Comprehensive two-dimensional gas chromatography with a TOF MS detector – An effective tool to trace the signature of grape varieties

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Supplementary Files

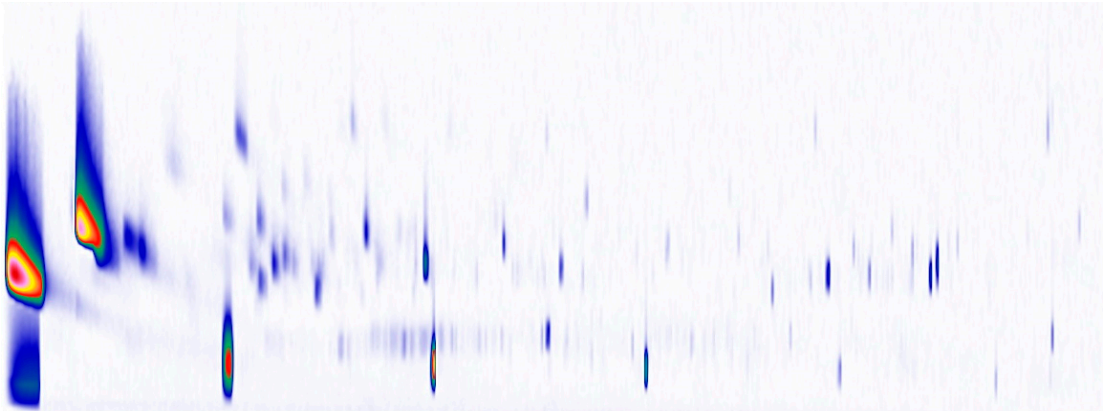

Figure S1. Example of a contour plot obtained through GC×GC-TOFMS analysis of a sample of grapes of Trincadeira.

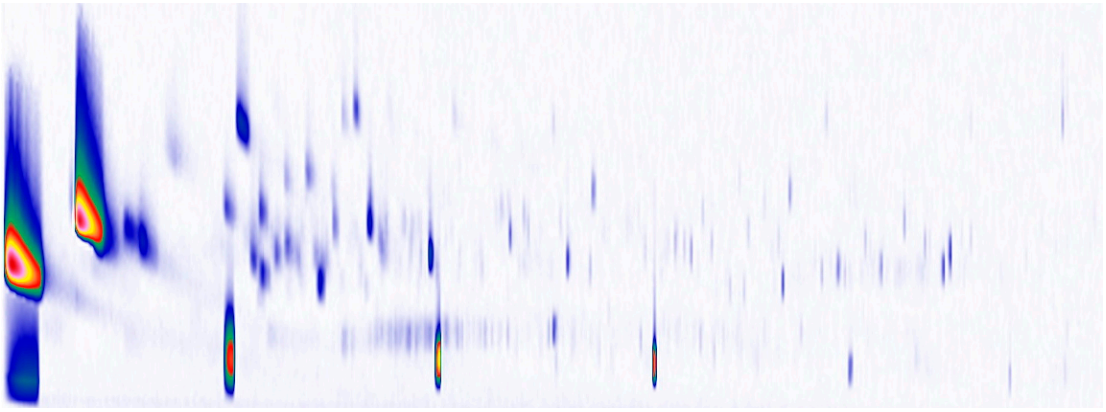

Figure S2. Example of a contour plot obtained through GC×GC-TOFMS analysis of a sample of grapes of Cabernet Sauvignon.

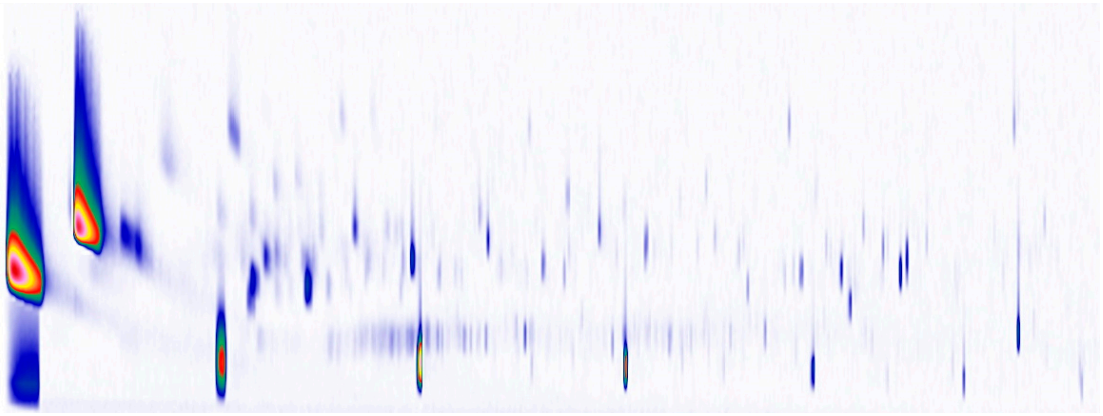

Figure S3. Example of a contour plot obtained through GC×GC-TOFMS analysis of a sample of grapes of Tinta Barroca.

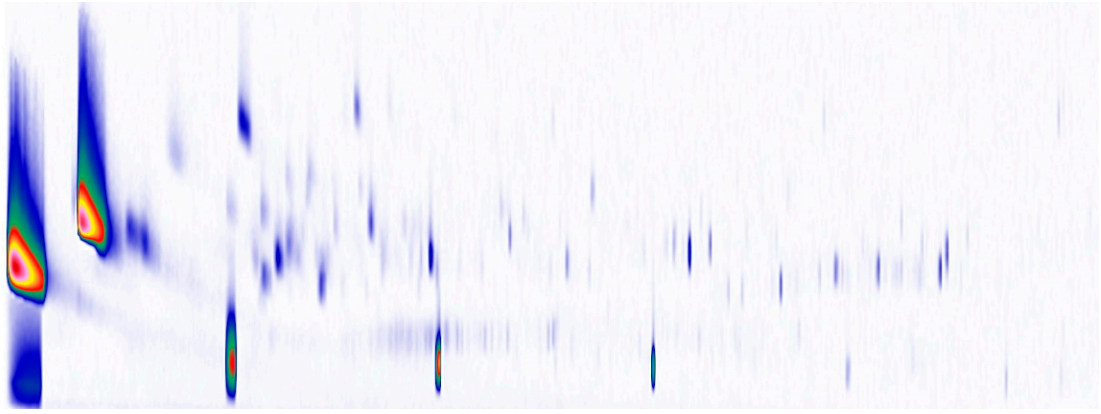

Figure S4. Example of a contour plot obtained through GC×GC-TOFMS analysis of a sample of grapes of Syrah.

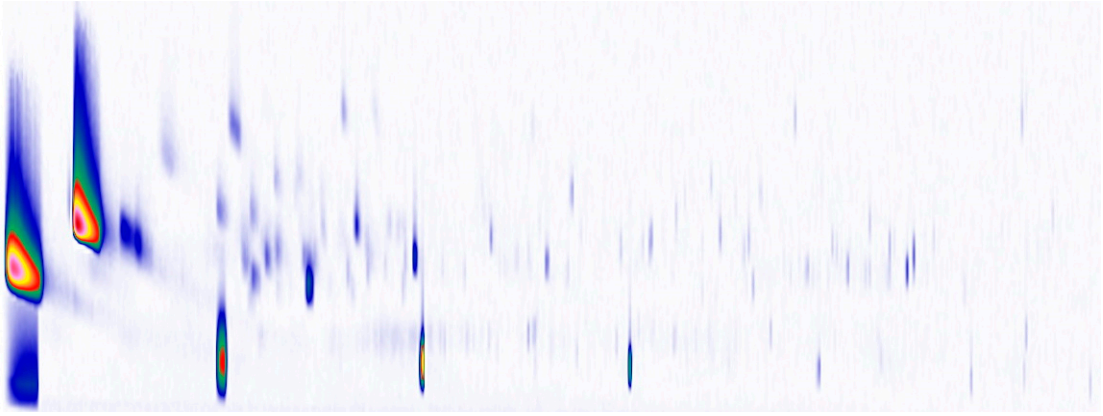

Figure S5. Example of a contour plot obtained through GC×GC-TOFMS analysis of a sample of grapes of Castelão.

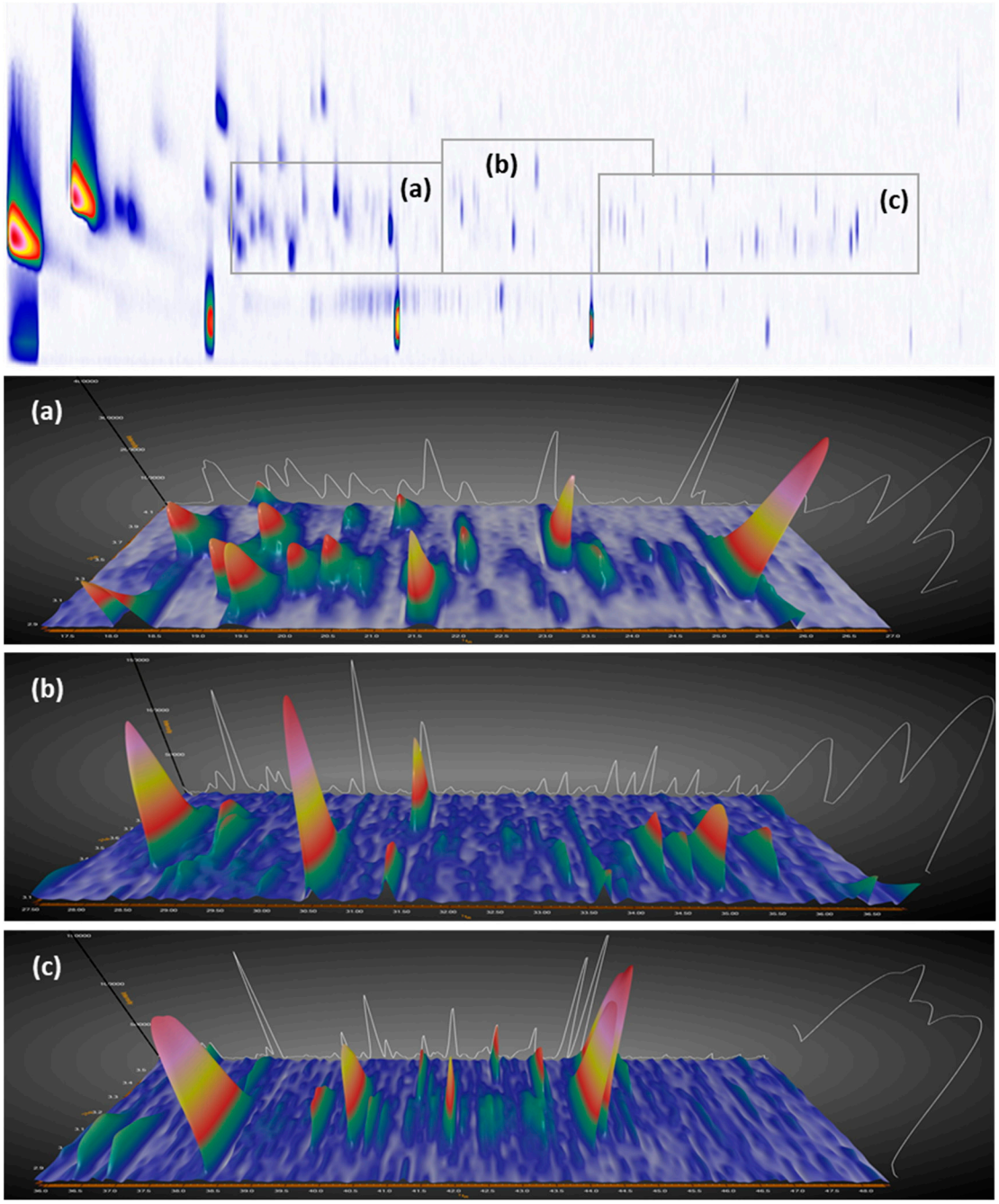

Figure S6. Example of a contour plot obtained through GC×GC-TOFMS analysis of a sample of grapes of CS, region of (a) monoterpenes, (b) C_{13}-norisoprenoids and (c) sesquiterpenes.

Table S1. The results of ANOVA and MANOVA for the free varietal compounds.

Compounds	ANOVA and MANOVA		
	Year	Variety	Year × Variety
β-Myrcene	NS	NS	NS
p-Cymene	**	***	***
d-Limonene	***	**	*
Ocimene	**	NS	**
γ-Terpinene	NS	NS	NS
Dihydromyrcenol	NS	NS	NS
α-Terpinolene	NS	NS	NS
p-Cymenene	NS	NS	*
Tetrahydrolinalool	**	*	NS
Linalool	**	***	***
Hotrienol	NS	NS	NS
γ-Terpineol	NS	NS	NS
Menthol	**	*	NS
α-Terpineol	*	NS	*
β-Citronellol	NS	NS	NS
Nerol [e]	NS	NS	NS
cis-Myrtanol	NS	*	NS
δ-Elemene	**	NS	NS
α-Cubebene	**	***	NS
α-Ylangene	*	NS	NS
α-Copaene	***	***	NS
β-Elemene	NS	NS	NS
Isocaryophyllene	NS	NS	NS
α-Gurjunene	**	***	NS
Longifolene	NS	NS	NS
α-Cedrene	*	NS	NS
β-Caryophyllene	NS	***	NS
γ-Elemene	***	***	*
Aromadendrene	NS	NS	NS
Aristolene	***	NS	NS
β-Coapene	***	***	***
α-Humulene	*	**	NS
β-Guaiene	*	NS	NS
γ-Selinene	NS	NS	NS
Valencene	NS	NS	NS
γ-Muurolene	***	***	**
α-Amorphene	NS	NS	NS
δ-Selinene	NS	NS	NS
Zonarene	***	***	***
α-Cadinene	***	***	*

Table S1. Cont.

Compounds	ANOVA and MANOVA		
	Year	Varieties	Year × Varieties
β-Cadinene	***	***	***
cis-Calamenene	***	***	***
m/z 105/161/189/204	**	NS	NS
α-Calacorene	***	***	*
Cadalene	NS	***	NS
β-Cyclocitral	NS	***	***
Vitispirane	NS	NS	NS
Theaspirane A	**	***	**
Theaspirane B	**	**	**
β-Damascenone	NS	***	NS
Geranylacetone	NS	***	***
β-Ionone	NS	**	*

Year×Variety: Interaction between year and varieties. Statistically significant at *$p \leq 0.05$, **$p \leq 0.01$ and ***$p \leq 0.001$, respectively. NS: Not significant.