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Analysis of Coffee Flavors by Purge & Trap Sampling

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Abstract:

Strong or weak, light or dark, black or with cream; everyone who drinks coffee has a preference. Today, there are not only the choices of what you would like in your coffee, but also how you would like it brewed. Do you prefer the old fashioned percolator or the straight forward brewed coffee? Or do you like the new coffee by the cup makers or the instant coffees? There are so many options! This study will analyze four different instant coffee blends for some of their respective flavors using a purge and trap concentrator.

Discussion:

Most of us who drink coffee know our preferences. We know which blend we like, what strength and definitely what we like in our coffee. However, most of us do not think about the flavors that go into our coffee that help us define our preferences. Coffee manufacturers, on the other hand are working diligently to create a new blend or a more satisfying flavor that would make us want to choose their coffee over another maker.

This study will look at four different blends of coffee and some of the compounds that contribute to the flavor of the blend. Using purge and trap sampling, the flavor compounds were purged out of the coffee and trapped onto an adsorbent trap. The analytes were then transferred to a Gas Chromatograph/Mass Spectrometer (GC/MS) for analysis. The study focused on six flavor compounds. The spicy smoky aroma of 2-methylfuran, the spicy caramel, almond odor of 5-methylfurfural, the buttery scent provided by the addition of 2,3-butanedione and 2,3-pentanedione and the impact of the two and three methyl butanals giving the dark chocolate malty flavor to the coffee.

Experimental:

The EST Analytical Encon Evolution Purge and Trap Concentrator and Centurion WS Autosampler were interfaced to a GC/MS. The Centurion WS was run in the soil mode and the purge and trap concentrator was configured with a Vocarb 3000 (K) analytical trap. The column selected for this study was an Rtx-1 60m x 0.25mm x 1µm. Listed in Tables 1 and 2 are the experimental parameters used for this study.

Purge and Trap Concentrator	EST Encon Evolution
Trap Type	Vocarb 3000
Valve Oven Temp.	150ºC
Transfer Line Temp.	150ºC
Trap Temp.	35ºC
Moisture Reduction Trap (MoRT) Temp.	39ºC
Purge Time	11 min
Purge Flow	40mL/min
Dry Purge Temp.	ambient
Dry Purge Flow	50mL/min
Dry Purge Time	1.0 min
Desorb Pressure Control	On
Desorb Pressure	5psi
Desorb Time	0.5 min
Desorb Preheat Delay	5 sec.
Desorb Temp.	260ºC
Moisture Reduction Trap (MoRT) Bake Temp.	230ºC
Bake Temp	260ºC
Sparge Vessel Bake Temp.	120ºC
Bake Time	8
Bake Flow	85mL/min
Purge and Trap Auto-Sampler	**EST Centurion WS**
Sample Type	Soil
Sample Fill Mode	loop
Sample Volume	10mL
Sample Prime Time	5 sec
Loop Equilibration Time	10 sec
Sample Transfer Time	15 sec
Sample Loop Rinse	Off
Sample Loop Sweep Time	15 sec
Number of Sparge Rinses	1
Rinse Volume	5mL
Rinse Transfer Time	20 sec
Rinse Drain Time	20 sec
Number of Foam Rinse Cycles	1
Water Heater Temp.	85°C
Sample Preheat Temp.	40°C
Soil Valve Temp.	85°C
Soil Transfer Line Temp.	150°C

Table 1: Purge and Trap Parameters

GC/MS	Agilent 7890/5975
Inlet	Split/Splitless
Inlet Temp.	200ºC
Inlet Head Pressure	16.041 psi
Mode	Split
Split Ratio	20:1
Column	Rtx-1 60m x 0.25mm I.D. 1.0µm film thickness
Oven Temp. Program	35ºC hold for 1.0 min., ramp 4ºC/min to 230ºC, total run time of 49.75 min.
Column Flow Rate	1.0ml/min
Gas	Helium
Total Flow	26.0ml/min
Source Temp.	230ºC
Quad Temp.	150ºC
MS Transfer Line Temp.	180ºC
Scan Range	m/z 35-265
Scans	3.12 scans/sec
Solvent Delay	0.0 min.

Table 2: GC/MS Parameters

The GC column was acquired from Restek while the instant coffees were purchased at a local retailer. The four roasts chosen for this study ranged from light to dark. One half of a gram of each coffee was dissolved in 40mls of de-ionized water at room temperature. The vials were shaken in order to fully dissolve the coffee. Next, 5mls of each coffee mixture were run in the soil mode using the Centurion WS autosampler and the Encon Evolution purge and trap concentrator. Each coffee was run in triplicate in order to verify the results. Figures 1 through 3 display a bar graph comparison of the flavors in each coffee blend. Chromatograms of the coffee blends are shown in Figures 4 through 7.

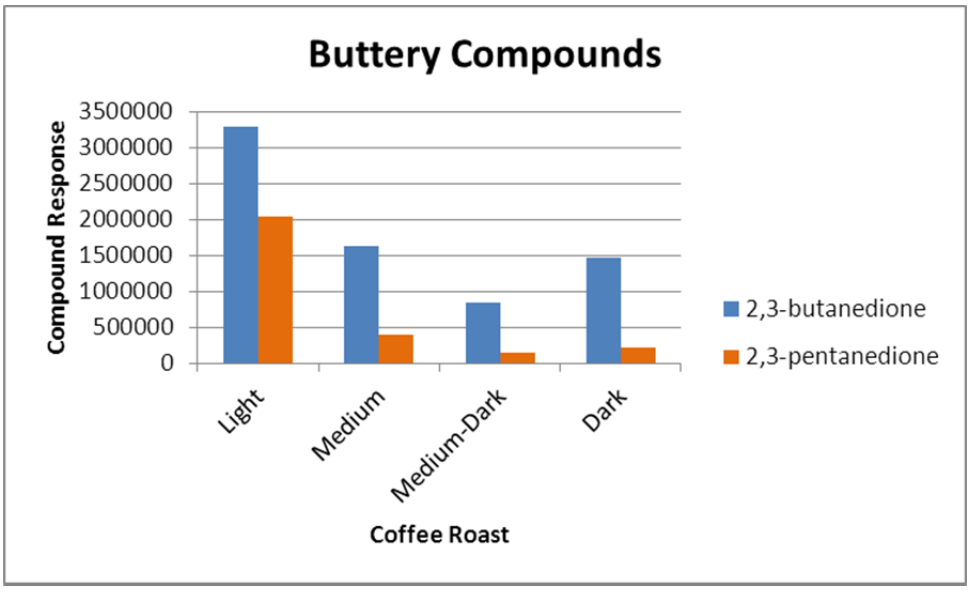

Figure 1: Buttery Compound Comparison

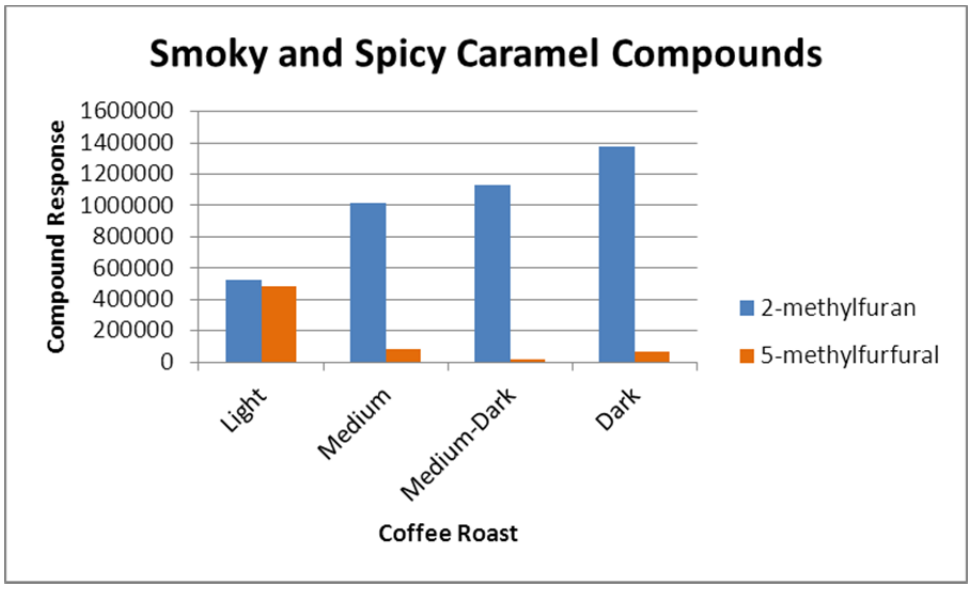

Figure 2: Smoky and Spicy Caramel Compound Comparison

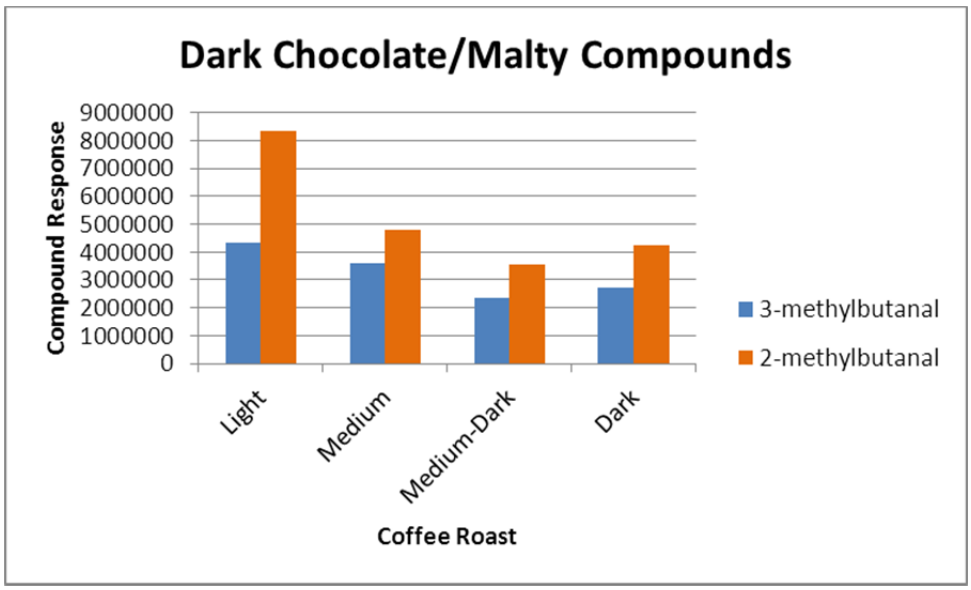

Figure 3: Dark Chocolate/Malty Compound Comparison

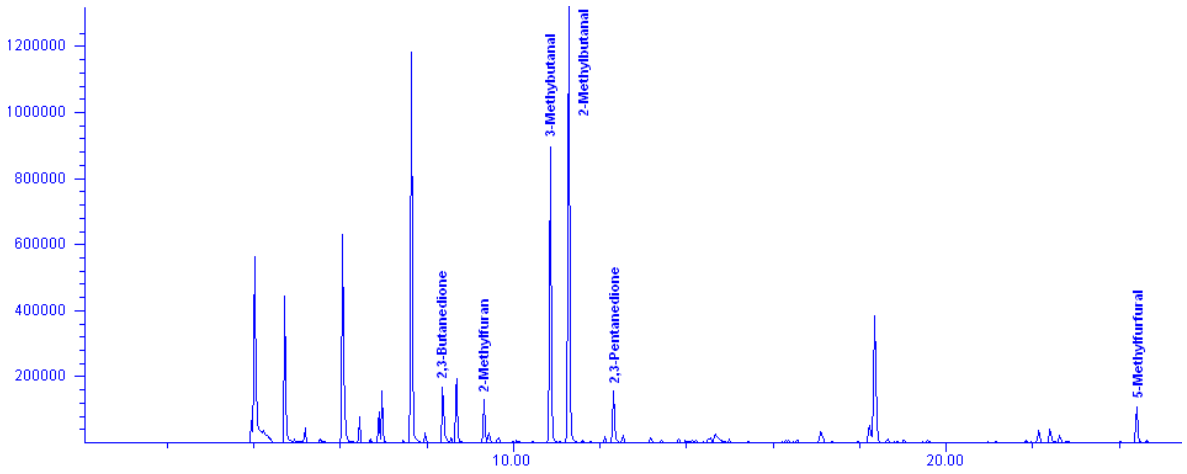

Figure 4: Light Roast Chromatogram

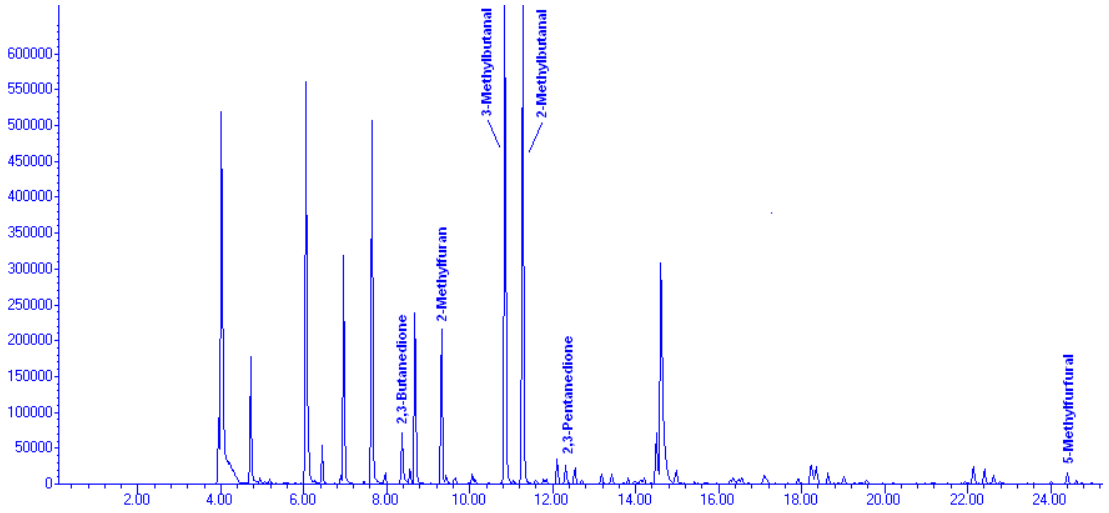

Figure 5: Medium Roast Chromatogram

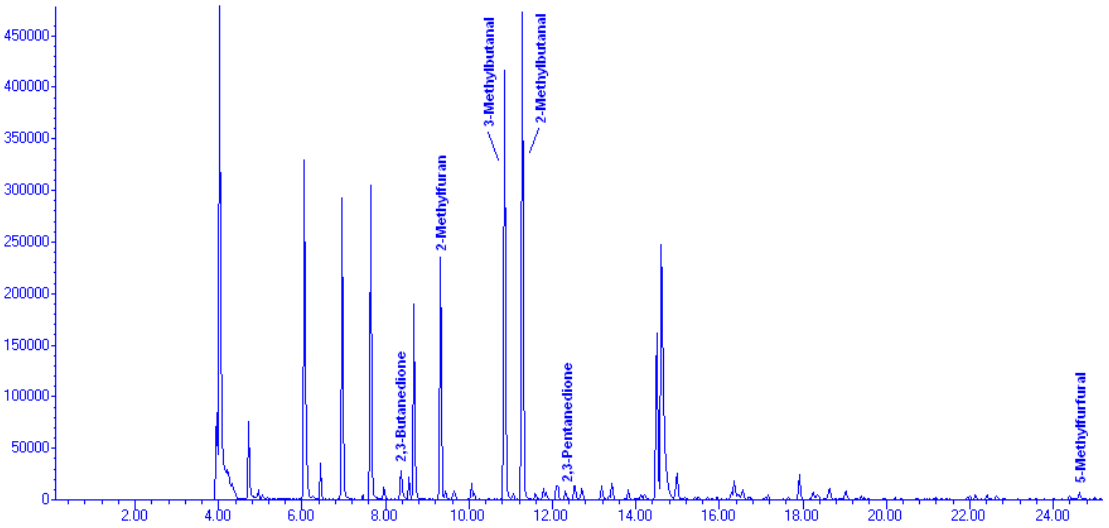

Figure 6: Medium Dark Roast Chromatogram

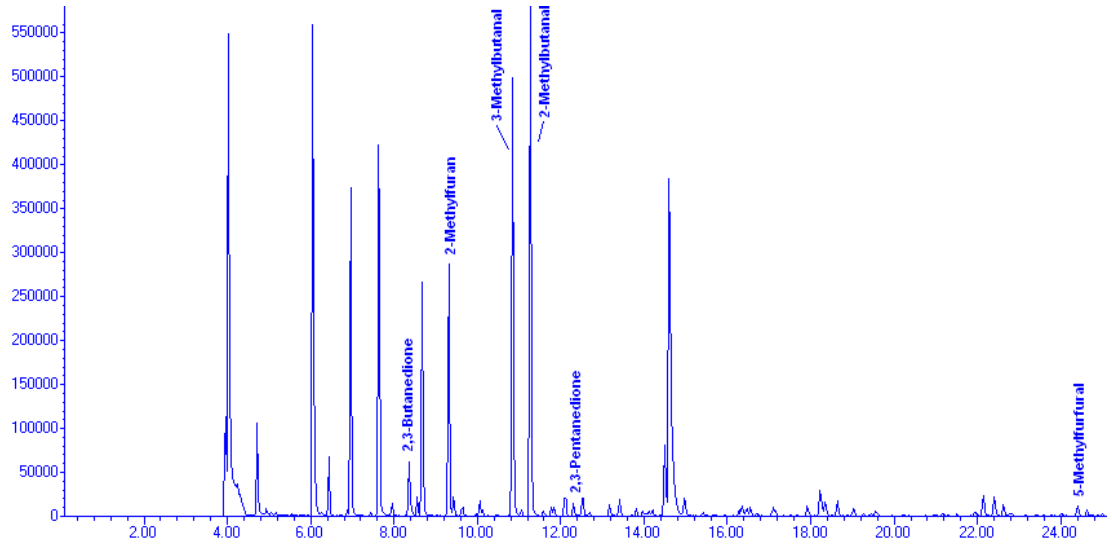

Figure 7: Dark Roast Chromatogram

Conclusion:

The lightest roast had the most buttery and dark chocolate/malty flavors while the darkest roast had more of the smoky flavor. Surprisingly, the darkest roast and the medium roast had similar proportions of the flavor compounds with the exception of the smoky flavor. While the light roast had large amounts of the flavors tested for, the chromatography of the light roast was much simpler than that of the darker roasts. Overall, the Encon Evolution Purge and Trap Concentrator in conjunction with the Centurion WS Autosampler proved to be an excellent system for sampling coffee. The results were reproducible and provided a lot of information on the flavors of the respective coffees.

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