The role of chemometrics in the characterization of coffee quality

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RATIONALE
Coffee analysis is a fundamental step to guarantee its quality, safety and traceability and to comply with legal/regulatory standards and consumers’ demand. The ever-increasing requirement of analytical controls, in the “omics” era, has made chemometrics an indispensable tool to manage the huge amount of data and extract relevant information to meet the demand to characterize industrial products.

METHODS
Analytical platforms on-line combining high concentration capability sampling techniques with either separative GC-MS (HS-SPME-GC-MS) or non-separative (HS-SPME-MS) techniques together with suitable chemometrics (PCA, PLS, PLS-DA, SIMCA) are here used to correlate aroma chemical profile and/or fingerprints with sensory properties, for coffee traceability and as a tool to monitor roasting process.

RESULTS
Prediction models of the coffee sensory notes based on analytical measurements have been studied for quality control. The chemical signatures enable to define sensory quality of in-cup coffee, although with some compromises. The most reliable models are those obtained for bitter, acid, spicy and woody properties, whose volatile fingerprint is representative of the sensory note. Chemometrics also provide tools to monitor the coffee roasting through correlation of chemical fingerprints with beans color, and/or profiling of aroma indices such as the 5-methylfurfural/2-acetylfuran ratio. Classification of Arabica mono-origin from blend of different origins through SIMCA algorithms affords to identify several volatiles characteristic of their origins.

CONCLUSIONS & PERSPECTIVES
Chemometrics with its discriminative, informative and predictive role can be a bridge between the complexity of coffee aroma and industrial requirements giving answers to challenge topics, and confirming and reinforcing relevance and significance of studying the relationships between coffee volatiles, aroma and quality in view of coffee sustainability.

References: