Food Chemistry 153 (2014) 298–314

Contents lists available at ScienceDirect

Food Chemistry

journal homepage: www.elsevier.com/locate/foodchem

Volatile fingerprint of Brazilian defective coffee seeds: corroboration of potential marker compounds and identification of new low quality indicators

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ARTICLE INFO

Article history:
Received 13 August 2013
Received in revised form 30 November 2013
Accepted 9 December 2013
Available online 14 December 2013

Keywords:
Coffee
Quality
Defective seeds
Volatile compounds
Volatile markers
Volatile fingerprint

ABSTRACT

In the present work, the volatile profiles of green and roasted Brazilian defective coffee seeds and their controls were characterised, totalling 159 compounds. Overall, defective seeds showed higher number and concentration of volatile compounds compared to those of control seeds, especially pyrazines, pyrroles and phenols. Corroborating our previous results, butyrolactone and hexanoic acid, previously considered as potential defective seeds' markers, were observed only in raw and roasted defective seeds, respectively, and not in control seeds. New compounds were suggested as potential defective seeds' markers: hexanoic acid (for raw and roasted defective seeds in general), butyrolactone (for raw defective seeds in general), and 3-ethyl-2-methyl-1,3-hexadiene (for raw black seeds); β-linalool and 2-butyl-3,5-dimethylpyrazine (for roasted defective seeds in general), and 2-pentylfuran (for roasted black seeds). Additional compounds suggested as low quality indicators were 2,3,5,6-tetramethylpyrazine,2,3-butanediol and 4-ethylguaiacol, β-linalool, 2-,3-dimethylbutyl butanoate, 2-phenylethyl acetate, 2,3-butanedione, hexanedioic acid, guaiacol, 2,3-dihydro-2-methyl-1H-benzopyrrol, 3-methylpiperidine, 2-pentylpiperidine, 3-octen-2-one, 2-octenal, 2-pentylfuran and 2-butyl-3-methylpyrazine.

1. Introduction

The sensory quality of coffee brew is strictly related to the chemical composition of raw seeds and post-harvest processing conditions (drying, storage and roasting). The criteria commonly used to evaluate the quality of green coffee includes seeds size, colour, shape, processing method, crop year, cup quality, and presence of defective seeds and of strange matters (Bee et al., 2005; Toci & Farah, 2008). Among those, the last two are the most important criteria employed worldwide in coffee trading.

Coffee brew is most usually prepared by percolation of roasted and ground seeds. Among a number of defects that may be included in coffee, the most detrimental ones to the brew's flavor, in order of predominance, are immature, sour and black seeds. Immature seeds derive from immature fruits, sour seeds derive mainly from ripe or immature fruits that are fermented on the ground or due to improper processing conditions and black seeds derive mainly from over-ripened fruits which are often also fermented. Black seeds may as well derive from carbohydrate deficiency caused by poor agricultural practices (Bee et al., 2005; Toci & Farah, 2008). Because of the harvesting procedures used to reach high yields, such as manual striping of the branches or mechanical shaking, about 20% of coffee production (8 million bags) corresponds to defective seeds. They are highly incorporated into the internal market so as to reduce the production costs, because defective coffee seeds are considered to be inappropriate for exportation (Farah, Monteiro, Calado, Franca, & Trugo, 2006). Although the percentage of black seeds is usually low in commercial mixtures of defects, this is said to be the most potentially detrimental type of defect to both cup quality and human health, the later due to a high incidence of ochratoxin A (Farah, 2012; Silva, Schwan, Dias, & Wheals, 2000). The second most detrimental defect is considered to be the sour seed, also due to microorganisms growth (Silva et al., 2000).

In order to enable the identification of large amounts of defects in coffee blends, in the last years, there has been a growing interest in the characterization of the chemical composition of defective coffee seeds, which varies considerably, especially in regards to volatile compounds, since the volatile composition of raw and roasted defective seeds may vary not only with genetics (species and cultivars) but also with soil composition (including the

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0308-8146/$ - see front matter © 2014 Published by Elsevier Ltd.
http://dx.doi.org/10.1016/j.foodchem.2013.12.040

Table 1
Volatile compounds (mg/kg) identified in SPME-headspace gas of raw coffee samples.

N	Compounds	IK[α]	ID[β]	Group 1				Group 2				Group 3					
				Control	Black	Immature	Sour	Control	Black	Immature	Sour	Control a	Black a	Control b	Immature b	Control c	Sour c
Alcohol																	
1	3-Methylbutanol	1219	A	9.3	*t*	14.4	*t*	7.6	–	37.8	5.9	14.7	20.7	20.0	29.3	11.2	14.6
2	Pentanol	1267	C	–	7.7	*t*	2.0	*t*	6.6	*t*	1.6	–	10.3	*t*	16.7	*t*	1.7
3	5-Methylhexanol	1337	A	10.7	4.1	8.1	6.9	–	3.2	7.4	9.9	–	8.5	6.2	15.0	––	*t*
4	Hexanol	1365	A	3.9	10.3	4.6	1.9	1.9	4.8	3.0	0.7	6.8	14.0	6.2	10.0	7.2	7.7
5	3-Octanol	1405	C	–	–	*t*	–	–	–	*t*	–	*t*	–	–	2.6	–	–
6	1-Octen-3-ol	1442	B	–	15.1	2.1	*t*	–	14.7	2.1	3.0	4.7	4.9	–	1.0	*t*	1.7
7	2,3-Butanediol (*meso*)	1588	A	32.2	*t*	13.8	170.6	20.7	34.0	0.2	59.4	47.7	48.3	18.6	65.3	*t*	41.8
8	3,7-Dimethyl-1,6-octadien-3-ol (β-linalool)	1562	A	–	*t*	9.9	3.9	–	23.1	4.0	2.4	–	80.5	2.0	4.0	–	–
9	Cyclohexaneomethanol	1566	C	–	–	–	3.3	–	–	–	–	–	–	–	–	–	–
10	2,3-Butanediol (leso)	1588	A	27.1	*t*	58.7	198.4	–	30.5	32.4	65.3	40.3	47.7	34.7	53.0	*t*	72.2
11	Benzenemethanol	1884	A	*t*	–	2.3	3.9	–	–	3.1	0.1	2.2	4.3	3.2	4.2	*t*	1.2
12	2-Phenyl-1-ethanol (phenylethyl alcohol)	1918	B	2.2	–	7.7	32.2	–	–	7.8	1.8	2.4	7.3	4.6	7.4	*t*	–
Acids																	
13	Acetic acid	1446	B	11.5	12.8	13.8	61.6	–	14.5	12.1	18.3	12.7	21.8	13.3	14.7	*t*	12.2
14	2-Methylpropanoic acid	1582	C	–	–	*t*	14.1	10.4	–	–	*t*	–	–	–	–	–	–
15	butanoic acid	1640	C	–	–	–	13.5	–	*t*	–	–	–	–	–	–	–	–
16	3-Methylbutanoic acid	1684	C	11.2	–	11.5	34.7	–	9.3	10.6	13.5	11.0	11.4	13.3	10.6	*t*	10.3
17	Hexanoic acid	1857	A	–	12.2	*t*	10.1	–	11.6	*t*	11.8	–	11.0	–	*t*	–	9.4
18	Cyclohexanecarboxylic acid	2089	C	–	–	–	11.6	–	–	–	–	–	–	–	–	–	–
Esters																	
19	2-Methyl-3-methylbutyl butanoate	1306	C	–	–	–	3.8	–	–	*t*	*t*	–	*t*	–	*t*	–	–
20	Methyl salicilate	1780	C	–	–	0.5	2.2	–	–	1.2	0.5	–	1.1	*t*	0.9	–	–
21	Ethyl-2-hydroxy-benzenoate	1816	C	–	–	*t*	1.0	–	–	0.7	*t*	–	*t*	–	0.5	*t*	–
22	2-phenylethyl acetate	1825	C	–	–	–	0.8	–	–	–	*t*	–	–	–	*t*	–	–
23	Monoethyl phtalate	2259	C	–	–	–	–	–	–	–	–	0.5	0.5	0.4	–	–	–
24	Diethyl 1,2-benzenedicarboxylate (diethyl phthalate)	2291	C	1.9	–	0.9	0.6	–	*t*	*t*	*t*	1.6	1.4	1.4	1.5	0.5	0.5
Ketones																	
25	2-Heptanone	1191	C	*t*	10.0	*t*	2.8	–	*t*	*t*	*t*	–	–	2.4	5.2	*t*	–
26	1-Methoxypropanone	1291	C	*t*	–	1.6	3.7	–	*t*	*t*	*t*	–	*t*	*t*	*t*	–	*t*
27	2-Nonanone	1403	C	–	0.9	1.0	101.4	0.9	3.2	*t*	*t*	*t*	2.1	*t*	*t*	*t*	0.2
28	3-Octen-2-one	1420	C	–	5.1	–	–	–	4.5	–	*t*	–	1.2	–	–	–	*t*
29	2-Undecanone	1608	C	–	–	–	3.2	–	*t*	–	–	*t*	*t*	–	*t*	–	*t*
Pyrazines																	
30	2,3,5-Trimethylpyrazine	1407	B	–	–	–	2.7	–	–	–	2.0	–	4.7	–	–	–	–
31	2,3,5,6-Tetramethylpyrazine	1480	B	–	7.9	*t*	15.7	–	*t*	–	3.7	–	3.2	–	–	–	–
32	2-Methoxy-3-methylpyrazine	1534	C	*t*	–	3.3	9.1	4.5	–	2.0	2.2	2.9	4.3	*t*	*t*	3.3	2.7
33	6-Ethenyltetrahydro-2,2,6-trimethyl-2H-pyran-3-ol	1775	C	–	–	–	2.6	–	–	–	–	–	–	–	–	–	–
Furans																	
34	2-Penthylfuran	1267	B	–	294.5	–	43.2	–	188.9	–	76.4	–	213.4	–	*t*	–	–
35	5-Ethenyltetrahydro-α,α,5-trimethyl-2-furylmethanol	1450	C	*t*	–	*t*	132.6	*t*	–	7.0	20.2	–	27.9	20.8	21.1	–	*t*
36	2-Furylmethanol	1675	B	29.5	34.7	32.4	28.8	–	26.1	*t*	–	41.1	20.3	*t*	28.1	11.4	9.7
Aldehydes																	
37	Hexanal	1101	A	*t*	174.7	*t*	*t*	18.6	219.0	*t*	49.5	*t*	141.3	*t*	*t*	19.7	21.6
38	2-Octenal	1438	C	–	9.7	–	–	–	7.0	–	0.2	–	2.2	–	–	–	*t*
39	Benzaldehyde	1530	A	*t*	1.8	2.4	11.7	–	6.9	1.7	4.3	4.4	16.7	1.0	5.2	0.9	3.7

(*continued on next page*)