

Utility of comprehensive GC×GC gas chromatography in finding varietal markers among volatile compounds in non-aromatic red wines

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Supplementary Files

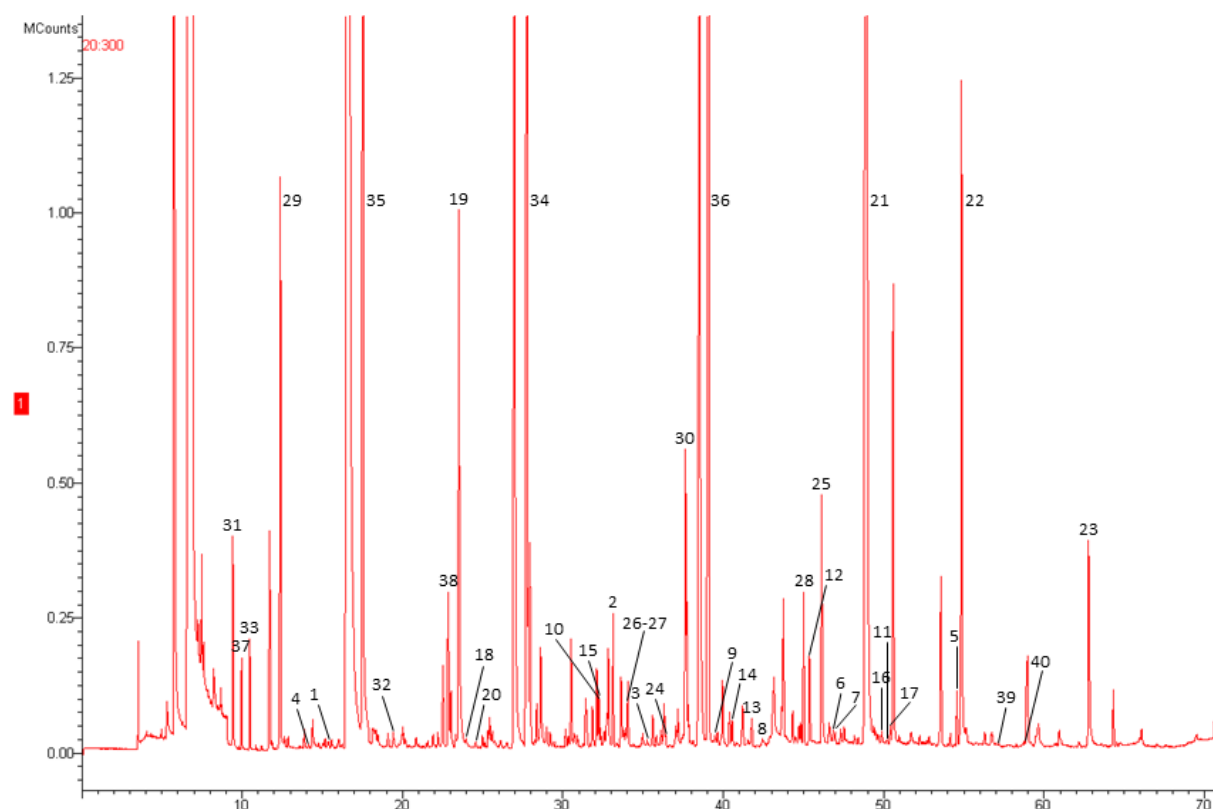


Figure S1. Example of a total ion current chromatogram obtained for a Teran monovarietal red wine using HS-SPME/GC-MS. The chromatographic peaks of the identified volatile compounds are numbered from 1 to 40 and correspond to those in Table 2.

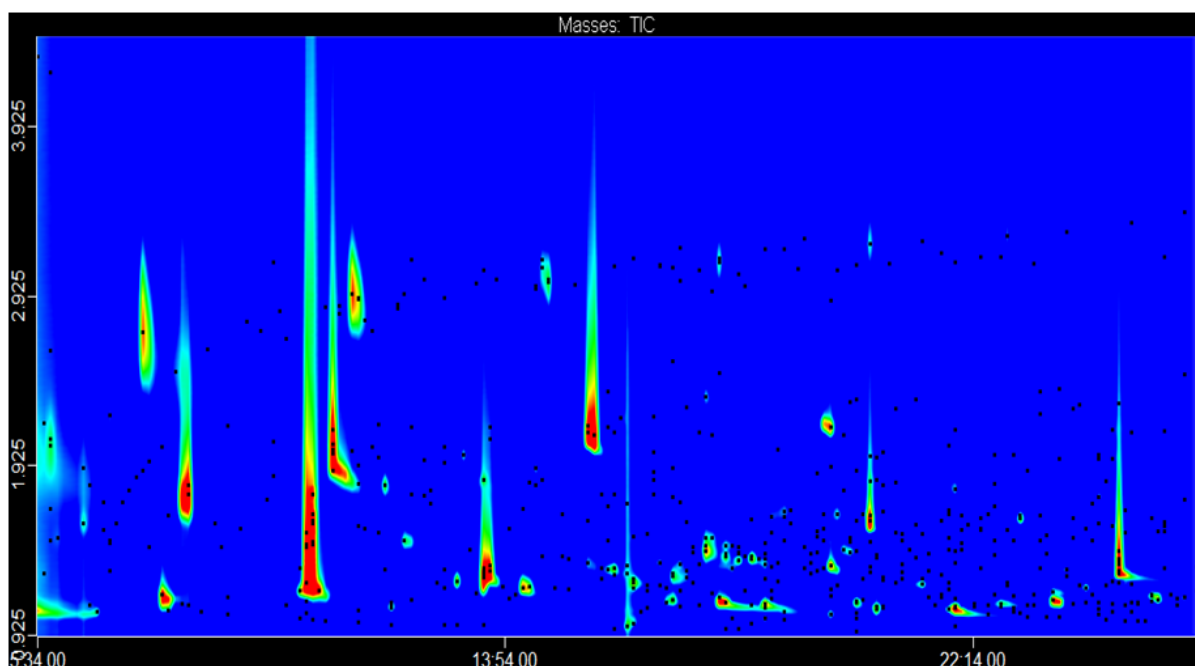


Figure S2. Example of a contour plot obtained for a monovarietal red wine using HS-SPME/GC×GC-TOF-MS. Colored areas represent more abundant volatile aroma compounds and black dots represent less abundant and trace volatile aroma compounds.

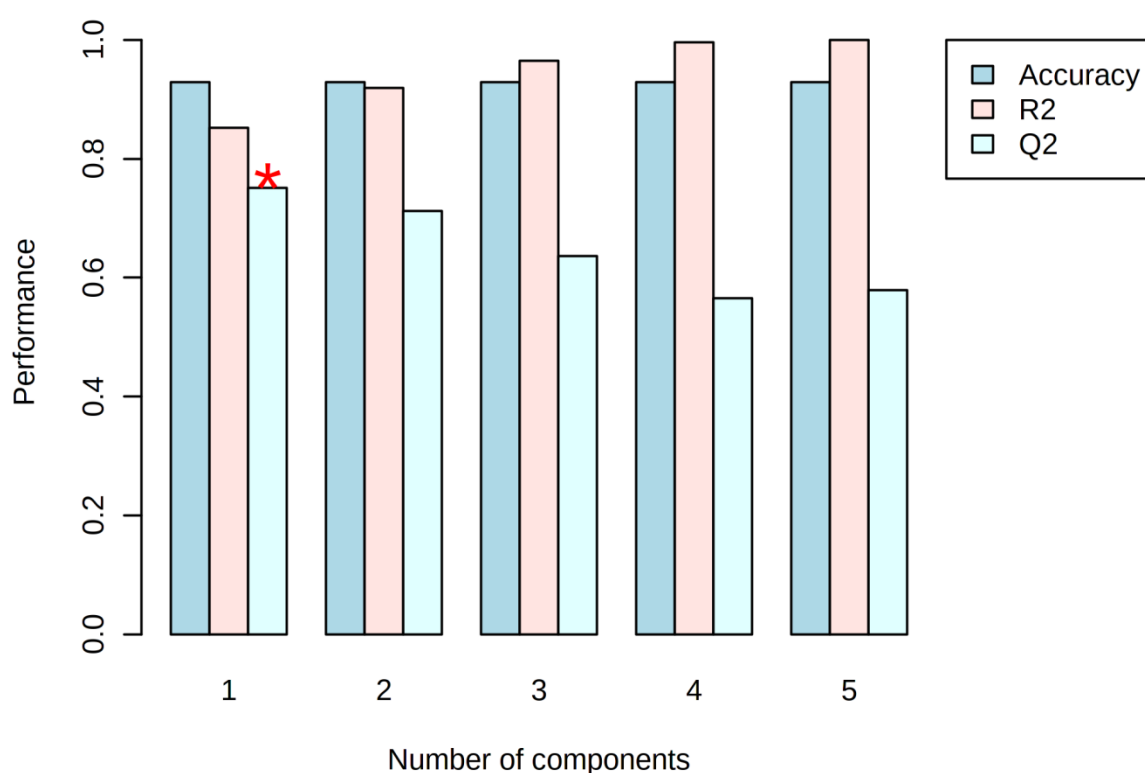


Figure S3. Evaluation of the PLS-DA model by a 10-fold cross-validation. Blue bars indicate the accuracy of the model, pink bars (R2) indicate the goodness of fit (explained variation), and light-blue bars (Q2) indicate the goodness of prediction. Good predictions with a high Q2 value are marked by *.

Table S1. Climate parameters in the Istria and Dalmatia regions of Croatia in 2015.

Parameter Region		Month (2015)											
		I	II	III	IV	V	VI	VII	VIII	IX	X	XI	XII
Temp. (°C)	Istria	6.4	5.7	9.0	12.0	17.6	22.1	26.3	23.9	19.2	13.7	9.3	6.8
	Dalmatia	9.1	8.9	11.4	14.2	19.9	23.9	28.3	26.8	22.4	17.3	13.4	10.9
Rainfall (mm)	Istria	51.3	53.5	44.8	23.8	37.7	51.7	22.7	77.5	64.0	162.8	28.0	0.5
	Dalmatia	93.8	157.5	61.3	47.8	66.1	37.4	9.2	73.8	68.8	241.4	45.1	0.1

Table S2. Odor perception thresholds (OPT, $\mu\text{g/L}$), odor descriptors, and average odor activity values (OAV = concentration/OPT) of the main odorants among volatile aroma compounds found in Plavac mali and Teran monovarietal red wines after headspace solid-phase microextraction followed by gas chromatography-mass spectrometry (HS-SPME-GC-MS), sorted by compound class and descending Fisher *F*-ratio (as reported in Table 2).

No.	Volatile compounds	OPT (matrix)‡	Odor descriptors‡	Variety	
				PM	TE
Terpenes					
2	Linalool	15 (10% v/v ethanol)	Roses, lychee	0.56	0.80
6	Geraniol	30 (10% v/v ethanol)	Roses, geranium	0.41	0.61
8	Citronellol	18 (10% v/v ethanol)	Citrus fruit	0.55	0.58
9	α-Terpineol	250 (synthetic wine*)	Lilac, camphor	0.01	0.02
C13-Norisoprenoids					
11	β-Ionone	0.09 (synthetic wine*)	Violet	1.33	1.78
12	β-Damascenone	0.05 (10% v/v ethanol)	Sweet, fruity, stewed apple	21.00	16.80
Alcohols					
19	1-Hexanol	8000 (10% v/v ethanol)	Fresh cut grass	0.17	0.18
20	cis-3-Hexen-1-ol	400 (10% v/v ethanol)	Green grass	0.18	0.20
21	2-Phenylethanol	10000 (10% v/v ethanol)	Rose	4.16	4.17
Acids					
22	Octanoic Acid	500 (synthetic wine*)	Cheese, rancid, fat	2.71	2.17
23	Decanoic Acid	1000 (synthetic wine*)	Rancid, waxen, plasticine	0.20	0.14
24	Butyric acid	173 (synthetic wine*)	Aged cheese, rancid	5.40	6.23
25	Hexanoic acid	420 (synthetic wine*)	Cheese, rancid	3.78	3.80
Esters					
28	2-Phenethyl acetate	250 (10% v/v ethanol)	Fruity, honey, floral	5.48	3.65
29	Isoamyl acetate	30 (10% v/v ethanol)	Banana	29.30	21.97
30	Ethyl decanoate	200 (synthetic wine*)	Grapes, fruity	0.28	0.20
31	Ethyl butyrate	20 (10% v/v ethanol)	Fruity	11.80	9.86
33	Ethyl-3-methylbutyrate	3 (10% v/v ethanol)	Berry, blackberry	5.76	7.86
34	Ethyl octanoate	2 (10% v/v ethanol)	Fruity	76.85	48.25
35	Ethyl hexanoate	5 (10% ethanol)	Green apple	56.80	33.02
36	Diethyl succinate	6000 (10% ethanol)	Overripe melon, vinous	0.56	0.68
37	Ethyl 2-methylbutyrate	1 (10% v/v ethanol)	Sweet fruit	11.15	15.83
38	Ethyl lactate	100000 (14% v/v ethanol)	Buttery	0.78	0.72
Benzenoids and phenols					
39	Ethyl cinnamate	1 (10% v/v ethanol)	Honey, cinnamon	0.36 ^a	0.14 ^b
40	Eugenol	5 (10% v/v ethanol)	Cloves	0.16	0.22

*Synthetic wine: 11% v/v ethanol, 7 g/L glycerol, 5 g/L tartaric acid, pH 3.4

[‡]Odor perception thresholds ($\mu\text{g/L}$) and odor descriptors reported in the literature [11,34,35,38,42-44].