- ***FLASH COMMUNICATION FOR 1ST OR 2ND YEAR STUDENTS (7 MIN)***

"DEVELOPMENT OF AN ARTIFICIAL INTELLIGENCE METHOD BASED ON CHEMICAL FINGERPRINTS ABLE TO DISCRIMINATE DEFECTIVE COCOA BEANS AND LIQUORS "

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Introduction

Cocoa is one of the most economically important commodities in the world, and it is considered a comfort food due to its mood-enhancing and biological benefits. Since the flavor is an indicator of the cocoa quality and is strongly influenced by climate change and the subsequent introduction of foreign cocoa varieties, it is necessary to ensure a high level quality raw material standards [1].

To date, food flavor analysis relies on visual monitoring and sensory panels, whom produce results that are subject to some variability. Thus, objective tools for monitoring sustainable cocoa production and identifying chemical markers to assess the sensory consistency of incoming beans are crucial [2-3]. This study, in collaboration and supported by Ferrero Italia, explores innovative methodologies to standardize flavor quality amidst these challenges and aims to develop an AI-based method built on chemical fingerprints and data fusion to discriminate between defective and high-quality cocoa beans and liquors [5].

Materials and Methods

The first part of my PhD project involved the use of non-targeted fingerprinting and profiling approaches combined with machine learning to produce detailed cocoa flavour profiles correlated with sensory characteristics, enabling objective evaluation in quality control [4].

Therefore, we proceeded with the work aimed to develop an AI method for routine quality control of incoming cocoa beans in the supply chain. Starting from the sensory panel data for the qualitative characterization of the samples, we performed an Automated Headspace Solid Phase Microextraction (HS-SPME) integrated with a GC-MS system to explore the chemical fingerprints of the samples volatilome while, for the analysis of the non-volatile fraction, we applied the Folin-Ciocâlteu assay for the Total Phenolic Content (TPC) and, through an LC-UV-DAD system, we investigated deeper at molecular level.

Results and Discussion

Our results showed distinct clustering by origin (Fig. 1), with the NEAR index identifying Ecuadorian cocoa as most similar to the industry reference flavour (Fig. 2) and PLS-DA modeling facilitated the creation of blends with different proportions of Ecuadorian cocoa, achieving the reference flavor standard.

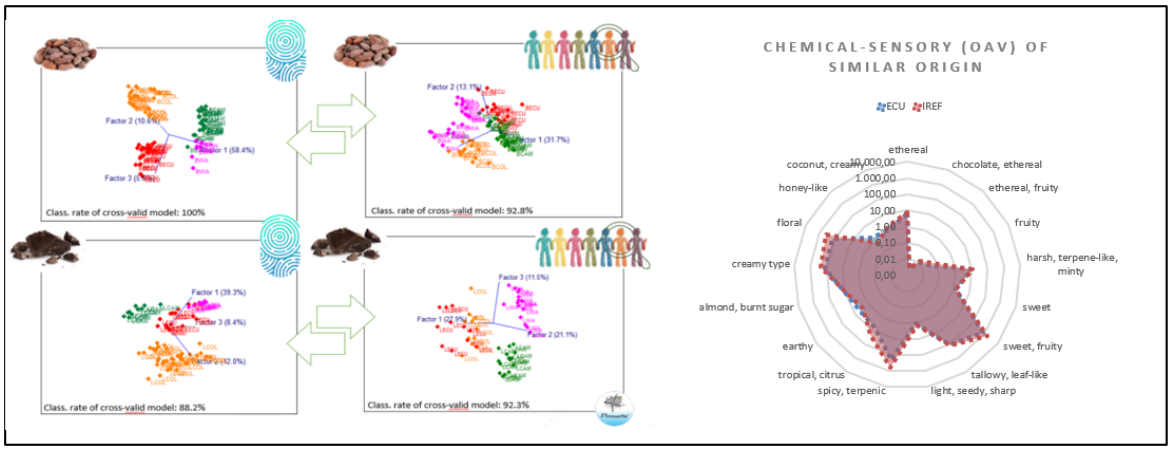
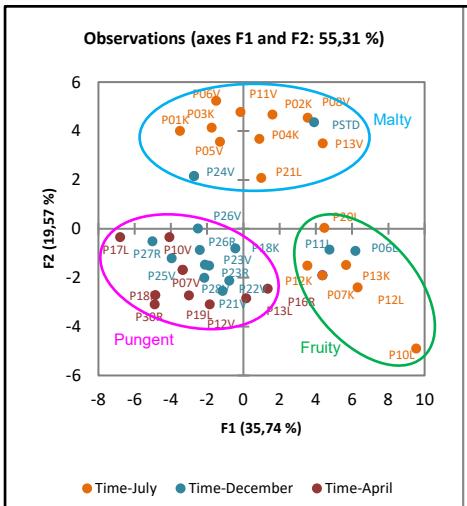


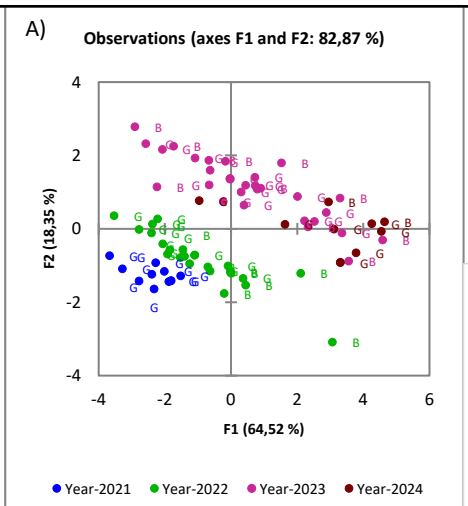
Fig. 1: 3D view of OPLS-DA by untargeted fingerprint and profiling of beans and liquors

Fig.2: Chemical-sensory (OAV) of similar origin compared to the reference standard

Figure 3 show the results of the chemical fingerprint of forty-five CCN51 liquors with a discrimination along positive values of the second principal component (PC2) for samples containing higher amounts of malty aromatic notes compounds such as 3-Methyl-butanal, 2-Methyl-butanal and 3-Methyl-1-butanol. Towards negative values of the PC2 and positive values of the PC1, we find samples characterized by more acidic,

floral, fruity, and sweet aromatic notes. At negative values of the PC1, we find some samples characterized by higher contents of Hexanoic Acid and n-Nonanoic acid, responsible for more pungent and sweaty notes.
Considering the non-volatile fraction (Fig. 4), the results of the Folin-Ciocâlteu test show a higher total phenolic content in the Bad samples, with statistically significant differences for the amount of epicatechin, catechin, procyanidin B2 and procyanidin C1, responsible for more bitter and astringent notes in the samples. Furthermore, a discrimination along the second principal component is observed based on the analysis year, showing a higher content of phenolic compounds and alkaloids in more recent samples compared to those analyzed before the quality defect.
We will continue to monitor these results with further analysis to better define the quality characterization of these samples, expanding our dataset to mitigate the effects of annual variability in discriminating the samples.





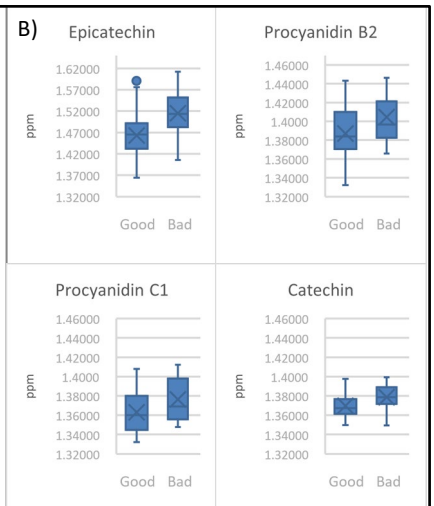


Fig. 3: Volatilome PCA of 45 liquors CCN51 analysed in July, December and April 2023-2024

Fig. 4: A) Non-volatile fraction PCA of 71 liquors CCN51 analysed from November 2021 to April 2024
Fig. 4: B) Statistically different phenols compounds between Good and Bad samples (α < 0,05)

Conclusions

This research successfully discriminated between the origins of cocoa beans and liquors, providing robust tools for long-term flavor standardization and underscores the necessity for advanced analytical tools to monitor and ensure the quality of cocoa products, addressing both environmental and political challenges [9-10]. By leveraging AI-based tools and comprehensive datasets, this study offers robust classification models and discriminative capabilities for long-term flavor quality studies in the chocolate industry, helping to maintain product excellence and consumer satisfaction in the face of global cocoa production challenges.

References

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