Affect Of Roasting On Coffee Essence

Sensus Technical Note (SEN-TN-0011) 11/26/2008

Kevin L, Goodner, Ph.D.

ABSTRACT

Low, medium, and high roast coffee essences were compared. Using the low roast as the reference point, compounds were identified and semi-quantified based on the relative change from the low roast coffee essence. A total of 36 compounds were identified as either the relative concentration decreasing or increasing by at least a factor of 2.

INTRODUCTION

Coffee beans are roasted to provide the unique and characteristic aroma of coffee. There are many variables in the roasting process such as time and temperature. Sensus has settled on 2 main roasting levels, medium and high. A low roasting condition was tested and analyzed in this report. A comparison of the 3 roasts to determine the compounds that change the most relative to the low roast is a valuable starting point to determining the key differences that drive flavor perception. This report details the chemicals that changed the most due to the roasting process.

MATERIALS AND METHODS

A Gerstel MultiPurposeSampler (MPS-2) (Baltimore, MD) was used with a 1-cm 3-phase (divinylbenene, Carboxen, Polydimethylsiloxane) for sample preparation. A 10-min incubation followed by a 40-min exposure was used to capture the volatiles on the fiber for injection into the GC. Samples were stirred using a 3x12mm stirbar in the 20mL vial. The fiber was desorbed for 5-min in the GC injector for 5 min. An Agilent 7890A gas chromatograph (Palo Alto, CA) was used for the analysis. Analysis was performed in the splitless mode with a helium flow rate of 1.25mL/min through a 60mx0.25mmx0.25μm RTX-5ms column. The initial oven temperature was 50°C immediately followed by a 4°C/min temperature ramp to 170°C which was followed by a 100°C/min ramp to 250°C and held for 5min in order to ensure no sample to sample contamination. The transfer line to the Leco TruTOF MS (St. Joseph, MN) was held at 240°C. Data was collected for 30-250 *m/z* at an acquisition rate of 10 spectra per sec. Identification was based on a combination of MS library matching along with reported retention indices.

7255 Hamilton Enterprise Park Drive
Hamilton, OH 45011
Tel: 513-892-7100
www.sensusflavors.com

RESULTS AND DISCUSSION

Table 1 is a list of 37 compounds that changed by at least a factor of 2 from the light roast coffee essence to the medium or high roast coffee essence. Many of the compounds are as one would expect from increased roasting. Pyrazine, pyridine, furan (not listed due to less than 2x increase) and their derivatives. Sulfur containing compounds such as dimethyl sulfide, 2-furfurylthiol, and others are also present. Some of the compounds increase or decrease going from light to medium to high roast while others decrease then increase or vice versa. Figure 1 is an overlay of *m/z* 94 to show the relative difference of dimethyl sulfide and how it increases with roast. This is fairly typical of the compounds that increase with roast. Figure 2 is also an overlay of *m/z* 94, but the peak is methyl pyrazine. This is fairly typical of a compound that increases from low to medium, but has little change from medium to high. This list will help serve as a launching point for further studies.

Figure 1. m/z 94 of dimethyl sulfide of light, medium, and high roast coffee.

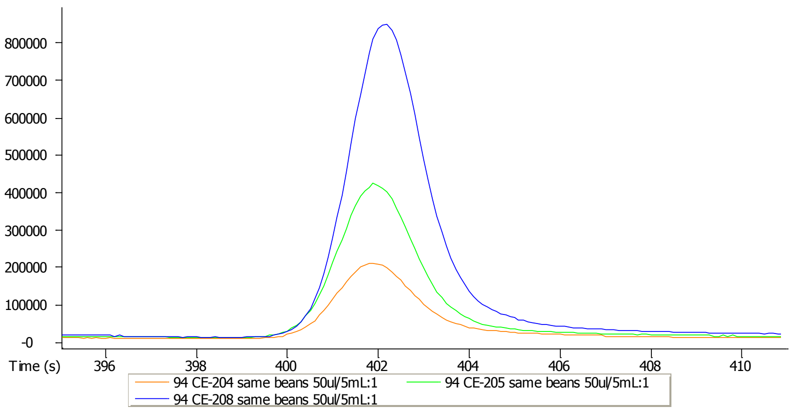
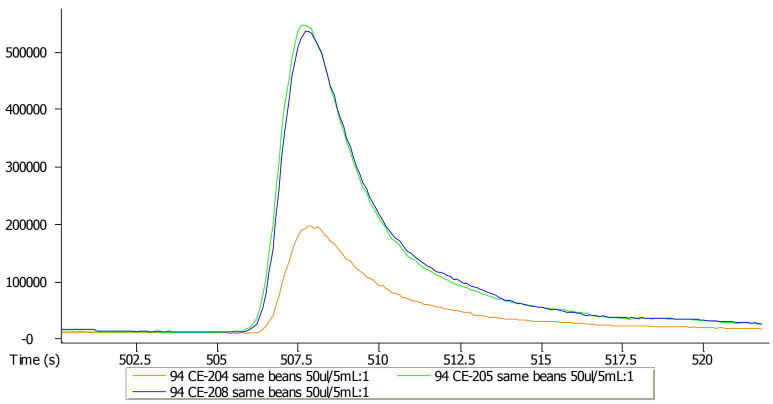


Figure 2. . m/z 94 of dimethyl sulfide of light, medium, and high roast coffee.



7255 Hamilton Enterprise Park Drive
Hamilton, OH 45011
Tel: 513-892-7100
www.sensusflavors.com

Table 1. Compounds and relative concentration as compared to light roast coffee essence.

Peak #	Name	Ret. Ind.	Relative Concentration	
			Medium	High
1	Pyrazine	728	19	39
2	Pyridine	739	159	227
3	Dimethyl Sulfide	742	127	211
4	2-Butenoic acid, methyl ester, (E)-	754	977	1391
5	Thiophene, 2,5-dihydro-	761	465	568
6	3-Methyl-3-butene-1-thiol	772	411	782
7	Pyrazine, methyl	820	204	172
8	Furan, (2-methoxymethyl)	824	213	190
9	Thiophene, 2,3-dihydro-5-methyl-	843	-	703
10	3-Furanmethanol	852	1268	782
11	3,4-Dimethylthiophene	877	523	-
12	Thiazole, 2,4-dimethyl-	884	242	617
13	2,5-Dimethylpyrimidine	910	674	150
14	2-Furfurylthiol	911	146	48
15	2-Furanmethanol, tetrahydro-, acetate	927	520	828
16	Pyridine, 2,4-dimethyl-	984	238	44
17	Benzene, 1,2,3-trimethyl-	995	42	46
18	2-Cyclohexen-1-one, 3-methyl-	1000	31	251
19	Octanal	1000	11	136
20	4(H)-Pyridine, N-acetyl-	1020	678	-
21	1H-Pyrrole-2-carboxaldehyde, 1-ethyl-	1052	839	814
22	2-Furanmethanethiol, 5-methyl-	1063	1062	121
23	2-Cyclopenten-1-one, 3-ethyl-2-hydroxy-	1096	661	508
24	5,9-Undecadien-2-one, 6,10-dimethyl-, (E)-	1107	597	523
25	Benzeneacetaldehyde, à,à-dimethyl-	1149	604	341
26	Naphthalene	1194	34	47
27	Furan, 2-[(methyldithio)methyl]-:2	1220	517	90
28	Ethanone, 1-(2-hydroxy-5-methylphenyl)-	1316	1929	661
29	1,4-Benzenediamine, N,N-dimethyl-	1348	902	98
30	Undecanal, 2-methyl-	1475	40	127
31	Diethyltoluamide	1587	46	27
32	Diethyl Phthalate	1598	47	33
33	Bis(2-furfuryl)disulfide:5	1700	58	17
34	Benzoic acid, 2-ethylhexyl ester	1714	47	35
35	2-Ethylhexyl salicylate	1815	59	45
36	1,2-Benzenedicarboxylic acid, bis(1-methylethyl) ester	1874	45	36

*Tentative IDs

7255 Hamilton Enterprise Park Drive
Hamilton, OH 45011
Tel: 513-892-7100
www.sensusflavors.com