CHARACTERIZATION OF ROASTED COFFEE BEAN
AROMA PROFILES BY SPME

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ABSTRACT
The investigation of the volatile compounds from 10 varieties of coffee beans obtained from
different geographical origins was carried out in cooperation with a local coffee roastery. In an
try to better understand the coffee bean roasting process and the emitted aromas, the
different coffee beans were sampled using solid-phase microextraction (SPME) with a
DVB/carboxen/PDMS fiber. The volatiles captured on the fiber were analyzed using gas
chromatography mass spectrometry (GC/MS) methods. There were about 50 different
components identified with about 20 of these exceeding 0.5% of the total integrated area for all
peaks as part of the coffee bean aroma profiles in the 10 types of coffee beans. Other studies
have found from 60 to 80 components in various coffee bean preparations with 8-10 comprising
greater than 80% of the total quantified volatiles (1). The compounds that were found to be
shared by the most bean varieties were furanmethanol, 2,5-dimethylpyrazine, pyridine, 2,3-
pentadione, furanmethanol acetate, 2-methylfuran, and 2,3-pentadione. These compounds are
formed from the reaction between amino acids and reducing sugars within the coffee bean as it is
roasted (the Maillard reaction). The characterization of the aroma profile and the relative
abundances of the volatiles will be presented for each variety.

INTRODUCTION
Coffee has its history as far back as the 9th century. It is thought to have originated in the
highlands of Kefa, Ethiopia and spread to the rest of the world via Egypt and Europe. The plant
is a woody perennial evergreen and is produced mainly in economically developing countries.
There are two main species of the coffee plant, Coffea arabica being the older one. While more
susceptible to disease, arabica is considered by most to taste better than the second species, Coffea canephora (robusta). Robusta, which contains about 40-50% more caffeine, can be cultivated in environments where arabica will not thrive. Research dedicated to the volatile fraction of roasted coffee beans has been extensive. The roasted bean aroma profile is extremely complex and can include several hundred components in a wide concentration range. The coffee bean chemical composition depends on numerous factors that affect the growth of the plant, how the beans are stored, and time and temperature of roasting for example. Gas chromatography-mass spectrometry (GC-MS) is commonly utilized for the identification of the volatile fraction of the roasted beans. The methods of isolating the volatile fractions prior to introduction into the GC-MS are varied and often involve solvent extraction or distillation. Solid phase microextraction (SPME) has proved to be a valuable tool for headspace sampling and was chosen as the method utilized during this investigation (2, 3).

**EXPERIMENTAL PROCEDURES**

**Coffee Samples.** Roasted coffees of different origins and different blends of coffees were supplied by Parisi Artisan Roasted coffees of Kansas City. Samples of each coffee variety or blend were obtained at the roastery after roasting and sealed in 20 mL glass vials until used for chemical analysis. Solid samples of the roasted whole coffee beans were weighed into 13x100 mm test tubes and the test tubes were fitted with a rubber septum.

**SPME Device.** The SPME device was from Supelco (Sigma Aldrich) as were the fused-silica fibers coated with a DVB/carboxen/PDMS film for headspace sampling.

**HS-SPME Sampling.** Samples were preheated at 65°C for 15 min. Extraction was performed for 40 min in the oven at 65°C by inserting a DVB/Carboxen/PDMS fiber to absorb the volatiles in the sample headspace. Before sampling, the fiber was conditioned for 30 min in the GC injection port at 250 °C. The fiber was pushed out of its stainless steel housing and exposed to the sample headspace. After extraction, the SPME device was retracted into its housing, removed from the sample vial, immediately inserted into the GC injector, pushed outside its housing, and thermally desorbed for 5 min at 250 °C.
**GC-MS Analysis.** The GC utilized for the analysis was an Agilent 5890 equipped with a Zebron ZB-1 column (15m x 0.25mm x 0.25um) (Phenomenex Torrance, CA). The mass spectrometer used was an unmodified benchtop quadrupole Agilent 5971 Mass Selective Detector (Agilent Technologies, Inc., Palo Alto California). The 5971 was controlled by ATX-EIGHTY-X data system (CSS Analytical Co. Inc.) with Agilent G1701BA Chemstation running on Microsoft Windows XP. The conditions for the GC were initial oven temperature of 40°C, injector 250°C, transfer line 280°C, a solvent delay of 0.00 min, the temperature was ramped at 10°C/min to a final temperature of 230°C and held for 1.00 min. Carrier gas was helium. The data collected from the GC-MS was analyzed with AMDIS (Automated Mass Spectral Deconvolution and Identification System), version 2.1, DTRA/NIST, 2002. Figure 1 is representative of a GC profile for the coffee volatiles.

**RESULTS AND DISCUSSION**

The SPME sampling of the coffee volatiles proved to be an effective method by which to characterize the differences in the roasted coffee beans. The results of the different volatiles present and their relative abundances are listed in Table 1. Eleven of the identified components were present in 50% of the coffee bean varieties. Of the eleven, five components were found in all of the varieties. While there was a significant similarity as to the major volatiles, there was a notable difference in the abundance of the corresponding compounds. Furanmethanol was found in and was the prevalent volatile in all 10 coffees with percentages as high as 58% with one exception which had as its major volatile a related derivative, furanmethanol acetate. 2,3-butanedione was also present in all 10 coffees, but at much lower levels than furanmethanol and with a 10-fold difference with respect to its relative percentage (10.7% in French Roast and 0.1% in Ethiopian). The varying amounts of volatile compounds present in the different varieties of beans could be responsible for the distinct aromas of some of the beans. For example, pyrazine-containing compounds are known to be partially responsible for the nutty notes in some beans. 2,5-dimethylpyrazine in particular has a characteristic aroma described as strong nutty, musty, meaty roast or green (like fresh mown grass). Furanmethanol has been characterized as caramel-like or burnt sugar-like aroma. While pyridine is associated with
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