APPLICATION NOTE

Gas Chromatography/
Mass Spectrometry

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Rapid Fingerprinting of Volatile Components in Coffee Varieties Using the Portable Torion T-9 Portable GC/MS System

Introduction

Coffee is widely consumed as a beverage because of the stimulating effect it produces in humans. The aroma of coffee contributes to the flavor and taste of the beverage and has consequently led to extensive research on coffee. Hundreds of volatile/semi-volatile aroma and flavor compounds have been identified in coffee using traditional laboratory based headspace GC/MS systems[1]. We present a study for rapid fingerprinting of coffee volatile/semi-volatile compounds using solid phase micro-extraction (SPME) coupled to a portable GC/MS system for separation and detection.

The on-site analysis of coffee using portable technology can be used for quick quality control check of raw and finished products, comparison of competitor products, analysis of storage conditions or for process development.

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Experimental

Sample Preparation

Coffee (1 gm) was placed in headspace vials (20 mL vial volume), capped and placed at room temperature for at least an hour to allow for saturation of the aroma volatiles in the headspace. The SPME fiber was directly exposed to the headspace vapors in the vial for 15 seconds prior to analysis.

Table 1. GC and MS conditions.

Sampling	SPME
SPME Phase	Divinylbenzene/Polydimethylsiloxane (DVB/PDMS, 65 µm)
GC Injector Temp	270°C
GC Column:	MTX-5, 5 m X 0.1 mm, 0.4 µ df
GC Carrier Gas	Helium, 0.2 ml/min
GC Column Temp	50-270 °C at 2 °C/sec, end hold time for 60 sec
Transfer Line	250 °C
Injector Split ratio	10 to 1
Mass analyzer	Toroidal ion trap
Mass Range	42-500 Da
Detector	Electron multiplier

Results and Discussion

Triplicate analysis of coffee (variety #1) is shown in Figure 1. The overlay of the Total Ion Current (TIC) suggests the analysis is very reproducible between injections.

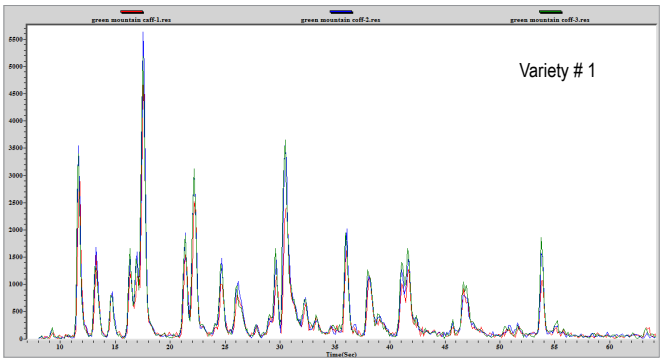

Figure 1. Overlay of the TIC of triplicates analysis of headspace vapors of coffee sample (variety #1).

The decaffeinated form of variety #1 coffee was similarily analyzed in triplicates (Figure 2) and also showed excellent reproducibility of analysis.

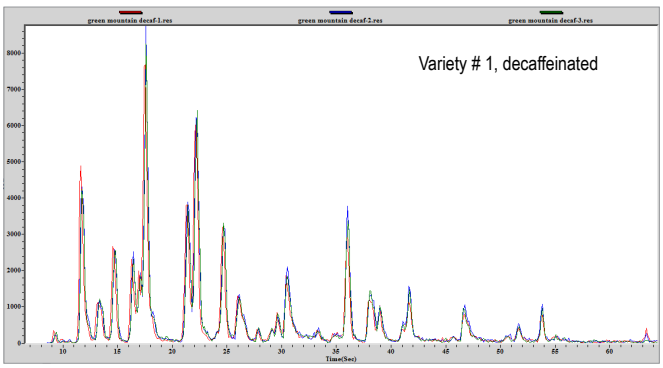

Figure 2. Overlay of the TIC of triplicates analysis of headspace vapors of decaffeinated coffee sample (variety #1).

The overlay of TIC of caffeinated and decaffeinated samples of coffee (variety #1) showed peaks with similar retention time but in many cases with varying intensities suggesting similar compounds are present in the two samples but at different concentrations (Figure 3). An extra peak was observed in the caffeinated sample that was not observed in the decaffeinated coffee.

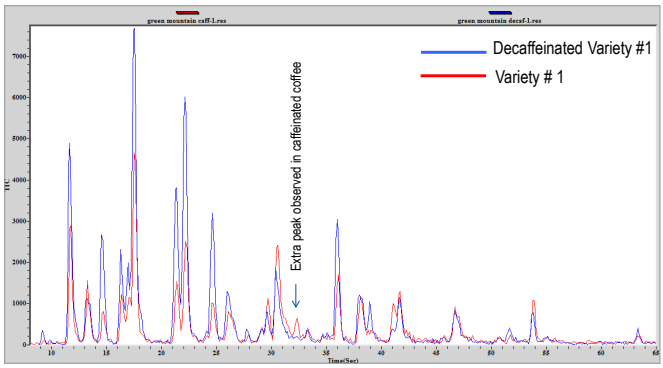

Figure 3. Overlay of the TIC of caffeinated and decaffeinated coffee variety #1 samples.

The extraneous peak observed in the caffeinated coffee resembled the spectra of toluene and comparisons confirmed its identification (Figure 4). The presence of toluene in the caffeinated sample is not surprising as literature suggests toluene can be produced in roasted coffee[2].

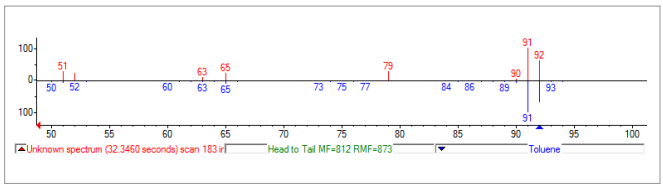

Figure 4. Mass spectra of peak observed at retention time at 32.3 sec in coffee sample (variety #1, Figure 3) matched with spectra of toluene (head to tail comparison) with a match factor of 98.5.

Two other varieties of coffee (variety #2 and #3) were analyzed and the TIC overlay of three coffee types (Figure 5) showed some distinct profiles between the samples. For instance, a peak at ~30 secs was common to #1 and #2 and not observed in #3. The spectra of this peak, was matched against NIST library and the probability of the match suggested it was likely methyl pyrrole.

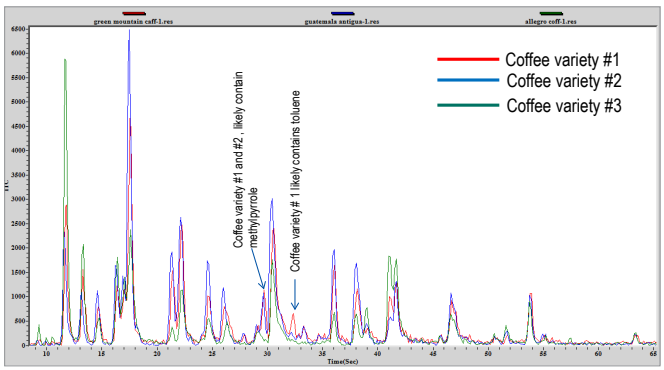

Figure 5. Overlay of the TICs of three different coffee varieties.

Literature studies suggest that methyl pyrrole degradation is accelerated in coffee with high moisture content[3], which may be the reason for variety #3 having little or no methyl pyrrole.

Conclusion

A brief study of coffee fingerprinting using the Torion T-9 coupled to SPME sampling resulted in reproducible profiles for triplicate analysis. Separation of the volatile/semi-volatile compounds by GC and the specificity of detection provided by MS along with spectral matching to the NIST library helped identify differences in coffee varieties. The Torion T-9 portable GC/MS provides a rapid and reliable screening technology to study coffee aroma profiles within a matter of a couple of minutes making it an ideal tool for on-site analysis.

References

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