

# Supplementary material

## Multi-sensor characterization of sparkling wines based on data fusion

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**Table S1.** Average, standard deviation, RSD (%), maximum and minimum concentrations of polyphenols in the set of samples under study. Standard deviation and relative standard deviation indicated the variability of concentrations as a measure of discriminating capacity among samples.

Compound	Average concentration (mg L <sup>-1</sup> )	Standard deviation	RSD (%)	Maximum value (mg L <sup>-1</sup> )	Minimum value (mg L <sup>-1</sup> )
FRAP index	5.45	1.71	31.36	10.72	2.64
FC index	1.52	0.37	24.23	2.62	1.06
Gallic acid	60.8	50.7	83.48	174.7	10.7
Protocatechuic acid	1.66	7.93	478.3	43.03	<LOD
Homogentisic acid	0.56	2.72	488.0	15.87	<LOD
Gentisic acid	21.7	5.64	25.96	30.16	<LOD
(+)-catechin	72.0	34.6	48.09	127.9	<LOD
Caffeic acid	116.0	43.9	37.85	235.1	54.2
Syringic acid	22.1	26.3	119.0	92.65	<LOD
Ethyl gallate	13.2	9.29	70.27	33.52	<LOD
<i>p</i> -Coumaric acid	120.5	45.9	38.07	215.0	56.4
Ferulic acid	13.2	3.21	24.35	20.75	7.55
Caftaric acid	259.9	93.8	36.10	398.9	71.1

**Table S2.** Average, standard deviation, RSD (%), maximum and minimum concentrations of organic acids in the set of samples under study from enzymatic and HPLC methods.

<b>Compound</b>	<b>Average concentration (g L<sup>-1</sup>)</b>	<b>Standard deviation</b>	<b>RSD (%)</b>	<b>Maximum value (g L<sup>-1</sup>)</b>	<b>Minimum value (g L<sup>-1</sup>)</b>
Lactic acid – enz.	1.47	0.46	31.24	2.19	0.51
Lactic acid - HPLC	2.35	0.81	34.47	3.76	0.44
Gluconic acid – enz.	0.07	0.04	49.92	0.14	0.02
Gluconic acid - HPLC	0.37	0.05	12.58	0.43	0.26
Malic acid – enz.	0.19	0.30	159.8	1.02	0.02
Malic acid - HPLC	0.56	0.41	73.42	1.69	0.11
Acetic acid – enz.	0.23	0.03	14.86	0.30	0.19
Citric acid - HPLC	0.14	0.04	31.61	0.26	0.08
Succinic acid - HPLC	0.51	0.12	23.99	0.76	0.33
Tartaric acid - HPLC	5.58	0.45	8.04	6.38	4.50

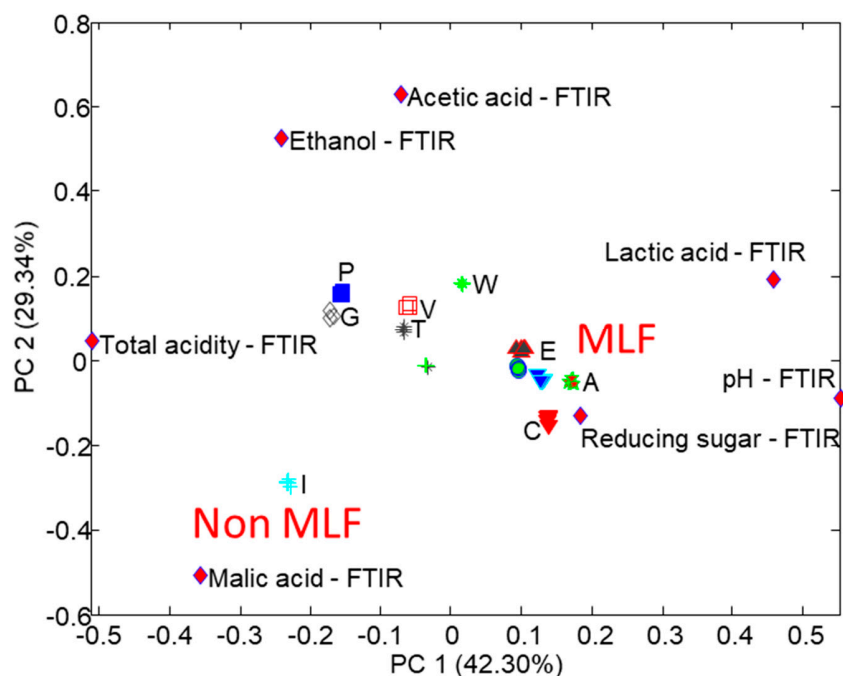
**Table S3.** Average, standard deviation, RSD (%), maximum and minimum values from FTIR, potentiometric and volumetric methods in the set of samples under study.

<b>Compound</b>	<b>Average concentration (g L<sup>-1</sup>)</b>	<b>Standard deviation</b>	<b>RSD (%)</b>	<b>Maximum value (g L<sup>-1</sup>)</b>	<b>Minimum value (g L<sup>-1</sup>)</b>
Reducing sugar - FTIR	8.99	2.05	22.7	10.31	1.43
pH – FTIR (*)	3.04	0.07	2.34	3.13	2.90
pH – potentiometry (*)	2.98	0.06	2.16	3.09	2.85
Acetic acid - FTIR	0.23	0.08	36.8	0.37	0.11
Total acidity - FTIR	6.25	0.43	6.89	6.97	5.48
Total acidity – vol.	6.25	0.42	6.75	7.10	5.50
Malic acid - FTIR	0.30	0.67	221	2.20	0.00
Lactic acid - FTIR	1.20	0.75	62.7	2.19	0.00
Ethanol - FTIR	11.3	0.30	2.61	11.9	10.9

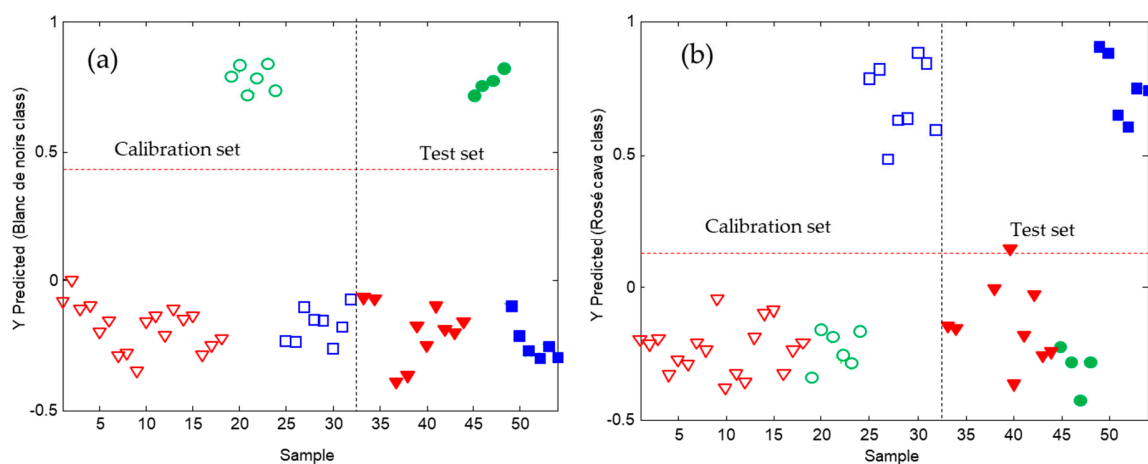
\* pH data values

**Table S4.** Summary of classification results by PLS-DA with 3 LVs for the assignation of white, blanc de noirs and rosé cava samples using the data fusion set.

Target class	Calibration		Validation	
	Sensitivity (%)	Selectivity (%)	Sensitivity (%)	Selectivity (%)
White	100	100	100	100
Blanc de noirs	100	100	100	100
Rosé	100	100	100	90



**Figure S1.** PCA results showing the biplot of PC1 vs PC2 from the study of FTIR data. Plot of scores (a) and plot of loadings (b). Cava class assignment: see Table 1.



**Figure S2.** Classification plots from PLS-DA for the assignment of (a) blanc de noirs and (b) rosé cava samples. Sample assignment: triangle = white; square = rosé; circle = blanc de noirs; Empty symbols = calibration samples; Solid symbols = validation samples. Red line indicated the classification threshold.

