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### The chemistry of the temporal evolution of coffee flavor quality

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Florence (Italy), October 5 - 7, 2022

# The chemistry of the temporal evolution of quality coffee flavor



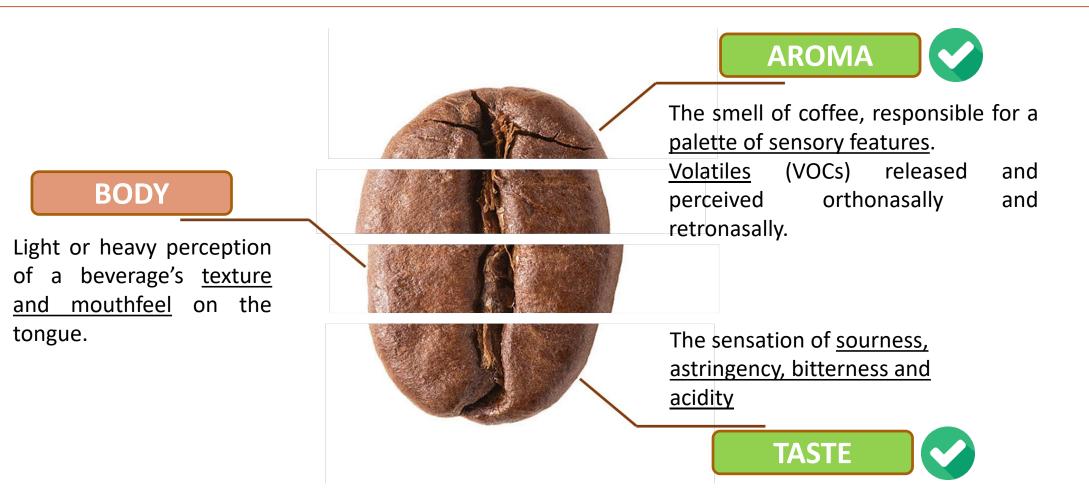
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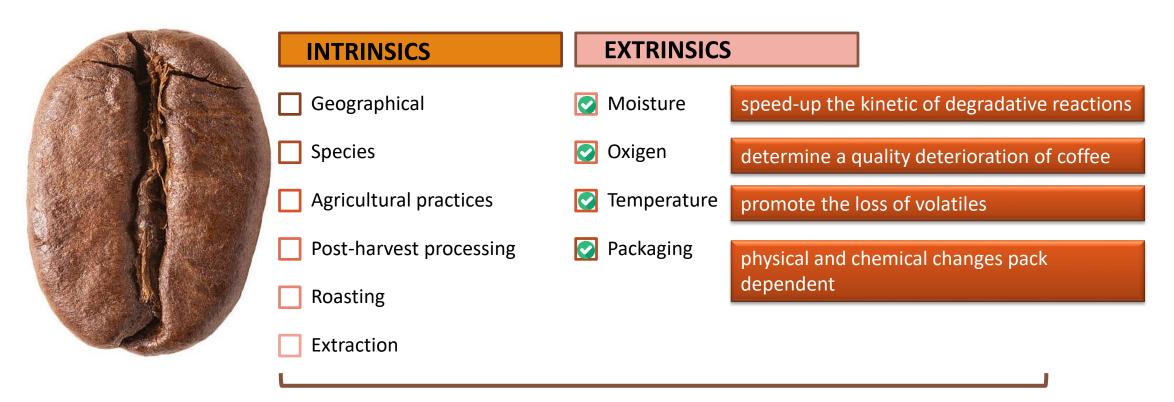
## **Aim and Scope**



The pleasure related to drink a good cup of coffee is due to its unique sensory **quality**. This is due to the potent taste and aroma given off by coffee during the roasting process. The balance of the these two chemical senses constitutes the most important determinant of what is defined as **flavour** perception [2,5-7].



Due to coffee sensory properties and its important financial value, it is essential to preserve and maintain its quality, especially during storage [1-4].



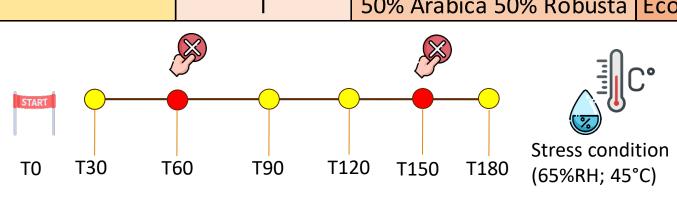
### Impacting on the quality of coffee flavour

The quality of coffee flavor is a key step of the coffee production, since it determines the consumer's acceptability and delineate the shelf-life of the product. Nowadays the estimation is made by using cupping protocols, but this kind of procedure is time-consuming requiring panel training and aligned professional panelists and often it suffers of a too subjective evaluation. Due to the ever-increasing demand of coffee, there is a need for analytical techniques suitable for routine control (QC). For these reasons, nowadays, we are looking for potential alignment with the analytical instrumental measurements, capable to sample, separate, identify and extrapolate chemical information in a complex food matrix [2,8,9]. In particular, gas chromatography coupled with mass spectrometry is used in foodomics for the quality control, authentication and characterization of the products of interest.

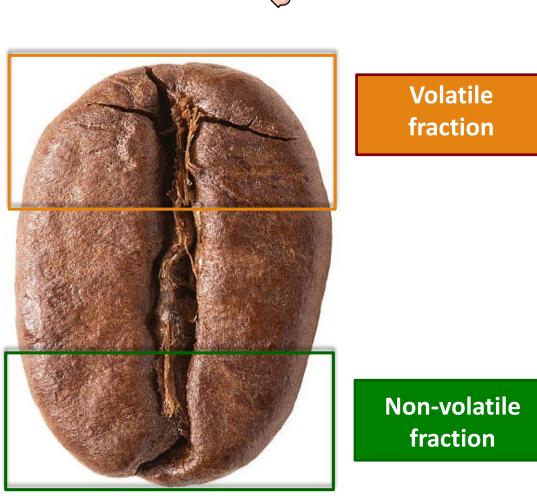
This work aims to study the chemical changes of coffee flavour investigating the contemporary evolution over time of the coffee volatilome and of its lipid fraction.

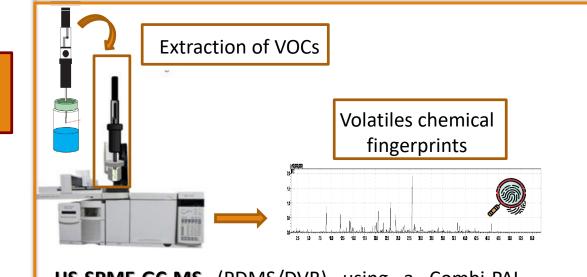


(III	Coffee Type	Blends	Species	Packs	
3 lots each					
1		В	100% Arabica	Eco, standard	
Capsule	sules available for Espresso coffee	Р	100% Arabica	Eco, standard	
		1	50% Arabica 50% Robusta	Eco, standard	



Sensorially not good, at T60 for Eco caps, at T150 for standard caps



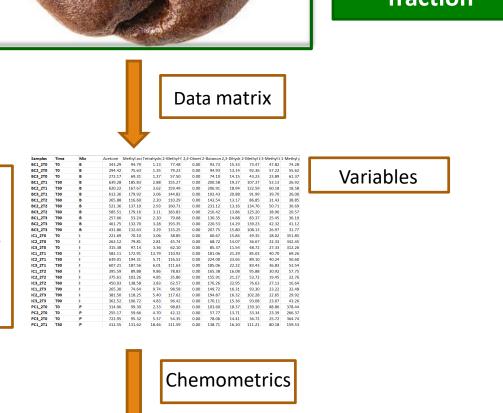


**HS-SPME-GC-MS** (PDMS/DVB) using a Combi-PAL AOC 5000 assembled on-line in a Shimadzu QP2010 GC-MS system, capillary column SGE SolGelwax 30 m x 0.25 mm  $d_c$  x 0.25  $\mu$ m  $d_f$ .

GC-MS Agilent 6890 GC-MS system, capillary

column Supelco SLB™-IL 76

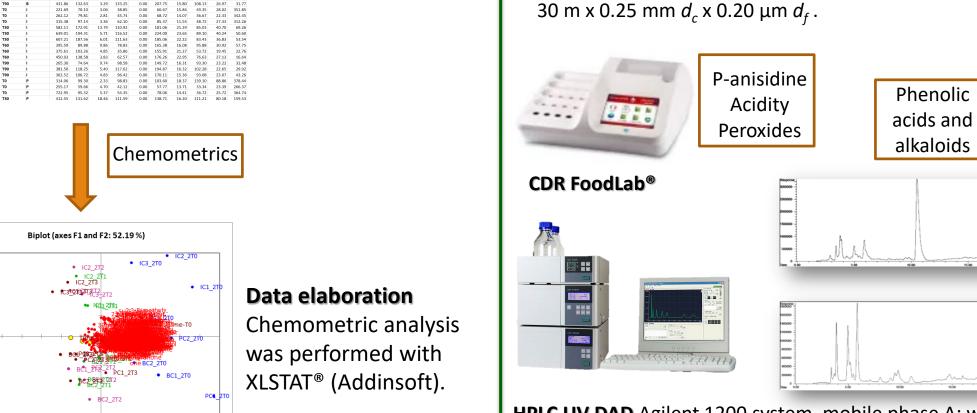
EFAs and FFAs (esterified fatty acids and free fatty acids)



-3 -2.5 -2 -1.5 -1 -0.5 0 0.5 1 1.5 2 2.5

• Time-T0 • Time-T30 • Time-T60 • Time-T90 • Centroids • Active variables

F1 (31.88 %)



**HPLC UV DAD** Agilent 1200 system, mobile phase A: water/formic acid (999: 1, v/v) and B: acetonitrile/formic acid (999: 1, v/v). Column Platinum EPS C18 reversed phase (250 x 4.6 mm, 80 Å, 5 μm), (Alltech, Deerfield).

276 nm

325 nm

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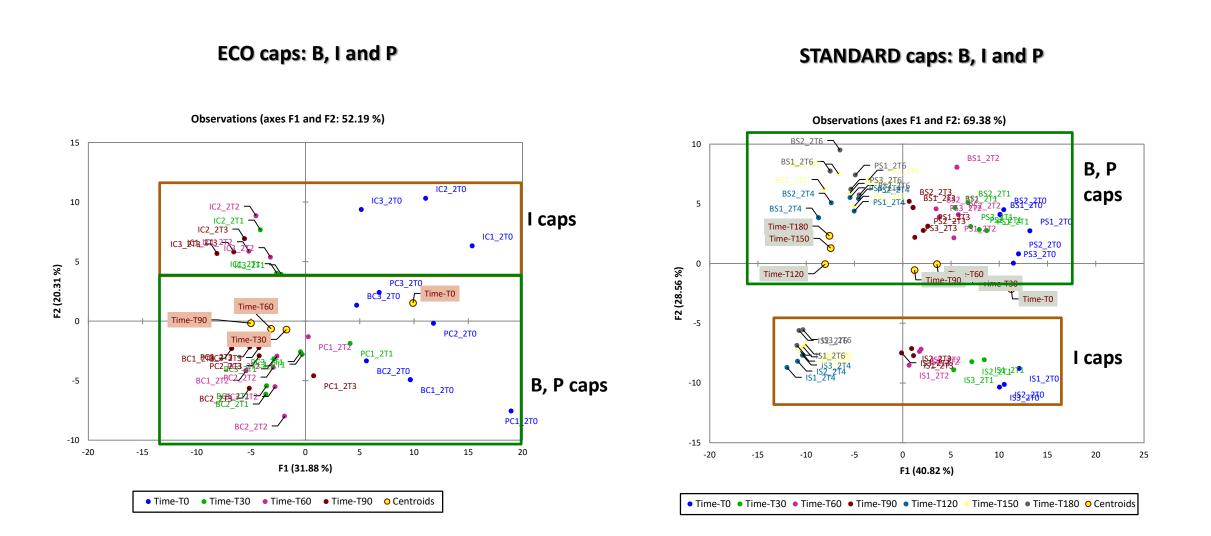
[7] Wenny B. Sunarharum W.B., Williams D.J., Smyth H. E. Food Research International 62 (2014) 315–325 [8] D. Bressanello, E. Liberto, C. Cordero, B. Sgorbini, P. Rubiolo, G. Pellegrino, M. Ruosi, C. Bicchi. (2018) Journal of Agricultural and

Food Chemisty. 66(27): 7096–7109 [9] G. Strocchi, E. Bagnulo, M. R. Ruosi, G. Ravaioli, F. Trapani, C. Bicchi, G. Pellegrino, E. Liberto, Food Chemistry submitted

# **Results and Discussion**



GC-MS data set were explored by **unsupervised multivariate analysis** to investigate diagnostic patterns.



PCA (Principal component analysis) score plots on **Eco caps** 

PCA (Principal component analysis) score plots on **Standard caps** 

The analytical data of the normalized responses for the Eco and standard capsules report a spread, along the F1 component from right to left, between the reference (T0) and the samples aged from T30:

In the **Eco caps**, at the initial monitoring time (T0), it is possible to notice a heterogeneous distribution, subsequently, however, from the time T30 the samples tend to cluster. In **standard caps**, samples result more homogeneous although a tendency to stand out among the starting times (from TO

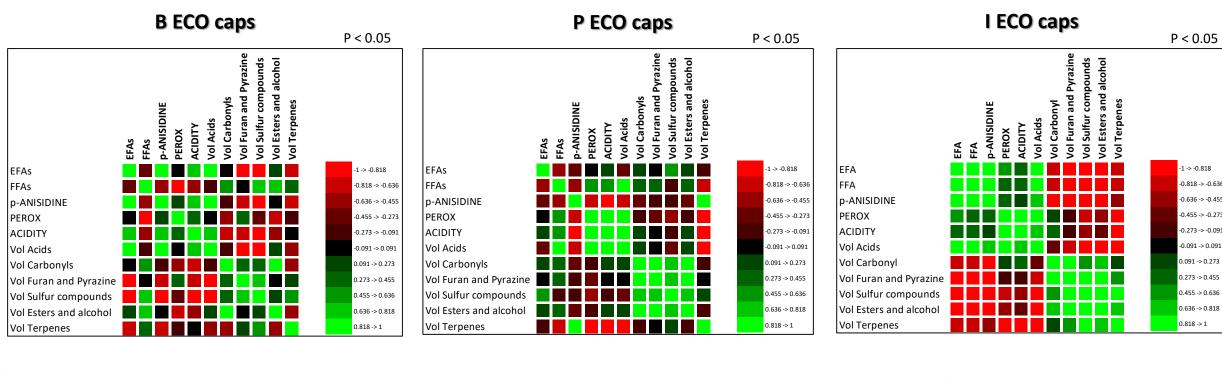
to T90) and aged samples (from T120 to T180). PCA of the Eco and standard caps, highlighted discrimination in terms of blends. I samples (50% of Robusta and 50% of

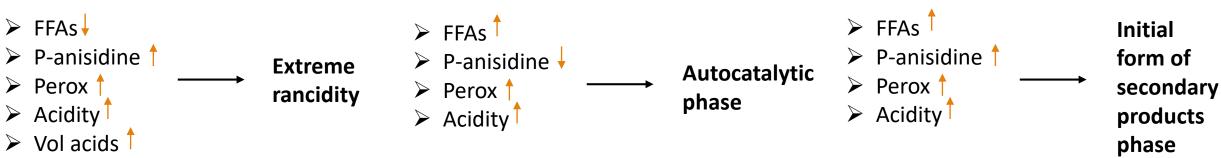
Arabica), in brown, are separated from the other blends, P and B, in green, that are 100% Arabica.





## Correlation between lipid fraction and aromatic fraction

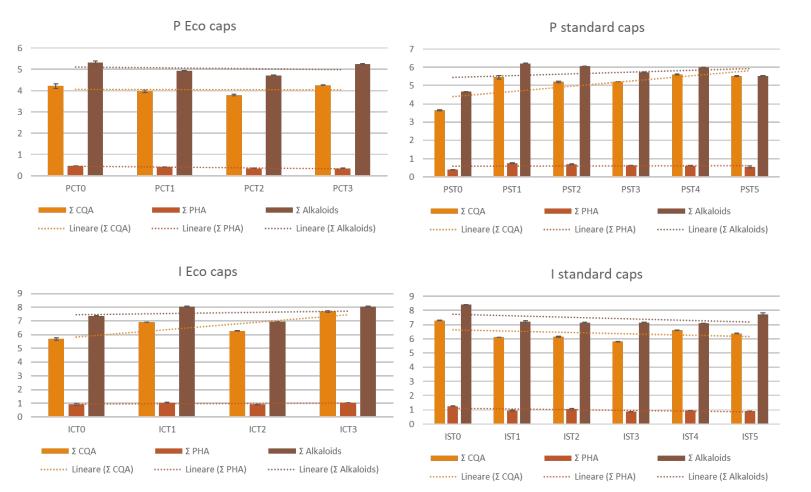




In **B caps** FFAs decreased for oxidative reactions conseguently to hydroleses of TAGs while anisidine together with Peroxides measures and vol acids increased.

**P and I** presented a comune trend in which FFAs increases together with the peroxides. What distinguishes the two blends is the different behaviour of anisidine.

## Phenolic fraction and alkaloids



In the phenolic fraction, composed by chlorogenic acids (CQAs), phenolic acids (PHA) and alkaloids, the compounds do not vary significantly (p>0.05). The fraction is very stable during time independently to the packaging and blend.

## **Conclusions**



This project investigated the sample volatile and non-volatile fractions. Among the volatiles constituting the coffee aroma, some markers describing the coffee aging independently from blends and packaging have been identified and also monitored over time in stress conditions. About the lipid fraction, it was evidenced the significant role played by the FFAs degradation and their derivatives on aging of samples. In any case, a different behaviour between blends and packaging was observed. About the phenolic acids and alkaloids, the fraction is very stable during the time independently to the packaging and the blend.

The next step would be to apply a fusion of data from the above analytical approaches in order to have a more comprehensive knowledge (omic approach) of the chemistry of coffee aging and the relationship of the interactions between taste and aroma at molecular level