









### Computer vision based on GCxGC-MS/FID for Coffee origin authentication

Giorgio Felizzato<sup>1</sup>, Andrea Caratti<sup>1</sup>, Chiara Cordero<sup>1</sup>, Luciano Navarini<sup>2</sup>, Erica Liberto<sup>1</sup> <sup>1</sup> Department of Science and Drug Technology, University of Turin, Italy <sup>2</sup> Illycaffè S.p.A., via Flavia 110, Trieste I-34147, Italy

Introduction: Coffee quality is determined by complex chemical profiles shaped by origin, variety, processing, and storage conditions. These profiles influence sensory properties and are key markers of authenticity, traceability, and overall quality. Computer Vision, a proven Artificial Intelligence (AI) technique, is effectively applied to authenticate coffee origin by extracting meaningful patterns from complex chromatographic data.

Two-dimensional gas chromatography (GC  $\times$  GC) captures the detailed chemical fingerprints of coffee samples. The multidimensional data are converted into 2D maps and analysed using a Computer Vision workflow that combines untargeted and targeted (UT) fingerprinting, producing composite class images representing geographical origins and enabling reliable, scalable coffee origin authentication.

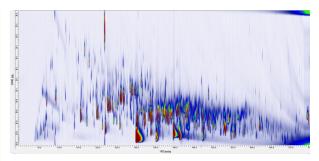
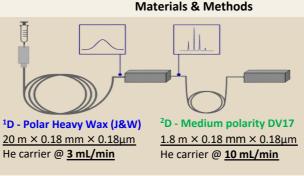


Figure 1: GCxGC chromatogram

## **Headspace SPME DVB/CAR/PDMS** $d_f 50/30 \, \mu m - 2 cm$ 50 °C - 40 minutes Sample

 $500 \pm 0.1 \, \text{mg}$ 

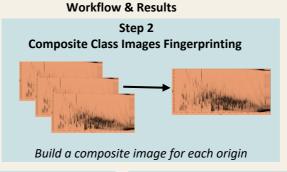


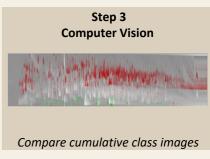
- GC Oven ramp: 50 °C (2 min) to 200 °C (5 min) at 2.5 °C/min and from 200 °C to 260 °C (5 min) at 5 °C/min
- S/SL injector: 250°C, split mode, split ratio
- MS Transfer line: 270°C GC-MS in EI ionisation mode: 70 eV
- MS acquisition: Mass range 35-350 m/z;
  - frequency 50 Hz

Step 5

Optimode settings: P<sub>M</sub> **2.5**, pulse 250 ms

# Step 1 **Untargeted Fingerprinting** Generate a template of untargeted peaks





**Targeted Template Construction** 

Identify peaks consistently contributing to origin-based differences Build a targeted template

# **Unsupervised and Supervised statistics**

Selection of informative chemicals (targeted analytes) Implementation and evaluation of supervised machine learning models

Conclusion: The integrated GC×GC-Computer Vision workflow provides a rapid and effective strategy for assessing compositional differences among coffees of different origins. Through cumulative image construction, pairwise comparison, and peak selection, the method highlights key chemical variations in a highly visual and intuitive manner. Computer vision enables the identification of peaks that differ between origins, which are then used to build a targeted template containing the compounds responsible for these differences. Coupled with statistical analysis, this approach support rapid and objective evaluation of incoming batches, ensuring consistency with declared origin and guiding decisions on overall product quality.

#### References:

- Caratti, A., Squara, S., Bicchi, C., Tao, Q., Geschwender, D., Reichenbach, S. E., Ferrero, F., Borreani, G., & Cordero, C. (2023). Augmented visualization by computer vision and chromatographic fingerprinting on comprehensive two-dimensional gas chromatographic patterns: Unraveling diagnostic signatures in food volatilome. Journal of Chromatography A, 1699. https://doi.org/10.1016/j.chroma.2023.464010
- Mondello, L., Cordero, C., Janssen, H. G., Synovec, R. E., Zoccali, M., & Tranchida, P. Q. (2025). Comprehensive two-dimensional gas chromatography–mass spectrometry. Nature Reviews Methods Primers, 5(1). https://doi.org/10.1038/s43586-024-00379-3