids
d) the contents of flavan-3-ols
e) the contents of flavonols
f) the contents of luteolin and apigenin
g) the contents of main monomeric anthocyanins in the form of glycosides
h) the contents of monomeric anthocyanins in the form of 3-acetyl glycosides
i) the contents of anthocyanins in the form of 3-*p*-cumaroylglycosides and malvidin-vinylglucosides
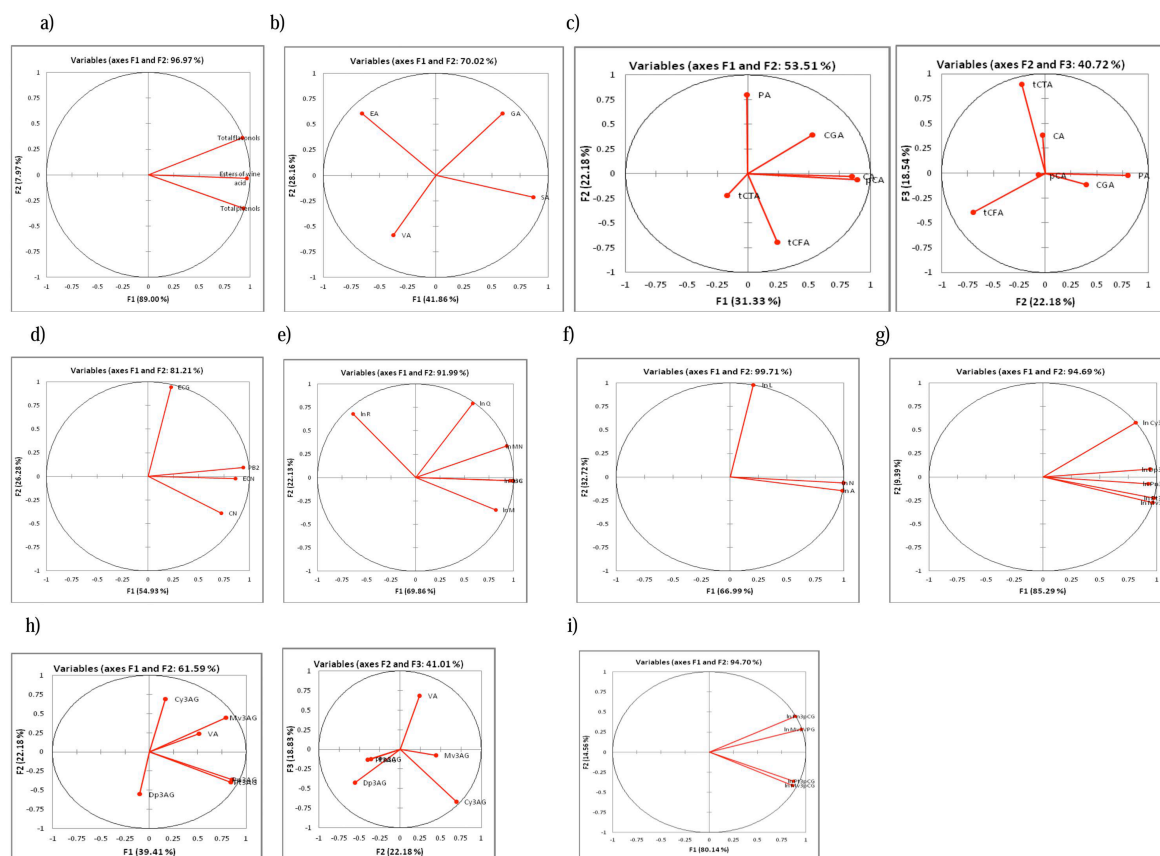
Fig. S2. Loading plots of data in Cabernet Sauvignon samples

a) the contents of total phenols, esters of wine acid and flavonols
b) the contents of hydroxybenzoic acids
c) the contents of hydroxycinnamic acids
d) the contents of flavan-3-ols
e) the contents of flavonols
f) the contents of luteolin and apigenin
g) the contents of main monomeric anthocyanins in the form of glycosides
h) the contents of monomeric anthocyanins in the form of 3-acetyl glycosides
i) the contents of anthocyanins in the form of 3-*p*-cumaroylglycosides and malvidin-vinylglucosides