

SPEX CertiPrep App Note

How Much Lightning is in Your Morning Jolt?

A study of the concentration of caffeine and other organic coffee marker molecules in fast food and home brewed

Introduction

Coffee is a major world commodity with 7 million metric tons of coffee produced annually. Roasted coffee beans can contain well over a thousand different compounds. In most cases, the most important of those chemicals are the flavor compounds (i.e. chlorogenic acids, polyphenols, terpenes, etc.) and caffeine. Other compounds, such as methyl cafestol and homostachydrine, can be important in fingerprinting the authenticity and adulteration of coffee and coffee species.

This study created chemical profiles of coffee around targeted groups of chemical markers in coffee to determine: caffeine content and decaffeination by-products), coffee or species authenticity, and adulteration and safety of coffee using LC/MS. Brewed regular roast and decaffeinated coffee was purchased from multiple chain fast food restaurants, coffee purveyors and convenience stores.

Samples of regular home brewed and pod brewed regular coffee were also tested for caffeine content, authenticity and flavor markers. Chemical profiling of some coffee samples showed misrepresentation of coffee species in some brewed coffees as well as the presence of higher than expected levels of caffeine in some samples. Also present were chemicals which indicated signs of either degraded coffee flavor or potential adulteration.

Methods & Materials

Samples

- Coffee tested from 5 fast food/coffee restaurants, local deli, in-office brewed and in-office 'cup' system (see Table 1)
- 10 'regular' caffeine coffees
 - One java extreme
 - One breakfast blend
 - One Columbian
- 7 'regular' decaffeinated coffees
 - One French Vanilla
- All FF, cup varieties stated 100% Arabica beans
- Deli & Brewed - Unknown

Table 1. Coffee Samples

Code	Type	Caffeine
DDR	Regular	Caffeinated
DEJE	Java Extra	Caffeinated
DER	Regular	Caffeinated
KEB	Breakfast Blend	Caffeinated
MCR	Regular	Caffeinated
QCR	Regular	Caffeinated
RDR	Regular Brewed	Caffeinated
SBR	Regular	Caffeinated
WWC	Columbian	Caffeinated
WWR	Regular	Caffeinated
DDD	Regular	Decaffeinated
KEVD	Decaf French Vanilla	Decaffeinated
MCD	Regular	Decaffeinated
QCD	Regular	Decaffeinated
RDD	Regular	Decaffeinated
SBD	Regular	Decaffeinated
WWD	Regular	Decaffeinated

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Materials

- HPLC Grade Acetonitrile
- LCMS Grade Water
- Formic Acid
- SPEX CertiPrep Standards
 - S-705 Caffeine
 - S-11265 Trigonelline
 - S-6659 Chlorogenic acid

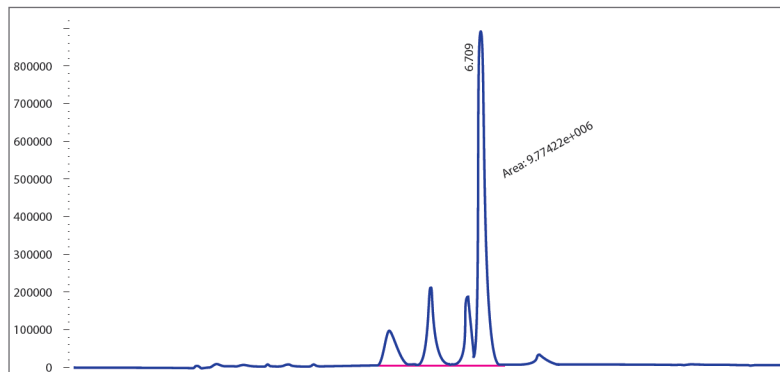
Sample Preparation

Coffee samples were allowed to settle and filter, the caffeinated coffee was diluted 2x before analysis and the decaffeinated coffee was analyzed as served.

Instrument Conditions

- LC Conditions
 - C18 2.6 μm 100 x 3.00 mm
 - 0.5 ml/min
 - 10 μL injection
 - Gradient: Water (0.1% formic) & Acetonitrile (0.1% Formic)
 - 98% Water to 98% Acetonitrile over 30 minutes
- MS Conditions
 - ESI
 - Pos & Neg modes
 - TIC & EIC (see Figure 1)

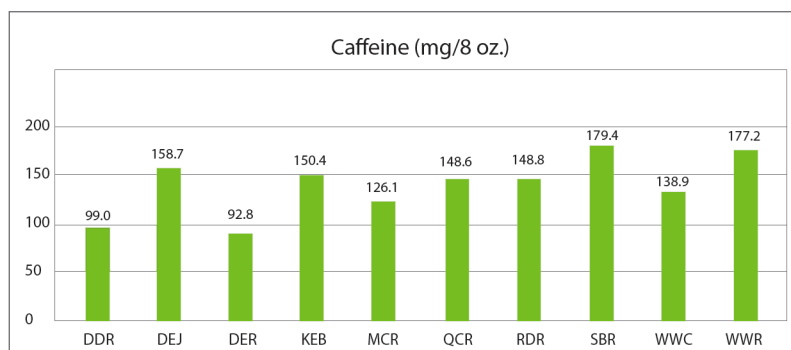
Figure 1. Extracted Ion Chromatography of CGA (Chlorogenic Acid)



Results and Discussion

Caffeinated Coffee

Figure 2. Caffeine Content in 8 oz. of Regular American Coffee (mg/serving)



The average cup of coffee is reported to be eight ounces with between 95 to 150 milligrams of coffee. Half of the regular coffees tested had over 150 mg of caffeine in an eight ounce cup with the average caffeine concentration in an 8-oz cup at 142 mg of caffeine (see Figure 2). The coffee industry reports that an average American consumes between 2 1/2 to 3 cups of coffee between 8 to 9 ounces in size.

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Examining common coffee purveyors coffee sizes, most of the popular coffee sellers have coffee sizes larger than eight ounces, including the small sizes (see Table 2). The average size of home coffee cups range between six and ten ounces and coffee mugs often have larger than a ten ounce serving. The suggested daily limit for caffeine is 400 mg per day. If the average coffee drinker consumes 3 'medium' (16 oz.) tested coffees with an average tested concentration of caffeine at 17.75 mg/oz. The drinker would have consumed over 850 mg of caffeine or more than twice the recommended allowance.

Table 2. Common Coffee Provider's Coffee Sizes (oz.)

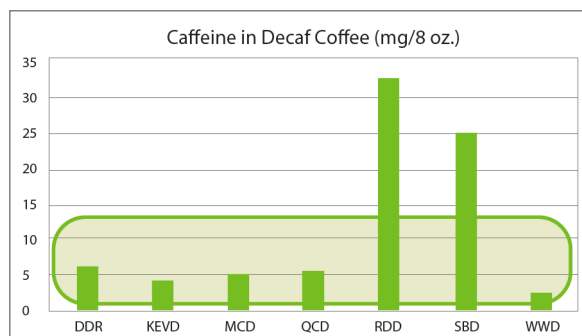
US Coffee Size (oz.)	Dunkin Donuts	McDonalds	Wawa	Starbucks
S	10	12	12	8
M	14	16	16	12
L	20	21	20	16
XL	24	N/A	24	20

Decaffeinated Coffee

Decaffeinated coffee is created by using solvent extraction to remove caffeine from green or pre-roasted beans. This process must remove more than 97% of caffeine in decaffeinated coffee in the United States and 99.99% of caffeine in the UK. The resulting caffeine level is usually between 2 to 13 mg per eight ounce serving.

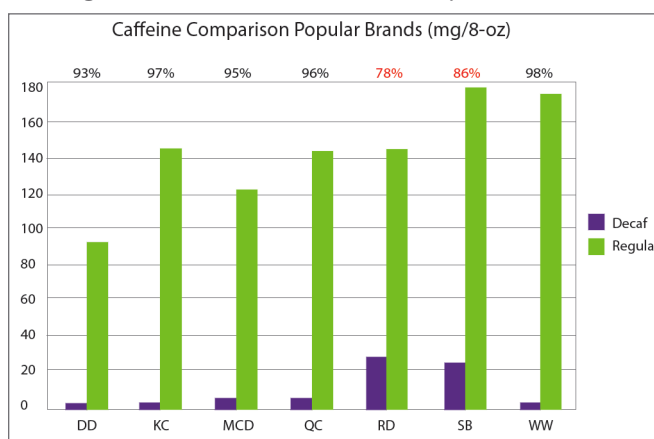
In our study, most of the decaffeinated coffees did not have reduced amounts of caffeine (see Figure 3). Two coffees had more than double the allowable level of caffeine in decaffeinated coffee.

Figure 3. Caffeine Levels in Decaffeinated Coffee (mg/8-oz serving)



In comparison with the regular coffee provided by each coffee purveyor, two brands out of seven had the minimum 97% decaffeination required by law (see Figure 4).

Figure 4. Comparison of Caffeine Levels Between Regular and Decaffeinated Coffee of Popular Brands



Chlorogenic Acid & Trigonelline

Chlorogenic acid (CGA) and Trigonelline are large chemical marker components in coffee. The concentration of these markers are dependent on the type of coffee (see Figure 5).

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Figure 5. Comparison of Coffee Components in Arabica and Robusta Coffee

	Chlorogenic Acids (CGA)	Trigonelline
Arabics	5.5 - 8% 200 - 400 mg / 8 oz.*	0.6 - 1.3% 60 - 140 mg / 8 oz.*
Robusta	7 - 10% > 300 mg / 8 oz.* More brewed coffee flavor	0.3 - 0.9% 30 - 100 mg / 8 oz.*

Arabica coffee is considered to be a higher and better flavor coffee than Robusta. The presence and concentration could potentially be used as a marker of identity. Both markers have bitter flavors and abundance of either marker could lead to a bitter flavor.

Both compounds were found more often in the decaffeinated coffee rather than the regular coffee possibly contributing to the reported bitter flavors found in decaffeinated coffee. The difference, however, was not pronounced enough between brands to use these compounds as identity markers (see Figures 6 & 7).

Figure 6. Chlorogenic Acid in Popular Coffee Brands (mg/8 oz.)

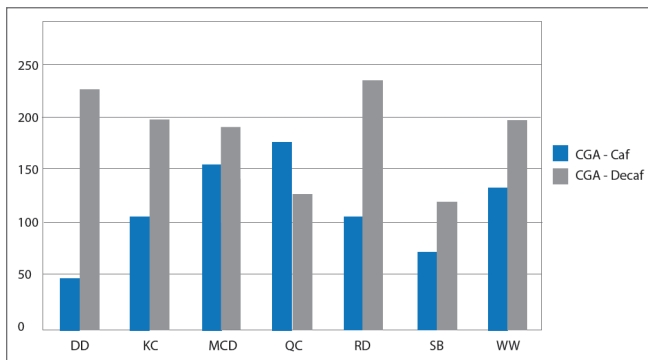
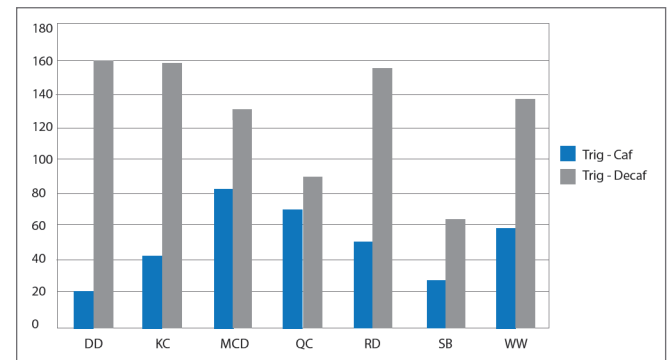


Figure 7. Trigonelline in Popular Coffee Brands (mg/8 oz.)



Conclusion

The highest caffeine contents were found in a very popular brand with almost 180 mg of caffeine in an eight ounce serving. Three commercial medium cups of coffee (16 oz. each) of any of the samples tested would exceed the allowable daily limit for caffeine.

The organic markers in coffee did not show any trend between brands which would suggest that these compounds indicated coffee identity. The marker compounds were generally higher in the decaffeinated coffees compared to the regular coffees.

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