Chemical signature characterization of different coffee aroma notes

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GLOBAL SPECIALTY COFFEE EXPO APRIL 20 - 23 2017 SEATTLE WASHINGTON STATE CONVENTION CENTER

Aim and Scope

The perception when drinking a cup of coffee is a complex multisensory experience. The perception of a cup of coffee involves all our senses, emotions and cognitive processes [1, 2] Figure 1. Aroma is a primary hedonic aspect of a coffee and plays a fundamental role in addressing the choice [3]; its composition can therefore be considered as a signature of the products [4, 5].

A pleasant multisensory experience

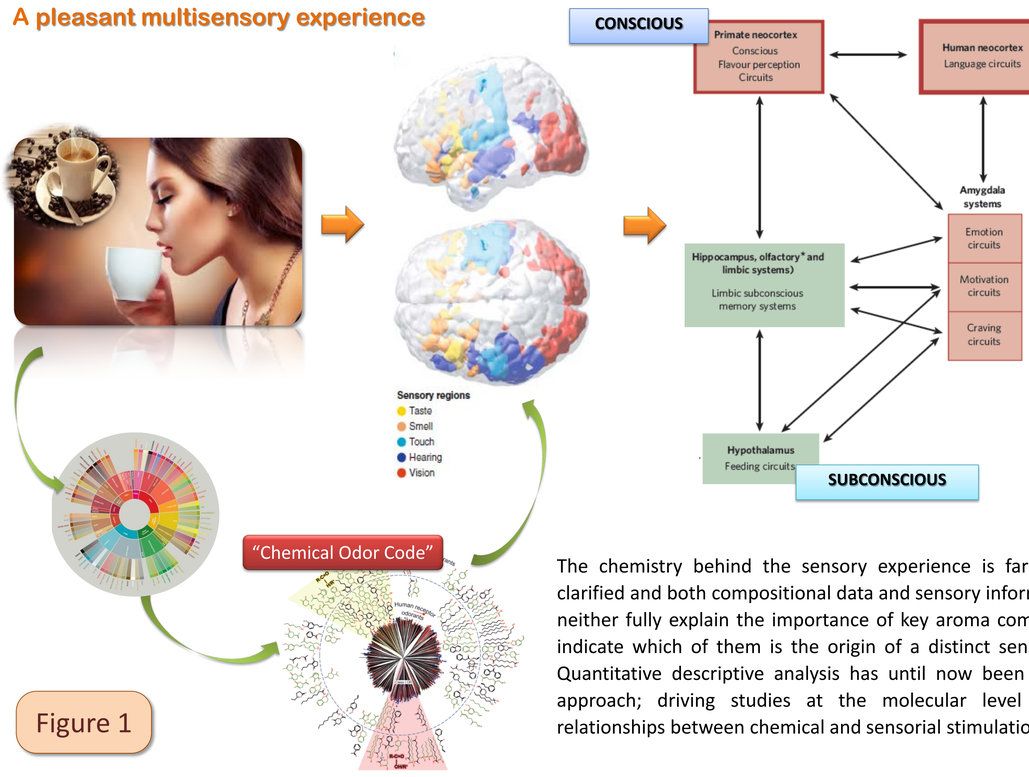


Figure 1

The chemistry behind the sensory experience is far from being clarified and both compositional data and sensory information alone neither fully explain the importance of key aroma compounds, nor indicate which of them is the origin of a distinct sensory note(s). Quantitative descriptive analysis has until now been the sensory approach; driving studies at the molecular level to disclose relationships between chemical and sensorial stimulation.

The sensory lexicon relating to coffee is a descriptive tool employed worldwide to define aroma and flavor attributes in a quantifiable manner, i.e. through scaled scores, and it can validly be used by trained professionals to evaluate a coffee; two different panels will obtain the same intensity score for each attribute [6]. Nevertheless, consumers are not familiar with these descriptors, and are mainly attracted by sensory emotions deriving from consumption of this enjoyable food. Moreover, individual perceptions differ because of genetic variability, which influences codification by the odor and taste receptors. In this context, sensometrics becomes a bridge linking these two sensory properties, providing the chemical information behind them; it can be used in product/blend development, benchmarking new products and evaluating their probable market impact, quality assurance and control, and in predicting preferences based on formulation changes.

The aim of this study is to reveal the chemical odor code (the signature) of different coffee aroma notes through a sensometric investigation of the relationships between volatiles compounds of coffees and sensory evaluations [7-8].

Coffee samples were sensorially evaluated through monadic profiling and analyzed by HS-SPME-GC-MS to obtain the fingerprints of their volatile fraction, and the results correlated through a statistical analysis.

Results show a high degree of association between chemical components and sensory evaluation affording the quali-quantitative identification of the volatiles related to a peculiar note and, thereby, to its chemical odor code.

Sensometric discipline unites sensory perception with mathematic and statistic tools studying for the relationship between several sensory attributes and chemical descriptors as a guide to the consumer behavior and consumer likings.

Sensometrics as a driver tool? Flowchart

Coffee samples
Peculiar sensory characteristics
indipendently from species, origins, post-harvest treatments

CHEMO-SENSORY EXP DESIGN STANDARDIZATION	Sensory evaluation by Quantitative Descriptive Analysis (QDA)	Chemical analysis Targeted coffee aroma fingerprinting HS-SPME-GC-MS
DISCRIMINATIVE & INFORMATIVE	1-way ANOVA of the sensory scores by trained assessors	PCA and Heat Map exploration of the relationship between sensory attributes and note-related compounds
	Samples' Qualitative Descriptive Analysis and sensory comparison between coffees	LDA and refining in the extraction of most significant note related odor-actives
PREDICTIVE		PLS regression to develop a note sensory prediction model and confirmation of its predictive ability
	Sensory confirmation	Quantitation and Model note formulation

Materials & Methods

Coffee Samples

100 roasted ground coffee samples with distinctive sensory notes, *Coffea arabica* L. (Arabica) and *Coffea canephora* Pierre (Robusta), originating from different countries and suitable for a coffee-filter machine were analyzed.

The roasting degree of each sample was carefully measured by ground bean light reflectance, with a single-beam Neuhaus Neotec Color Test II instrument (Genderkesee, Germany) at a wavelength of 900 nm, on 25-30g of ground coffee. Roasting degree was set at 55°Nh, to be close to the international standardization protocol for cupping (SCAA, 2015). Samples were roasted within 24 hours prior to cupping, and left for at least 8 hours to stabilize.

SPME sampling and GC-MS conditions

SPME fibres coated with 65-µm thick polydimethylsiloxane/divinylbenzene (PDMS/DVB) were purchased from Supelco (Bellefonte U.S.A). 1.5g of roasted coffee powder was sampled at 50 °C for 40 min after ISTD (C13) pre-loading. Analyses were run on a GCMS-QP2010 system equipped with an autosampler combi-PAL AOC 5000 Autoinjector (Shimadzu - Milano, Italia).

The GC column was a SGE SolGelwax (100% polyethylene glycol) 30 m L x 0.25 mm d*c* x 0.25 µm d*f* (SGE- Melbourne, Australia). Helium (2mL/min) was used as carrier gas. The oven temperature was programmed as follow: 40°C (1 min.) - 3°C/min. - 200°C - 10°C/min. – 250°C (5 min.). The injector was fitted with a liner suitable for SPME analyses and was set at 230°C in split mode (split ratio: 5/1).

The MS spectrometer was set as follow: ionization mode: electron impact, ionization energy: 70eV, m/z interval 35-350 m/z, transfer line temperature: 250°C, ion source temperature: 200°C.

Quantitative Descriptive Analysis

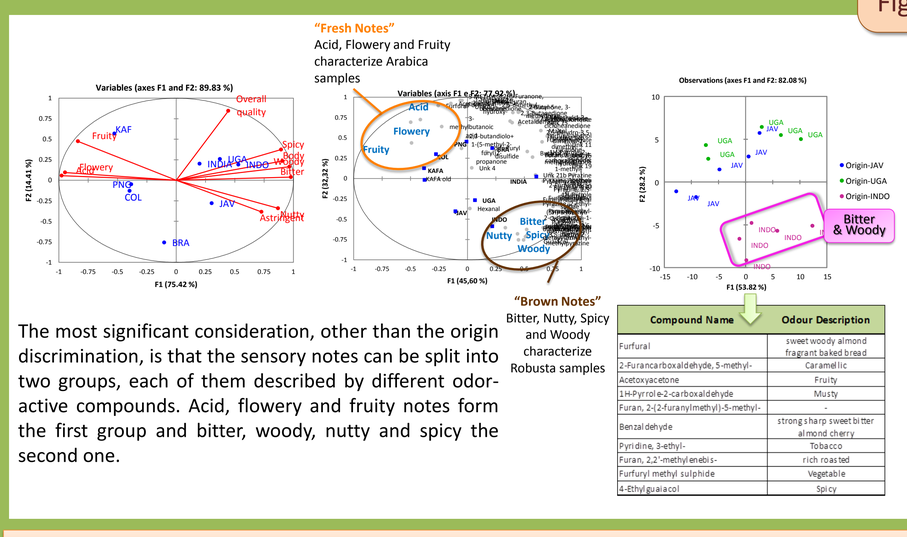
The samples were submitted to sensory evaluation by a panel of five experts following the SCA protocol. The protocol entails three tasting steps, after roasting to a set color (55-60° Nh) and eight hours of sample stabilization: i) evaluation of the aroma by sniffing the dry ground coffee, ii) evaluation of the aroma by sniffing the brew three minutes after its preparation and stirring, and iii) flavor evaluation after 8-10 minutes . Other attributes such as aftertaste, acidity, body, and balance are evaluated by tasting the brew, spraying it into the mouth to maximize retro-nasal vapors. Cup quality was assessed for several attributes. Those considered for this study were: flavor (flowery, fruity, woody, nutty, spicy), acidity, bitterness, body, astringency and aroma intensity. Quality and intensity of each attribute were evaluated simultaneously, upon a scale from 1 to 10. Chemometrics was run by XLSTAT (version 2015.5.01.23164) software, copyright Addinsoft 1995-2015.

Results and Discussion

Qualitative Descriptive Analysis (QDA)

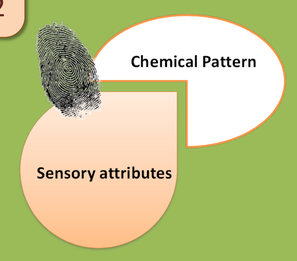
In QDA, a panel of trained assessors rates, for a number of products, the perceived intensities of distinct attributes on scales according to reference documents for specific food commodities (e.g. coffee, olive oil) or depending on the panel experience and on the complexity of the products. By averaging these intensity ratings and replicates it is possible to obtain a data matrix where rows represent the food samples and columns the relative sensory attributes used to describe them. The analysis of this data matrix by PCA can give information on how coffee samples are related and which sensory attributes better describe each sample Figure 2.

Figure 2



The most significant consideration, other than the origin discrimination, is that the sensory notes can be split into two groups, each of them described by different odor-active compounds. Acid, flowery and fruity notes form the first group and bitter, woody, nutty and spicy the second one.

Compound Name	Odour Description
Furfural	sweet woody almond fragrant baked bread
2-Furancarboxaldehyde, 5-methyl-	Caramellic
Acetoxyacetone	Fruity
1H-Pyrrole-2-carboxaldehyde	Musty
Furan, 2-(2-furanylmethyl)-5-methyl-	-
Benzaldehyde	strong sharp sweet bitter almond cherry
Pyridine, 3-ethyl-	Tobacco
Furan, 2,2'-methylenebis-	rich roasted
Furfuryl methyl sulphide	Vegetable
4-Ethylguaiacol	Spicy



The percentage contribution on the whole aroma fingerprint of each compound resulted highly correlated with a particular attribute and has been monitored across the different samples in order to investigate the relationship between these compounds and the expression of each peculiar sensory characteristic between samples. Figure 2

Quali-Quantitative chemical information

The "Heat Map" of the samples scored by the percentage contribution of the compounds resulted highly correlated respectively with the woody, nutty and "fresh" notes (acid, flowery/fruity) Figure 3. The slots in each row are colored according to the magnitude of their values, from dark (low percentage) to light color (high percentage); for instance, compound #82 (guaiacol) mainly contributes to the profiles of INDO, UGA and JAVA samples. INDO samples had the highest contribution from variables related to woody. INDIA samples, despite of their origin (i.e. Arabica), show sensory characteristics similar to Robusta confirming also from a chemical point of view the sensory scores given by the panel.

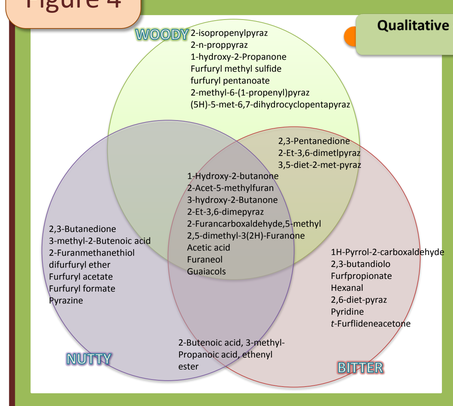
Figure 3

Woody	BRA	COL	JAV	UGA	PNG	INDIA	INDO	KAFA
82	0.38	0.42	1.01	1.56	0.48	0.74	2.02	0.44
81	1.05	1.05	1.67	1.37	1.12	1.32	1.71	1.03
38	0.1	0.08	0.13	0.12	0.08	0.12	0.14	0.07
93	0.32	0.3	1.19	1.25	0.3	0.61	2.22	0.17
67	0.18	0.15	0.35	0.29	0.15	0.34	0.4	0.18
91	0.27	0.29	0.53	0.66	0.3	0.4	0.71	0.29
21	2.87	2.67	3.64	3.4	2.54	3.52	3.98	3.45
54	0.2	0.17	0.37	0.33	0.18	0.32	0.46	0.19
32	0.29	0.22	0.4	0.38	0.24	0.31	0.43	0.18
58	0.23	0.17	0.42	0.37	0.19	0.41	0.57	0.2
65	0.37	0.31	0.56	0.46	0.31	0.45	0.5	0.34
43	0.04	0.03	0.09	0.08	0.03	0.1	0.14	0.04
28	1.59	1.35	2.64	2.27	1.36	2.46	2.98	1.57
27	1.26	1.12	2.23	1.89	1.09	1.78	2.26	1.37
22	3.46	3.09	4.51	4.02	3.13	4.3	4.68	3.53
39	0.15	0.12	0.39	0.31	0.13	0.32	0.45	0.17
30	0.05	0.04	0.09	0.07	0.04	0.07	0.11	0.04
51	0.15	0.12	0.28	0.22	0.12	0.21	0.32	0.13
33	0.91	0.75	1.84	1.5	0.66	1.65	1.99	0.66
38	0.17	0.19	0.2	0.24	0.22	0.3	0.42	0.2
95	1.83	1.94	5.54	5.35	1.61	1.88	5.4	1.02
55	0.88	0.74	0.82	0.89	0.86	0.94	0.98	1.09
44	0.54	0.34	0.64	0.57	0.4	0.65	0.69	0.33
87	0.16	0.1	0.14	0.32	0.13	0.19	0.27	0.09
23	1.44	1.21	2.22	1.96	1.22	1.78	2.19	1.35
24	0.64	0.51	0.9	0.82	0.54	0.89	1.08	0.55
35	0.35	0.29	0.73	0.6	0.3	0.62	0.9	0.36
26	0.12	0.08	0.12	0.13	0.1	0.2	0.23	0.1

Qualitative chemical variables related to sensory notes

Quantitative chemical variables related to sensory notes

Figure 4



Note-related compounds were studied using a supervised chemometric tool, named PLS-DA. Samples with the lowest score (for each target note) were assigned to class 1, while those with the highest score were assigned to class 2. PLS-DA describes samples by calculating new variables that maximize separation among groups while minimizing variability within groups. The impact of each compound on the separation of the pool of samples in the two classes (1 and 2) was evaluated by VIP (Variable Impact On Projections). Figure 4 reports the Venn Diagram of note-related compounds extracted from PLS-DA used to build the note prediction model for woody, bitter, and nutty attributes.

The compounds determined by PLS-DA for each sensory attribute were used to study the correlation between chemical and sensory data, by constructing a note prediction model through Partial Least Square Regression (PLS). Figure 5 lists the parameters used to build the model (a), together with the fit of the regression curve and validation set (b) and the sensory score prediction capability for the woody note on test samples (c).

Sensory scores Prediction by the "chemical odor code defined" variables

Prediction reliability was evaluated through deviation (Residues) from the predicted *vs.* experimental scores. The model showed close correlation between odor-active compounds selected and sensory scores.

The predictive capability was good, i.e. Q^2= 0.66, with a prediction error of 0.59 (woody). Similar results were also obtained for the other sensory attributes considered.

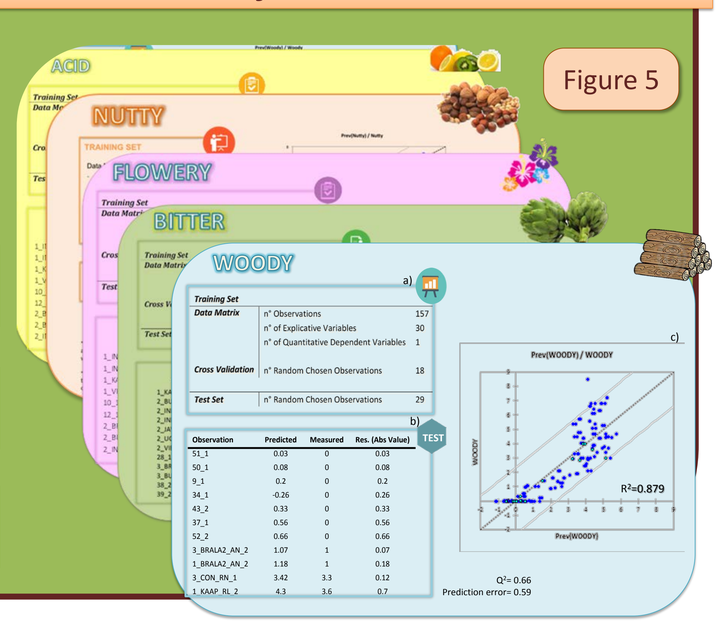
The sensometric-driven approach was found to be discriminative, informative, and predictive in revealing the chemical signature of the different coffee aroma notes.

Discriminative
Description of samples with peculiar aroma independently of the species, post-harvest treatments and origins

Informative
Association between chemical compounds, sensory evaluation and the quali-quantitative identification of the volatiles related to a peculiar attribute

Predictive
It can be used to predict a specific aroma sensory attribute

Figure 5



Conclusions

The good sensory score prediction, based on this sensometric approach, confirms and reinforces the relevance and significance of the odor-active compounds selected by this procedure. Moreover, considering all aroma notes at once, the sensometric method can also be used to develop a predictive model that is complementary and objective for sensory evaluation, comprehensively defining the sensory quality of coffee aroma.

On-going research into the quantitation of key odorants for each specific aromatic note should make it possible to create single note models. These results may, for example, be useful to study the neurological and physiological effects of each sensory attribute of coffee, their relationship with the hedonic processing (i.e. emotional, craving etc.), and/or with inflammation or other physiological responses.

Complementary tool to sensory evaluation
This tool will be useful to develop a sensory predictive model as a complementary and objective tool for the comprehensive evaluation of coffee aroma.

Notes modelization
Quantitation of the meaningful odor-active compounds able to chemically describe the aroma notes will enable to create aroma models.

Testing of the aroma models
Aroma models might be tested on in vitro olfactory receptors in order to study the brain and the body answers and to create new value in coffee and in consumer's preference.

FUTURE

References

[1] Chiralertpong A. et al. Chemosensory Perception (2008), 2, 147.
[2] Prescott J. Current Opinion in Food Science (2015), 3, 47.
[3] Sunarharum W.B. et al. Food Research International (2014), 62, 315.
[4] Ruosi M.R. et al. Journal of Agricultural and Food Chemistry (2012), 60, 11283.
[5] Liberto E. et al. Journal of Agricultural and Food Chemistry (2013), 61, 1652.
[6] https://worldcoffeeresearch.org/
[7] Bressanello D. et al. Food Chemistry (2017), submitted.
[8] Cevallos-Cevallos J.M. et al. Trends in Food Science & Technology (2009), 20, 557.