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The role of chemometrics in the characterization of coffee quality

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Introduction

Coffee analysis is a paramount tool to guarantee its quality, safety and traceability and to be in compliance with legal standards and consumers' demand. With the ever-increasing requirement of analytical controls in the "*omics*" sciences era chemometrics became an indispensable tool to manage huge amount of data and extract relevant information to meet the industries demand in the characterization of their products also in view of the regulatory agencies.

Materials/Methods

Different chemometric tools (PCA, PLS, PLS-DA, SIMCA) were used to correlate aroma chemical profile (or fingerprint) and sensory properties, or used as a tool to monitor roasting process and for coffee traceability.

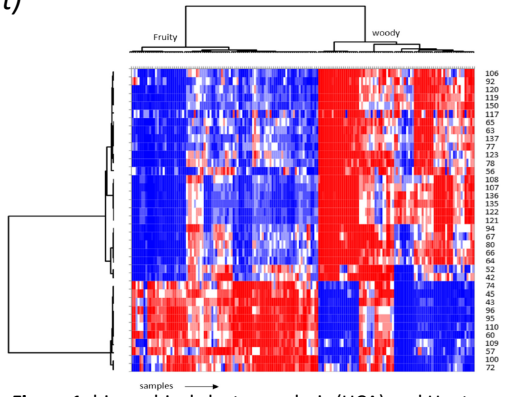

Figure 1: hierarchical cluster analysis (HCA) and Heat-map of a group of coffee that present woody and fruity features

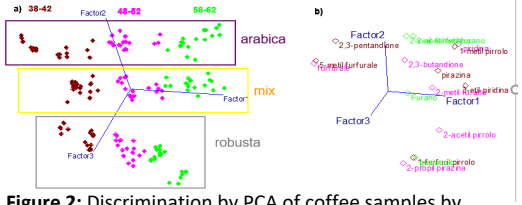

Figure 2: Discrimination by PCA of coffee samples by roasting color and blends

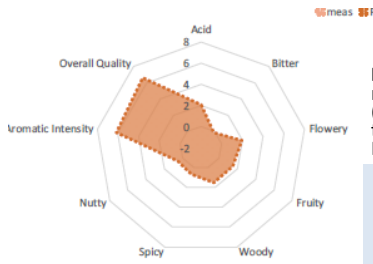

Figure 3: Comparison of the measured coffee sensory profiles (from the panel) and predicted by the chemical fingerprints through PLS.

Results/Discussion

The chemical signature of some coffee sensory have been studied for developing prediction models based on analytical measurements to be adopted at control level. In particular, the sensory profile was linked with the chemical composition accurately defined by HS-SPME-GC-MS or HS-SPME-MS platforms (fig.1). The most effective aroma index defined by correlate the chemical fingerprint with the coffee color in monitoring the coffee roasting resulted in the 5-methylfurfural/2-acetylfuran (fig. 2). Prediction models are capable to define sensory quality of coffee in cup and can be exploited in quality control procedures (fig. 3)

Conclusion/Perspectives

This approach resulted to be a) discriminative, because it was able to point out samples with different origins or roasting degree; b) informative, because it entails the odorants complementary and simultaneous use of sensory and chemical data to define odorants able to describe the chemistry of aroma notes, or volatiles linked to origin; and c) predictive, because the panel-coherent sensory score prediction, despite the limitations, confirms and reinforces the relevance and the significance to study the relationships between coffee volatiles and aroma quality.

References:
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