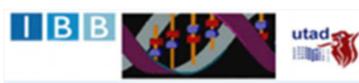


Mass spectrometry-based fingerprinting of proteins/peptides in wine quality control

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During the last third of the twentieth century the world wine market became significantly more competitive. Consumption declined in the traditional wine producing and consuming countries, while competition emerged from such 'New World' nations as the United States, Australia and Chile, and prosperous consumers chose quality rather than quantity in consumption.

Wineries work in an aggressive market and the need to improve productivity and produce the best quality wines makes it mandatory for them to invest resources in wine research. In addition, food traceability is essential to preserve the identity of unique quality traits against fraud or commercial disputes. Therefore, there is a growing demand for new fast methodologies for the collection of information related to units/batches of wine ingredients and products [1].

Proteins present in the wine and their related peptides can supply a characteristic mass spectrometry-based fingerprint, MS-FP, which can be used, in conjunction with informatics and statistics tools, for traceability and quality control in the wine industry [2]. Despite its potential for wine control purposes, protein and/or peptide MS-FP has not yet been fully exploited [3].

INTRODUCTION

A rapid method to characterize and to classify wines is the so called wine fingerprint. Each wine has a characteristic pattern of compounds that makes it unique. Such patterns are obtained from wine components such as volatile compounds, proteins, peptides, or other type of organic molecules, such as tannins. These patterns are generally known as wine fingerprint.

The use of mass spectrometry based on Matrix Assisted Laser Desorption Ionization, MALDI, to obtain fingerprints has been extensively used to classify samples such as plasma or serum. MALDI can be used in direct mode after a simplified sample treatment. In this manner the sample is directly placed onto the MALDI-target and analyzed. It is well known that there is no universal matrix for MALDI analysis. As a general rule matrixes are chosen experimentally. Wine is a complex matrix that includes peptides, proteins, alcohols, sugars, etc.

In the present work it is shown the potential of using peptide mass fingerprint, PMF, derived from whole wine protein tryptic digests to distinguish different wines.

METHODS

Protein content of two different white wines, (i) "Pazo Serantellos", grape type Albariño; (ii) "Fiuza", grape type Sauvignon Blanc, was extracted by precipitation with a mixture of 20% (W/V) TCA/Acetone. Protein digestion was carried out overnight with Trypsin. From the common matrices generally used in MALDI analysis we tried 2,5-dihydroxybenzoic acid, DHB; sinapinic acid and α -Cyano-4-hydroxycinnamic acid, α -Cyano. Mass spectrometry was performed using a MALDI-TOF/TOF instrument. The mass list of 20 technical replicates of each wine were used to perform a clustering analysis with Euclidean distance and it was generated a Heatmap, Figure 1.

RESULTS AND CONCLUSIONS

The inspection with classification algorithms of the MALDI spectra obtained with sinapinic acid, DHB and α -Cyano demonstrated that a better classification was obtained when spotting was carried out with the α -Cyano matrix. As demonstrated in Figure 1, it appears to be possible to differentiate wines through their protein content, once it is evident two major branches in the cluster heat map. However, it will be necessary to increase the number of wines used since a few representative samples have been analyzed.

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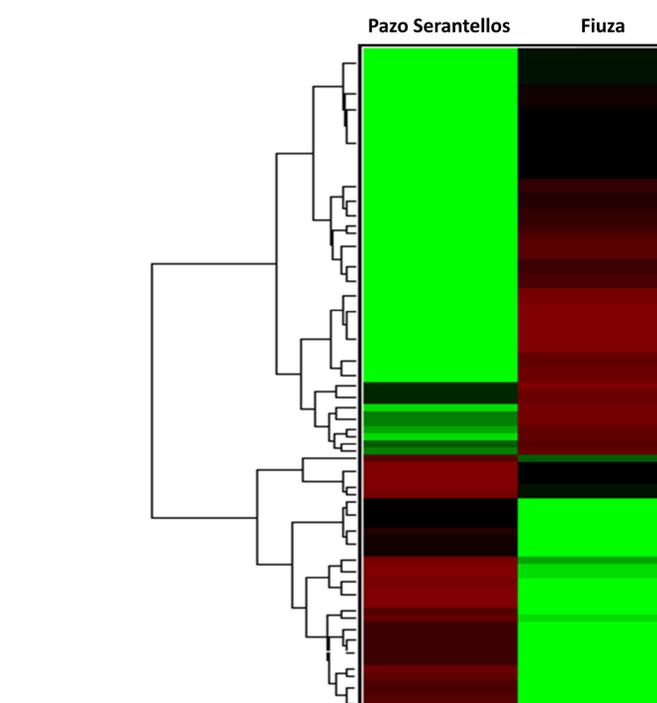


Figure 1. Cluster Heatmap. Cluster analysis (Euclidean distance) of two different wines. The qualitative presence or absence of peptide m/z values were used as variables for the analysis. It was established a peptide mass tolerance of 50 ppm. Green means the total absence and red means total presence of the peak in all replicates of the wine.

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