

Objective

Competitive benchmarking, which consists of comparing one's products or processes to the leaders' ones, is a technique commonly employed by companies. This type of studies allows to position one's products in the market versus competitors and to give indications in order to improve, re-engineer or re-formulate products.

In this study, an Electronic Nose and an Electronic Tongue were used to analyze and compare several varieties of coffees from two brands of coffee capsules. The objective was to get detailed sensory information about these two brands of coffee capsules and compare them to each other on the coffee intensity scale.



Materials & Methods

Samples

Twelve samples of coffee were prepared in "real" conditions using a Senseo coffee machine, then analyzed with HERACLES electronic nose and ASTREE electronic tongue.

Brand	Label	Intensity	Origin
Senseo	SD00	Decaffeinated	
	SB05	5	Brazil
	SE06	6	
	SK06	6	Kenya
	SC07	7	Colombia
	SU08	8	
	CD03	3	
	CC04	4	Colombia
Carte Noire	CK06	6	Kenya
	CE08	8	
	CE09	9	
	CE11	11	

Each brand defined its own intensity scale:

- -1 to 10 for Senseo
- 3 to 11 for Carte Noire.



E-Sensing Instruments

Tests on odor and taste attributes were conducted respectively with HERACLES electronic nose and ASTREE electronic tongue (Alpha MOS, France).

The HERACLES is based on the technology of ultra fast chromatography, with two metal columns of different polarities (MXT-5 and MXT-1701, length = 10m, diameter = $180\mu m$, Restek) in parallel and coupled to 2 Flame Ionization Detectors (FID).

Two chromatograms are obtained simultaneously, allowing a sharper identification of the chemical compounds.

The integrated solid adsorbent trap thermoregulated by Peltier cooler (0-260°C) achieves an efficient pre-concentration of light volatiles and shows a great sensitivity (in the pg range). The electronic nose is coupled to an autosampler (PAL3 RSI CTC Analytics) to automate sampling and injection. The analysis was conducted with headspace injection mode. The HERACLES e-nose was additionally equipped with AroChemBase module (Alpha MOS, France). It consists of a library of chemical compounds with name, formula, CAS number, molecular weight, Kovats retention sensory attributes and bibliography. It allows pre-screening chemical compounds and giving sensory features directly clicking the chromatograms' peaks generated by HERACLES e-nose.

The ASTREE electronic tongue analyzes organic and inorganic compounds dissolved in liquids that are responsible for taste. The detection principle is based on a potentiometric measurement with seven ChemFET (Chemical modified Field Effect Transistor) sensors.



Data acquisition and data processing was achieved with AlphaSoft software (Alpha MOS, France) for the two instruments. The analytical parameters optimized for this analysis are described in table 1.



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HERACLES electronic nose parameters					
Sample mass	1g of coffee solution in a 20mL vial				
Head space generation	20 min at 70°C				
Injected volume	5 mL				
Trap temperature	60°C / 240°C (desorption)				
Columns program	50°C to 80°C by 1°C/s and 80°C to 280°C by 3°C/s				
FID temperature	260°C				
ASTREE electronic tongue parameters					
Sample preparation	Coffee preparation with one capsule and deionised water				
Sample volume	25 mL				
Acquisition time	120 s				

Table 1: Analytical parameters of the instruments

Odor analysis

The comparison of the chromatograms obtained with HERACLES e-nose shows some significant differences between the flavor profiles of the two brands and the intensity of the coffee (Figure 1).

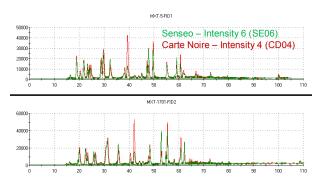


Figure 1. Superimposed chromatograms of 2 samples of coffee capsules, obtained with HERACLES e-nose

An odor map based on Principal Components Analysis (PCA) was generated based on all volatile compounds detected in the headspace of coffees (Figure 2). The Carte Noire coffees show a large difference of intensity on odor map, whereas Senseo coffees seem to have a closest odor fingerprint.

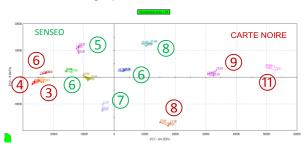


Figure 2: odor map of coffees based on Principal Components Analysis (PCA) with all peaks

The nature of the most discriminant volatile compounds involved in coffee flavor was investigated using their Kovats index and the ArochemBase (Table 2).

Discriminant compounds are evaluated based on a comparison of peaks' area (Figure 3).

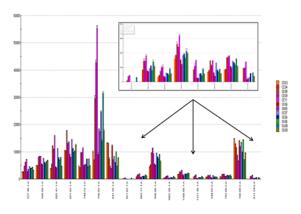


Figure 3. Concentration of various volatile compounds responsible for the discrimination between the 12 samples



A correlation between the sensory information about coffee intensity available on the packaging and the HERACLES results can be done (Figure 4). The model shows a high correlation (correlation coefficient = 0.9316), which allowed to project the decaffeinated sample on this model to estimate its intensity: it is close to the intensity of Senseo n°5.

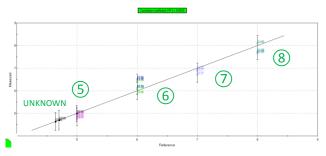


Figure 4. Sensory score correlation with the HERACLES results on Senseo samples – Projection of SD00 as an unknown sample

RT MXT-5 (± 0.1s)	RT MXT-1701 (±0. 1s)	KI MXT-5 (± 20)	KI MXT-1701 (± 20)	Possible identification	Descriptors
16.4	18.3	446	545	Ethanol	Alcoholic
20.3	20.03	527	593	Methyl acetate*	Etheral, fruity
24.0	26.4	599	692	2,3-butanedione	Butter, caramelized, creamy
24.6	23.3	605	645	2-methylfuran*	Burnt, chocolate, metallic, musty
28.7	30.8	652	742	3-methylbutanal	Almond, fruity, green, toasted
29.7	30.8	662	742	2-methylbutanal	Almond, cocoa, green, malty
31.3	35.0	678	782	n-butanol*	Fruity
32.4	35.7	693	790	2,3-pentanedione	Butter, caramelized, sweet
36.2	38.9	729	822	Pyrazine	Nutty, roasted hazelnuts
38.1	40.5	745	840	Pyridine*	Rancid, acid
39.0	41.9	757	856	2-Methyl-1-butanol	Butter, malty
45.9	47.1	821	911	Ethyl 2-methylbutyrate	Fruity, green, sweet
47.8	53.0	841	985	Furfural	Almond, bread, sweet
48.8	55.5	851	1021	3-methylbutanoic acid	Rancid, acid
59.7	58.1	983	1062	Ethyl hexanoate	Apple, fruity, sweet
60.7	60.9	997	1106	3-octanol	Nutty, mushroom
66.1	68.4	1083	1249	4-hydroxy-2,5-dimethyl-3(2H)-furanone	Baked, burnt sugar, caramelized
67.7	65.2	1107	1186	Tetramethylpyrazine	Chocolate, cocoa, coffee, nutty, roast
68.4	65.7	1121	1196	Nonanal	Floral, fruity, green, sweet

^{*} Most correlated to coffee intensity

 $\label{thm:compounds} \textbf{Table 2: identification of the most discriminant compounds using ArochemBase}$

Taste analysis

Based on ASTREE measurements, it can be observed that the 2 brands of coffees show very different taste profiles (Figure 5).

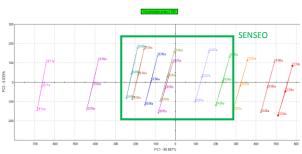


Figure 5. Principal Components Analysis (PCA) on ASTREE measurements for all coffee samples

There is a clear difference between the Carte Noire samples but the Senseo products are more homogeneous and show a closer taste profile.

The taste of the coffees proves also to be well differentiated, especially on sour attributes and a taste ranking is created (Figure 6).



Figure 6. Taste ranking of Carte Noire samples on sourness intensity

Odor and taste analysis

HERACLES and ASTREE data are merged to make an overall profile comparison of coffee products: odor and taste information are associated to the different samples. A PCA is created with this data fusion (Figure 7).

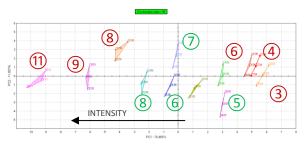


Figure 7. Principal Components Analysis (PCA) on Data Fusion



Conclusion

This benchmarking study conducted on various brands of coffees with sensory analysis instruments (e-nose and e-tongue) showed that the major differences were related to odor and flavor characteristics.

The SENSEO coffees have close profiles on taste and odor. On the opposite, we have a clear discrimination among the CARTE NOIRE coffees.

A scale of the coffee intensity is made and could be used to evaluate other coffees from these brands.