CHEMOMETRICS AS A TOOL TO ANSWER TO THE CHALLENGES OF THE CLIMATE CHANGE AND POLITICAL SITUATIONS ON THE CONSISTENCY OF COCOA FLAVOUR QUALITY

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Abstract for posters

Cocoa is one of the most economically important commodities in the world and currently the main producers are West and East Africa (three-quarters of world production) and Latin America and Asia [1-2]. Cocoa production is strongly influenced by socio-political balances in farm areas and especially by climate change which affects both the amount of cocoa production and the flavour quality of the final products [3-6]. Since the flavour of cocoa products is the main property that directs the consumer's choice, as well as acting as an indicator of the quality of the product itself, it is necessary to ensure a high level of raw material quality standards [5]. Therefore, tools to track sustainable cocoa production are of paramount importance, especially due to climate change and the introduction of foreign varieties to support the high global demand for cocoa-derived products, which heavily influence cocoa production, quality and purity. With this in mind, the study we report is part of a broader project aimed at analysing the flavour profiles of cocoa from different origins and defining their chemical-sensory identity card aimed at a constant quality standard supply by also considering cocoa from different origins to cope with climate change and political conflicts. The volatilome of one hundred sixty cocoa samples was analyzed by HS-SPME-GC-MS in combination with chemometrics for origin "identitation"[7-9]. To achieve the above-mentioned objectives, fingerprinting (non-targeted) and profiling (targeted) approaches were used, which were able to decipher the information contained in the complex volatilome dataset of both beans and liquor from different origins and validate the results, allowing the origins studied to be discriminated with successful classification models for their informative, discriminative and classification capacity. The results indicate a coherent, clear clustering of samples according to their origin with the two analytical strategies, both on raw beans and on cocoa liquors, albeit with differences at the molecular level. Predicting the classification of cocoa beans with the untargeted fingerprint on an external test set gave excellent results for beans with a classification rate of 100% and very good results for liquors (88%), despite the processing they underwent. Better results were obtained for targeted approaches with a classification rate above 92% (i.e. 92.86% for beans and 92.31% for liquors).

References

- Somarriba, E.; Peguero, F.; Cerda, R.; Orozco-Aguilar, L.; López-Sampson, A.; Leandro-Muñoz, M. E.; Jagoret, P.; Sinclair, F. L. (2021) Rehabilitation and Renovation of Cocoa (Theobroma Cacao L.) Agroforestry Systems. A Review. *Agron. Sustain. Dev.*, 41 (5), 1–19.
- ICCO. Statistics International Cocoa Organization https://www.icco.org/ (accessed Sep 5, 2022).
- Boeckx, P.; Bauters, M.; Dewettinck, K. (2020) Poverty and Climate Change Challenges for Sustainable Intensification of Cocoa Systems. *Curr. Opin. Environ. Sustain.*, 47, 106–111.
- (4) Aprotosoaie, A. C.; Vlad Luca, S.; Miron, A. (2016)Flavor Chemistry of Cocoa and Cocoa Products-An Overview. *Compr. Rev. Food Sci. Food Saf.*, 15 (1), 73–91.
- (5) CABISCO/ECA/FCC. (2015) Cocoa Beans: Chocolate & Cocoa Industry Quality Requirements.
- (6) Perotti, P.; Cordero, C.; Bortolini, C.; Rubiolo, P.; Bicchi, C.; Liberto, E. (2020) Cocoa Smoky Off-Flavor: Chemical Characterization and Objective Evaluation for Quality Control. *Food Chem.*, 309, 125561.
- Magagna, F.; Liberto, E.; Reichenbach, S. E.; Tao, Q.; Carretta, A.; Cobelli, L.; Giardina, M.; Bicchi, C.; Cordero, C. (2018) Advanced Fingerprinting of High-Quality Cocoa: Challenges in Transferring Methods from Thermal to Differential-Flow Modulated Comprehensive Two Dimensional Gas Chromatography. J. Chromatogr. A., 9, 122-136.
- (8) Medina, S.; Perestrelo, R.; Silva, P.; Pereira, J. A. M.; Câmara, J. S. Current Trends and Recent Advances on Food Authenticity Technologies and Chemometric Approaches (2019). *Trends Food Sci. Technol.*, 85, 163–176.
- (9) Cuadros-Rodríguez, L.; Ortega-Gavilán, F.; Martín-Torres, S.; Arroyo-Cerezo, A.; Jiménez-Carvelo, A. M. (2021) Chromatographic Fingerprinting and Food Identity/Quality: Potentials and Challenges. *Cite This J. Agric. Food Chem*, 69, 14428– 14434.