



CASE STUDY :

Coffee Aroma

This study performed for MaxiCoffee quantified ground coffee aroma degradation during the first few hours after grinding. Aryballe also examined the characteristics of the aroma and how it evolved over time after grinding.



In this study, Aryballe worked with MaxiCoffee, a French group specializing in the world of coffee, to study the degradation of aroma of coffee beans immediately after they are ground. The goal of the study was to analyze and quantify the differences between aroma of fresh ground beans and pre-ground and packaged coffee.





Determining aroma loss post-grinding

This study examined three different coffee brands provided by MaxiCoffee. The samples were provided to Aryballe in sealed packs with 250 g of coffee beans each.

To prepare the samples for measurement, coffee beans were ground immediately after opening of a sealed package. The same grinder with the same amount of coffee and the same grain size was selected for the grinding. This allowed us to maintain consistency throughout the grinding phase—which means that the initial aromatic loss due to the friction generated by the grinding wheels remained constant.

Approximately 100g of coffee beans were poured into the beans tray of a professional coffee grinder provided and preconfigured by MaxiCoffee; beans were then ground; first few tens of grams of coffee powder were discarded (used to clean up the grinder); finally, 20 g of coffee powder was poured into 100 ml sampling vials.

An artificially aged coffee powder was used as a negative control. To achieve aging effect, a normally prepared coffee powder sample was left open for 3 days under the laboratory hood. This negative control sample was measured alongside the fresh coffee samples.

The table below details the samples and their notations used throughout this report.

Sample Name (Brand)
Coffee A
Coffee B
Coffee C
Negative control (aged 3+ days)

Table 1: Coffee Samples Details





Coffee powder samples are hygroscopic and absorb humidity from the surrounding air when measured. Thus, measurements of these samples required the use of the Amplifier to acquire a stronger signal than in the case of direct

measurement and to separate humidity from odor VOCs. The HeptaValve Mini was used during the coffee powder samples to ensure reproducibility of the results over a few days.

Results

A typical measure of a coffee sample (with Amplifier) is shown on Figure 1. Three peaks (zones) are highlighted. First - a valve switch artifact, second - the humidity zone where water

molecules desorb from Tenax resin and contribute to the signal, and finally a third - the region of interest where the odor molecules create a peak signal for the sensor.

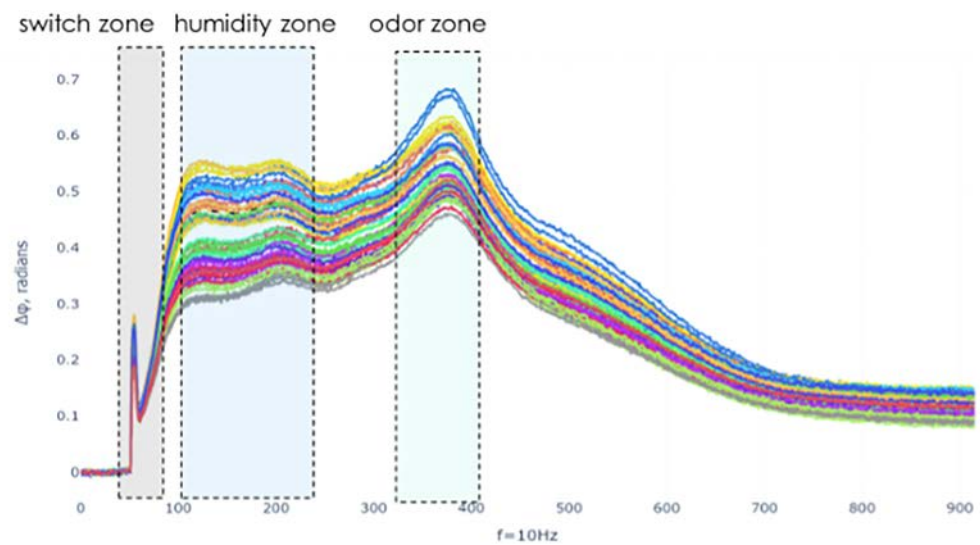


Figure 1: Typical raw signal (all peptides) profile of a coffee sample acquired with the amplifier.



This measurement cycle was repeated over the course of the study for each of the coffee powder samples to capture the change in intensity of the odor over time.

The intensity of the odor for each sample over time is represented as percentage of initial odor intensity after subtracting the residual signal (negative control). This normalized graph is shown on Figure 2.

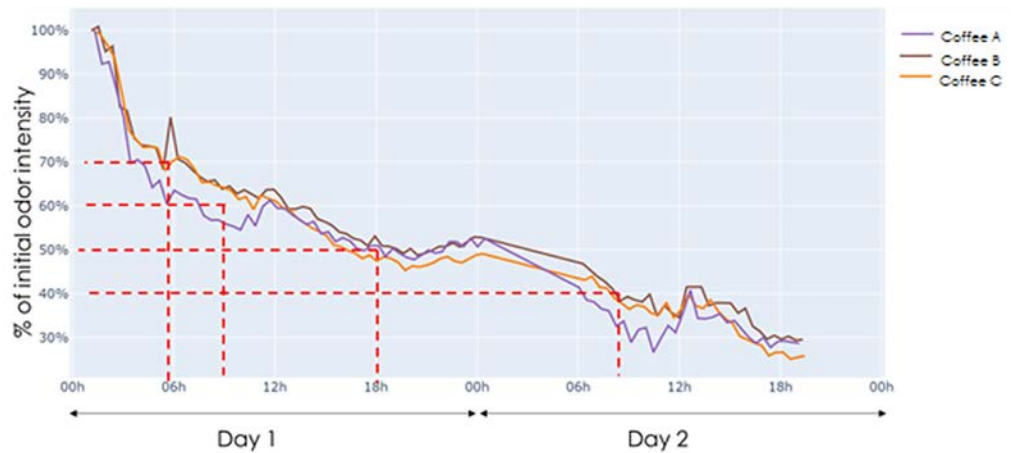


Figure 2: Coffee samples normalized mean peak values over time. Normalized between each of the sample's initial (maximum) value and negative control mean value (minimum).

Figure 2 shows that the odor intensity decrease has an asymptotical behavior: intensity drops dramatically over the first hours, then stabilizes and reaches equilibrium towards the end of experiment. The red dotted lines in figure 2 show percentiles for different amount of odor loss.

In looking at the change in aroma over a 24-hour period for the different type of storage, the results showed that freshly ground coffee loses significant intensity over a period of 24 hours.



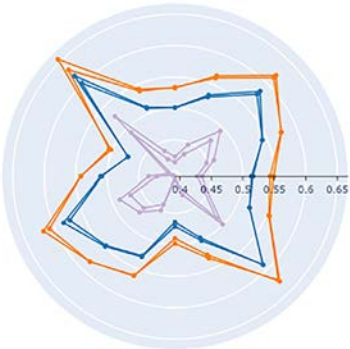


Figure 3: Absolute intensity

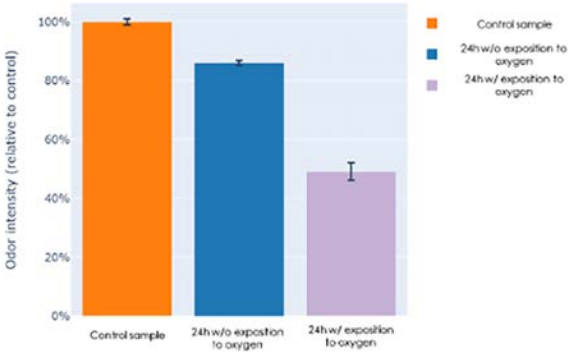


Figure 4: Relative intensity

We can conclude that freshly ground coffee will lose greater than 15% of its aroma in just 24 h without

exposition to oxygen and will lose greater than 50% of its aroma in just 24 h when left in open container.





Examining changes in aroma character

In the second part of this study, reference VOCs (molecules) were used to construct a database of the pure signatures of some of the well-known coffee odor notes. The relation between certain odor notes and their underlying chemical compound responsible was investigated by numerous contributors and overviewed by Buffo et al . For this study, five major notes were targeted. Their corresponding chemical names and reference CAS numbers are detailed in the table below.

Odor Note	VOC (chemical compound)	Phase	Reference (CAS)
Caramel, sweet	Strawberry furanone	Solid, easily melting hygroscopic powder	strawberry furanone, 3658-77-3
Cocoa, nutty, almond	2-methyl furan	Clear liquid	2-methyl furan, 534-22-5
Fruit, honey	Beta-damascone	Clear liquid	beta-damascone, 35044-68-9
Toast, roast, sulfurous	Furfuryl mercaptan	Yellow oily liquid	furfuryl mercaptan, 98-02-2
Smoke, spice, woody	Guaiacol	Clear liquid	ortho-guaiacol, 90-05-1

Table 2: Reference compound details





Chemicals were purchased in sample quantities at Sigma-Aldrich specifically for the study. 0.2 ml of each liquid compound (1 mg of strawberry furanone) were poured into 100 ml vials and connected to HeptaValve Mini for measurements.

Chosen pure chemicals have strong distinct odor and do not require amplification or humidity removal so they were measured directly by the NeOse Advance. The HeptaValve Mini was used to automate the acquisition. The obtained signatures were stored in the database and were later used in analysis.

Specific peptide response variation

To study how different specific odor notes behave, we mapped Aryballe sensor peptides responses to specific chemical compounds that attribute

to different aroma notes. The peptide normalized responses on five major reference compounds are shown on Figure 5.



Figure 5: Signatures of five reference compounds represented as a colored table (green - low, magenta - high). Prominent peptides are marked with yellow asterisks.





In Figure 5, rows are reference compounds and columns represent peptides. Values are color mapped (green – low response, magenta – high response). Using this reference

database, we can conclude on which peptide pairs contribute the most to which compounds. These prominent peptides were mapped for each compound and shown in the Table 3.

Odor Note	VOC (chemical compound)	Prominent Peptides
Caramel, sweet	Strawberry furanone	24, 66
Cocoa, nutty, almond	2-methyl furan	23, 63
Fruit, honey	Beta-damascone	22
Toast, roast, sulfurous	Furfuryl mercaptan	20, 28
Smoke, spice, woody	Guaiacol	25, 29

Table 3: Prominent peptides for each of the reference compounds

We then studied the normalized signatures for each coffee power sample to see how the response of

the targeted peptides changed over time. These results can be seen in Figure 6.

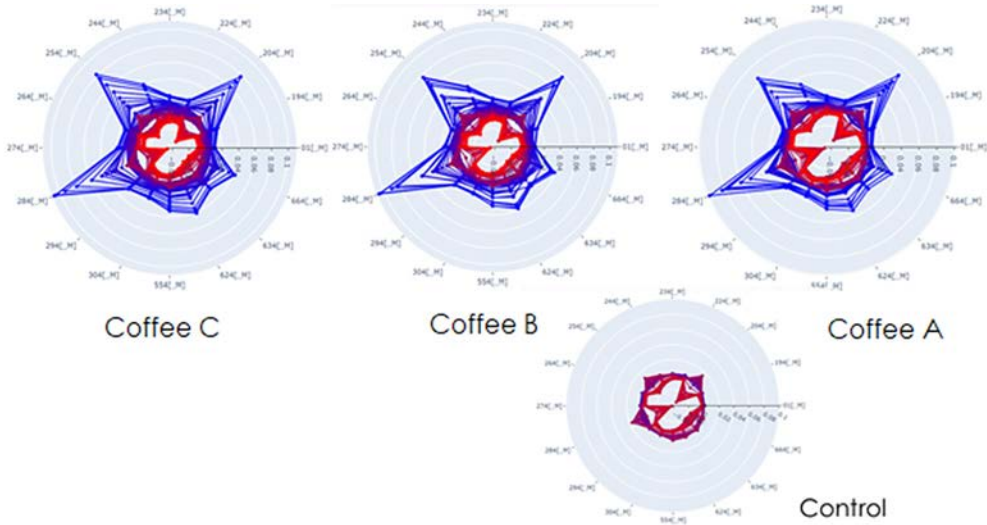


Figure 6: Coffee samples' normalized signatures over time with blue showing the initial signature and red the signature at the end of the study. It is observed that different peptides' responses decay with different rate. Peptides 254, 284 and 204 show the most variation.





These peptide intensity variations are linked to the odor note mapping we created in Figure 5. Figure 7

shows the intensity drop for different peptides grouped using the odor note mapping.

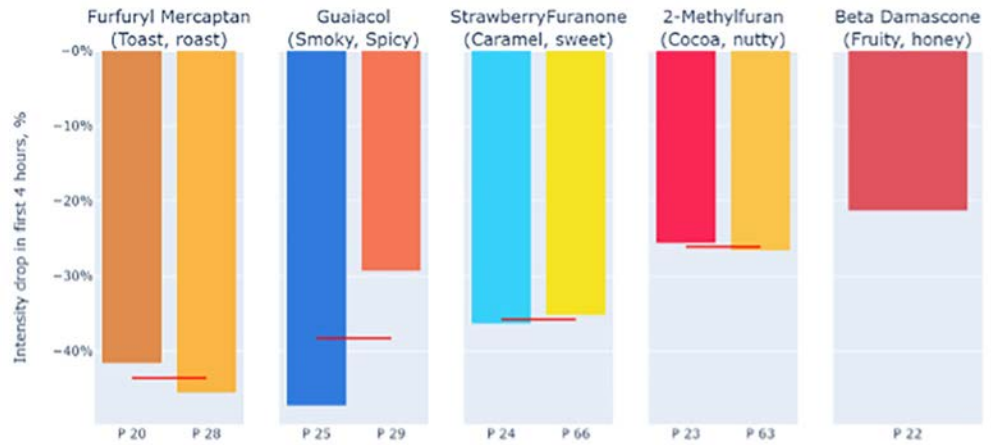


Figure 7: Intensity drop during the first 4 hours for one of the coffee samples (Coffee B), grouped by odor notes and their prominent peptides (each subplot corresponds to a note and bars denote peptides). Red horizontal line on each subplot denotes a peptide average per odor note.

This part of the study showed that toast/roast odor notes degrade twice as fast as fruity/honey ones

while caramel and nutty notes behave somewhere in between.





Conclusion

Part one of this study found that ground coffee odor degrades over time and the rate of this degradation was quantified. **Fifty percent of initial flavor is lost during the first 24 hours after grinding.** The second phase of the study found that different aroma notes degrade at different rates.

Armed with this data, MaxiCoffee can confidently point to the higher quality coffee experience enjoyed by consumers who buy whole beans and grind them before brewing rather than purchasing pre-ground and packaged coffee products. Aroma and flavor notes are a critical part of the coffee-drinking experience, and not only does this study show that intensity is lost over time but that the aroma profile actually changes significantly as different flavors degrade faster than others, potentially leading to a much different cup of coffee than the roaster and producer intended.





About Aryballe

The best human noses can distinguish 10,000 odors. Unlike color and sound, smell does not fall along a clear spectrum, making it hard to compare various odors. But Aryballe is helping to change this by evaluating characteristics of individual scent molecules and testing them against a data-base of known smells using a combination of biochemistry, advance optics and machine learning.

Based in Grenoble, France and founded in 2014, Aryballe combines biochemistry, advanced optics and machine learning to mimic the human sense of smell. The company's premier product offering, NeOse Advance, uses silicon photonics technology to detect, record and recognize odor data, which powers improved decision making for R&D, quality control, manufacturing and end-user experiences. Aryballe Suite, the company's cloud-enabled software, enables customers to intuitively access and customize analysis of odors based on their unique needs. With operations in France, South Korea and the USA, Aryballe works with global leaders in automotive, consumer appliances, food manufacturing and flavor & fragrances.

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