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# DETERMINATION AND CORRELATION OF VOLATILE AND NONVOLATILE COMPOUNDS WITH COFFEE QUALITY

Jackson Wood
jman56@siu.edu

# DETERMINATION AND CORRELATION OF VOLATILE AND NONVOLATILE COMPOUNDS WITH COFFEE QUALITY

**Jackson Wood**

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## Abstract

Coffee is one of the most popular drinks around the world and as such is a very active area of research. This research used HS-SPME - GCMS and HPLC to correlate volatile and nonvolatile coffee components with flavor profiles generated by professional coffee tasters. Coffee was also tasted and ranked by amateur volunteers culled from SIU students and faculty population. Results indicated the professionally established overall coffee scores correlated with coffee cost per ounce, and there were differences between professional and amateur tasters. Professional tasters were trained to recognize subtle differences in flavor attributes such as fruity, floral, and sweet, while amateur tasters were strongly influenced by factors affecting acidity and bitterness. Correlations were observed between the volatile compounds 2,5-dimethylpyrazine, 5-methyl-2-furaldehyde, 2-furanmethanol acetate, guaiacol, 4-ethylguaiacol, p-cyanobenzaldehyde, a cinnamaldehyde derivative, and a 2-methylphenol derivative and several flavor notes including sweet, acidity and bitter rating. The nonvolatile compounds nicotinic acid, trigonelline, chlorogenic acid, and caffeine also exhibited correlations sweet, caramel, and bitter ratings. Future research on this topic should include stable isotope ratio mass spectrometry to determine the proper geographic origins of the coffees from Kroger, Seattle’s Best, Starbucks, and Folgers. This will allow for a comparison across geographic locations. Principle component analysis can also be explored evaluate if groups of two or more volatile and nonvolatile compounds work together synergistically to affect the coffees’ distinct tasting notes.

## ACKNOWLEDGEMENTS

The researcher would like to sincerely thank Café Imports for providing professional tasting services. Also, thanks go to the SIU Mass Spectrometry Facility and Graduate Student Lee Elliot. Thank you to the SIUC REU Program for funding under NSF and DoD (Department of Defense, Air Force Office of Scientific Research) grants DMR 1757954 and 1461255. Finally, a huge thank you to Drs. Mary and Gary Kinsel for all their advice, expertise, and guidance over three and a half years of being an undergraduate researcher.

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# CHAPTER 1 - Introduction and Background

Coffee is one of the world's bestselling commodities with over 2.25 billion cups sold per day worldwide.[1] With that selling potential it is obvious why coffee is such a hot topic in research. Coffee has been a popular drink for 6 centuries with the earliest account of coffee as we know it today (roasted and brewed) coming from the 15$^{th}$ century. There are two main species of coffee that are commercially available today. *Coffea canephora* typically known today as "Robusta." *Coffea arabica* is the most popular species known generally just as "Arabica". Coffee beans are grown around the world with the five leading countries being Brazil, Vietnam, Columbia, Indonesia, and Ethiopia.

Coffee is a very complex mixture consisting of over 1000 compounds. These consist of both volatile and non-volatile compounds. Volatile compounds typically make up the aroma and the non-volatile compounds make up the flavors. Together the interactions of these compounds make up the overall distinctive flavor of coffee. Numerous studies have been performed to identify key compounds contributing to the aroma of coffees. Key categories of volatile compounds often found include furans, pyrazines, aldehydes, ketones, alcohols/phenols, pyrroles, and esters among others. Expansive lists have been created showing these common compounds[9,10,11,17] and some have begun correlating them with their aroma profiles.[12] Volatile furans exhibit malty and sweet flavor notes. Aldehydes are primarily responsible for major fruity flavor notes. Ketones commonly contribute to buttery flavor notes. The pyrazines are recognized as the volatiles associated with roasted and burnt aromas. Phenolic compounds often lend spicy flavor notes. Trigonelline, nicotinic acid, chlorogenic acid, and caffeine are major non-volatile compounds in coffee.

Among the most abundant volatiles present in coffee are 2-furanmehanol, phenylacetaldehyde, 4-ethylguaiacol, 4-vinylguaiacol, and isoeugenol (Figure 1). 2-Furanmethanol and phenylacetaldehyde are important to the development of caramel and fruity flavor notes, respectively. 4-Ethylguaiacol, 4-vinylguaiacol, and isoeugenol are all phenolic-based compounds and contribute to spicy flavor notes. 4-Ethylguaiacol has a clove-like profile nuanced with sweet vanilla. The aroma of 4-vinylguaiacol has been described as reminiscent of cloves. The origin of these compounds is via the thermal degradation of the chlorogenic acids.[12]

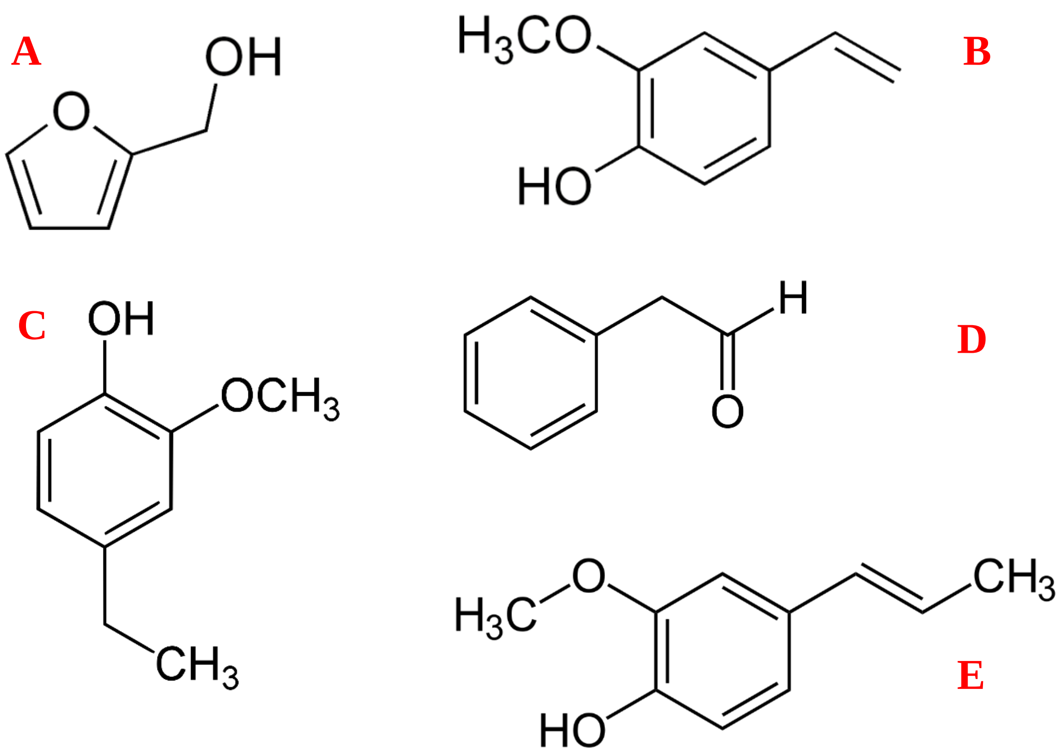


**Figure 1:** Selected volatile compounds. A) 2-furanmethanol, B) 4-vinylguaiacol, C) 4-ethylguaiacol, D) phenylacetaldehyde, E) isoeugenol.

Caffeine is the most well-known of the nonvolatile compounds and for good reason. The average 8 fl. oz. cup of coffee has around 95mg of caffeine according to the United States Department of Agriculture (USDA)'s National Nutrient Database for Standard Reference.[2] Caffeine is known to be a stimulant of the Central Nervous System (CNS) and in high doses can cause heart arrythmias. Another important molecule in coffee is chlorogenic acid (CGA). Chlorogenic acid is an ester of caffeic acid and quinic acid, it has been shown that CGA has a wide range of health benefits including helping maintain a healthy blood pressure.[3]

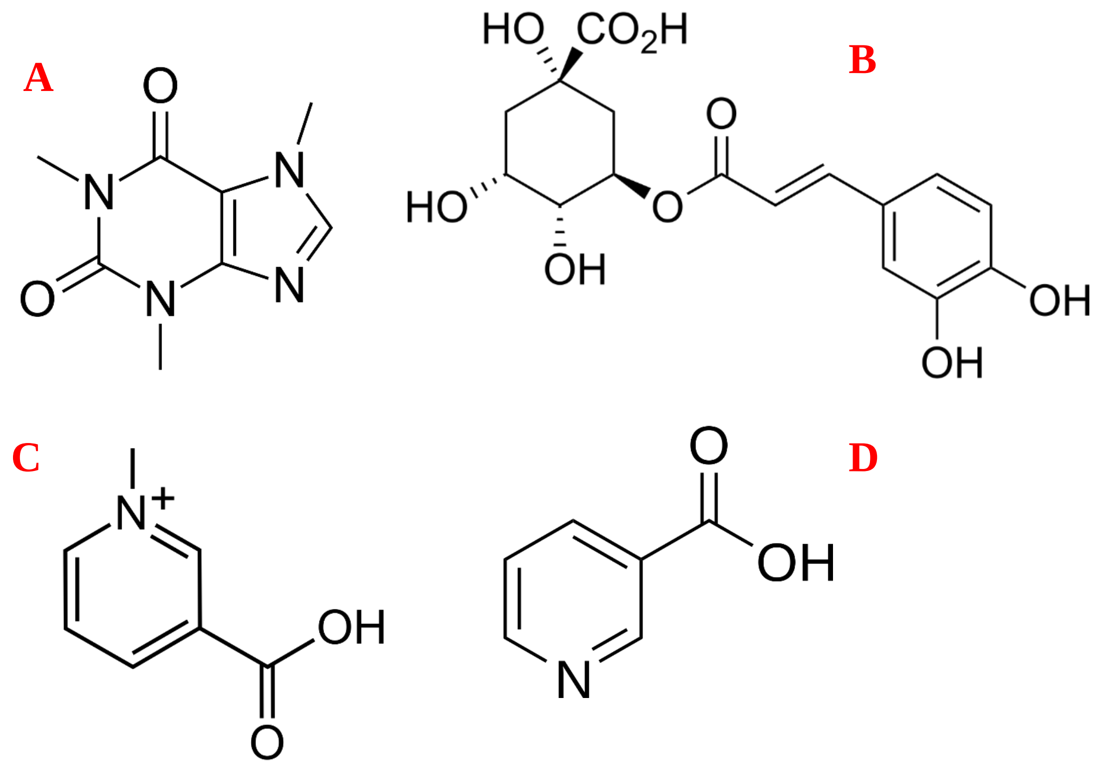


**Figure 2:** Selected non-volatile compounds. A) caffeine, B) chlorogenic acid, C) trigonelline, D) nicotinic acid.

Nicotinic acid, also known as niacin or vitamin $B_3$, is an essential vitamin. It serves as a precursor for the coenzymes nicotinamide adenine dinucleotide (NAD) and nicotinamide adenine dinucleotide phosphate (NADP) which function in many oxidation-reduction reactions in the body. Nicotinic acid is found in most arabica coffees and has been shown to have anti-inflammatory effects.[4] Nicotinic acid is a precursor for the synthesis of trigonelline in the coffee plant. Trigonelline is degraded during roasting to form nicotinic acid and other pyrroles and pyridine-derivatives important to aroma. Trigonelline has been suggested to act as a neuroprotective compound in Alzheimer's and Parkinson's diseases.[5,6] It has also been shown to help control diabetes in rats.[7]

The goal of this project was to determine the volatile and nonvolatile compounds in coffee that create the subtle differences between different cups of coffee using the analytical techniques Head Space - Solid Phase Micro Extraction (HS-SPME) with Gas Chromatography Mass Spectrometry (GC-MS) and High-Performance Liquid Chromatography (HPLC) with ultraviolet – visible detection. GCMS and HPLC are each highly suited for the analysis of coffee due to the ability of these instruments to separation complex mixture of compounds. GCMS combines chromatography and electron impact mass spectrometry separate and detect volatile compounds responsible for coffee aroma. HPLC combines liquid chromatography and ultra-visible detection to separate, detect and quantitate the nonvolatile (water soluble).[13,14,15,16] This volatile and nonvolatile compound information was compared and correlated with professional flavor profiles and coffee rankings provided by Café Imports of Minneapolis, Minnesota, and amateur tasters recruited from Southern Illinois University (SIU) student and faculty population.

# CHAPTER 2 – Materials and Methods

Eight medium roast coffee were purchased from Kiva Han (Columbian Supremo), King's Coast (Aztec Reserve, EZ Morning, Lifeline), Kroger (Premium Blend), Seattle's best (Breakfast Blend), Folgers (Classic Roast), and Starbucks (House Blend). Each coffee was chosen to have a variation in coffee bean origin. Four (4) cups of each coffee were brewed from 4 tablespoons of grounds and 4 cups tap water using a Cuisinart DCC-3200 and were analyzed by GCMS and HPLC with UV-visible detection. Each coffee was numbered 1-8 and was from the following geographic origins. 1: Kroger (origin unknown), 2: Starbucks (origin unknown), 3: Seattle's Best (origin unknown), 4: Kiva Han (Columbia), 5: Folgers (origin unknown), 6: Aztec Reserve (Chiapas, Mexico), 7: EZ Morning (Costa Rica and Sumatra), 8: Lifeline (Sumatra, Ethiopia, and Guatemala).

## Coffee Taste Testing

Each coffee was tasted professionally by Café Imports of Minneapolis, Minnesota, and amateur tasters recruited from Southern Illinois University (SIU) student and faculty population. Each of the professional tasters (n=7) from Café Imports were presented about 1.5oz of each coffee in a 5.5oz glass (52.7 grams ground coffee brewed to yield 30oz coffee). Coffee was scored using the standard Café Imports scoring sheets, which are based off of a modified Specialty Coffee Association (SCA) standard cupping form and with a maximum score of 100 points (Figure 3).

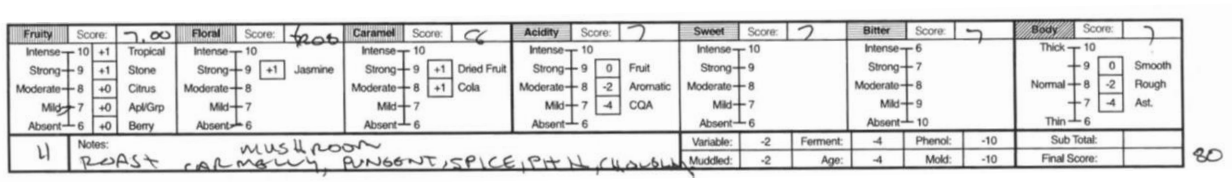


**Figure 3:** Sample scoring sheet from Café Imports based of a modified sheet from the SCA.

The amateur tasters were presented with about 2oz of each coffee, 4 coffees per sitting, in a 3oz Dixie cup (one tablespoon (approx. 4.6g) ground coffee brewed for each cup of coffee). Coffees were scored using a simplified scoring sheet approved by the SIU Human Subject Committee (Figure 4). Coffees 1 and 2 were tasted by 16 individuals, coffees 3 and 4 by 14 individuals, coffees 5 and 6 by 15 individuals, and coffees 7 and 8 by 17 individuals.

Coffee Analysis

Solvents and reagents were purchased from Fisher Chemical and Sigma-Aldrich: caffeine (ReagentPlus®; Sigma-Aldrich, C0750-100G); trigonelline (Analytical standard, Sigma-Aldrich, T5509-1G); nicotinic acid ($\geq$ 98%, Sigma-Aldrich, N4126-5G); chlorogenic acid ($\geq$ 95%, Sigma-Aldrich, C3878-1G); o-phosphoric Acid (85%, Fisher Chemical, A242-1); methanol (HPLC grade, Fisher Chemical, A452-1); octanesulfonate ($\geq$ 99%, Sigma-Aldrich, 74884-10G); acetonitrile (HPLC Grade, Fisher Chemical, A998-4)). All chemicals were stored at room temperature. Purified (18 MegOhm) water sourced from a Millipore Direct-Q™ 5 system.

*Identification of volatile compounds by GCMS:* This method was optimized from a combination of methods previously published.[9,10,11] For each coffee three 11-mL aliquots were transferred to three separate 15-mL sample vials, a micro stir bar was added, and closed with threaded caps having Teflon-lined silicone septa.

## Coffee Survey Data Sheet

Are you a coffee drinker? ☐Yes ☐No

If yes, how many cups per day? ☐ 1 – 2 ☐ 3 – 4 ☐ 5 or more

If yes, how do you typically drink your coffee? (Check all that apply.)
☐ Black ☐ with sugar ☐ with milk, cream or half and half

### Rating Coffee Attributes

**Sweetness:** If it is extremely sweet rate it 1 and if its balanced rate it a 5. Or anywhere in between.
**Acidity:** If it tastes extremely sour rate it 1 if it tastes very balanced rate it 5. Or anywhere in between.
**Mouth Feel:** If it feels thin like tea rate it 1 or if "thicker" and full-bodied rate it 5. Or anywhere in between.
**Bitterness:** Do not confuse "strength" with "bitterness." If it is extremely bitter rate it 1. If it tastes smooth rate it 5. Or anywhere in between.

| Coffee # | | | | |
|---|---|---|---|---|
| Sweetness (1-5) | | | | |
| Taste (1-5) | | | | |
| Mouth Feel (1-5) | | | | |
| Bitterness (1-5) | | | | |

**Did you like the coffee?** Rate it 1 if you dislike intensely. Rate it 10 if you like it best. Or anywhere in between.

| Coffee # | | | | |
|---|---|---|---|---|
| Rating (1-10) | | | | |

Additional Comments:
Use the back of this page for any additional comments.

This project has been reviewed and approved by the SIUC Human Subjects Committee. Questions concerning your rights as a participant in this research may be addressed to the Committee Chairperson, Office of Sponsored Projects Administration, SIUC, Carbondale, IL 62901-4709. Phone (618) 453-4533. E-mail: siuhsc@siu.edu

Revised 7/5/2018 1

**Figure 4:** Sample scoring sheet approved by the SIU Human Subjects Committee to be used by the amateur tasters.

The three sample vials were then equilibrated at 85°C on a stirring hotplate (ThermoFisher Scientific, Isotemp). Head Space Solid Phase Micro Extraction (HS-SPME) coupled with GCMS was used to sample the volatile compounds, separate and identify the aroma compounds. The SPME fiber (Supelco, 65μm PDMS/DVB, stableflex, 24-gauge, manual) was exposed in the head space of the coffee for 20 minutes. Immediately following exposure, the fiber was inserted into the inlet of the GCMS (ThermoFisher Scientific, TraceGC Ultra PolarisQ Ion Trap Mass

Spectrometer with a 0.8mm ID straight glass liner (SGE Analytical Science, 092148) and the compounds allowed to desorb at 230°C for 5 minutes. A DB5-MS capillary column (J&W Scientific, 30m x 0.250mm x 0.25 micron) was used. The GC oven temperature was programmed from 40°C (2 min hold), increased to 130°C at 10°C/min (1 min hold), increased again to 175°C at 5°C/min (1 min hold), then rose to a final temperature of 250°C at 15°C/min (3 min hold). The helium carrier gas flowed at 1mL/min, and the MS transfer line was heated to 275°C. The resulting chromatogram and mass spectra were used to identify the compounds that change significantly from one medium roast coffee brand to the next brand.

*Identification of water-soluble compounds by HPLC:* The HPLC method was adapted from Arai et al.[13] Three 1-mL aliquots of coffee were filtered and transferred to three separate 2-mL autosampler vials fitted with a screw top caps containing Teflon-lined septa. The aliquots were immediately loaded into an autosampler for separation and quantitation by HPLC with UV-visible detection (Agilent 1200 Series with an Agilent Eclipse XDB-C18 column (4.6mm x 150mm x 5µm)). The mobile phase was 0.1% phosphoric acid, 15% methanol, 4mM octanesulfonate in 18MegOhm water. The mobile phase flowrate was 1mL/min, injection volume was 10µL, and the column temperature was maintained at 35°C. Absorption was recorded at 220nm and 320nm. Standards of caffeine (753.7µM, 1507µM, 3015µM, 4220µM, 4823µM, 5426µM, and 6029µM), trigonelline (25.52µM, 51.05µM, 102.1µM, 204.1µM, 408.2µM, 612.3µM, 816.4µM, and 4539µM), nicotinic acid (103.4µM, 206.7µM, 413.4µM, 826.6µM, 1240µM, 1653µM, and 2066µM), and chlorogenic acid (24.34µM, 48.68µM, 97.35µM, 194.6µM, 389.2µM, 583.9µM, 778.5µM, and 4121µM) were prepared having concentrations indicated.

CHAPTER 3 – Results and Discussions

The results of the professional coffee tastings are contained in Tables 1 and 2.

**Table 1:** Table of professional coffee tasters' responses for each flavor profile for each coffee.

| Response \| Coffee | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 7 | 7.5 | 6 | 7 | 6.5 | 6 | 6 | 6 | Fruity |
| 2 | 6 | 6 | 6 | 7.5 | 6 | 6 | 6 | 6.5 | |
| 3 | 6 | 6 | 6 | 7 | 6 | 6 | 6 | 6 | |
| 4 | 6 | 6 | 7 | 6 | 6 | 6 | 7 | 6 | |
| 5 | 6 | 6.5 | 6 | 7.5 | 5 | 7 | 7 | 6 | |
| 6 | 6 | 6 | 6 | 6 | 6 | 6 | 6 | 6 | |
| 7 | 6 | 6 | 6 | 6 | 6 | 6.5 | 6 | 6 | |
| Average | 6.14 | 6.29 | 6.14 | 6.71 | 5.93 | 6.21 | 6.29 | 6.07 | |
| StdDev | 0.35 | 0.52 | 0.35 | 0.65 | 0.42 | 0.36 | 0.45 | 0.17 | |
| 1 | 6 | 6 | 6 | 6 | 6 | 6 | 6 | 6 | Floral |
| 2 | 6.5 | 6 | 6 | 6 | 6 | 6 | 6 | 6 | |
| 3 | 6 | 6 | 6 | 6 | 6 | 6 | 6 | 6 | |
| 4 | 6 | 6 | 6 | 6 | 6 | 6 | 6 | 6 | |
| 5 | 6 | 6 | 6 | 7 | 5 | 6 | 6 | 6 | |
| 6 | 6 | 6 | 6 | 6 | 6 | 6 | 6 | 6 | |
| 7 | 6 | 6 | 6 | 6 | 6 | 6 | 6 | 6 | |
| Average | 6.07 | 6.00 | 6.00 | 6.14 | 5.86 | 6.00 | 6.00 | 6.00 | |
| StdDev | 0.17 | 0.00 | 0.00 | 0.35 | 0.35 | 0.00 | 0.00 | 0.00 | |
| 1 | 8 | 8 | 7 | 8 | 7.5 | 7 | 8 | 6 | Caramel |
| 2 | 7.5 | 7 | 7 | 7.5 | 6 | 6.5 | 6.5 | 7 | |
| 3 | 6.5 | 7 | 7 | 7.5 | 6.5 | 7 | 6.5 | 7 | |
| 4 | 7 | 7 | 7 | 6 | 6 | 7 | 7 | 7 | |
| 5 | 7 | 8 | 6 | 7 | 5 | 7 | 6.5 | 7 | |
| 6 | 6 | 7 | 6 | 7 | 6 | 6.5 | 6.5 | 7 | |
| 7 | 6.5 | 7 | 6.5 | 7.5 | 6.5 | 7 | 7.5 | 6.5 | |
| Average | 6.93 | 7.29 | 6.64 | 7.21 | 6.21 | 6.86 | 6.93 | 6.79 | |
| StdDev | 0.62 | 0.45 | 0.44 | 0.59 | 0.70 | 0.23 | 0.56 | 0.36 | |
| 1 | 6.5 | 7.5 | 6.5 | 7 | 7 | 7 | 7.5 | 6 | Acidity |
| 2 | 6.5 | 6 | 6 | 7 | 6.5 | 6.5 | 6 | 7 | |
| 3 | 6.5 | 7 | 6.5 | 8 | 6.5 | 7 | 6.5 | 7 | |
| 4 | 6 | 7 | 7 | 7 | 6 | 7 | 7 | 7 | |
| 5 | 6 | 6.5 | 6 | 7.5 | 6 | 6.5 | 7 | 7 | |
| 6 | 6 | 7 | 8 | 7 | 8 | 7 | 7.5 | 7 | |
| 7 | 6.5 | 7 | 6 | 7.5 | 6 | 6.5 | 7.5 | 7.5 | |
| Average | 6.29 | 6.86 | 6.57 | 7.29 | 6.57 | 6.79 | 7.00 | 6.93 | |
| StdDev | 0.25 | 0.44 | 0.68 | 0.36 | 0.68 | 0.25 | 0.53 | 0.42 | |

**Table 1:** Table of professional coffee tasters' responses for each flavor profile for each coffee (continued).

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 6.5 | 7.5 | 6.5 | 7 | 7 | 6.5 | 7.5 | 6 | Sweet |
| 2 | 7 | 6.5 | 7 | 7.5 | 6 | 7 | 6.5 | 7 | |
| 3 | 6 | 7 | 6.5 | 7 | 6.5 | 6.5 | 6.5 | 6.5 | |
| 4 | 6 | 7 | 7 | 6 | 7 | 7 | 7 | 7 | |
| 5 | 6.5 | 7.5 | 5 | 7.5 | 5 | 7 | 7 | 6 | |
| 6 | 6 | 6.5 | 6 | 7 | 6 | 6 | 6.5 | 6 | |
| 7 | 6.5 | 7 | 6.5 | 7.5 | 6 | 7 | 7.5 | 7 | |
| Average | 6.36 | 7.00 | 6.36 | 7.07 | 6.21 | 6.71 | 6.93 | 6.50 | |
| StdDev | 0.35 | 0.38 | 0.64 | 0.49 | 0.65 | 0.36 | 0.42 | 0.46 | |
| 1 | 6 | 6.5 | 7 | 7 | 6 | 6 | 6.5 | 6 | Bitter |
| 2 | 6 | 5 | 6 | 6.5 | 4 | 6 | 5 | 6.5 | |
| 3 | 6 | 7 | 7 | 7 | 6 | 6 | 6 | 6.5 | |
| 4 | 6 | 6 | 7 | 6 | 6 | 6 | 7 | 7 | |
| 5 | 6 | 7 | 5 | 7 | 5 | 6.5 | 7.5 | 5 | |
| 6 | 6 | 6 | 6 | 6 | 6 | 6 | 6 | 7 | |
| 7 | 6 | 6 | 6 | 6.5 | 6 | 6.5 | 7 | 6 | |
| Average | 6.00 | 6.21 | 6.29 | 6.57 | 5.57 | 6.14 | 6.43 | 6.29 | |
| StdDev | 0.00 | 0.65 | 0.70 | 0.42 | 0.73 | 0.23 | 0.78 | 0.65 | |
| 1 | 7 | 7 | 7 | 7 | 7 | 7 | 6.5 | 6 | Body |
| 2 | 6.5 | 7.5 | 7 | 7 | 7 | 6 | 7 | 7 | |
| 3 | 6 | 7 | 7 | 7.5 | 7 | 7 | 7 | 6.5 | |
| 4 | 7 | 6 | 9 | 7 | 7 | 6.5 | 7 | 7 | |
| 5 | 7.5 | 7.5 | 7 | 7 | 7 | 7.5 | 7.5 | 8 | |
| 6 | 7 | 8 | 8 | 8 | 7 | 8 | 8 | 7 | |
| 7 | 6 | 6 | 7.5 | 7.5 | 8 | 7.5 | 8 | 8 | |
| Average | 6.71 | 7.00 | 7.50 | 7.29 | 7.14 | 7.07 | 7.29 | 7.07 | |
| StdDev | 0.52 | 0.71 | 0.71 | 0.36 | 0.35 | 0.62 | 0.52 | 0.68 | |

**Table 2:** Professional tasters' overall ratings for each coffee.

| Response | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 71 | 80 | 75 | 80 | 77 | 75.5 | 79 | 72 | Overall Score |
| 2 | 76 | 74 | 75 | 79 | 71.5 | 74 | 73 | 77 | |
| 3 | 73 | 78 | 75 | 81 | 74.5 | 75.5 | 74.5 | 75.5 | |
| 4 | 67 | 70 | 70 | 76 | 74 | 75 | 76 | 76 | |
| 5 | 75 | 77.5 | 69 | 80.5 | 68 | 77.5 | 79 | 74 | |
| 6 | 67 | 74.5 | 72 | 77 | 65 | 74.5 | 75.5 | 76 | |
| 7 | 73 | 75 | 74 | 75 | 74.5 | 77 | 80 | 77 | |
| Average | 71.71 | 75.57 | 72.86 | 78.36 | 72.07 | 75.57 | 76.71 | 75.36 | |
| StdDev | 3.33 | 3.03 | 2.36 | 2.18 | 3.90 | 1.18 | 2.45 | 1.66 | |

The results of the amateur coffee tastings are contained in Table 3.

**Table 3:** Amateur tasting averages for each flavor profile and overall, with standard deviations.

| | Average | | | | |
|---|---|---|---|---|---|
| Average | Sweetness | Acidity | Mouth Feel | Bitterness | Rating |
| 1 | 4.03 | 3.94 | 2.38 | 3.38 | 6.00 |
| 2 | 3.94 | 3.44 | 2.47 | 3.09 | 4.36 |
| 3 | 4.36 | 3.50 | 3.71 | 3.07 | 5.75 |
| 4 | 4.36 | 3.71 | 2.93 | 3.57 | 5.86 |
| 5 | 4.20 | 3.33 | 3.33 | 3.13 | 5.53 |
| 6 | 4.40 | 4.07 | 2.80 | 3.13 | 5.90 |
| 7 | 3.47 | 3.79 | 2.65 | 3.53 | 6.18 |
| 8 | 3.94 | 2.68 | 3.41 | 2.41 | 4.92 |
| | Standard Deviation | | | | |
| Average | Sweetness | Acidity | Mouth Feel | Bitterness | Rating |
| 1 | 0.67 | 0.90 | 0.63 | 1.05 | 2.06 |
| 2 | 0.97 | 0.86 | 0.89 | 0.94 | 2.04 |
| 3 | 0.89 | 1.05 | 1.03 | 1.03 | 1.40 |
| 4 | 0.97 | 0.88 | 0.88 | 0.98 | 1.36 |
| 5 | 0.91 | 1.01 | 0.79 | 0.96 | 1.75 |
| 6 | 0.71 | 1.06 | 0.91 | 0.96 | 1.86 |
| 7 | 1.19 | 1.20 | 1.28 | 0.98 | 2.48 |
| 8 | 1.11 | 1.20 | 1.29 | 1.33 | 2.39 |

Table 4 summarizes the overall ranking of the eight coffees as determined by the professional coffee tasters and the amateur coffee tasters. It is worth noting that 3 of the 4 highest ranked coffees and 3 of the 4 lowest ranked coffees are the same between the professional tasters and the amateur tasters. Those that differ are Kroger and Starbucks, the amateur tasters really liked Kroger's blend but did not like Starbucks' blend. An analysis of the cost per ounce of coffee versus the average overall professional rating was also performed. The results show a strong positive correlation, however, without more information a proper conclusion cannot be drawn as to why this correlation is present.

**Table 4:** Summary of overall professional and amateur ratings.

| Professional | | | Amatuer | | |
|---|---|---|---|---|---|
| Coffee | Average | StdDev | Coffee | Average | StdDev |
| 4 | 78.36 | 2.18 | 7 | 6.18 | 2.48 |
| 7 | 76.71 | 2.45 | 1 | 6.00 | 2.06 |
| 6 | 75.57 | 1.18 | 6 | 5.90 | 1.86 |
| 2 | 75.57 | 3.03 | 4 | 5.86 | 1.36 |
| 8 | 75.36 | 1.66 | 3 | 5.75 | 1.40 |
| 3 | 72.86 | 2.36 | 5 | 5.53 | 1.75 |
| 5 | 72.07 | 3.9 | 8 | 4.92 | 2.39 |
| 1 | 71.71 | 3.33 | 2 | 4.36 | 2.04 |

**Table 5:** Cost per ounce analysis of all 8 coffees.

| Coffee | Cost ($) | Amount (oz) | Cost/Amount ($/oz) |
|---|---|---|---|
| 1 - Kroger | $5.49 | 29 | $0.189 |
| 2 - Starbucks | $6.49 | 12 | $0.541 |
| 3 - Seattle's Best | $4.99 | 12 | $0.416 |
| 4 - Kiva Han | $11.99 | 12 | $0.999 |
| 5 - Folgers | $7.99 | 30.5 | $0.262 |
| 6 - Aztec Reserve | $14.99 | 12 | $1.249 |
| 7 - EZ Morning | $12.99 | 12 | $1.083 |
| 8 - Lifeline | $12.99 | 12 | $1.083 |

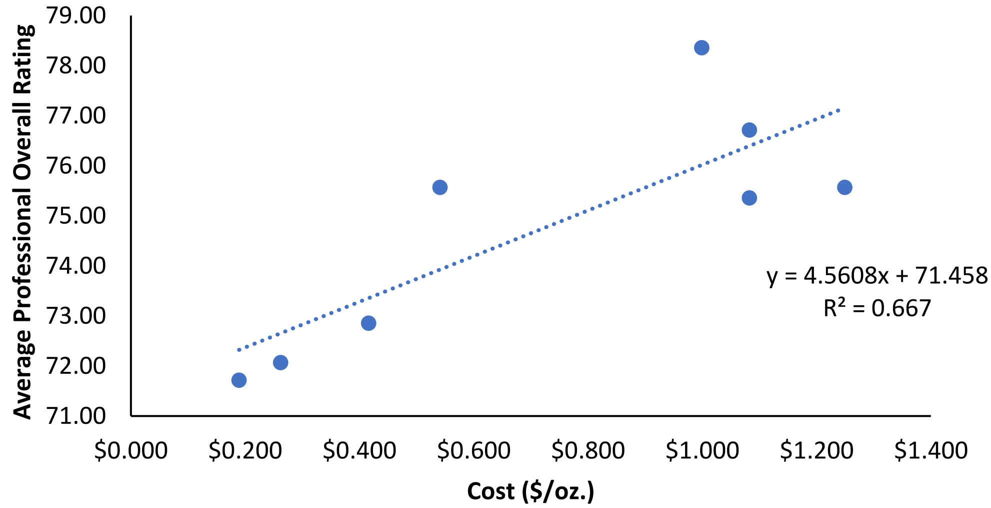


**Figure 5:** Average professional overall rating as a function of cost per ounce of coffee.

Table 6 summarizes retention times and percent overall observed peak area of the chromatographic peaks detected by GCMS.

Representative volatile compound profiles are shown in Figure 6.

**Table 6:** Raw GCMS data showing average peak areas across three trials for of each coffee with standard deviations. Note: Peaks highlighted red were identified as column/fiber bleed.

| | % Area | | | | | | | | StdDev | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| RT | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 |
| 6.56 | 1.14 | 2.00 | 1.45 | 1.27 | 1.43 | 1.39 | 1.28 | 1.43 | 0.15 | 0.90 | 0.10 | 0.03 | 0.52 | 0.13 | 0.15 | 0.25 |
| 7.45 | 0.97 | 1.68 | 0.97 | 2.15 | 1.15 | 1.48 | 2.09 | 1.60 | 0.13 | 0.03 | 0.04 | 0.11 | 0.08 | 0.14 | 0.18 | 0.30 |
| 7.71 | 0.71 | 1.01 | 0.75 | 1.12 | 0.57 | 0.89 | 0.78 | 0.68 | 0.07 | 0.23 | 0.04 | 0.05 | 0.06 | 0.10 | 0.04 | 0.04 |
| 7.98 | 0.71 | 0.99 | 1.24 | 0.85 | 0.54 | 0.57 | 0.69 | 2.22 | 0.53 | 0.62 | 1.08 | 0.75 | 0.42 | 0.42 | 0.49 | 2.19 |
| 8.07 | 0.99 | 1.17 | 1.11 | 0.97 | 0.71 | 1.28 | 1.01 | 1.43 | 0.16 | 0.05 | 0.13 | 0.09 | 0.03 | 0.05 | 0.05 | 0.34 |
| 8.15 | 1.06 | 1.39 | 0.71 | 0.88 | 0.91 | 1.18 | 0.91 | 1.12 | 0.18 | 0.11 | 0.02 | 0.04 | 0.03 | 0.08 | 0.05 | 0.18 |
| 9.38 | 2.05 | 2.77 | 1.44 | 1.78 | 1.74 | 2.42 | 1.80 | 2.55 | 0.40 | 0.19 | 0.13 | 0.11 | 0.07 | 0.14 | 0.08 | 0.58 |
| 9.46 | 1.81 | 1.70 | 3.30 | 2.01 | 1.37 | 2.65 | 2.36 | 3.70 | 0.33 | 0.07 | 0.65 | 0.28 | 0.03 | 0.09 | 0.16 | 1.40 |
| 9.58 | 1.55 | 1.13 | 1.66 | 1.24 | 1.87 | 1.40 | 1.17 | 1.91 | 0.32 | 0.08 | 0.04 | 0.20 | 0.12 | 0.08 | 0.03 | 0.37 |
| 10.19 | 1.32 | 1.14 | 1.43 | 1.56 | 0.94 | 1.28 | 1.27 | 1.31 | 0.17 | 0.14 | 0.18 | 0.09 | 0.07 | 0.07 | 0.07 | 0.17 |
| 10.62 | 1.56 | 1.93 | 1.20 | 1.38 | 1.25 | 1.61 | 1.32 | 1.87 | 0.28 | 0.10 | 0.13 | 0.10 | 0.03 | 0.02 | 0.01 | 0.47 |
| 10.78 | 1.87 | 1.89 | 1.66 | 1.74 | 1.74 | 2.02 | 1.80 | 2.33 | 0.37 | 0.08 | 0.18 | 0.14 | 0.05 | 0.10 | 0.10 | 0.55 |
| 11.02 | 5.46 | 5.67 | 7.09 | 5.77 | 4.27 | 6.29 | 6.06 | 7.89 | 0.80 | 0.11 | 1.07 | 0.55 | 0.05 | 0.11 | 0.08 | 2.02 |
| 11.22 | 1.90 | 2.81 | 1.60 | 2.07 | 1.44 | 2.02 | 2.35 | 2.73 | 0.43 | 0.25 | 0.30 | 0.42 | 0.05 | 0.08 | 0.07 | 0.78 |
| 11.29 | 1.61 | 2.05 | 1.69 | 1.61 | 1.30 | 1.51 | 1.68 | 1.97 | 0.31 | 0.04 | 0.19 | 0.13 | 0.05 | 0.05 | 0.06 | 0.40 |
| 12.74 | 9.14 | 4.87 | 7.74 | 4.04 | 13.24 | 5.99 | 5.43 | 6.78 | 0.53 | 0.21 | 0.57 | 0.19 | 0.27 | 0.10 | 0.28 | 0.53 |
| 13.07 | 2.68 | 4.42 | 3.79 | 5.21 | 2.31 | 3.53 | 4.77 | 3.76 | 0.37 | 0.42 | 0.67 | 1.19 | 0.92 | 0.68 | 0.86 | 0.63 |
| 13.18 | 3.79 | 3.42 | 5.74 | 3.32 | 3.36 | 5.24 | 4.35 | 5.27 | 0.04 | 0.06 | 0.39 | 0.15 | 0.04 | 0.15 | 0.20 | 0.12 |
| 13.52 | 28.59 | 18.21 | 14.01 | 16.94 | 25.77 | 12.35 | 17.34 | 12.41 | 1.65 | 0.42 | 1.11 | 0.54 | 1.34 | 0.35 | 0.16 | 0.27 |
| 14.53 | 3.47 | 4.03 | 6.43 | 5.21 | 3.66 | 5.69 | 4.29 | 8.35 | 0.49 | 0.27 | 0.60 | 0.59 | 0.33 | 0.15 | 0.50 | 1.55 |
| 14.88 | 3.10 | 3.95 | 3.91 | 3.66 | 3.29 | 4.09 | 3.29 | 2.77 | 0.32 | 0.37 | 0.33 | 0.37 | 0.32 | 0.20 | 0.20 | 0.97 |
| 15.06 | 2.28 | 1.96 | 2.28 | 1.81 | 2.84 | 2.22 | 2.15 | 1.93 | 0.30 | 0.22 | 0.33 | 0.23 | 0.28 | 0.15 | 0.20 | 0.77 |
| 15.60 | 2.03 | 2.93 | 2.67 | 3.53 | 1.83 | 3.73 | 3.33 | 2.93 | 0.28 | 0.26 | 0.31 | 0.52 | 0.16 | 0.29 | 0.24 | 1.30 |
| 16.03 | 1.16 | 1.39 | 1.06 | 1.29 | 1.26 | 1.55 | 1.27 | 1.11 | 0.20 | 0.26 | 0.24 | 0.22 | 0.18 | 0.17 | 0.16 | 0.49 |
| 16.12 | 0.92 | 0.99 | 1.90 | 0.86 | 0.93 | 1.59 | 1.14 | 1.48 | 0.15 | 0.04 | 0.23 | 0.10 | 0.07 | 0.13 | 0.05 | 0.61 |
| 16.25 | 1.86 | 2.52 | 2.60 | 2.77 | 2.25 | 3.14 | 2.54 | 2.35 | 0.29 | 0.41 | 0.39 | 0.34 | 0.24 | 0.44 | 0.23 | 0.50 |
| 16.56 | 4.16 | 7.25 | 6.47 | 9.51 | 4.52 | 6.50 | 8.27 | 4.53 | 1.11 | 0.63 | 0.92 | 1.81 | 1.66 | 1.81 | 2.68 | 0.87 |
| 16.93 | 2.79 | 3.28 | 3.97 | 3.50 | 3.44 | 3.87 | 3.92 | 2.09 | 0.77 | 0.60 | 0.87 | 0.81 | 0.56 | 0.55 | 0.70 | 0.76 |
| 17.13 | 1.17 | 0.98 | 1.22 | 1.00 | 1.18 | 1.17 | 0.95 | 0.96 | 0.25 | 0.16 | 0.25 | 0.24 | 0.24 | 0.10 | 0.14 | 0.34 |
| 17.91 | 2.31 | 2.78 | 1.69 | 2.29 | 2.52 | 2.80 | 2.28 | 2.24 | 0.59 | 0.46 | 0.44 | 0.53 | 0.50 | 0.53 | 0.25 | 0.77 |
| 18.76 | 1.89 | 1.65 | 2.58 | 2.57 | 2.37 | 2.87 | 2.32 | 2.32 | 0.76 | 0.43 | 1.15 | 1.27 | 0.85 | 0.54 | 0.34 | 1.12 |
| 19.17 | 1.60 | 2.20 | 1.95 | 2.26 | 1.87 | 2.50 | 2.66 | 1.99 | 0.47 | 0.47 | 0.50 | 0.75 | 0.43 | 0.52 | 0.53 | 0.85 |
| 20.13 | 2.33 | 3.85 | 2.68 | 3.83 | 2.11 | 3.18 | 3.13 | 1.98 | 0.79 | 0.19 | 0.97 | 0.42 | 0.16 | 1.00 | 0.63 | 0.56 |

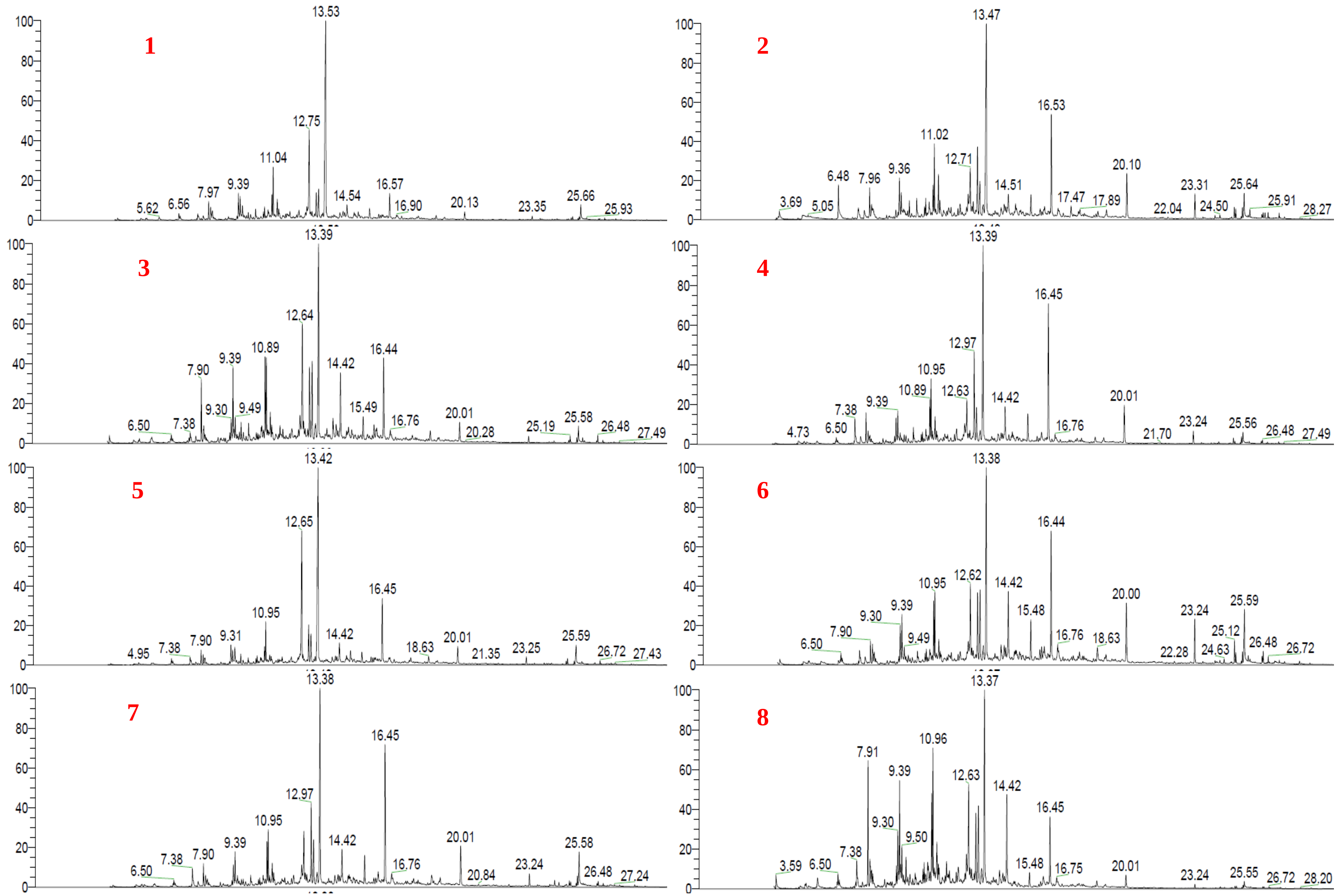


**Figure 6:** GCMS chromatograms of each coffee labeled with its respective identifying number.

The professional taster's rankings (Tables 1 and 2) and the amateur tasters' rankings (Table 3) were plotted as a function of GCMS peak areas (Table 6). The peak areas in Table 6 are percent areas calculated as the percent of the total peak area of the 33 peaks of interest (Figure 6). These 33 peaks were chosen initially due to noticeable differences across all 8 coffees. Correlations between the peak areas and flavor profiles were noted and the corresponding mass spectra were used to identify the compounds. The following compounds were identified: 2,5-dimethylpyrazine (RT 6.65), 5-methyl-2-furaldehyde (RT 7.45), 2-furanmethanol acetate (RT 7.98), guaiacol (RT 9.58), 4-ethylguaiacol (RT 12.74), p-cyanobenzaldehyde (RT 15.06), cinnamaldehyde derivative (RT 15.60), and 2-methylphenol derivative (RT 19.17).

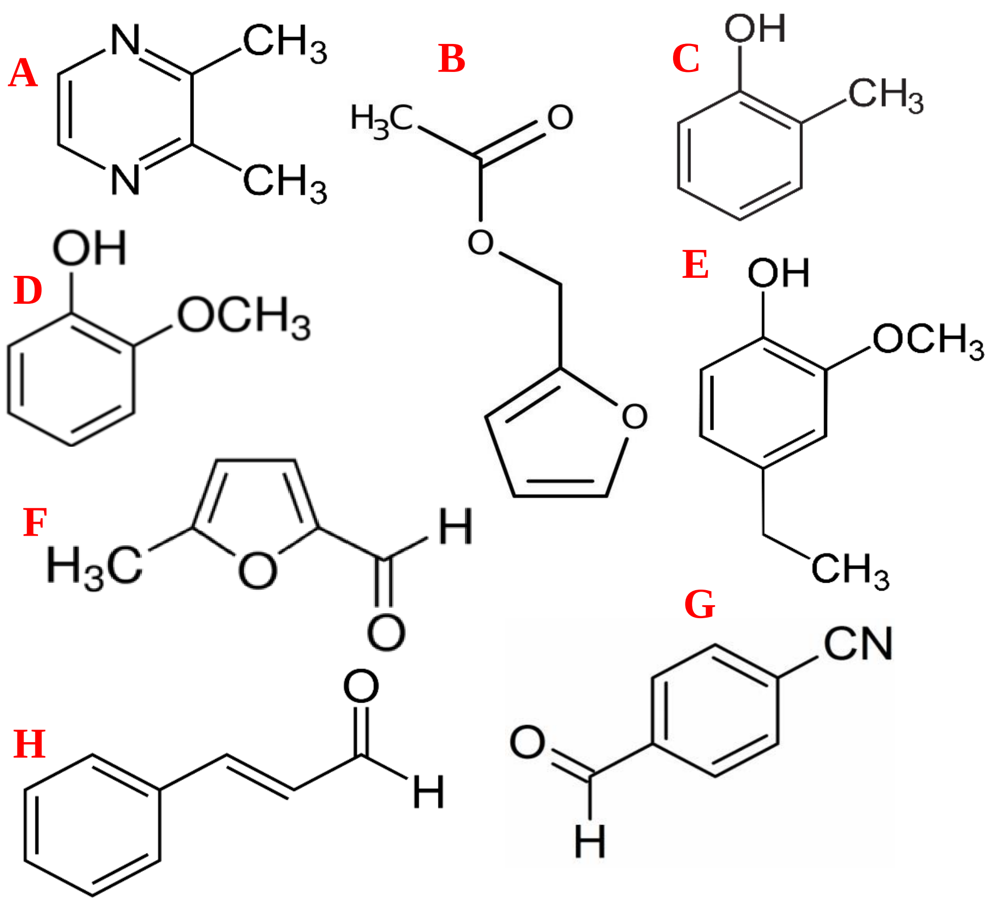


**Figure 7:** Structures of identified compounds by GCMS. A) 2,3-dimethylpyrazine, B) 2-furanmethanol acetate, C) 2-methylphenol, D) guaiacol, E) 4-ethylguaiacol, F) 5-methyl-2-furaldehyde, G) p-cyanobenzaldehyde, H) cinnamaldehyde.

2,5-Dimethylpyrazine was found to have a strong negative correlation with the amateur average overall rating (Figure 8). 2-Furanmethanol acetate was found to have a strong negative correlation with average amateur acidity (Figure 9), and average amateur bitterness (Figure 10) meaning that the more 2-furanmethanol acetate present the more acidic and bitter the coffee tasted. 5-Methyl-2-furaldehyde shows a strong positive correlation with average professional sweet (Figure 11A), average professional acidity (Figure 11B), and average professional overall rating (Figure 11C). This means that the more 5-methyl-2-furaldehyde present the sweeter and more acidic the coffee tasted. 4-ethylguaiacol shows a strong negative correlation with average professional caramel rating (Figure 12A), average professional sweet rating (Figure 12B), and average professional overall rating (Figure 12C). It also shows a strong negative correlation with average professional bitter rating (Figure 12D), because of the way bitterness is graded this means that as the relative concentration increases so does the bitterness of the coffee. Guaiacol was found to have a strong negative correlation with average professional sweet rating (Figure 13A). The cinnamaldehyde derivative shows a strong positive correlation with average professional overall rating (Figure 13B). The 2-methylphenol derivative shows a similar correlation with average professional overall rating (Figure 13C) as the cinnamaldehyde derivative. *p*-Cyanobenzaldehyde shows similar correlations with professional caramel (Figure 14A) and professional bitterness (Figure 14B) as 4-ethylguaiacol.

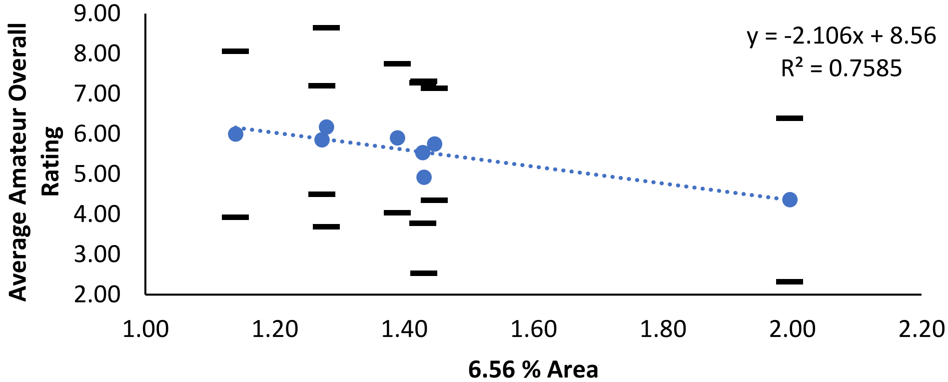


**Figure 8:** Average amateur overall rating as a function of 2,5-dimethylpyrazine relative concentration.

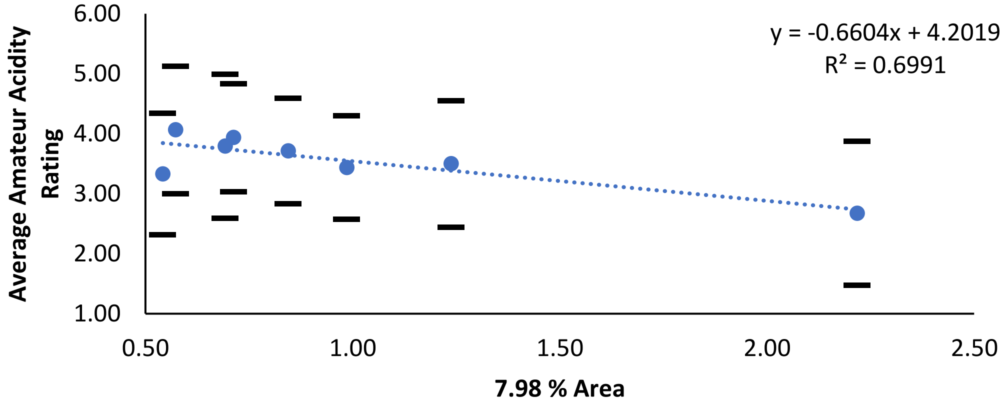


**Figure 9:** Average amateur acidity rating as a function of 2-furanmethanol acetate relative concentration.

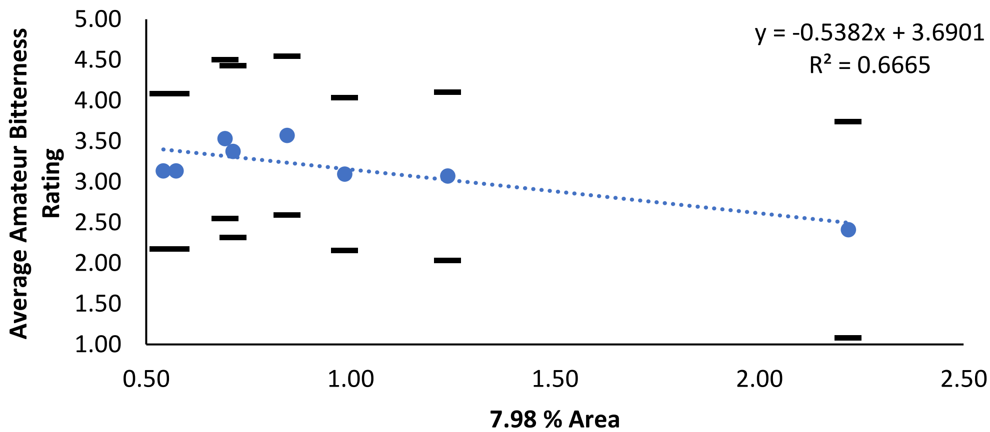


**Figure 10:** Average amateur bitterness rating as a function of 2-furanmethanol acetate relative concentration.

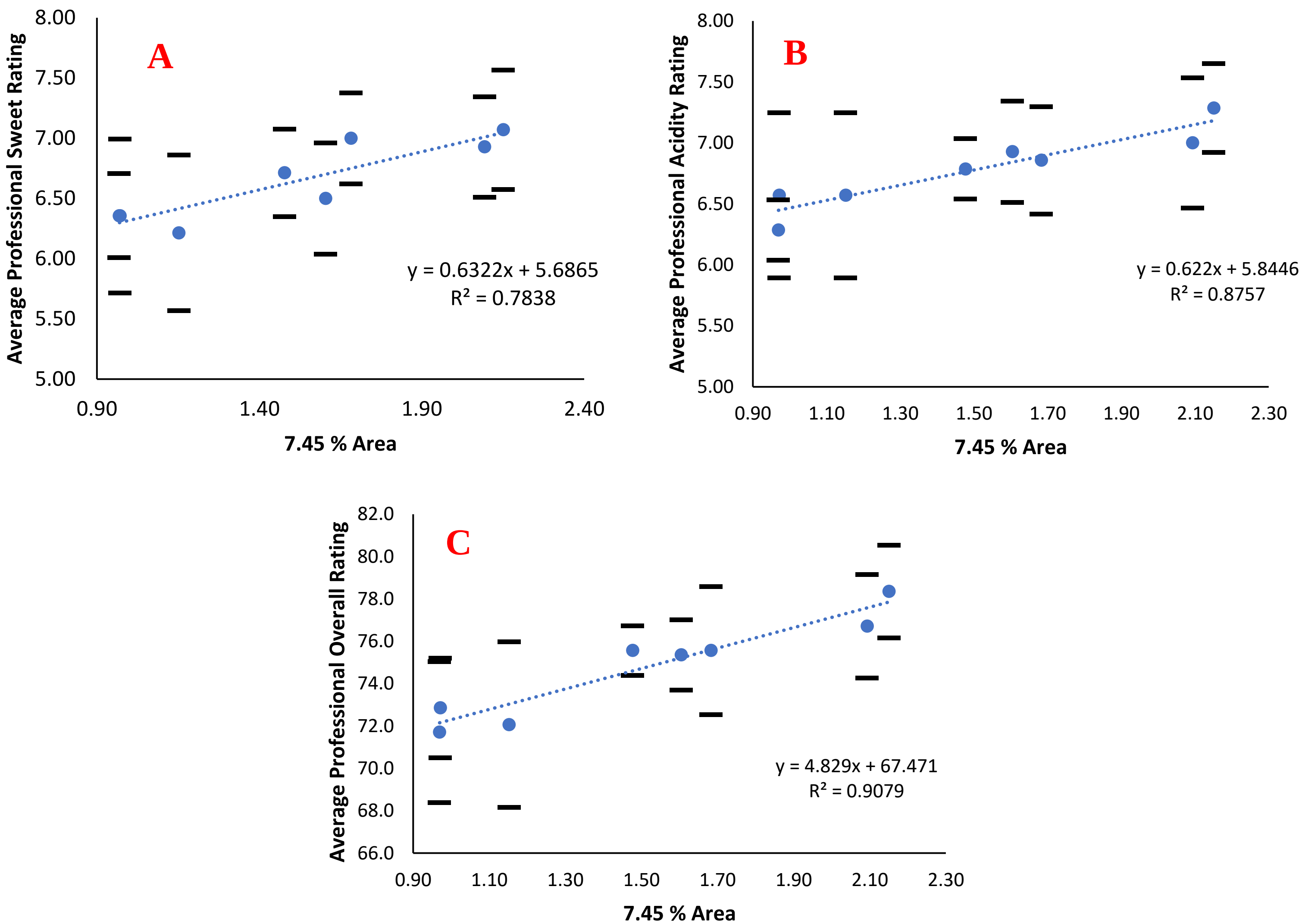


**Figure 11:** A) Average professional sweet rating, B) average professional acidity rating, and C) average professional overall rating, all as a function of 5-methyl-2-furaldehyde relative concentration.

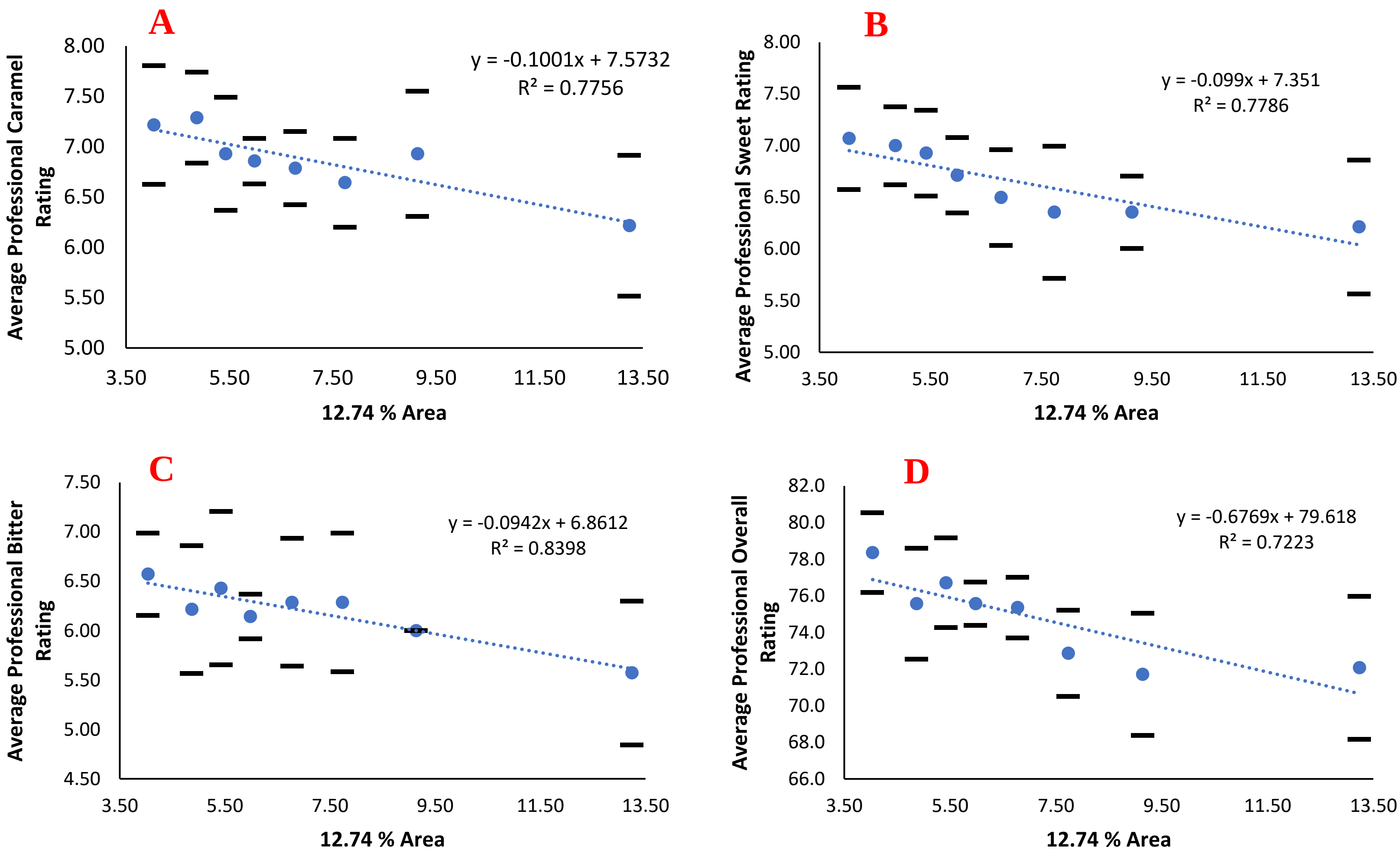


**Figure 12:** A) Average professional caramel rating, B) average professional sweet rating, C) average professional bitterness rating, and D) average professional overall rating, all as a function of 4-ethylguaiacol relative concentration.

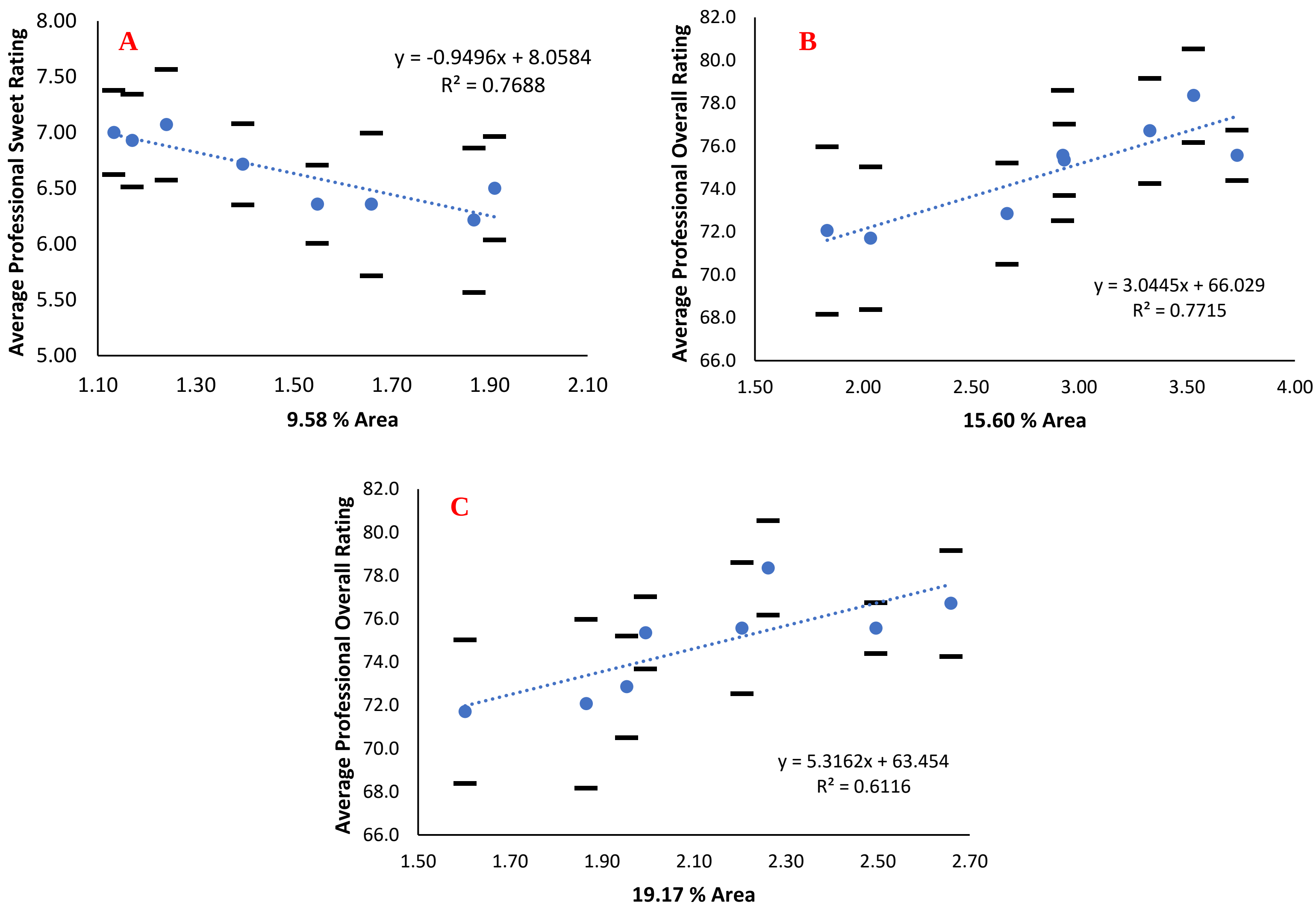


**Figure 13:** A) Average professional rating as a function of guaiacol relative concentration. B) Average professional overall rating as a function of cinnamaldehyde derivative relative concentration. C) Average professional overall rating as a function of 2-methylphenol derivative relative concentration.

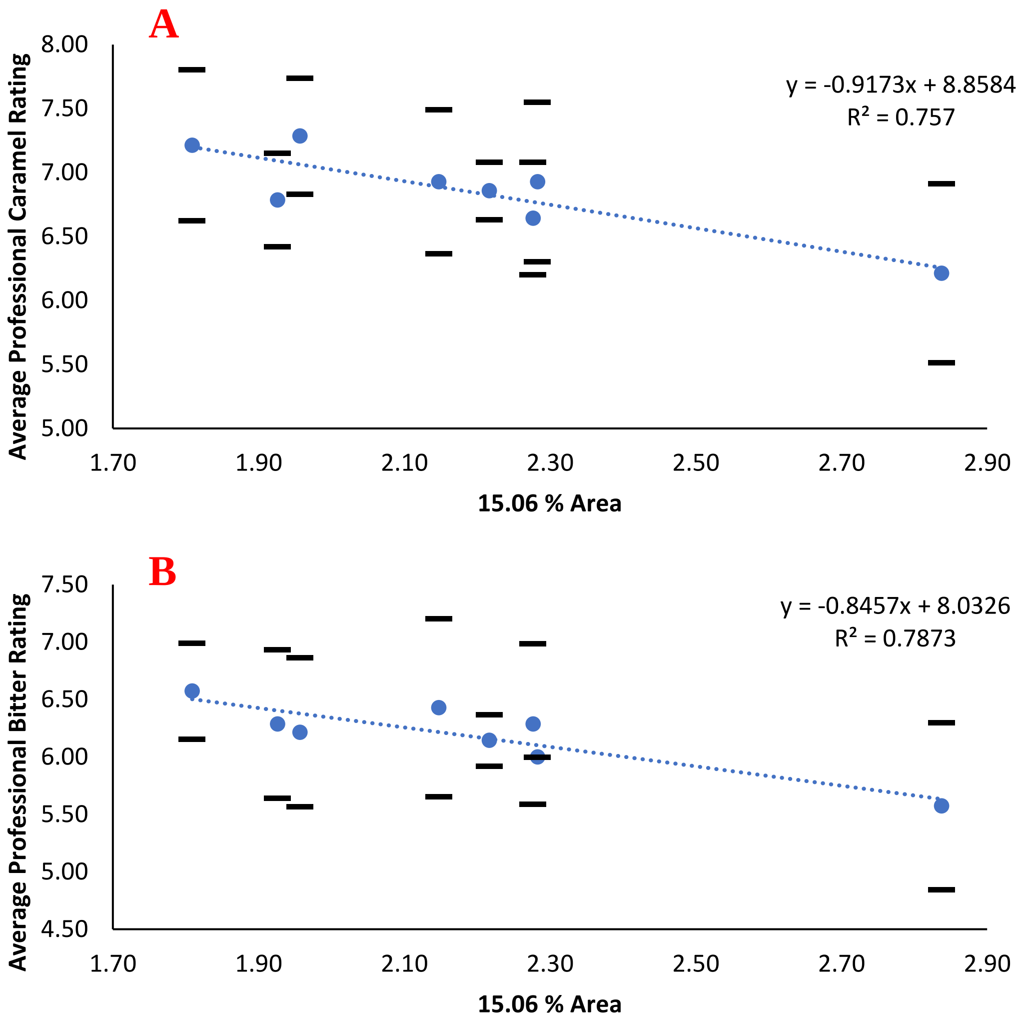


**Figure 14: A)** Average professional caramel rating and B) average professional bitterness rating both as a function of p-cyanobenzaldehyde relative concentration.

Peak areas collected from the HPLC chromatograms (Figures 16-23) were used to find the average concentrations of the four nonvolatile compounds in the 8 coffees (Table 5) using the beers law standard equations (Figure 15 and Table 8). The professional tasters' data (Tables 1 and 2) and the amateur tasters' data (Table 3) were then plotted as a function of the calculated peak areas (Table 5) to find correlations between the average concentration and the average rating. Caffeine was determined to have a strong negative correlation with average professional bitter rating (Figure 24, $R^2$ =.6756). Because bitterness is considered a negative attribute by the SCA, the lower the rating the more bitter the coffee tasted. This means that overall the more caffeine present in the coffee, the more bitter it tastes. This correlation is confirmed in published literature.[18] Trigonelline and chlorogenic acid on the other hand both have a strong positive correlation with professional sweet rating (Figure 25 (A and B respectively), $R^2$ =.7532, $R^2$ =.8032). It was determined that nicotinic acid has a strong positive correlation with amateur mouth feel rating (Figure 26C, $R^2$ =.9107) meaning that the more nicotinic acid the fuller bodied the coffee tasted. Nicotinic acid also has a strong negative correlation with both professional caramel (Figure 26A, $R^2$ =.7098) and professional sweet ratings (Figure 26B, $R^2$ =.8938) meaning that the more nicotinic acid present the less caramel or sweet the coffee tasted. Nicotinic acid is a degradation product of trigonelline that results loss of methyl during heating.

**Table 7:** HPLC standard data showing calculated concentrations with peak area.

| | Nicotinic Acid | | Trigonelline | | Chlorogenic Acid | | Caffeine | |
|---|---|---|---|---|---|---|---|---|
| Standard | Concentraion (µM) | Peak Area | Concentraion (µM) | Peak Area | Concentraion (µM) | Peak Area (220nm) | Concentraion (µM) | Peak Area |
| 0.25 | 103.354 | 228.83763 | 25.5225 | 65.79673 | 24.338 | 143.66147 | 753.65575 | 4587.02246 |
| 0.5 | 206.708 | 453.4198 | 51.045 | 133.98944 | 48.676 | 285.55936 | 1507.3115 | 8964.46094 |
| 1 | 413.416 | 945.02423 | 102.090 | 270.34586 | 97.352 | 662.81580 | 3014.623 | 17093.70 |
| 2 | 826.584 | 1884.44275 | 204.099 | 539.73083 | 194.623 | 1321.78833 | 4220.472 | 23094.70 |
| 3 | 1240.000 | 2812.27661 | 408.199 | 1061.56177 | 389.246 | 2634.64600 | 4823.397 | 25742.70 |
| 4 | 1653.416 | 3718.12915 | 612.298 | 1568.29248 | 583.869 | 3911.40332 | 5426.321 | 28313.40 |
| 5 | 2065.840 | 4631.63965 | 816.397 | 2086.15894 | 778.492 | 5203.34766 | 6029.246 | 30752.60 |
| 7 | | | 4539.170 | 11230.90000 | 4120.690 | 27606.10000 | | |

**Table 8:** HPLC data for each of the four non-volatile compounds. Note: Nicotinic acid was below the level of detection for coffees 1, 4, and 7.

| | Nicotinic Acid | | Trigonelline | | Chlorogenic Acid | | Caffeine | |
|---|---|---|---|---|---|---|---|---|
| Coffee | Concentration | StdDev | Concentration | StdDev | Concentration | StdDev | Concentration | StdDev |
| 1 | | | 1437.28687 | 0.959294563 | 642.3084286 | 7.098136247 | 3035.156041 | 3.196616589 |
| 2 | 168.7772075 | 3.935817201 | 2883.6419 | 10.10136135 | 1296.408745 | 9.703981894 | 3179.199454 | 16.56483288 |
| 3 | 204.1537295 | 7.49183005 | 1211.603521 | 6.278031946 | 488.7283228 | 2.262220706 | 2755.486858 | 10.5134507 |
| 4 | | | 2385.434058 | 12.75784337 | 1245.608967 | 11.46606163 | 2780.077351 | 18.61956189 |
| 5 | 199.1690333 | 1.382320753 | 1741.964917 | 1.255643828 | 814.6500821 | 5.321374924 | 3771.806916 | 6.131274538 |
| 6 | 186.7809526 | 1.936008239 | 1887.361081 | 4.268885303 | 886.7556234 | 3.363299437 | 3193.732937 | 7.598130648 |
| 7 | | | 2424.700702 | 9.321276396 | 1259.098217 | 8.405916545 | 3141.393662 | 12.13051451 |
| 8 | 194.5721374 | 5.652162773 | 1849.918473 | 13.48885743 | 816.951867 | 9.556002066 | 2819.883839 | 22.66360776 |

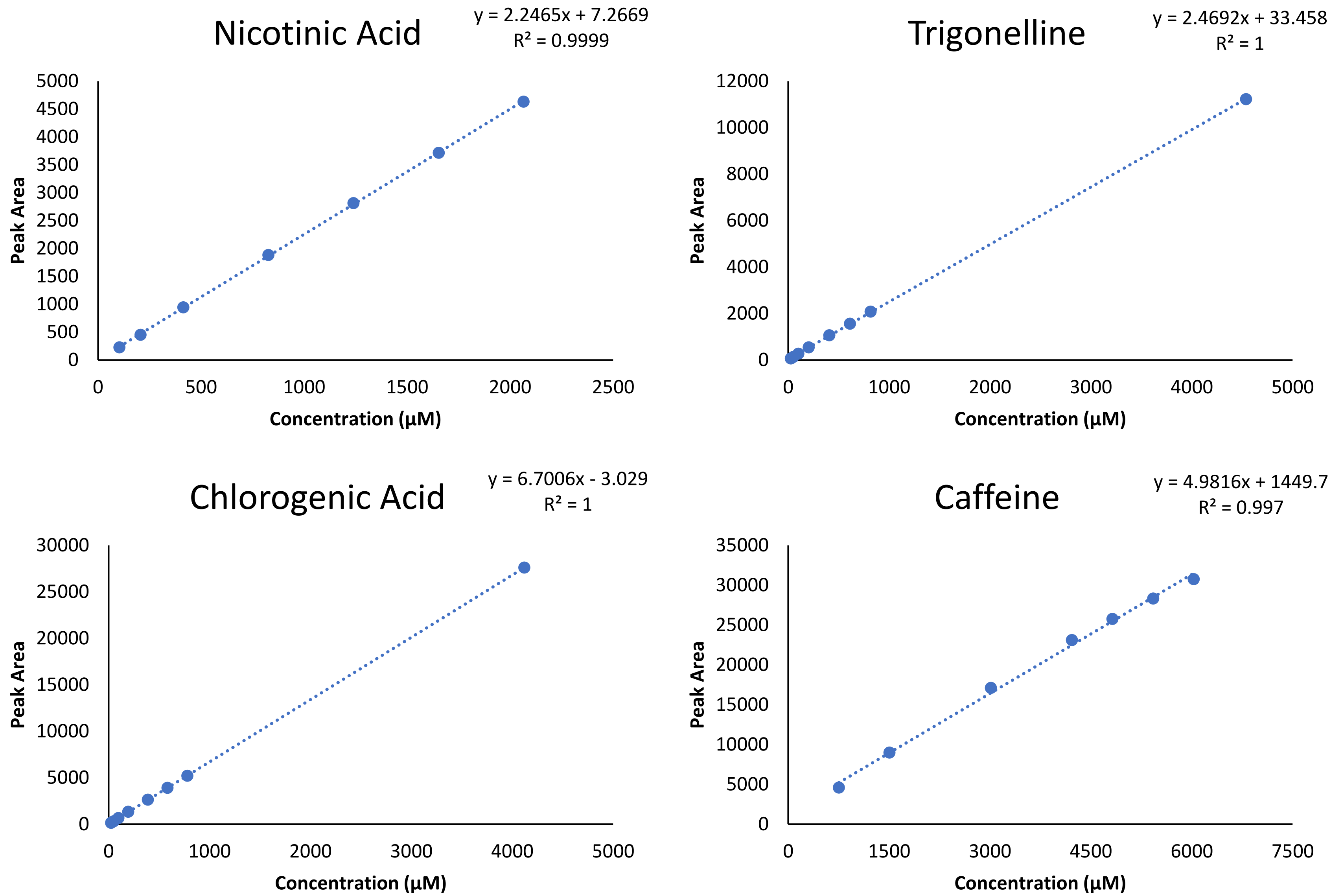


**Figure 15:** Plots with equations and R-squared values for each of the four nonvolatile standards.

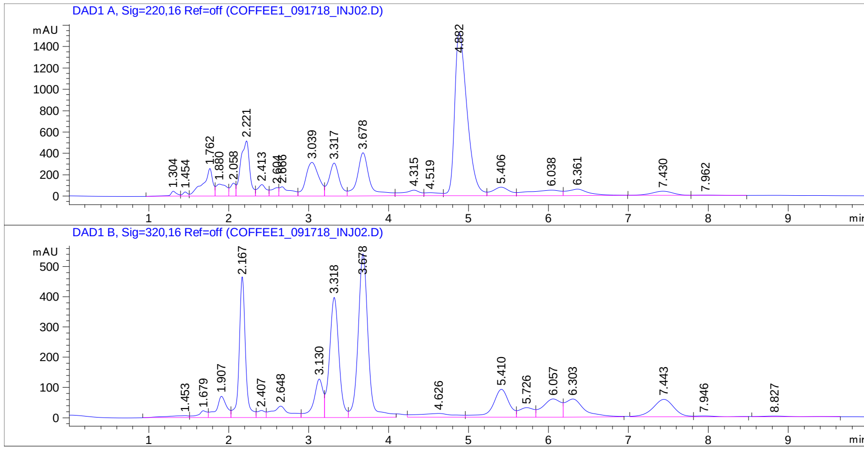


**Figure 16:** HPLC chromatogram of Kroger brand coffee.

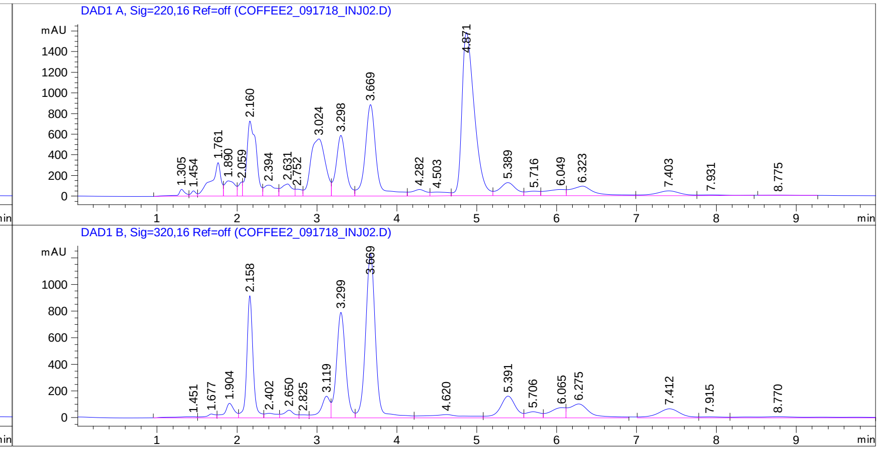


**Figure 17:** HPLC chromatogram of Starbucks brand coffee.

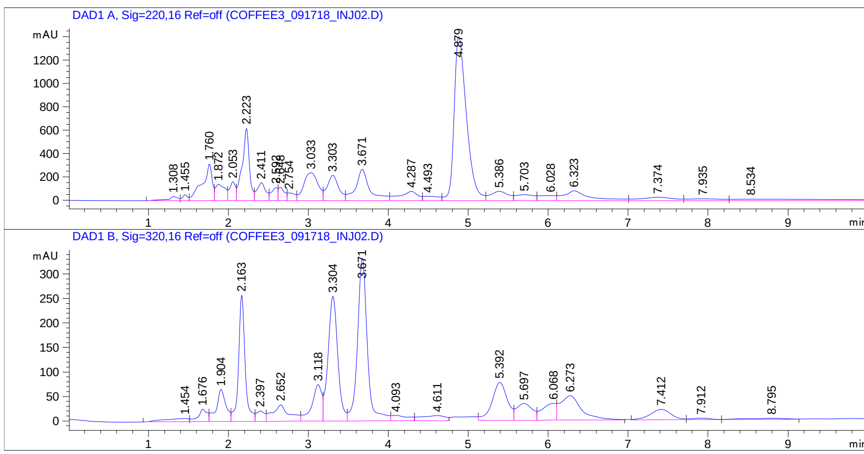


**Figure 18:** HPLC chromatogram of Seattle's Best brand coffee.

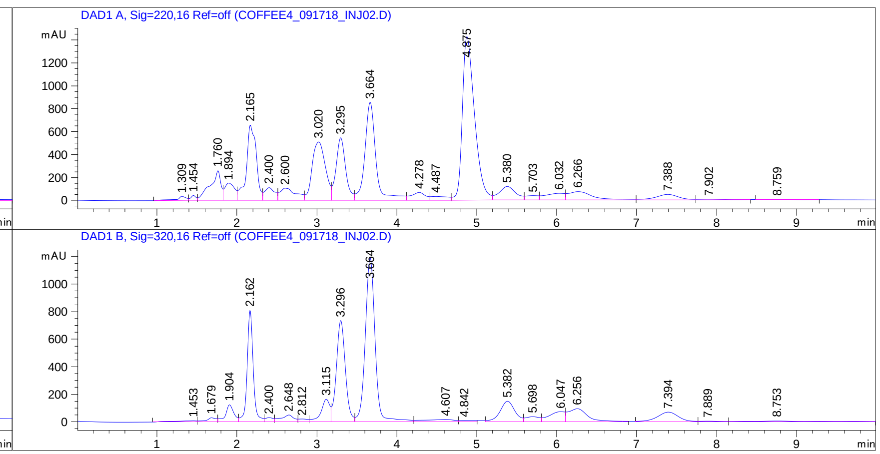


**Figure 19:** HPLC chromatogram of Kiva Han's Columbian Supremo coffee.

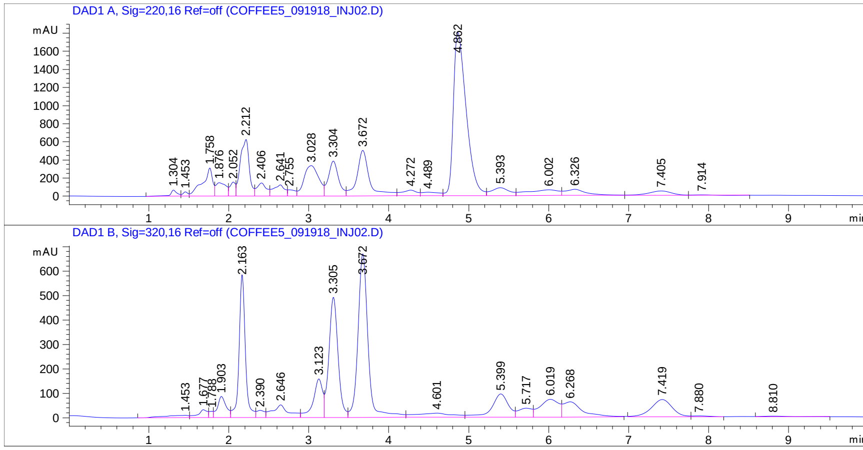


**Figure 20:** HPLC chromatogram of Folgers brand coffee.

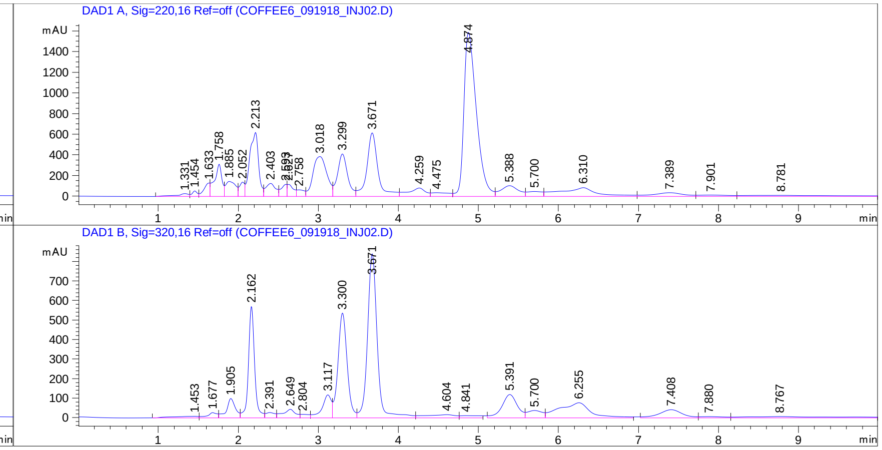


**Figure 21:** HPLC chromatogram of Kings Coast's Aztec Reserve Coffee.

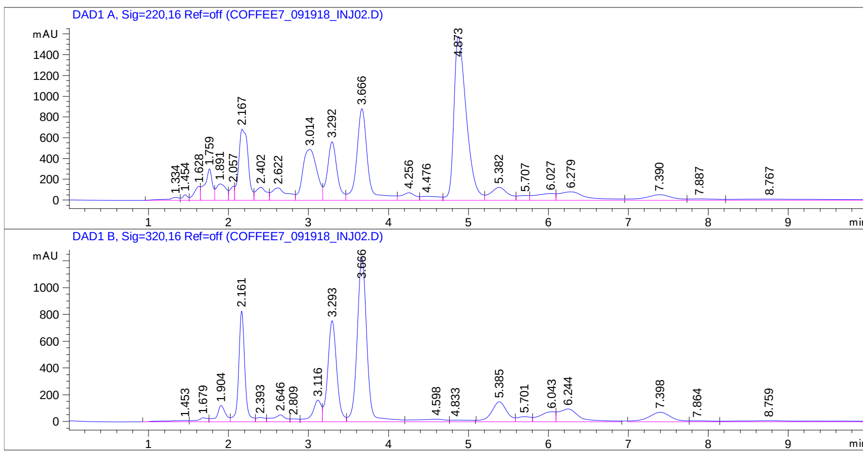


**Figure 22:** HPLC chromatogram of Kings Coast's EZ Morning coffee.

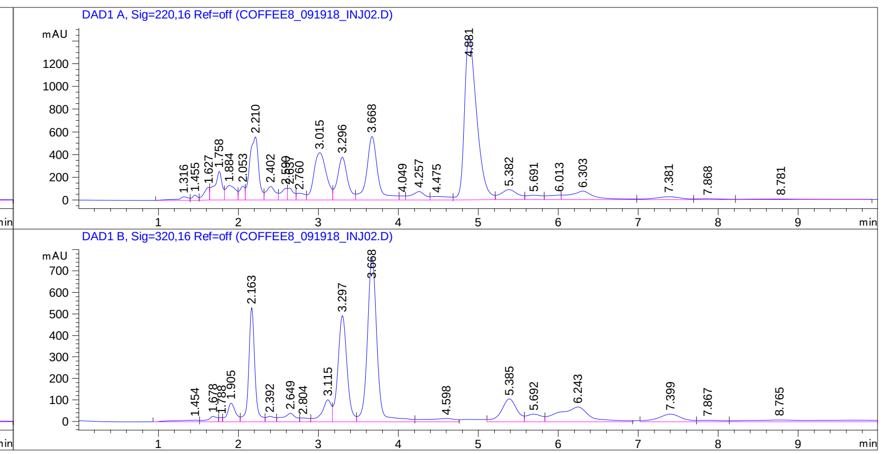


**Figure 23:** HPLC chromatogram of Kings Coast's Lifeline coffee.

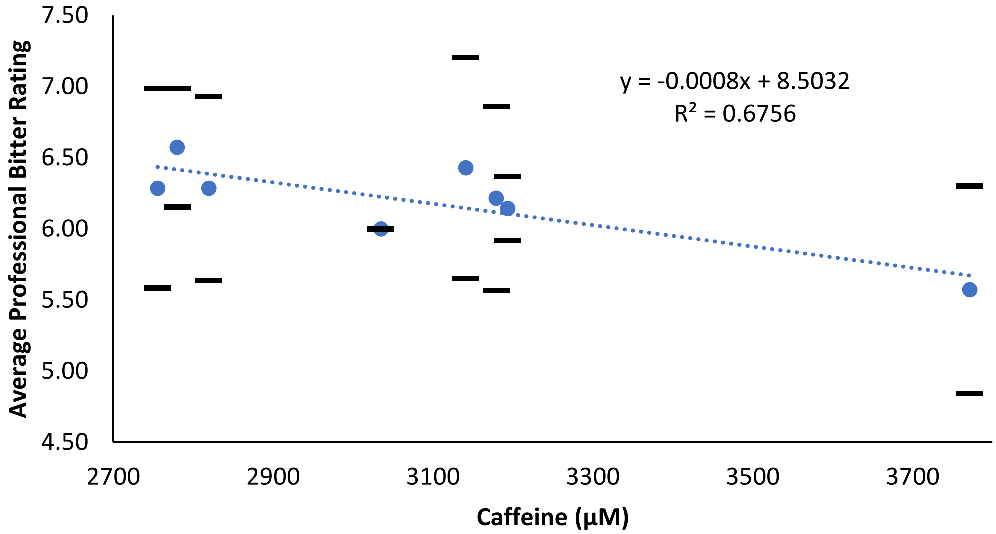


**Figure 24:** Average professional bitter rating as a function of caffeine concentration. Note: A lower rating means more bitter less balanced flavor.

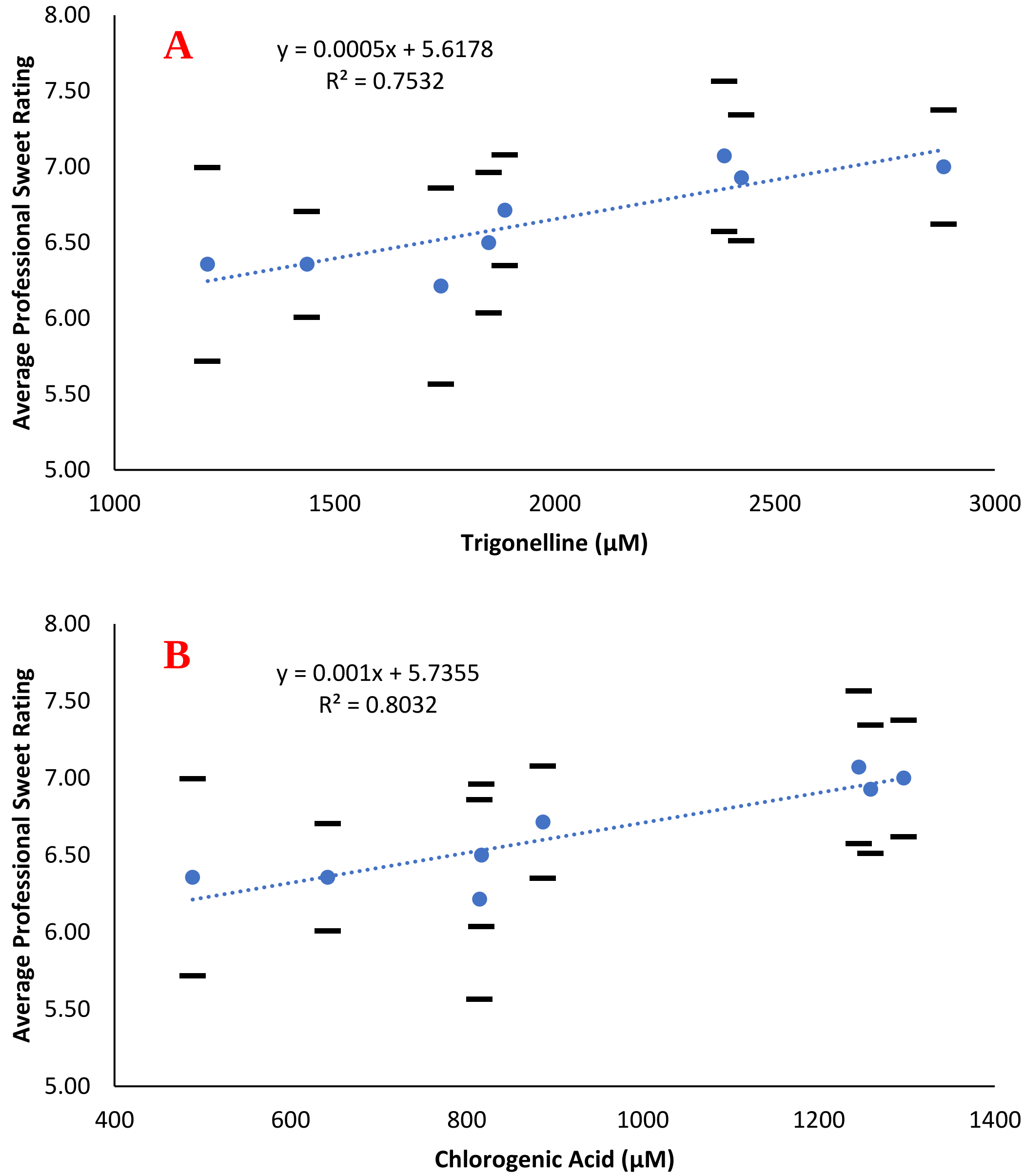


**Figure 25:** A) Average professional sweet rating as a function of trigonelline concentration and B) chlorogenic acid concentration.

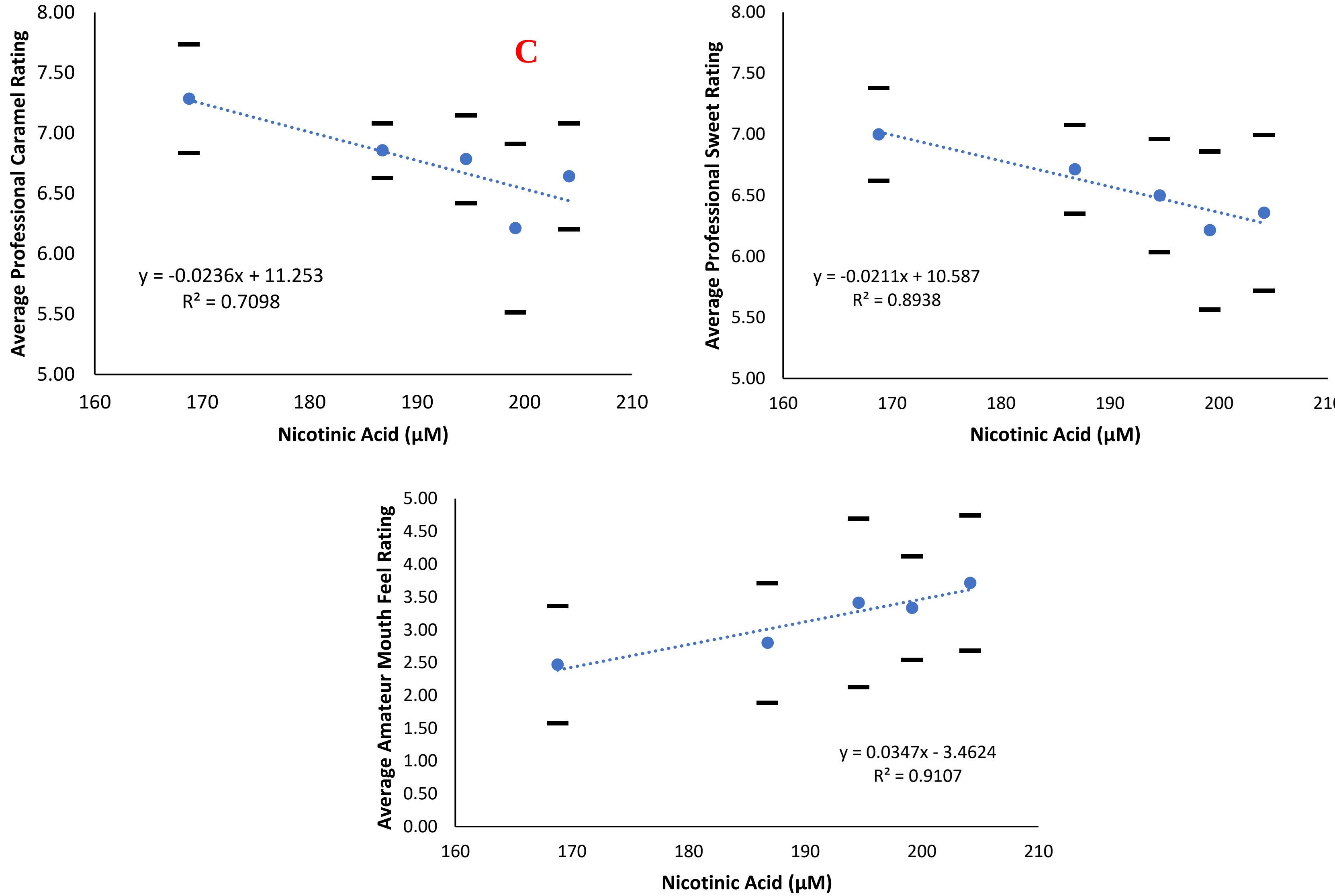


**Figure 26:** A) Average professional caramel rating, B) average professional sweet rating, and C) average amateur mouth feel rating, all as a function of nicotinic acid concentration.

# CHAPTER 4 – Conclusions

Amateur tasters are much more sensitive to those flavor profiles which they are familiar with (i.e. acidity and bitterness) which show some strong correlations. Professional coffee tasters, on the other hand, are specially trained to differentiate and recognize subtle flavor and aroma notes that the average person does not notice. It has been observed that there are significantly more correlations between professional tasting notes and chemical components. The relationship between trigonelline and nicotinic acid is also illustrated in the correlation plots. When trigonelline concentration is high, the nicotinic acid concentration is low. This correlation shows strongest with the sweet rating where the professional tasters rate the coffee more balanced when trigonelline is low and nicotinic acid is high. Professional tasters also rank the coffee as more balanced when there is less caffeine. Future research on this topic should include stable isotope ratio mass spectrometry to determine the proper geographic origins of the coffees from Kroger, Seattle's Best, Starbucks, and Folgers. This will allow for a comparison across geographic locations. Principle component analysis can also be explored evaluate if groups of two or more volatile and nonvolatile compounds work together synergistically to affect the coffees' distinct tasting notes.

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