Coffee sensory HS-SPME-GC-MS fingerprints for the "identitation" of the coffee oxidized note

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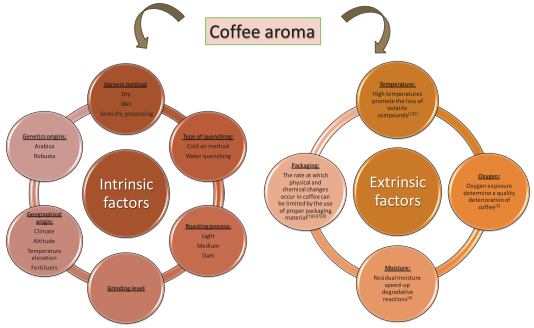
BACKGROUND

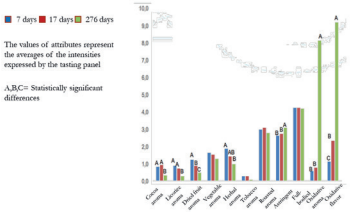
Good quality coffee flavor has been described as a balanced combination of flavor, body and aroma in the absence of faults. Flavor perception is represented by two feelings that strongly interact each other: aroma, perceived through the sense of smell perceived at the level of the oral cavity and related with non-volatile compounds. However, aroma results dominant in the flavor perception and can modulate the taste intensity. Behind the pleasure consumption, there is a deep investigation on coffee aroma as qualitative determinants of the product.



The quality of coffee flavor is a key step of the coffee production. Despite the relative stability of coffee in comparison to other foods, during the shelf-life of roasted coffee it was evidenced a variation in concentration and sensory potency of volatile compounds that brings to a loss of sensorial quality.
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 quality coffee study, there is a need for analytical techniques suitable for routine control (QC).

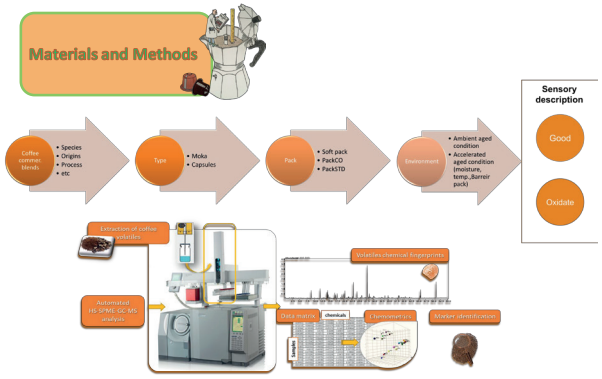
Aim

The project aims to the chemical characterization of the aroma and in particular, the target is the research of one or more chemical markers, that present a low acceptability, linked to the evolution of aromatic quality over time on coffees

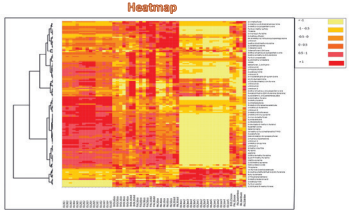


Sensory data, highlight a modification on sour taste, bitterness and aroma. In particular for aroma emerged an intense oxidized note that significantly increases over time. From here we started our work focusing on identifying the markers correlated with oxidation.

Materials and Methods



Results and Discussion



The HS-SPME-GC-MS revealed clearly a loss of some volatile components in aged samples as visualised on the heatmap. In particular, it is clear that the Moka samples are more oxidized than the caps in aged samples, visible by the yellow intensity related to the loss of compounds such as compounds containing sulfur, but also pyrazines, pyrroles and alcohols. The caps have a richer chemical profile in the good samples than the moka. What appears from the heatmap is also the different behavior between the two types of caps packaging: Eco caps show a poor profiles just in good samples, compared to packSTD one that become poorer in aged samples

References

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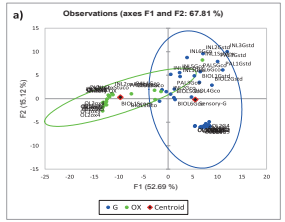
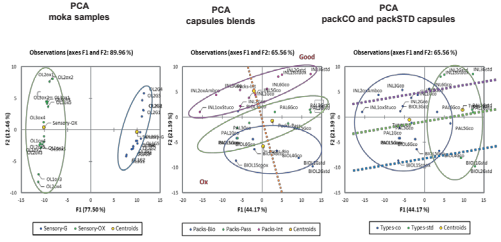
Chemometric unsupervised investigation: PCA



Principal component analysis (PCA), has shown two cluster of the samples, good and aged, as displayed here in the score plot.
Obviously the variability inside the groups is influenced by the variability of the samples.

The exploration within the different packaging reveals, a good separation between good samples and aged ones. Moka samples and-1t0he three Eco-caps blend showed that oxidized samples are separated on the first PC in function of the blends. Distribution of packCO and packSTD capsules shows that exists a diversity on the volatile profile between these two kind of packs and it is differently expressed depending from the blends. In the table are reported volatiles with a variation higher than 20% in aged samples. Here, it is visible that the aging trend of the volatiles is different and depends from the type of pack and storage conditions.



Chemometric supervised investigation: PLS-DA

Common volatile components of the different packaging higher in aged samples and their % of variation

	OL	BIO	PASS	INT	
	37°C 50%W	37°C 50%W	37°C 50%W	Room T	37°C 50%W
Acetic acid	82	90	115	29	94
Propanoic acid	165	103	95	28	112
1H-Pyrrole-2-carboxaldehyde	133	59	46	-14	21
5-(Hydroxymethyl)dihydro-2(3H)-furanone	228	71	25	-20	47

Supervised chemometrics method through Partial least square discriminant analysis (PLS- DA), confirm the volatiles highlighted in the PCA, showing that, some of them, are highly correlated with oxididation as displayed by the Pearson correlation. Among these, 4 chemical components, neither of them reported in literature yet, show common increased trends in oxidized samples independently of the packaging, blends or coffee preparation.

Conclusions and perspectives

These preliminary results show that the HS-SPME-GC-MS fingerprints combined with chemometrics is promising to study chemicals involved in the changes of coffee aroma during its shelf life. The chemical fingerprints affords to identify and define a "chemical identity" of the oxidized note in compliance with sensory evaluation.