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Identification of potential aroma markers of coffee oxidized note

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Aim and Scope

Coffee is considered a stable product with a long shelf-life, although, after roasting, it is still an effective 'chemical reactor' because of the high reactivity of its components. During storage, roasted coffee undergoes chemical and physical changes that can affect its quality. The changes in sensory properties are generally due to the loss of volatile compounds characteristic of the aroma of roasted coffee, and the appearance of ordidation products that can cause unpleasant flavours [2-4]. The loss of aroma freshness during storage, known as "staling", i.e. ".a sweet but unlovely flavour and marginal constel coffee which reflects the oxidization of many of the pleasant volatiles and the loss of others; a change in the flavour and the acid constituents causing a partial bland tone.." [5], mainly depends on temperature, humidity, presence of oxygen and barrier capacity of the packaging. Despite the number the studies in this field, they have always focused on one or two compounds in the expression of coffee loss of freshness and not on the synergism between the components responsible to give an oxidised perception in the whole coffee volatilome. Furthermore, due to the complexity and the dynamicity of the chemistry involved, coffee degradation studies have mainly been conducted on a single species, package or condition.

Therefore, defining the oxidation chemical footprint of coffee can be an objective valuable tool to be used in screening as a support to the sensory panel in testing new and more sustainable packaging. This study investigates the volatilome of good quality (from now "good" for short) and oxidised coffees (i.e. Coffea arabica (Arabica) and Coffea canephora, (Robusta)) in different packaging (i.e. standard with metallic barrier and Eco-caps) by combining HS-SPME-GC-MS/FPD with a machine learning approach to define a potential fingerprint describing the oxidised note of roasted coffee

Materials and Methods

Samples included thirty R&G (roasted and ground) coffees for moka preparation from three lots packed under vacuum in a multilayer film with a metallic barrier (M samples); a set of Eco-caps in modified atmosphere for espresso coffee (5 caps) from different lots of different blends named B and P (100% Arabica of different origins) and I (50/50 Arabica and Robusta) for a total of 30 samples.

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A portion of the coffee samples was maintained at room temperature and the other was submitted to accelerated ageing under stressed storage conditions in oven at 37°C and 50% relative humidity

> The samples were classified as good (G) and oxidised (OX) by a trained industrial sensory panel. The reference standard to define the oxidative note was a moka coffee that had been kept open for 4 months.

The oxidised note was defined as the intensity of the smell/aroma attributable to rancid notes, walnut oil, peanut shell, old dried fruit, and "old" coffee, also often referred to as a cardboard note, e.g. damp, or closed/stale pizza box directly/indirectly perceived by the olfactory organ. _____







GC-MS/FPD instrument set-up Injector temperature: 240°C; injector mode: splitless; gas carrier: Helium; flow rate: 1µl/min; fiber desorption time and reconditioning: 5 min;

column: SGE SolGelwax (100% polyethylene glycol) 30 m x 0,25 mm dc x 0,25 μm df (SGE- Melbourne, Australia); temperature program: from 40°C (2 min) to 200°C at 3,5°C/min, then to 240°C (5 min) at 10°C/min. Ionization mode: EI (70 eV); temperatures: Ion source: 200 °C; Quadrupole: 150°C; Transfer line: 260°C; Scan range: 35-350 amu. FPD detercor: 260°C.

Data elaboration Machine learning analysis was performed with Pirouette® (Infometrix) and XLSTAT® (Addinsoft). The heat map was created by gene-e (https://software.broadinstitute.org/GENE-E/)



3. Potential markers of the

oxidised coffee note

1. Chemical profiling of good and oxidised

Results and discussion

The analysed coffee samples were described by the 147 volatiles. In figure 1 is reported an illustrative pattern of the chemical signatures of the good and oxidised moka samples (M) visualized with a heat map of the normalized volatile responses versus the IS (n-C13). Samples are clustered using ascendant hierarchical clustering based on Euclidean distances using the average linkage agglomerative method. The samples in the heat map are clustered into two groups, good (MG) and oxidised samples (MOX). A comparison of the two groups enables us to distinguish the pool of components in lower abundance (in orange), i.e. those that are lost or degraded with the oxidation of coffee, from the components that are more abundant in the MOX samples (in brown), indicating their possible formation or increase with oxidation





71/147 volatiles were found with a VIP (variable importance in projection) > 1 in describing the oxidised samples (Figure 2).

VIP scores estimate the importance of variables in the projection used in the PLS-DA model and are often used to select variables; when a variable presents a VIP that is close to or greater than 1, it can be considered important in the given model.

Twenty-five highly significant volatiles describing the oxidised coffees with a similar trend in all of the investigated blends and packaging, and with a CV% of at least 20, were identified as potential markers of oxidised coffees.

Most of them are present in lower amounts in oxidised samples, few are already known to decrease over time and others behave differently from previous studies. These components are all heterocycles and are highly reactive, in particular in the presence of moisture and oxygen, which may explain their decrease in oxidised coffees

The coffee volatilome includes both odourant and nonodourant compounds, the latter of which contribute to synergism in the aroma perception. In figure 3 is reported the 'sensory footprint" of volatiles describing oxidized note.



These data show that several volatiles are more abundant in oxidised samples and, some of them, are common to all packaging. Although the coffee aroma is the result of synergism between several volatiles, some of those that are better correlated to oxidation have been described as having an unpleasant odour

Conclusions and future perspectives

enty-five target components of the coffee volatilome have been identified as markers of coffee oxidation because they present the same behaviour and statistical meaning in all of the investigated samples, The literature survey suggests several compounds although not standardized as markers of decrease of aroma quality of R&G coffee auring storage. However, most of the suggested markers and indices seem to be more closely related to the freshness of the coffee aroma. These data provide information on the oxidised note and demonstrate that artificial intelligence can successfully be used to define instrumentally define the evolution of the quality of coffee aroma over time, and can be an objective valuable tool to be used in screening as a support to the sensory panel [6-8] in testing new and more sustainable packaging, driving the research toward the developing of Artificial Smelling Machine tools.

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