Characterization and classification of musts, wines and sparkling wines by their elemental composition determined by ICP-OES and ICP-MS

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INTRODUCTION

The control of the composition of food products with Protected Designation of Origin, such as wines and sparkling wines, is essential to prevent fraudulent practices and adulterations. A wide range of compounds can be used as tentative biomarkers for characterization and authentication purposes, being elemental composition one of the most successful sources of information, especially for dealing with geographical origin and varietal issues. Currently, Inductively Coupled Plasma with Optical Emission Spectrometry (ICP-OES) and Inductively Coupled Plasma Mass Spectrometry (ICP-MS) are the techniques of choice to carry out multi-elemental analysis of this kind of beverages in a rapid and simple way.

IN THIS WORK

In our study, samples from the different processing stages in the elaboration of sparkling wine (cava) -including must, base wine, and sparkling wine- of Pinot Noir and Xarel·lo grape varieties have been analyzed by ICP techniques to determine the elemental composition. The resulting data has been used to classify these products according to oenological practices, and product qualities. For this purpose, Principal Components Analysis, box plot diagrams and bar charts have been used with the aim to found markers and sample patterns dealing with changes resulting from the different steps of the production process of cava wines and sample patterns that allow their classification.

EXPERIMENTAL

SAMPLES

40 samples of must, wine and sparkling wine

	Quality	Must	Base wine	Stabilized wine	3 months sparkling wine	7 months sparkling wine
Pinot Noir	A	MPA	BWPA	SWPA	C3PA	C7PA
	B	MPB	BWPB	SWPB	C3PB	C7PB
	C	MPC	BWPC	SWPC	C3PC	C7PC
	D	MPD	BWPD	SWPD	C3PD	C7PD
Xarel·lo	A	MXA	BWXA	SWXA	C3XA	C7XA
	B	MXB	BWXB	SWXB	C3XB	C7XB
	C	MXC	BWXC	SWXC	C3XC	C7XC
	D	MXD	BWXD	SWXD	C3XD	C7XD

Quality code: A to D, being A the best and D the poorest.

PRETREATMENT

- Preliminary studies on sample dilution and filtration of samples
- Same treatment for all musts, wines and sparkling wines:

Dilution with 1% HNO_3 ← simpler, quicker, cleaner

1 mL sample + 9 mL of 1% HNO_3 → ICP tubes

MEASUREMENT

Multi-elementary techniques that offer accurate and fast determination at trace and ultra-trace level: ICP-OES and ICP-MS

RESULTS

38 elements measured by ICP-OES and ICP-MS.

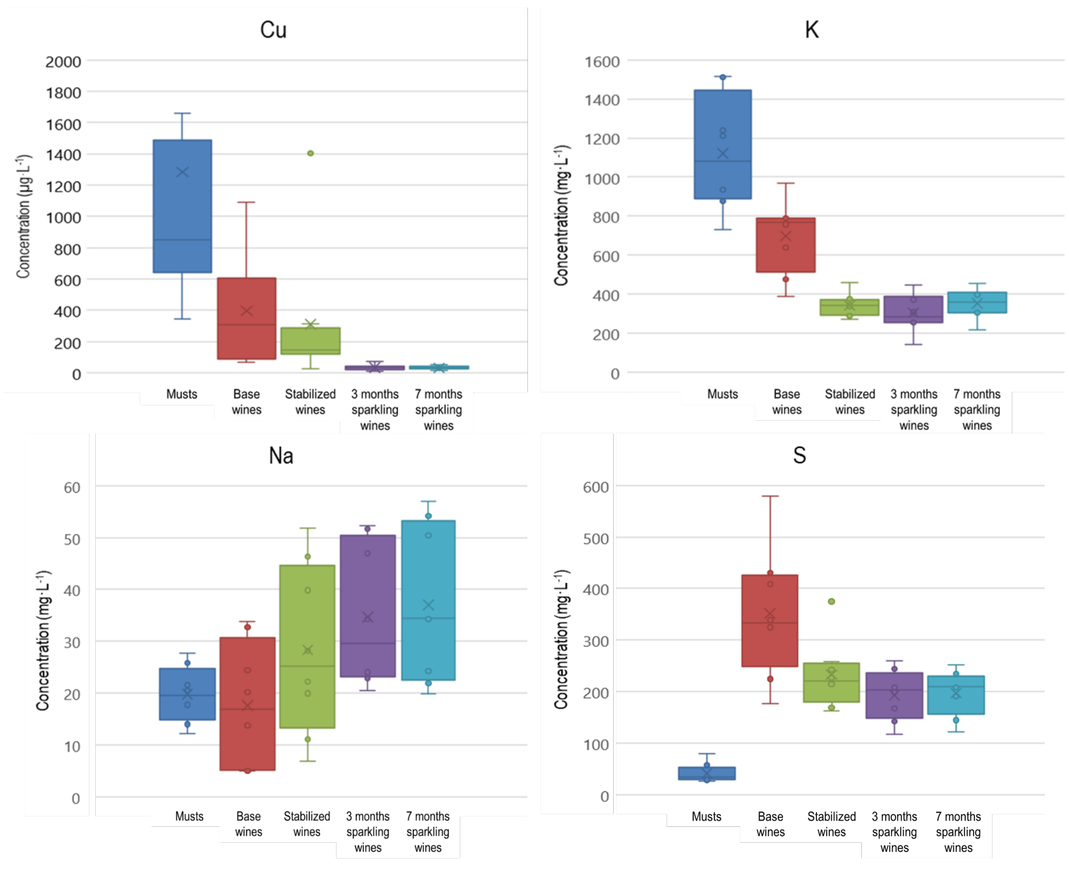
- **26 elements** had signals **over the detection limits** of the instrument and the method.

(Al, As, B, Ba, Ca, Co, Cs, Cu, Fe, K, Li, Mg, Mn, Mo, Na, Ni, P, Rb, S, Sb, Si, Sr, Ti, V, Zn and Zr)

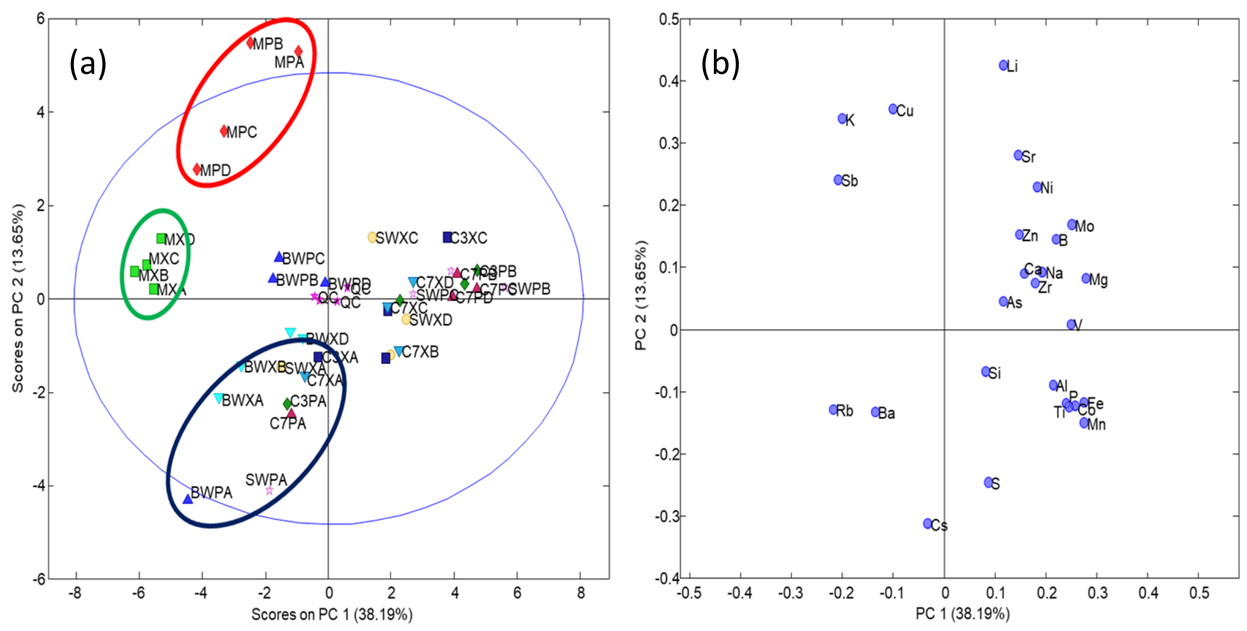
- 9 elements had signals under the detection limit of the instrument, plus other 3 under the quantification limit of the method.

(Cr, Cd, Ce, Ga, La, Nd, Pb, Sc, Sn, U, W and Y)

BOXPLOTS OF SIGNIFICANT ELEMENTS



PRINCIPAL COMPONENT ANALYSIS



Application of PCA to the characterization of must, wine and cava samples. (a) Map of samples: scatter plot of scores of PC1 vs PC2; (b) Map of variables: scatter plot of loadings of PC1 vs PC2. Sample assignation is given in the table.

CONCLUSIONS

- The elemental composition of the musts, wines and sparkling wines was successfully determined by ICP-OES and ICP-MS.
- The resulting compositional data was used as the data for characterization purposes based on chemometric methods.
- PCA models showed a clear difference among the metal composition of A quality and the lower ones (B, C and D qualities).
- Some elements were initially present in the must, thus coming from the grape (e.g. Cu and K), while others were introduced throughout the cava production (e.g. Na, Mn, Al, and S coming from clarification and sulfite addition).

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