

Role of Roasting Conditions in the Profile of Volatile Flavor Chemicals Formed from Coffee Beans

JOON-KWAN MOON AND TAKAYUKI SHIBAMOTO*

Department of Environmental Toxicology, University of California, Davis, One Shields Avenue, Davis, California 95616

The volatile chemicals in dichloromethane extracts from green coffee beans, roasted at 230 °C for 12 min (light), at 240 °C for 14 min (medium), at 250 °C for 17 min (city), or at 250 °C for 21 min (French), were analyzed by gas chromatography and gas chromatography–mass spectrometry. Among the 52 volatile compounds identified, the major compounds were 5-hydroxymethylfurfural, furfuryl alcohol, and 6-methyl-3,5-dihydroxy-4*H*-pyran-4-one in light-roasted beans; furfuryl alcohol, 5-hydroxymethylfurfural, and γ -butyrolactone in medium-roasted beans; furfuryl alcohol, γ -butyrolactone, and 2-acetylpyrrole in city-roasted beans; and γ -butyrolactone, furfuryl alcohol, and catechol in French-roasted beans. Furfural derivatives and furanones were yielded in relatively high concentrations under mild roasting conditions and then reduced at higher roasting intensities. More pyridines and pyrroles were formed by high roasting intensities than by mild roasting intensities. Chlorogenic acid degradation products, phenols, and a lactone were produced more by high roasting intensities than by low roasting intensities. The results of the present study suggest that controlling the roasting conditions according to the formation of particular chemicals can prepare a roasted coffee with preferable flavor.

KEYWORDS: Coffee volatiles; brewed coffee; γ -butyrolactone; roasted coffee; roasting conditions

INTRODUCTION

Coffee is one of the most popular beverages in the world. Since the beginning of the last century, the chemical components of coffee, in particular, flavor chemicals, have been studied intensively and continuously. The number of volatile chemicals identified in brewed coffee has reached over 1000 (1). Among volatile chemicals found in brewed coffee, over 300 are heterocyclic compounds, which include pyrroles, oxazoles, furans, thiazoles, thiophenes, imidazoles, and pyrazines (2). It has been known that some of these heterocyclic compounds contribute toasted or roasted flavors to heat-treated foods and beverages, including brewed coffee (3). Consequently, the role of heterocyclic compounds in brewed coffee flavor has been intensively studied and reported in many papers (4). A sensory assessment of model systems indicated that some heterocyclic compounds, such as furans, pyridines, pyrroles, and alkylpyrazines, as well as non-heterocyclic compounds such as cyclotens and furanones contributed significantly to the characteristic coffee flavor (5).

Green coffee beans do not have the characteristic color and flavors of roasted coffee. Therefore, roasting produces various coffee flavors, and its conditions have a major impact on the formation of roasted coffee flavors (6). There have been many reports on the role of roasting conditions in the formation of various coffee components, including chlorogenic acids (7) and volatile compounds (8). It is, therefore, important to investigate

the formation of medicinal components, including volatile chemicals with antioxidant activity, produced during roasting to assess the possible beneficial effects from coffee drinking. The present study investigates the formation of volatile chemicals in coffee beans under various roasting conditions.

MATERIALS AND METHODS

Materials and Chemicals. HPLC grade water and dichloromethane were bought from Fisher Co. (Pittsburgh, PA). Authentic volatile chemicals were bought from reliable commercial sources or were gifts from TAKATA Koryo Co., Ltd. (Osaka, Japan). All other chemicals and solvents were bought from reliable commercial sources.

Various brands of commercially roasted ground coffees (Dunkin, Fine Puroast, GOUD, and San Francisco Bay Area) were purchased from a local market (Davis, CA). Organic green coffee beans (Ethiopian Yirgacheffe, Nicaraguan, and Sumatran) were bought from Napa Valley Coffee Roasting Co. (Napa, CA).

Sample Preparations for Green Coffee Beans Roasted under Various Conditions. Ethiopian Yirgacheffe, Nicaraguan, and Sumatran green coffee beans (100 g each) were roasted with a Gene Café coffee bean roaster (Fresh Beans Inc., Park City, UT) at 230 °C for 12 min (light), at 240 °C for 14 min (medium), at 250 °C for 17 min (city), or at 250 °C for 21 min (French). The terms for the roasting conditions (light, medium, city, and French) were derived from descriptions shown on the roaster.

After roasting, the coffee beans were ground with a Starbucks Barista coffee grinder (Seattle, WA). Roasted–ground coffee (12.5 g) was brewed with 450 mL of deionized water using a Mr. Coffee NCX-20 model coffee maker (Sunbeam Product, Inc., Boca Raton, FL).

The brewed coffee (200 mL) was extracted with 200 mL of dichloromethane using a liquid–liquid continuous extractor for 6 h. After the

*Corresponding author [telephone (530) 752-4523; fax (530) 752-3394; e-mail tshibamoto@ucdavis.edu].

Table 1. Amount of Total Volatile Chemicals Obtained from Coffee Beans (Milligrams per Gram of Coffee Beans)^a

coffee bean origin	roasting condition			
	light roast	medium roast	city roast	French roast
Ethiopian	19.6 ± 0.8	21.5 ± 1.4	32.4 ± 0.3	33.3 ± 1.2
Nicaraguan	19.3 ± 0.6	29.6 ± 5.3	32.7 ± 0.6	35.0 ± 5.3
Sumatran	16.4 ± 0.7	27.2 ± 7.3	30.0 ± 2.9	35.4 ± 3.6

^a Values are mean ± SD (*n* = 3).

extract was dried over anhydrous sodium sulfate, the solvent was removed using a rotary flash evaporator under reduced pressure until the volume of the sample was reduced to approximately 3 mL. The solvent was further removed under a purified nitrogen stream until the volume was reduced to exactly 1 mL. The prepared sample was stored at 5 °C until used for analysis of volatile chemicals.

Sample Preparations for Commercial Roasted–Ground Coffee.

Commercially obtained roasted–ground coffees (12.5 g each) were brewed and extracted exactly according to the method described above. The samples prepared (1 mL each) were stored at 5 °C until used for analysis of volatile chemicals.

Identification of Volatile Chemicals in Samples. Chemicals in the dichloromethane extract were identified by comparison with the Kovats gas chromatographic retention index *I* and by the mass spectral fragmentation pattern of each component compared with those of authentic compounds. The identification of the GC components was also confirmed with the NIST AMDIS version 2.1 software.

An Agilent model 6890 GC equipped with a 60 m × 0.25 mm i.d. (*d_f* = 0.5 μm) DB-Wax bonded-phase fused silica capillary column (Agilent, Folsom, CA) and an FID was used for measurement of the Kovats index and routine analysis of volatiles. The helium carrier gas flow rate was 1.0 mL/min at a split ratio of 20:1. The injector and detector temperatures were 250 and 280 °C, respectively. The oven temperature was programmed from 40 °C (held for 5 min) to 210 at 2 °C/min and then held for 70 min.

An Agilent model 6890 GC interfaced to an Agilent 5971A mass selective detector (GC-MS) was used for mass spectral identification of the GC components at MS ionization voltage of 70 eV. GC column conditions were exactly the same as the ones used for GC-FID.

RESULTS AND DISCUSSION

Table 1 shows the total amount of volatile chemicals recovered from each sample of coffee beans. The results of the analysis of volatile chemicals in the extracts from Ethiopian coffee beans (**Table 2**), Nicaraguan coffee beans (**Table 3**), and Sumatran coffee beans (**Table 4**) roasted under four different conditions are shown in **Tables 2–4**. A total of 52 volatile chemicals were positively identified. They were 4 pyridines, 9 pyrazines, 5 pyrroles, 7 furanones, 7 furans, 4 cyclopentenes, 4 phenols, and 12 other miscellaneous compounds.

The absolute concentration of each chemical in **Tables 2–4** should be able to be roughly estimated from the total amount of volatile chemicals found in each sample (**Table 1**). A standard curve for the quantitation of each chemical must be prepared using the corresponding authentic chemical to obtain its absolute concentration. However, it is common practice to use GC peak area % as concentration to assess the flavor profile of foods and beverage. In the case of light roasting, 5-hydroxymethylfurfural is found in the greatest concentrations (26.77 ± 0.48% in Ethiopian, 24.82 ± 1.62% in Nicaraguan, and 23.09 ± 2.13% in Sumatran). In the case of medium roasting, the concentration of furfuryl alcohol was the highest (28.19 ± 1.82% in Ethiopian, 28.27 ± 1.19% in Nicaraguan, and 27.51 ± 2.40% in Sumatran). Furfuryl alcohol remained in the highest concentration in the case of city roasting (18.31 ± 0.80% in Ethiopian, 22.75 ± 1.63% in Nicaraguan, and 26.29 ± 1.38% in Sumatran). However, in the case of French roasting, the concentrations of these furan

derivatives decreased considerably and those of γ -butyrolactone became the highest (13.29 ± 1.56% in Ethiopian, 13.81 ± 0.73% in Nicaraguan, and 15.22 ± 0.23% in Sumatran).

The compositions and concentrations of chemicals in the extracts from coffee beans roasted under four different conditions did not, however, differ significantly among the three brands. Therefore, further discussion is mainly focused on the results from Ethiopian coffee beans (**Table 2**). The concentrations of volatile chemicals in the extracts from Ethiopian coffee beans changed according to the different roasting conditions. For example, the total concentration of pyridines increased from 1.9 to 10.6%. On the other hand, the total concentration of furans decreased from 52.6% (light roasting) to 10.2% (French roasting). The greatest concentration of total pyrroles was obtained by city roasting (7.6%).

Figure 1 shows concentrations of the chemicals significantly influenced by roasting conditions found in extracts obtained from Ethiopian coffee beans roasted under four different conditions. The concentration of 5-hydroxymethylfurfural decreased significantly with increase in the intensity of the roasting condition from 26.8% (light roasting) to 0% (French roasting). The concentrations of the other main furfural derivatives, furfuryl alcohol and furfural, also decreased from 20.7% (light roasting) to 8.3% (French roasting) and from 2.8% (light roasting) to 0.1% (French roasting), respectively. These results were consistent with previous reports. For example, the concentration of furfural decreased significantly from 19.9 to 2% when coffee beans were roasted at 230 °C for 25 and 30 min, respectively (9). The decrease in furfural concentrations at higher roasting intensity may be due to decomposition (10) or polymerization (11).

Furfural derivatives, such as furfural and furfuryl alcohol, have been known since the 1930s to form from monosaccharide (12), and their flavor characteristics were known as sweet, bread-like, and caramellic (13). Later, it was found that they were formed readily from the reaction between a sugar and an amino acid at elevated temperatures (14), suggesting that the composition of coffee beans is an ideal matrix to form furfurals upon roasting. The furfurals shown in **Tables 2–4** have been found in coffee previously (1). 2-Furfurylthiol, which has a characteristic coffee flavor and was reported in coffee (15, 16), was detected in the present study, but it is not listed in **Tables 2–4** because its GC peak area % was <0.01.

Reduction of the concentration when the intensity of roasting conditions increased was also observed in the formation of 2,5-dimethyl-4-hydroxy-3(2*H*)-furanone (DMHF) and 3,5-dihydroxy-2-methyl-4*H*-pyran-4-one (DMP) (**Figure 1**). The concentration of DMHF was reduced from 2.7% (light roasting) to 0.5% (French roasting). Significant reduction from 9.8% (light roasting) to 0.6% (French roasting) was also observed in the case of DMP.

The formation of DMHF in the Maillard reaction systems was first reported in the early 1960s (17), and it became known as one of the main Maillard reaction products (18). Later, various furanone derivatives, including DMHF, were found in coffee volatiles (1, 19). In the meantime, DMHF, which possesses a strong caramellic–fruity flavor (13), was reported as a flavor component in various fruits, such as pineapples (20), strawberries (21), grapes (22), and citrus juice (23). DMHF has been studied as a component with medicinal activity, specifically, as an antioxidant, in addition to being studied as a flavor component in food and beverages (24). DMP is also known as a product of sugar degradation in the Maillard reaction systems (25) and also possesses a characteristic caramel-like flavor (13). DMP was also reported in coffee in the late 1970s (19).

Table 2. Volatile Chemicals Identified in Brewed Coffee Prepared from Ethiopian Green Beans Roasted at Different Conditions

compound	<i>i</i> ^b	GC peak area % ^a			
		light roast	medium roast	city roast	French roast
pyridines					
pyridine	1202	0.30 ± 0.04	1.20 ± 0.26	3.57 ± 0.52	6.45 ± 2.23
2-methylpyridine	1240	— ^c	—	—	0.04 ± 0.01
6-methyl-3-pyridinol	2430	—	0.18 ± 0.06	0.58 ± 0.07	0.58 ± 0.12
3-hydroxypyridine	2450	1.60 ± 0.35	3.53 ± 0.92	4.48 ± 0.66	3.50 ± 0.71
pyrazines					
pyrazine	1231	—	0.02 ± 0.01	0.07 ± 0.02	0.08 ± 0.03
2-methylpyrazine	1286	0.65 ± 0.08	0.95 ± 0.18	0.77 ± 0.08	0.67 ± 0.21
2,5-dimethylpyrazine	1346	0.50 ± 0.01	0.60 ± 0.03	0.37 ± 0.02	0.30 ± 0.06
2,6-dimethylpyrazine	1352	0.43 ± 0.01	0.59 ± 0.04	0.45 ± 0.02	0.38 ± 0.07
2-ethylpyrazine	1357	0.13 ± 0.01	0.19 ± 0.02	0.15 ± 0.03	0.16 ± 0.04
2,3-dimethylpyrazine	1371	0.08 ± 0.00	0.11 ± 0.00	0.14 ± 0.00	0.14 ± 0.02
2-ethyl-6-methylpyrazine	1408	0.15 ± 0.00	0.21 ± 0.01	0.29 ± 0.01	0.42 ± 0.05
2-ethyl-5-methylpyrazine	1415	0.12 ± 0.00	0.16 ± 0.00	0.11 ± 0.00	0.09 ± 0.01
2,3,5-trimethylpyrazine	1429	0.37 ± 0.01	0.37 ± 0.01	0.21 ± 0.01	0.19 ± 0.02
pyrazine-2-carboxylic acid amide	1740	0.25 ± 0.00	0.24 ± 0.01	0.26 ± 0.01	0.24 ± 0.01
pyrroles					
1-methylpyrrole	1542	0.11 ± 0.00	0.31 ± 0.01	0.17 ± 0.01	0.08 ± 0.01
1-methyl-1 <i>H</i> -pyrrole-2-carboxaldehyde	1651	0.15 ± 0.00	0.38 ± 0.02	0.26 ± 0.01	0.22 ± 0.02
2-acetyl-1-methylpyrrole	1683	0.12 ± 0.00	0.24 ± 0.03	0.45 ± 0.02	0.43 ± 0.02
2-acetylpyrrole	2022	0.61 ± 0.01	0.92 ± 0.08	5.60 ± 0.56	4.66 ± 0.15
pyrrole-2-carboxaldehyde	2059	1.18 ± 0.00	2.38 ± 0.19	1.13 ± 0.05	0.94 ± 0.06
furanones					
dihydro-2-methyl-3(2 <i>H</i>)-furanone	1282	0.32 ± 0.09	0.66 ± 0.28	0.27 ± 0.04	0.18 ± 0.07
5-methyl-2(5 <i>H</i>)-furanone	1707	0.13 ± 0.00	0.19 ± 0.01	0.20 ± 0.01	0.20 ± 0.00
2(5 <i>H</i>)-furanone	1787	0.71 ± 0.00	0.86 ± 0.06	0.13 ± 0.01	0.10 ± 0.00
dihydro-4-methyl-2(3 <i>H</i>)-furanone	1847	—	0.18 ± 0.01	0.77 ± 0.04	0.80 ± 0.04
2,5-dimethyl-4-hydroxy-3(2 <i>H</i>)-furanone	2062	2.70 ± 0.05	2.03 ± 0.10	0.58 ± 0.00	0.48 ± 0.14
5-acetyldihydro-2(3 <i>H</i>)-furanone	2096	0.54 ± 0.02	0.75 ± 0.04	0.58 ± 0.02	0.46 ± 0.01
dihydro-5-(hydroxymethyl)-2(3 <i>H</i>)-furanone	2516	0.42 ± 0.24	0.82 ± 0.08	1.18 ± 0.18	1.04 ± 0.33
furans					
furfural	1482	2.28 ± 0.34	2.54 ± 0.33	0.19 ± 0.01	0.09 ± 0.04
2-acetylfuran	1527	0.56 ± 0.02	1.01 ± 0.03	0.81 ± 0.04	0.74 ± 0.01
furfuryl acetate	1552	0.14 ± 0.01	0.52 ± 0.03	0.85 ± 0.04	0.70 ± 0.11
5-methylfurfural	1596	1.70 ± 0.04	3.12 ± 0.05	0.46 ± 0.02	0.13 ± 0.02
furfuryl alcohol	1678	20.68 ± 0.11	28.19 ± 1.82	18.31 ± 0.80	8.31 ± 0.95
5-methylfuran-2-carboxylic acid, methyl ester	2044	0.52 ± 0.01	0.48 ± 0.03	0.23 ± 0.03	0.25 ± 0.00
5-hydroxymethylfurfural	2528	26.77 ± 0.48	9.11 ± 0.33	0.32 ± 0.02	—
cyclopentenes					
4,4-dimethyl-2-cyclopenten-1-one	1511	—	—	—	0.04 ± 0.01
2,3-dimethyl-2-cyclopenten-1-one	1573	—	0.03 ± 0.02	0.15 ± 0.01	0.19 ± 0.01
2-hydroxy-3-methyl-2-cyclopenten-1-one	1857	1.01 ± 0.01	1.62 ± 0.11	1.53 ± 0.06	1.56 ± 0.05
3-ethyl-2-hydroxy-2-cyclopenten-1-one	1924	0.25 ± 0.00	0.41 ± 0.03	0.69 ± 0.03	0.84 ± 0.04
phenols					
2-methoxyphenol	1886	0.19 ± 0.00	0.45 ± 0.03	1.01 ± 0.05	1.32 ± 0.08
phenol	2030	0.25 ± 0.00	0.52 ± 0.03	1.94 ± 0.07	3.36 ± 0.16
2-methoxy-4-vinylphenol	2225	2.22 ± 0.09	2.47 ± 0.10	1.54 ± 0.03	0.93 ± 0.03
catechol	2718	—	—	8.86 ± 0.78	10.02 ± 2.75
other miscellaneous compounds					
acetoin	1303	0.19 ± 0.05	0.38 ± 0.14	0.20 ± 0.04	0.10 ± 0.03
hydroxyacetone	1319	2.10 ± 0.54	1.85 ± 0.75	0.49 ± 0.11	0.43 ± 0.10
1-ethoxy-2-methylpropane	1364	0.10 ± 0.01	0.19 ± 0.04	0.11 ± 0.01	0.07 ± 0.02
1-hydroxy-2-butanone	1394	0.55 ± 0.08	0.79 ± 0.14	0.26 ± 0.02	0.21 ± 0.05
acetic acid	1468	0.19 ± 0.07	1.09 ± 0.31	0.46 ± 0.06	0.46 ± 0.13
1-acetyloxy-2-propanone	1477	0.49 ± 0.03	1.43 ± 0.06	0.76 ± 0.04	0.37 ± 0.04
propionic acid	1557	0.34 ± 0.02	0.52 ± 0.12	0.17 ± 0.01	0.16 ± 0.02
γ-butyrolactone	1662	2.06 ± 0.02	4.26 ± 0.20	10.93 ± 0.57	13.29 ± 1.56
3-methylbutanoic acid	1687	4.03 ± 0.03	4.48 ± 0.06	2.15 ± 0.11	1.56 ± 0.18
3-methyl-2-butenic acid	1819	1.29 ± 0.01	1.46 ± 0.11	0.39 ± 0.01	0.54 ± 0.01
maltol	2004	1.52 ± 0.02	3.58 ± 0.23	1.34 ± 0.06	1.26 ± 0.03
3,5-dihydroxy-6-methyl-4 <i>H</i> -pyran-4-one	2309	9.80 ± 0.36	0.92 ± 0.09	0.52 ± 0.02	0.64 ± 0.02

^a Solvent peak is excluded. Values are mean ± SD, *n* = 3. ^b Kovats index on DB-Wax column. ^c GC peak area % <0.01.

The nitrogen-containing heterocyclic compounds, including pyridines, pyrazines, and pyrroles, are the major flavor chemicals found in coffee (1). They are also well-known as Maillard reaction

products and give characteristic roasted or toasted flavors to heat-treated foods and beverages (26). Alkylpyrazines identified in the present study were reported in the late 1960s as products of

Table 3. Volatile Chemicals Identified in Brewed Coffee Prepared from Nicaraguan Green Beans Roasted at Different Conditions

compound	<i>i</i> ^b	GC peak area % ^a			
		light roast	medium roast	city roast	French roast
pyridines					
pyridine	1202	0.19 ± 0.04	1.23 ± 0.18	3.99 ± 0.10	5.96 ± 0.92
methylpyridine	1240	— ^c	—	—	—
6-methyl-3-pyridinol	2430	0.09 ± 0.02	0.29 ± 0.02	0.75 ± 0.22	0.63 ± 0.05
3-hydroxypyridine	2450	1.86 ± 0.21	4.20 ± 0.25	4.59 ± 1.58	3.33 ± 0.23
pyrazines					
pyrazine	1231	—	0.06 ± 0.02	0.12 ± 0.00	0.08 ± 0.02
2-methylpyrazine	1286	0.47 ± 0.11	1.24 ± 0.16	1.13 ± 0.08	0.81 ± 0.11
2,5-dimethylpyrazine	1346	0.44 ± 0.06	0.69 ± 0.04	0.45 ± 0.04	0.34 ± 0.02
2,6-dimethylpyrazine	1352	0.41 ± 0.06	0.74 ± 0.04	0.61 ± 0.03	0.45 ± 0.03
2-ethylpyrazine	1357	0.11 ± 0.02	0.24 ± 0.02	0.24 ± 0.02	0.18 ± 0.04
2,3-dimethylpyrazine	1371	0.08 ± 0.01	0.14 ± 0.01	0.17 ± 0.02	0.17 ± 0.01
2-ethyl-6-methylpyrazine	1408	0.12 ± 0.07	0.28 ± 0.01	0.32 ± 0.03	0.45 ± 0.00
2-ethyl-5-methylpyrazine	1415	0.13 ± 0.01	0.18 ± 0.01	0.13 ± 0.01	0.11 ± 0.00
2,3,5-trimethylpyrazine	1429	0.38 ± 0.03	0.43 ± 0.02	0.23 ± 0.02	0.21 ± 0.00
pyrazine-2-carboxylic acid amide	1740	0.29 ± 0.01	0.25 ± 0.00	0.23 ± 0.03	0.24 ± 0.01
pyrroles					
1-methylpyrrole	1542	0.12 ± 0.02	0.30 ± 0.00	0.17 ± 0.02	0.08 ± 0.00
1-methyl-1 <i>H</i> -pyrrole-2-carboxaldehyde	1651	0.13 ± 0.02	0.36 ± 0.01	0.25 ± 0.03	0.20 ± 0.00
2-acetyl-1-methylpyrrole	1683	0.17 ± 0.33	0.28 ± 0.01	0.41 ± 0.04	0.44 ± 0.01
2-acetylpyrrole	2022	0.82 ± 0.05	0.79 ± 0.08	5.90 ± 0.57	5.89 ± 0.31
pyrrole-2-carboxaldehyde	2059	1.41 ± 0.10	2.07 ± 0.04	1.00 ± 0.10	0.98 ± 0.05
furanones					
dihydro-2-methyl-3(2 <i>H</i>)-furanone	1282	0.14 ± 0.05	0.77 ± 0.17	0.38 ± 0.04	0.20 ± 0.02
5-methyl-2(5 <i>H</i>)-furanone	1707	0.13 ± 0.01	0.18 ± 0.01	0.19 ± 0.02	0.17 ± 0.01
2(5 <i>H</i>)-furanone	1787	0.80 ± 0.04	0.82 ± 0.01	0.20 ± 0.01	0.14 ± 0.01
dihydro-4-methyl-2(3 <i>H</i>)-furanone	1847	0.03 ± 0.01	0.20 ± 0.04	0.53 ± 0.09	0.74 ± 0.04
2,5-dimethyl-4-hydroxy-3(2 <i>H</i>)-furanone	2062	2.33 ± 0.18	2.00 ± 0.01	0.42 ± 0.03	0.46 ± 0.02
5-acetyldihydro-2(3 <i>H</i>)-furanone	2096	0.58 ± 0.06	0.78 ± 0.04	0.54 ± 0.02	0.50 ± 0.05
dihydro-5-(hydroxymethyl)-2(3 <i>H</i>)-furanone	2516	0.57 ± 0.05	1.03 ± 0.22	1.26 ± 0.35	1.23 ± 0.07
furans					
furfural	1482	1.10 ± 0.23	2.14 ± 0.23	0.28 ± 0.03	0.13 ± 0.02
2-acetylfuran	1527	0.48 ± 0.06	0.92 ± 0.03	0.83 ± 0.08	0.73 ± 0.04
furfuryl acetate	1552	0.14 ± 0.03	0.53 ± 0.00	1.11 ± 0.14	0.75 ± 0.02
5-methylfurfural	1596	1.46 ± 0.04	2.80 ± 0.06	0.48 ± 0.03	0.14 ± 0.01
furfuryl alcohol	1678	23.00 ± 1.30	28.27 ± 1.19	22.75 ± 1.63	10.82 ± 0.81
5-methylfuran-2-carboxylic acid, methyl ester	2044	0.67 ± 0.06	0.50 ± 0.01	0.23 ± 0.03	0.25 ± 0.03
5-hydroxymethylfurfural	2528	24.82 ± 1.62	7.69 ± 0.07	0.26 ± 0.01	—
cyclopentenes					
4,4-dimethyl-2-cyclopenten-1-one	1511	—	—	—	—
2,3-dimethyl-2-cyclopenten-1-one	1573	—	—	0.13 ± 0.01	0.19 ± 0.01
2-hydroxy-3-methyl-2-cyclopenten-1-one	1857	1.26 ± 0.07	1.52 ± 0.06	1.27 ± 0.12	1.45 ± 0.07
3-ethyl-2-hydroxy-2-cyclopenten-1-one	1924	0.35 ± 0.02	0.42 ± 0.01	0.57 ± 0.06	0.85 ± 0.06
phenols					
2-methoxyphenol	1886	0.24 ± 0.02	0.40 ± 0.01	0.73 ± 0.12	1.12 ± 0.06
phenol	2030	0.38 ± 0.07	0.47 ± 0.07	1.36 ± 0.12	2.68 ± 0.13
2-methoxy-4-vinylphenol	2225	2.55 ± 0.39	2.81 ± 0.58	1.39 ± 0.08	1.17 ± 0.06
catechol	2718	—	—	6.87 ± 0.82	9.73 ± 0.58
other miscellaneous compounds					
acetoin	1303	0.10 ± 0.03	0.47 ± 0.08	0.29 ± 0.01	0.12 ± 0.02
hydroxyacetone	1319	0.85 ± 0.15	2.14 ± 0.28	0.65 ± 0.07	0.43 ± 0.07
1-ethoxy-2-methylpropane	1364	0.03 ± 0.01	0.22 ± 0.02	0.13 ± 0.01	0.08 ± 0.01
1-hydroxy-2-butanone	1394	0.31 ± 0.06	0.80 ± 0.06	0.30 ± 0.02	0.21 ± 0.02
acetic acid	1468	0.85 ± 0.08	1.08 ± 0.05	0.60 ± 0.15	0.52 ± 0.04
1-acetyloxy-2-propanone	1477	0.40 ± 0.06	1.35 ± 0.04	0.81 ± 0.09	0.36 ± 0.02
propionic acid	1557	0.33 ± 0.01	0.50 ± 0.04	0.20 ± 0.04	0.14 ± 0.01
γ-butyrolactone	1662	2.06 ± 0.16	4.17 ± 0.03	10.77 ± 1.00	13.81 ± 0.73
3-methylbutanoic acid	1687	2.10 ± 0.09	2.33 ± 0.09	1.00 ± 0.02	0.76 ± 0.05
3-methyl-2-butenic acid	1819	1.15 ± 0.06	1.07 ± 0.02	0.50 ± 0.05	0.47 ± 0.02
maltol	2004	2.91 ± 0.29	4.60 ± 0.05	1.07 ± 0.03	1.38 ± 0.18
3,5-dihydroxy-6-methyl-4 <i>H</i> -pyran-4-one	2309	8.38 ± 1.10	0.92 ± 0.09	0.42 ± 0.02	0.60 ± 0.08

^a Solvent peak is excluded. Values are mean ± SD, *n* = 3. ^b Kovats index on DB-Wax column. ^c GC peak area % <0.01.

a sugar–amino acid browning reaction (27). Pyrazines have become one of the most important chemicals in cooked flavors, and many comprehensive reviews have been published about

them (28). However, the alkylpyrazines found in the present study did not show significant changes under different roasting conditions.

Table 4. Volatile Chemicals Identified in Brewed Coffee Prepared from Sumatran Green Beans Roasted at Different Conditions

compound	<i>I</i> ^b	GC peak area % ^a			
		light roast	medium roast	city roast	French roast
pyridines					
pyridine	1202	0.13 ± 0.01	1.06 ± 0.14	2.87 ± 0.43	5.19 ± 0.74
2-methylpyridine	1240	— ^c	—	—	—
6-methyl-3-pyridinol	2430	—	0.11 ± 0.10	0.61 ± 0.18	0.60 ± 0.02
3-hydroxypyridine	2450	0.96 ± 0.38	2.55 ± 0.84	4.84 ± 1.45	3.25 ± 0.32
pyrazines					
pyrazine	1231	—	0.07 ± 0.02	0.07 ± 0.01	0.07 ± 0.02
2-methylpyrazine	1286	0.52 ± 0.05	1.31 ± 0.17	0.96 ± 0.09	0.74 ± 0.10
2,5-dimethylpyrazine	1346	0.54 ± 0.06	0.73 ± 0.03	0.47 ± 0.02	0.34 ± 0.02
2,6-dimethylpyrazine	1352	0.49 ± 0.05	0.82 ± 0.04	0.61 ± 0.03	0.47 ± 0.04
2-ethylpyrazine	1357	0.11 ± 0.01	0.25 ± 0.02	0.17 ± 0.01	0.17 ± 0.05
2,3-dimethylpyrazine	1371	0.09 ± 0.01	0.14 ± 0.01	0.16 ± 0.01	0.20 ± 0.01
2-ethyl-6-methylpyrazine	1408	0.19 ± 0.02	0.30 ± 0.01	0.34 ± 0.01	0.46 ± 0.02
2-ethyl-5-methylpyrazine	1415	0.15 ± 0.01	0.15 ± 0.00	0.11 ± 0.01	0.09 ± 0.03
2,3,5-trimethylpyrazine	1429	0.33 ± 0.04	0.43 ± 0.00	0.27 ± 0.01	0.22 ± 0.01
pyrazine-2-carboxylic acid amide	1740	0.37 ± 0.03	0.20 ± 0.01	0.24 ± 0.02	0.22 ± 0.01
pyrroles					
1-methylpyrrole	1542	0.04 ± 0.02	0.27 ± 0.01	0.21 ± 0.01	0.09 ± 0.01
1-methyl-1 <i>H</i> -pyrrole-2-carboxaldehyde	1651	0.06 ± 0.02	0.36 ± 0.05	0.33 ± 0.01	0.25 ± 0.01
2-acetyl-1-methylpyrrole	1683	0.14 ± 0.01	0.21 ± 0.01	0.47 ± 0.02	0.50 ± 0.02
2-acetylpyrrole	2022	0.83 ± 0.05	0.95 ± 0.08	6.72 ± 0.67	7.07 ± 0.37
pyrrole-2-carboxaldehyde	2059	0.94 ± 0.05	1.93 ± 0.15	1.38 ± 0.12	1.17 ± 0.06
furanones					
dihydro-2-methyl-3(2 <i>H</i>)-furanone	1282	0.08 ± 0.01	0.72 ± 0.17	0.29 ± 0.04	0.15 ± 0.03
5-methyl-2(5 <i>H</i>)-furanone	1707	0.05 ± 0.03	0.16 ± 0.01	0.17 ± 0.01	0.15 ± 0.03
2(5 <i>H</i>)-furanone	1787	0.63 ± 0.09	0.83 ± 0.06	0.20 ± 0.02	0.08 ± 0.03
dihydro-4-methyl-2(3 <i>H</i>)-furanone	1847	—	0.14 ± 0.01	0.51 ± 0.04	0.80 ± 0.01
2,5-dimethyl-4-hydroxy-3(2 <i>H</i>)-furanone	2062	3.11 ± 0.24	1.99 ± 0.21	0.52 ± 0.01	0.36 ± 0.01
5-acetyldihydro-2(3 <i>H</i>)-furanone	2096	0.37 ± 0.02	0.60 ± 0.06	0.60 ± 0.02	0.55 ± 0.05
dihydro-5-(hydroxymethyl)-2(3 <i>H</i>)-furanone	2516	0.40 ± 0.34	0.81 ± 0.22	0.84 ± 0.30	0.95 ± 0.04
furans					
furfural	1482	0.71 ± 0.09	2.69 ± 0.34	0.25 ± 0.02	0.13 ± 0.02
2-acetylfuran	1527	0.28 ± 0.04	0.99 ± 0.06	0.86 ± 0.03	0.74 ± 0.04
furfuryl acetate	1552	—	0.43 ± 0.04	0.92 ± 0.05	0.79 ± 0.04
5-methylfurfural	1596	0.82 ± 0.08	2.70 ± 0.23	0.50 ± 0.04	0.16 ± 0.02
furfuryl alcohol	1678	18.93 ± 3.09	27.51 ± 2.40	26.29 ± 1.38	12.35 ± 0.34
5-methylfuran-2-carboxylic acid, methyl ester	2044	0.51 ± 0.03	0.48 ± 0.03	0.28 ± 0.02	0.29 ± 0.01
5-hydroxymethylfurfural	2528	23.09 ± 2.13	9.68 ± 1.26	0.22 ± 0.02	—
cyclopentenes					
4,4-dimethyl-2-cyclopenten-1-one	1511	—	—	0.02 ± 0.00	0.04 ± 0.01
2,3-dimethyl-2-cyclopenten-1-one	1573	—	—	0.12 ± 0.00	0.17 ± 0.01
2-hydroxy-3-methyl-2-cyclopenten-1-one	1857	0.93 ± 0.05	1.34 ± 0.09	1.61 ± 0.11	1.68 ± 0.04
3-ethyl-2-hydroxy-2-cyclopenten-1-one	1924	0.23 ± 0.02	0.43 ± 0.03	0.69 ± 0.08	0.98 ± 0.04
phenols					
2-methoxyphenol	1886	—	0.34 ± 0.02	0.90 ± 0.07	1.36 ± 0.04
phenol	2030	0.13 ± 0.02	0.38 ± 0.10	1.21 ± 0.09	2.61 ± 0.05
2-methoxy-4-vinylphenol	2225	3.51 ± 0.35	2.39 ± 0.26	1.71 ± 0.06	1.13 ± 0.06
catechol	2718	—	—	4.31 ± 0.98	7.56 ± 0.75
other miscellaneous compounds					
acetoin	1303	0.08 ± 0.01	0.41 ± 0.10	0.21 ± 0.03	0.11 ± 0.03
hydroxyacetone	1319	0.83 ± 0.12	2.38 ± 0.62	0.46 ± 0.08	0.39 ± 0.07
1-ethoxy-2-methylpropane	1364	0.02 ± 0.01	0.21 ± 0.03	0.12 ± 0.01	0.07 ± 0.01
1-hydroxy-2-butanone	1394	0.21 ± 0.04	0.92 ± 0.13	0.28 ± 0.01	0.21 ± 0.02
acetic acid	1468	0.73 ± 0.04	1.23 ± 0.15	0.44 ± 0.13	0.39 ± 0.05
1-acetyloxy-2-propanone	1477	0.23 ± 0.04	1.19 ± 0.08	0.96 ± 0.04	0.39 ± 0.03
propionic acid	1557	0.34 ± 0.04	0.64 ± 0.06	0.30 ± 0.05	0.15 ± 0.01
γ-butyrolactone	1662	2.54 ± 0.40	4.88 ± 0.33	11.06 ± 0.87	15.22 ± 0.23
3-methylbutanoic acid	1687	3.79 ± 0.38	3.55 ± 0.03	2.09 ± 0.23	1.36 ± 0.07
3-methyl-2-butenic acid	1819	1.23 ± 0.07	1.02 ± 0.04	0.67 ± 0.03	0.56 ± 0.02
maltol	2004	2.70 ± 0.24	3.44 ± 0.23	1.08 ± 0.10	0.97 ± 0.07
3,5-dihydroxy-6-methyl-4 <i>H</i> -pyran-4-one	2309	15.26 ± 1.09	1.66 ± 0.33	0.41 ± 0.03	0.60 ± 0.05

^a Solvent peak is excluded. Values are mean ± SD, *n* = 3. ^b Kovats index on DB-Wax column. ^c GC peak area % <0.01.

Pyridine, which has a pungent and diffusive odor but which gives a pleasant-burnt/smoky odor in extreme dilution (13), was first reported in coffee in 1946 (29). In the present study, the

concentration of pyridine increased steadily with the increase of the roasting intensity (Figure 1). This result was consistent with the previous paper (9), suggesting that higher intensity roasting

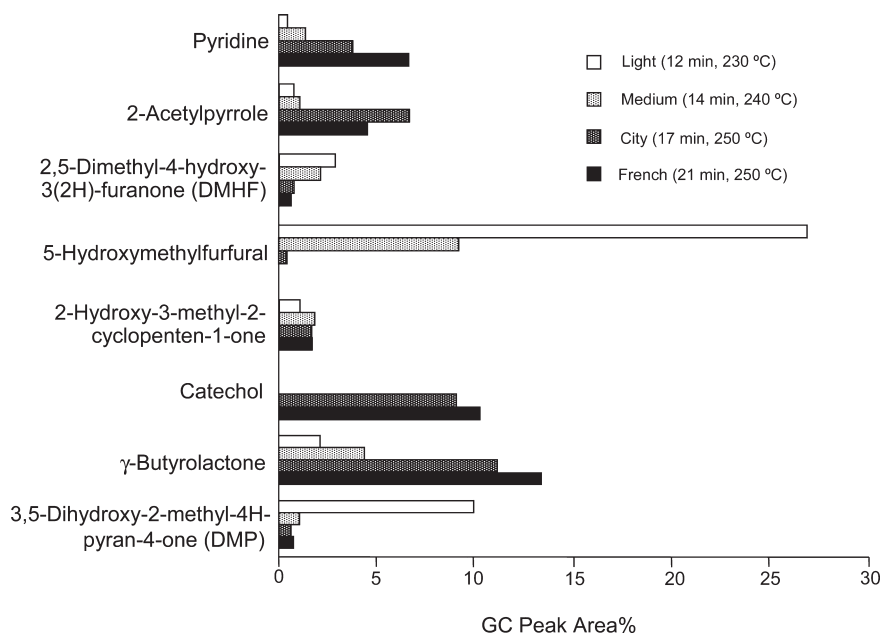


Figure 1. Concentrations of chemicals significantly influenced by four roasting conditions found in extracts obtained from Ethiopian coffee beans.

produces more pyridine. On the other hand, in the roasted Nicaraguan green coffee beans 3-hydroxypyridine was formed more in the coffee roasted by the city roasting condition ($4.59 \pm 1.58\%$) than in that by the French roasting condition ($3.33 \pm 0.23\%$). The same result was obtained from the roasted Ethiopian green coffee beans, whereas the concentration of 2-acetylpyrrole increased considerably from $0.92 \pm 0.08\%$ (medium roasting) to $5.60 \pm 0.56\%$ (city roasting) and then reduced to $4.66 \pm 0.15\%$ (French roasting).

The formation of γ -butyrolactone exhibited clear roasting-intensity response (**Figure 1**), ranging from $2.06 \pm 0.02\%$ (light roasting) to $13.29 \pm 1.56\%$ (French roasting). The result was also consistent with the previous paper (18). One study indicated that γ -butyrolactone formed from a chlorogenic acid lactone (30).

γ -Butyrolactone in coffee volatiles was reported in many studies in the 1960s (31), and since then it has been constantly reported in coffee volatiles (1, 32). Generally, γ -butyrolactone and its alkyl-substituted derivatives possess butter/coconut-like flavors and have been widely used for perfumes and food flavorings (13). Therefore, this compound may play an important role in the flavor of coffees roasted under different conditions.

Phenols were found in coffee in the relatively early years of flavor studies (33). Among phenols identified in the present study, 2-methoxyphenol and 2-methoxy-4-vinylphenol decreased with increasing roasting intensity. On the other hand, phenol and catechol increased with increasing roasting intensity. As **Figure 1** shows, catechol was found only in the coffee roasted under the relatively intense conditions of city ($8.86 \pm 0.78\%$) and French roasting ($10.02 \pm 2.75\%$). These results may be due to formation from different precursors. In fact, chlorogenic acids, which contain a phenolic moiety, readily degrade in coffee upon heat treatment (34).

The concentration of cyclopentenones found in the present study was relatively low and did not show significant changes under different roasting conditions (**Figure 1**). Their concentration increased slightly when the roasting intensity increased, which is consistent with a recent paper (35). Cyclopentenones, including 2-hydroxy-3-methyl-2-cyclopenten-1-one, have been known to be present in coffee volatiles since the mid 1960s (36). They were also known as a sugar caramelization product and have a sweet and caramellic-spicy odor (37).

Volatile chemicals always play an important role in the palatability and preferences for heat-treated foods and beverages. Also, the specific conditions of heat treatment significantly influence the final flavor of foods and beverages. The present study found that the roasting conditions significantly changed the concentrations of certain volatile chemicals in coffee beans. Flavor chemicals such as furfural derivatives and furanones, which form from components (e.g., sugars and lipids) of green coffee beans, were yielded in relatively high concentrations under mild roasting conditions but were reduced under higher roasting intensities. On the other hand, chemicals such as pyridines and pyrroles, which form from the Maillard reaction between an amino acid and a sugar, were formed more in coffee beans roasted under high roasting intensities than in those roasted under mild roasting intensities. Also, the chemicals formed from the degradation of chlorogenic acids, such as phenols and lactone, were produced more by high roasting intensities than by low roasting intensities. Therefore, formation differences of these volatile chemicals caused by roasting conditions must play an important role in the flavor characteristic of brewed coffees.

Another study on the role of roasting conditions in the formation of 16 aroma chemicals from Sumatran coffee beans reported that the concentrations of hexanal, pyridine, and dimethyl sulfide increased when the roasting temperature was increased, whereas the concentrations of the other 13 aroma chemicals were either reduced or kept constant when the roasting temperature was increased (16).

Table 5 shows the results of volatile analysis of four commercial roasted-ground coffees. The table also lists the compounds found in the coffee beans roasted under four different conditions in the laboratory (**Tables 2–4**). The amount of total volatile chemicals recovered from coffee beans was 24.3 ± 1.8 mg/g from Dunkin, 28.5 ± 6.6 mg/g from GOUD, 34.9 ± 5.5 mg/g from Puroast Fine, and 35.1 ± 3.4 mg/g from SF Bay.

Figure 2 shows the concentrations of coffee components that showed significant changes in concentration according to the roasting condition (refer to **Figure 1**). General profiles of volatile chemicals in the commercial roasted-ground coffee were similar to those in the laboratory-roasted coffees. Furans were found in the greatest concentrations in all four commercial roasted-ground coffees. The results suggest that GOUD coffee was

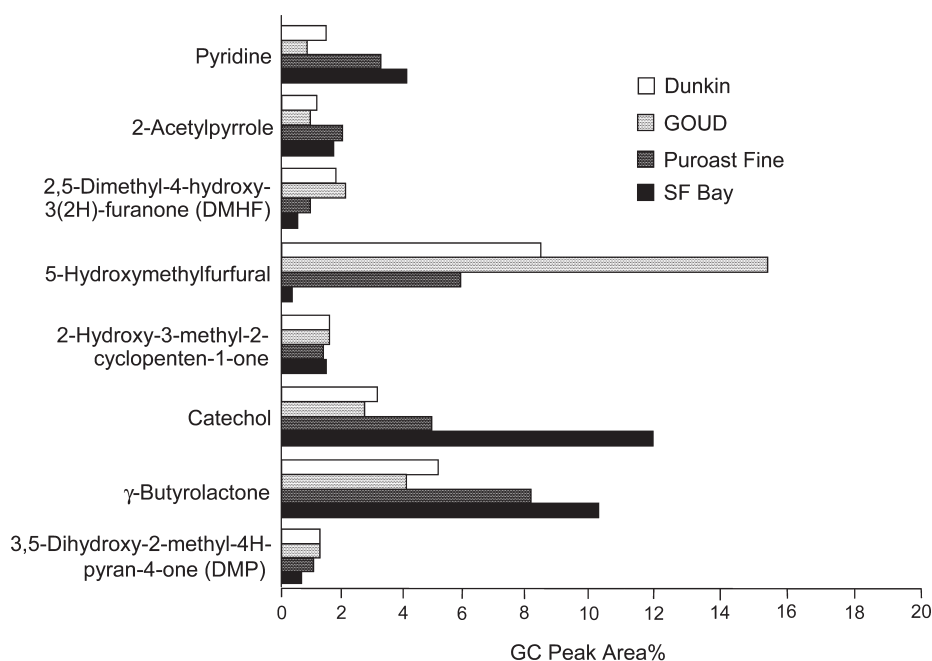
Table 5. Volatile Chemicals Identified in Brewed Coffee Prepared from Commercial Roasted–Ground Coffee

compound	<i>i</i> ^b	GC peak area % ^a			
		Dunkin	GOUD	Puroast Fine	SF Bay
pyridines					
pyridine	1202	1.32 ± 0.20	0.73 ± 0.15	3.07 ± 0.76	3.81 ± 0.25
2-methylpyridine	1240	— ^c	—	0.03 ± 0.00	0.03 ± 0.00
6-methyl-3-pyridinol	2430	0.22 ± 0.02	0.13 ± 0.09	0.66 ± 0.10	1.02 ± 0.14
3-hydroxypyridine	2450	3.17 ± 0.38	2.65 ± 0.54	6.42 ± 1.29	6.59 ± 0.89
pyrazines					
pyrazine	1231	0.12 ± 0.03	—	0.05 ± 0.02	0.10 ± 0.01
2-methylpyrazine	1286	1.48 ± 1.27	1.27 ± 0.23	0.57 ± 0.10	0.87 ± 0.05
2,5-dimethylpyrazine	1346	0.65 ± 0.05	0.58 ± 0.05	0.31 ± 0.01	0.36 ± 0.01
2,6-dimethylpyrazine	1352	0.69 ± 0.06	0.60 ± 0.06	0.34 ± 0.02	0.47 ± 0.02
2-ethylpyrazine	1357	0.24 ± 0.03	0.18 ± 0.02	0.15 ± 0.03	0.16 ± 0.01
2,3-dimethylpyrazine	1371	0.15 ± 0.01	0.13 ± 0.01	0.11 ± 0.01	0.15 ± 0.01
2-ethyl-6-methylpyrazine	1408	0.25 ± 0.02	0.18 ± 0.01	0.27 ± 0.01	0.32 ± 0.01
2-ethyl-5-methylpyrazine	1415	0.12 ± 0.01	0.10 ± 0.01	0.10 ± 0.02	0.09 ± 0.01
2,3,5-trimethylpyrazine	1429	0.35 ± 0.03	0.32 ± 0.01	0.19 ± 0.01	0.23 ± 0.01
pyrazine-2-carboxylic acid amide	1740	—	—	—	—
pyrroles					
1-methylpyrrole	1542	—	—	—	—
1-methyl-1 <i>H</i> -pyrrole-2-carboxaldehyde	1651	0.25 ± 0.02	0.17 ± 0.01	0.43 ± 0.03	0.25 ± 0.07
2-acetyl-1-methylpyrrole	1683	0.22 ± 0.01	0.16 ± 0.01	0.27 ± 0.02	0.37 ± 0.03
2-acetylpyrrole	2022	1.07 ± 0.05	0.87 ± 0.06	1.87 ± 0.16	1.48 ± 0.10
pyrrole-2-carboxaldehyde	2059	1.66 ± 0.03	1.37 ± 0.11	1.94 ± 0.14	1.01 ± 0.07
furanones					
dihydro-2-methyl-3(2 <i>H</i>)-furanone	1282	0.58 ± 0.13	0.42 ± 0.12	0.71 ± 0.19	0.25 ± 0.02
5-methyl-2(5 <i>H</i>)-furanone	1707	0.17 ± 0.01	0.19 ± 0.01	0.12 ± 0.01	0.12 ± 0.01
2(5 <i>H</i>)-furanone	1787	0.62 ± 0.03	0.66 ± 0.07	0.29 ± 0.02	0.12 ± 0.01
dihydro-4-methyl-2(3 <i>H</i>)-furanone	1847	—	—	—	—
2,5-dimethyl-4-hydroxy-3(2 <i>H</i>)-furanone	2062	1.58 ± 0.14	1.91 ± 0.21	0.83 ± 0.04	0.47 ± 0.02
5-acetyldihydro-2(3 <i>H</i>)-furanone	2096	—	—	—	—
dihydro-5-(hydroxymethyl)-2(3 <i>H</i>)-furanone	2516	1.40 ± 0.21	1.39 ± 0.22	1.57 ± 0.24	1.70 ± 0.22
furans					
furfural	1482	1.80 ± 0.21	2.50 ± 0.36	0.73 ± 0.08	0.17 ± 0.01
2-acetylfuran	1527	0.80 ± 0.05	0.82 ± 0.05	0.57 ± 0.01	0.65 ± 0.02
furfuryl acetate	1552	0.55 ± 0.06	0.36 ± 0.04	0.49 ± 0.07	0.92 ± 0.04
5-methylfurfural	1596	2.21 ± 0.12	2.34 ± 0.13	1.05 ± 0.06	0.28 ± 0.01
furfuryl alcohol	1678	29.35 ± 2.16	24.78 ± 1.28	19.75 ± 1.34	16.78 ± 0.47
5-methylfuran-2-carboxylic acid, methyl ester	2044	—	—	—	—
5-hydroxymethylfurfural	2528	8.06 ± 0.71	15.16 ± 1.69	5.55 ± 0.10	0.24 ± 0.02
cyclopentenes					
4,4-dimethyl-2-cyclopenten-1-one	1511	—	—	—	—
2,3-dimethyl-2-cyclopenten-1-one	1573	—	—	—	—
2-hydroxy-3-methyl-2-cyclopenten-1-one	1857	1.42 ± 0.08	1.47 ± 0.04	1.24 ± 0.12	1.28 ± 0.10
3-ethyl-2-hydroxy-2-cyclopenten-1-one	1924	0.25 ± 0.00	0.41 ± 0.03	0.69 ± 0.03	0.84 ± 0.04
phenols					
2-methoxyphenol	1886	0.16 ± 0.01	0.19 ± 0.03	0.17 ± 0.01	0.12 ± 0.01
phenol	2030	0.46 ± 0.02	0.46 ± 0.04	1.33 ± 0.12	1.35 ± 0.07
2-methoxy-4-vinylphenol	2225	—	—	1.19 ± 0.30	—
catechol	2718	2.91 ± 0.20	2.48 ± 0.26	4.63 ± 0.15	11.48 ± 0.60
other miscellaneous compounds					
acetoin	1303	—	—	—	—
hydroxyacetone	1319	2.73 ± 0.56	3.20 ± 0.88	1.09 ± 0.44	0.49 ± 0.08
1-ethoxy-2-methylpropane	1364	—	—	—	—
1-hydroxy-2-butanone	1394	0.60 ± 0.04	0.84 ± 0.13	0.38 ± 0.06	0.21 ± 0.01
acetic acid	1468	0.05 ± 0.07	—	0.07 ± 0.01	0.07 ± 0.01
1-acetyloxy-2-propanone	1477	1.47 ± 0.10	1.47 ± 0.10	0.84 ± 0.05	0.62 ± 0.02
propionic acid	1557	0.15 ± 0.02	0.05 ± 0.01	0.06 ± 0.01	0.05 ± 0.00
γ-butyrolactone	1662	4.82 ± 0.16	3.79 ± 0.30	7.76 ± 0.38	9.82 ± 0.51
3-methylbutanoic acid	1687	2.11 ± 0.02	2.53 ± 0.03	2.41 ± 0.08	0.89 ± 0.11
3-methyl-2-butenic acid	1819	0.60 ± 0.07	0.63 ± 0.04	0.02 ± 0.01	0.07 ± 0.01
maltol	2004	3.14 ± 0.13	2.50 ± 0.39	6.76 ± 1.10	4.97 ± 0.33
3,5-dihydroxy-6-methyl-4 <i>H</i> -pyran-4-one	2309	1.08 ± 0.19	1.12 ± 0.13	0.95 ± 0.06	0.54 ± 0.04

^a Solvent peak is excluded. Values are mean ± SD, *n* = 3. ^b Kovats index on DB-Was column. ^c GC peak area % <0.01.

prepared under the least intense conditions among the four commercial roasted–ground coffees because 5-hydroxymethylfurfural was found in high concentrations (15.16 ± 1.69%) and

catechol concentration was low (2.48 ± 0.26%). The presence of other chemicals was similar to that in the light roasted coffee. On the other hand, SF Bay coffee may be prepared by the most



1

Figure 2. Concentrations of coffee components that showed significant changes in concentration according to the roasting condition (refer to **Figure 1**).

intense conditions among the four commercial roasted—ground coffees because catechol and γ -butyrolactone were found in high concentrations of 11.48 ± 0.60 and $9.82 \pm 0.51\%$, respectively. The presence of other chemicals resulted in concentrations similar to those of the French roasted coffee.

The results of the present study suggest that controlling the roasting conditions according to the formation of particular chemicals can prepare a roasted coffee with preferable flavor.

LITERATURE CITED

- (1) Flament, I.; Bessiere-Thomas, Y. *Coffee Flavor Chemistry*; Wiley: New York, 2002.
- (2) Shibamoto, T. An overview of coffee aroma and flavor chemistry. In *Proceedings of the 14th International Scientific Colloquium on Coffee*, San Francisco, 1991; Association Scientifique Internationale du Café: Paris, France, 1992; pp 107–116.
- (3) Shibamoto, T. Heterocyclic compounds in browning and browning/nitrite model systems: Occurrence, formation mechanisms, flavor characteristics and mutagenic activity. In *Instrumental Analysis of Foods*; Charalambous, G., Inglett, G., Eds.; Academic Press: New York, 1983; Vol. I, pp 229–278.
- (4) Bastos, C. A.; Moreira, R. F. A.; Trugo, L. C. Volatile components in roasted coffee. Part I: Heterocyclic compounds. *Quim. Nova* **1999**, *22*, 209–217.
- (5) Czerny, M.; Mayer, F.; Grosch, W. Sensory study on the character impact odorants of roasted Arabica coffee. *J. Agric. Food Chem.* **1999**, *47*, 695–699.
- (6) Buffo, R. A.; Cardelli-Freire, C. Coffee flavour: an overview. *Flavour Fragrance J.* **2004**, *19*, 99–104.
- (7) Trugo, L. C.; Macrae, R. A study of the effect of roasting on the chlorogenic acid composition of coffee using HPLC. *Food Chem.* **1984**, *15*, 219–227.
- (8) Dorfner, R.; Ferge, T.; Uchimura, T.; Yeretian, C.; Zimmermann, R.; Kettrup, A. Laser/chemical ionization—mass spectrometry as an on-line analysis technique for monitoring the coffee roasting progress. *Colloque Sci. Int. Cafe* **2001**, *19*, 432–445.
- (9) Shibamoto, T.; Harada, K.; Mihara, S.; Nishimura, O.; Yamaguchi, K.; Aitoku, A.; Fukada, T. Application of HPLC for evaluation of coffee flavor quality. In *The Quality of Food and Beverages*; Charalambous, G., Ed.; Academic Press: New York, 1981; pp 312–334.
- (10) Silwar, R.; Lüllmann, C. Investigation of aroma formation in Robusta coffee during roasting. *Cafe Cacao The* **1993**, *37*, 145–151.
- (11) Zil'bergleit, M. A.; Glushko, T. V. Polymerization products of furfural and hydroxymethylfurfural in acetic acid. *Koksnes Kimija* **1991**, *1*, 66–68.
- (12) Bott, H. G.; Hirst, E. L. Formation of furfural from methylated pentoses. *J. Chem. Soc.* **1932**, 2621–2624.
- (13) Arctander, S. *Perfume and Flavor Chemicals*; published by the author: Montclair, NJ, 1969.
- (14) Nakama, A.; Kim, E. H.; Shinohara, K.; Omura, H. Formation of furfural derivatives in the amino-carbonyl reaction. *Biosci., Biotechnol., Biochem.* **1993**, *57*, 1757–1759.
- (15) Akiyama, M.; Murakami, K.; Ohtani, N.; Iwatsuki, K.; Sotoyama, K.; Wada, A.; Tokuno, K.; Iwabuchi, H.; Tanaka, K. Analysis of volatile compounds released during the grinding of roasted coffee beans using solid-phase microextraction. *J. Agric. Food Chem.* **2003**, *51*, 1961–1969.
- (16) Baggenstoss, J.; Poisson, L.; Kaegi, R.; Perren, R.; Escher, F. Coffee roasting and aroma formation: application of different time-temperature conditions. *J. Agric. Food Chem.* **2008**, *56*, 5836–5846.
- (17) Hodge, J. E.; Fisher, B. E.; Nelson, E. C. Dicarbonyls, reductones, and heterocyclics produced by the reactions of reducing sugars with secondary amine salts. *Am. Soc. Brew. Chem. Proc.* **1963**, 84–92.
- (18) Blank, I.; Fay, L. B.; Lakner, F. J.; Schlosser, M. Determination of 4-hydroxy-2,5-dimethyl-3(2H)-furanone and 2(or 5)-ethyl-4-hydroxy-6(or 2)-methyl-3(2H)-furanone in pentose sugar-based Maillard model systems by isotope dilution assays. *J. Agric. Food Chem.* **1997**, *45*, 2642–2648.
- (19) Tressl, R.; Bahri, D.; Köppler, H.; Jensen, A. Diphenole und Caramelkomponenten in Röstkaffees verschiedener Sorten. II. *Z. Lebensm. Unters. Forsch.* **1978**, *167*, 111–114.
- (20) Rodin, J. O.; Himel, R. M.; Silverstein, R. M.; Leeper, R. W.; Gortner, W. A. Volatile flavor and aroma components of pineapple (I) isolation and tentative identification of 2,5-dimethyl-4-hydroxy-3(2H)-furanone. *J. Food Sci.* **1965**, *30*, 280–285.
- (21) Perez, A. G.; Olias, R.; Olias, J. M.; Sanz, C. Biosynthesis of 4-hydroxy-2,5-dimethyl-3(2H)-furanone and derivatives in in vitro grown strawberries. *J. Agric. Food Chem.* **1999**, *47*, 655–658.
- (22) Rapp, A.; Knipser, W.; Engel, L.; Ullemeyer, H.; Heimann, W. Off-flavor compounds in the berry and wine aroma. *Vitis* **1980**, *19*, 13–23.
- (23) Haleva-Toledo, E.; Maim, M.; Zehavi, U.; Rouseff, R. L. 4-Hydroxy-2,5-dimethyl-3(2H)-furanone formation in buffers and model

- solutions of citrus juice. *J. Agric. Food Chem.* **1997**, *45*, 1314–1319.
- (24) Miyake, T.; Shibamoto, T. Inhibition of malonaldehyde and acetaldehyde formation from blood plasma oxidation by naturally occurring antioxidants. *J. Agric. Food Chem.* **1998**, *46*, 3694–3697.
- (25) Ledl, F. Z. Analysis of volatile sugar degradation products. *Lebens. Gerich. Chem.* **1987**, *41*, 83–87.
- (26) Shibamoto, T. Heterocyclic compounds in browning and browning/nitrite model systems: occurrence, formation mechanisms, flavor characteristics and mutagenic activity. In *Instrumental Analysis of Foods*; Charalambous, G., Inglett, G., Eds.; Academic Press: New York, 1983; Vol. I, pp 229–278.
- (27) Koehler, P. E.; Mason, M. E.; Newell, J. A. Formation of pyrazine compounds in sugar–amine reactions. *J. Agric. Food Chem.* **1969**, *17*, 393–396.
- (28) Maga, J. A. Pyrazine update. *Food Rev. Int.* **1992**, *8*, 479–558.
- (29) Hughes, E. B.; Smith, R. F. The nicotinic acid content of coffee. *J. Soc. Chem. Ind.* **1946**, *65*, 284–286.
- (30) Moreira, D. P.; Farah, A.; Donangelo, C. M. Kinetic behavior of chlorogenic acids and lactones during roasting of Brazilian *Coffea arabica* and *Coffea canephora*. *Colloque Sci. Int. Cafe* **2006**, *21*, 244–247.
- (31) Stoffelsma, J.; Pypker, J. Some new constituents of roasted coffee. *Recl. Trav. Chim. Pays-Bas* **1968**, *87*, 241–242.
- (32) Fujioka, K.; Shibamoto, T. Quantitation of volatiles and nonvolatile acids in an extract from coffee beverages: correlation with antioxidant activity. *J. Agric. Food Chem.* **2006**, *54*, 6054–6058.
- (33) Heins, J. T.; Maarse, H.; ten Noever de Brauw, M. C.; Weurman, C. Direct food vapour analysis and component identification by a coupled capillary GLC-MS arrangement. *J. Gas Chromatogr.* **1966**, *4*, 395–397.
- (34) Leloup, V.; Louvrier, A.; Liardon, R. Degradation mechanisms of chlorogenic acids during roasting. *Colloque Sci. Int. Cafe* **1995**, *16*, 192–198.
- (35) Akiyama, M.; Murakami, K.; Hirano, Y.; Ikeda, M.; Iwatsuki, K.; Wada, A.; Tokuno, K.; Onishi, M.; Iwabuchi, H. Characterization of headspace aroma compounds of freshly brewed Arabica coffees and studies on characteristic aroma compounds of Ethiopian coffee. *J. Food Sci.* **2008**, *73*, C335–C346.
- (36) Gianturco, M. A.; Giammarino, A. S.; Pitcher, R. G. The structures of five cyclic diketones isolated from coffee. *Tetrahedron* **1963**, *19*, 2051–2059.
- (37) Nishimura, O.; Mihara, S. Investigation of 2-hydroxy-2-cyclopentene-1-ones in roasted coffee. *J. Agric. Food Chem.* **1990**, *38*, 1038–1041.

Received April 6, 2009. Revised manuscript received May 17, 2009. Accepted May 18, 2009. This study was supported, in part, by a grant-in-aid from Puroast Co., Ltd., Woodland, CA.