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Determination of volatile marker compounds of common coffee roast defects

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ABSTRACT

Coffee beans from the same origin were roasted using six time-temperature profiles, in order to identify volatile aroma compounds associated with five common roast coffee defects (light, scorched, dark, baked and underdeveloped). Thirty-seven volatile aroma compounds were selected on the basis that they had previously been identified as potent odorants of coffee and were also identified in all coffee brew preparations; the relative abundance of these aroma compounds was then evaluated using gas chromatography mass spectrometry (GC–MS) with headspace solid phase micro extraction. Some of the 37 key aroma compounds were significantly changed in each coffee roast defect and changes in one marker compound was chosen for each defect type, that is, indole for light defect, 4-ethyl-2-methoxyphenol for scorched defect, phenol for dark defect, maltol for baked defect and 2,5-dimethylfuran for underdeveloped defect. The association of specific changes in aroma profiles for different roast defects has not been shown previously and could be incorporated into screening tools to enable the coffee industry quickly identify if roast defects occur during production.

1. Introduction

Coffee is one of the most popular hot beverages consumed around the world. It is drunk by millions of people every day and there continues to be an increasing demanding for high quality speciality coffees (Bhumiratana, Adhikari, & Chambers Iv, 2011). The production of coffee that is perceived to be of good quality is dependent on many factors, these include the quality of the green bean, roaster type, the extraction process and water type used during brewing (Ribeiro, Augusto, Salva, Thomaziello, & Ferreira, 2009). Furthermore, coffee's unique aroma profile is very closely related to the time-temperature profiles used during the roasting process (Baggenstoss, Poisson, Kaegi, Perren, & Escher, 2008; Fisk, Kettle, Hofmeister, Virdie, & Kenny, 2012; Gloess et al., 2014).

Many different methods have been proposed to determine the optimum degree of roast. These include colour generation, weight loss, moisture content, degradation of chlorogenic acid or the ratio of free amino acids (Baggenstoss et al., 2008). However, the nature of the roasting process is very complex and no clear universally accepted definitions exist. Colour, although imprecise, is therefore currently used as the industry standard (Şenyuva & Gökmen, 2005).

Unlike flavour defects which result directly from the green bean, its production, processing and storage (Mancha Agresti, Franca, Oliveira, & Augusti, 2008), the term roast defects indicates problems within the roasting process, directly resulting in the presence of off-flavours in the coffee brew. Variations in time-temperature profiles within the roasting process will directly impact the rate of moisture loss, internal bean temperature and local microchemistry. This will regulate the rate at which caramelisation, Maillard chemistry, oxidation and pyrolysis occurs, and the resultant development of colour and flavour in the final roasted coffee bean (Sunarharum, Williams, & Smyth, 2014).

More than 800 volatile compounds have been identified to be present in roast and ground coffee. The most common classes of compounds reported in the headspace include acids, aldehydes (Ullrich & Grosch, 1987), alcohols (Merritt & Robertson, 1966), sulphur compounds (Silwar, 1986), phenolic compounds (Pypker & Brouwer, 1970), pyrazines (Reymond, Muggler-Chavan, Viani, Vuataz, & Egli, 1966), pyridines (Balts & Bochmann, 1987), thiophenes (Vitzthum & Werkhoff, 1976), pyrroles and furans. Due to the high number of compounds and inherent complexity of aroma

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chemistry within the coffee bean, it is essential to have both a methodology and a source of markers available to the coffee industry to enable them to identify roast defects.

The overarching objective of this study was to demonstrate how aroma profiles were impacted when roast defects occurred during coffee roasting and to generate a list of marker compounds associated with five roast defects (light, scorched, dark, baked and underdeveloped). Gas chromatography mass spectrometry (GC–MS) with headspace solid phase micro extraction (SPME) was used to compare the changes in volatile aroma compounds present in the roast defect coffee. To the best of our knowledge this is the first study to present a methodology for the evaluation of, and generate a framework of compounds associated with, roast defects in the aroma profile of roasted coffee.

2. Materials and methods

2.1. Coffee samples

All the coffee beans were single-origin washed Kenya Arabica from the wet mill from crop years 2012/2013 and 2013/2014. They were supplied by Kontra Coffee (Dag Hammarskjölds Alle 36, 2100 Copenhagen, Denmark), and were roasted using a batch size of 1 kg through a Probat drum roaster (Probat-Werke, Germany) modified to include additional temperature probes to monitor bean temperature. Roast degree was measured with a Javalytics JAV-RDA-DN (Madison Instruments, Inc., United States) and Agtron number was used to indicate the colour of the roast- the smaller the number, the darker the roast.

The roasting parameters for the standard roast and five roasting defects were recorded (Table S1). When a popping sound is perceived during roasting, it is the first crack and the development time is defined as the time from first crack to the end of roasting in this study. The standard roasting started when the air temperature in the roaster was at 210 °C and its developing time was 2 min 40 s with the total roasting time of 11 min 25 s. The light roast defect had the same starting temperature (210 °C) but with only 10 s development time and total roasting time of 8 min 40 s. The scorched roast defect had a higher starting temperature (275 °C) and shorter total roasting time (7 min 40 s) than standard roast. The dark roast defect had longer developing time (4 min 45 s) than the standard roast, and resulted in an additional 2 min of total roasting time. Baked roast defect had a higher initial temperature (230 °C) than the standard roast, and longer development time (6 min 20 s). In the underdeveloped samples, coffee was roasted at a much lower initial temperature (135 °C) and a longer total roasting time (20 min 20 s) than the standard roast.

Roasted samples were individually packed in the odour-free airtight package. Beans from each type were weighed (90 g) and ground using an electronic coffee grinder (KG 49, Delonghi, Australia), then passed through a metal sieve (710 mm, Endecotts, Essex, UK). Ground coffee (11 g) was brewed with boiling water (200 mL) using a French press brewer (3 Cup Black Cafetiere, Argos, UK) using deionised water (Purite Ltd, Oxon, UK). The resulting coffee brew was stirred 5 times with a spoon and allowed to stand for 4 min before depressing the plunger. The brewed coffee (4 mL) was stored in amber glass vials (20 mL, 22.5 mm × 75.5 mm, Sigma-Aldrich, UK) and closed with crimp seals (Sigma-Aldrich, UK) for

Table 1
Detection of 37 volatile aroma compounds in the standard roast coffee and defect samples.

	Retention time	Aroma compound	Odour description[a]	Functional group
1	2.25	3-Methylbutanal	Malty	Aldehyde
2	2.28	2-Methylbutanal	Malty	Aldehyde
3	2.70	2,5-Dimethylfuran	Ethereal	Furan
4	3.08	2,3-Butanedione	Buttery, cheesy	Ketone
5	4.88	2,3-Pentadione	Oily buttery	Ketone
6	5.00	Dimethyl disulphide	Onion	Sulphide
7	5.22	2-vinylfuran	Ethereal, rum, cocoa note	Furan
8	5.35	Hexanal	Grassy, green oily	Aldehyde
9	5.54	3-Methylthiophene	Ash	Sulphide
10	7.33	2,3-Hexandione	Buttery, cheesy, sweet, creamy	Ketone
11	8.83	Pyridine	Bitter, astringent, roasted, burnt	Heterocyclic N
12	11.83	Furfuryl methyl ether	Nutty, coffee grounds-like, rich, phenolic	Ether
13	12.53	2-Methylpyrazine	Nutty, roasted, chocolate	Pyrazine
14	12.70	Dihydro-2-methyl-3-furanone	Sweet, roasted	Ketone
15	14.96	2,5-Dimethylpyrazine	Nutty, roasted, grassy, corn	Pyrazine
16	15.27	2,6-Dimethylpyrazine	Nutty, sweet, fried	Pyrazine
17	15.59	2-Ethylpyrazine	Nutty, roasted	Pyrazine
18	16.03	2,3-dimethyl-Pyrazine	Nutty, roasted, green	Pyrazine
19	17.42	Dimethyl trisulphide	Onion	Sulphide
20	17.86	2-Ethyl-6-methylpyrazine	Roasted, hazelnut-like	Pyrazine
21	18.59	Trimethyl pyrazine	Nutty, roasted	Pyrazine
22	21.81	2-Furfural	Bread, almond, sweet	Aldehyde
23	22.94	Acetic acid	Sour	Organic acid
24	23.37	2-Acetylfuran	Balsamic-sweet	Furan
25	24.11	Pyrrole	Nutty, hay-like, herbaceous	Heterocyclic N
26	30.13	Furfuryl alcohol	Burnt	Alcohol
27	31.30	Butanoic acid	Sour	Organic acid
28	31.30	Hexanoic acid	Fatty-rancid, acrid-acid	Organic acid
29	35.11	2-Furfuryl methyl disulphide	Coffee-like	Sulphide
30	36.22	1-Furfurylpyrrole	Hay-like, mushroom-like, green	Heterocyclic N
31	40.76	Maltol	Caramel	Alcohol
32	41.16	1-(1-H-pyrrol-2-yl)ethanone	Nutty, musty	Ketone
33	41.81	Difurfuryl ether	Coffee-like, toasted odour	Ether
34	42.65	Phenol	Smoky	Phenolic
35	43.21	4-Ethyl-2-methoxyphenol	Smoky, spicy	Phenolic
36	45.25	Octanoic acid	Sweet cheesy	Organic acid
37	55.02	Indole	Burnt, mothball	Heterocyclic N

[a] Flament (2002).