

Effect of drying technique on the volatile content of Ecuadorian bulk and fine-flavor cocoa

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Supplementary information

Table S1. Volatile compounds identified in fresh, and oven-dried (OD), sun-dried (SD) or sun-dried using a black plastic sheeting (SBPD) bulk (foratero (F) and CCN51 (C)) and fine-flavor (ETT103 (E) and LR14 (L)) cocoa, with the corresponding retention times (min), retention indexes (experimental and theoretical (NIST)) and ions of quantification.

		Fresh cocoa								OD				SD				SBPD			
	RT (min)	Compound	RI _{experimental}	RI _{NIST}	IonQ	F	C	E	L	F	C	E	L	F	C	E	L	F	C	E	L
Aldehydes																					
1	4.42	2-Methyl butanal	920	922	57	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x
2	7.79	Hexanal	1087	1086	56	x	x	x	x												
3	13.99	(E)-2-Octenal	1443	1443	70	x		x	x												
4	14.38	3-(Methylthio)propanal	1471	1471	104	x	x	x												x	
5	14.54	Furfural	1483	1483	96							x	x								
6	15.36	Benzaldehyde	1545	1545	77	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x
7	16.84	Benzacetaldehyde	1664	1663	91	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x
8	20.07	α-Ethylidenbenzeneacetaldehyde	1955	1961	117	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x
Alcohols																					
9	7.12	2-Methylbut-3-en-2-ol	1056	1058	71	x	x	x	x												
10	8.2	2-Methyl-propanol	1106	1105	74												x				
11	8.72	3-Methyl-2-butanol +	1131	1124	73																
12		2-pentanol	1131	1130	73	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x
13	10.35	3-Methyl-butanol	1213	1213	55	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x
14	10.57	2-Hexanol	1226	1226	69	x	x	x	x												
15	10.63	2-Methyl-butanol	1229	1224	57		x			x	x	x	x	x	x	x	x	x	x	x	x
16	11.09	1-Pentanol	1255	1255	55	x	x	x	x												
17	12.24	2-Heptanol	1324	1324	55	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x
18	12.6	4-Methyl-5-hexen-2-ol (probably)	1347	1344*/1348**	81	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x
19	12.79	1-Hexanol	1360	1360	56	x	x	x		x		x					x				x
20	13.71	2-Octanol	1422	1422	55	x	x	x	x		x		x	x	x	x	x			x	x
21	15.07	2-Nonanol	1522	1521	69	x	x	x	x	x	x	x	x	x	x	x	x	x	x		x
22	15.38	2,3-Butanediol	1547	1544	57								x	x	x	x					
23	18.69	α-Phenylethanol	1826	1827	79	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x
24	19.41	Benzyl alcohol	1893	1893	79	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x
25	19.8	Phenylethyl alcohol (2-Phenylethanol)	1930	1929	91	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x
Acids																					
26	14.24	Acetic acid	1461	1460	60					x	x	x	x	x	x	x	x	x	x	x	x
27	15.54	Propanoic acid	1556	1556	74					x	x	x	x	x	x	x	x	x	x	x	x
28	15.79	2-Methyl-propanoic acid	1578	1578	73					x	x	x	x	x	x	x	x	x	x	x	x
29	16.58	Butanoic_acid	1643	1642	60					x		x								x	x
30	17.23	2-/3-Methyl-butanoic acid	1685	1687/1685	74					x	x	x	x	x	x	x	x	x	x	x	x

						Fresh cocoa				OD				SD				SBPD			
RT (min)		Compound	RI _{experimental}	RI _{NIST}	IonQ	F	C	E	L	F	C	E	L	F	C	E	L	F	C	E	L
Ketones																					
31	5.62	2-Pentanone	986	985	86	x	x	x	x	x	x							x	x		
32	9.99	2-Heptanone +	1188	1188	58	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x
33		5-methyl-2-hexanone	1188	1188																	
34	11.7	2-Octanone	1290	1290	58	x	x	x	x	x	x	x	x	x	x	x	x	x		x	x
35	11.78	3-Hydroxy-2-butanone (acetoin)	1295	1295	88					x	x	x	x	x	x	x	x	x	x	x	x
36	12.97	2-Hydroxy-3-pentanone	1372	1370	57					x	x		x	x	x		x	x	x		x
37	13.23	2-Nonanone	1389	1389	58	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x
38	16	3,6-Heptanedione (probably)	1595	1592***	57	x	x	x	x	x			x	x			x				x
39	16.96	Acetophenone	1674	1671	105	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x
Esters																					
40	4.14	Ethyl acetate	904	904	61						x	x	x	x	x	x	x	x	x	x	x
41	7.6	2-Pentyl acetate	1078	1074	87					x				x	x		x	x	x		
42	8.6	2-/3-Methylbutyl acetate	1125	1126	70					x	x	x	x	x	x	x	x	x	x	x	x
43	10.9	Ethyl hexanoate	1245	1245	88					x	x	x	x	x	x	x	x	x	x	x	x
44	11.3	1-Methylhexyl acetate (2-heptanol acetate)	1273	1266	98					x	x	x	x	x	x	x	x	x	x	x	x
45	13.99	Ethyl octanoate	1443	1445	88					x	x	x	x	x	x	x	x	x	x	x	x
46	14.83	2,3-Butanedioldiacetate	1504	1501	87					x	x		x					x			
47	17.81	Benzyl acetate	1747	1747	108					x	x	x	x	x	x		x	x	x	x	x
48	18.43	Ethyl benzeneacetate	1802	1800	91					x	x	x	x	x	x	x	x	x	x	x	x
49	18.77	β-Phenylethyl acetate	1833	1833	104					x	x	x	x	x	x	x	x	x	x	x	x
50	18.78	Phenethyl pivalate	1833	1832	57						x	x		x	x	x			x		
51	19.03	Butyl benzoate	1857	1856	105	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x
Terpenes																					
52	9.32	β-Myrcene	1161	1161	93	x		x	x	x	x	x	x	x	x	x	x		x	x	x
53	10.16	D-Limonene	1202	1202	68	x							x	x		x	x				
54	10.78	Ocimene (isomers E and Z)	1236	1237	93	x		x	x		x	x	x			x	x			x	x
55	13.13	γ-Pyrone (1,3,5,5-tetramethyl- 1,3-cyclohexadiene)	1382	1406	121	x		x	x			x	x			x	x				x
56	14.09	Linalool oxide I	1450	1450	94	x	x	x	x	x	x	x	x	x	x	x	x		x	x	x
57	14.49	Linalool oxide II	1478	1478	94	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x
58	15.45	Linalool	1552	1552	71	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x
Lactones																					
59	16.49	Valerolactone	1635	1629	56						x	x	x			x				x	x
60	16.74	Butyrolactone	1656	1652	86					x	x	x	x	x	x	x	x	x	x	x	x
Miscellaneous																					
61	13.59	trimethyl-Pyrazine	1414	1414	122					x	x	x	x	x			x	x			x
62	16.29	Isophorone	1618	1615	138					x		x									x
63	16.42	Benzonitrile	1629	1629	103					x		x				x				x	
64	19.28	o-Guaiacol	1881	1886	109					x								x			

Compounds tentative identified according to the linear retention index (RI) calculated in previous works: 4-methyl-5-hexen-2-ol, *Costa Castro Alves et al. [21] and **Li [22]; 3,6-Heptanedione, ***Raffo et al. [23]. RI: retention index; Ion Q: ion of quantification.