

## Determination of the Caffeine Extraction Profile of Brewing Coffee

### Before lab:

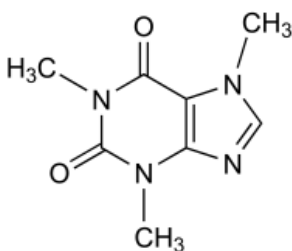
1. Write a procedure for the preparation of a 1000 ppm caffeine stock solution
2. Calculate the volumes needed to dilute the 1000 ppm caffeine stock solution in order to achieve 0, 100, 250, 400, and 500 ppm standards
3. Write a procedure similar to the example shown below describing what you want to do.

### Introduction:

When coffee is prepared, hot water is used to extract flavor components from ground, roasted coffee beans. Other molecules, such as caffeine are also extracted. Typical brewed coffee will have a concentration of 300 to 450 ppm caffeine. The caffeine molecule can be detected and quantified using High-Performance Liquid Chromatography (HPLC).



The purpose of this lab is to experimentally determine the caffeine extraction profile (a plot of mass of caffeine extracted versus volume of hot water passed through the ground beans) for the brewing of a typical pot of coffee. You will determine if the caffeine extraction profile is a good example of an exponential process and you will also address the long-standing question of what portion of the brew cycle to sample to maximize the caffeine content per cup.



The CRC Handbook of Chemistry and Physics notes that caffeine (1,3,7-trimethylxanthine) is slightly soluble in water, ethanol, acetone, and benzene. It is insoluble in ether; soluble in hot water and chloroform; and it sublimates readily. Its molar absorptivity at 274 nm is approximately  $2 \times 10^4$  in ethanol solution.

### Example Procedure:

#### Determine the Caffeine Elution Profile of a Brewed Pot of Coffee

4. Start brewing **4 cups** of coffee with the coffee pot and coffee grounds provided
5. Collect nine 70 mL aliquots of coffee spaced every 1 minute (total 9 minutes)
6. Filter each sample with their own individual 0.45 micron filter and syringe
7. Fill up an HPLC vial with portions of each of the filtered samples
8. Give the TA your labeled samples

**Calculations:**

1. Using Origin or some program like it, quantify the area under the caffeine elution peak of the HPLC chromatogram
2. Generate a calibration curve and use it to calculate the concentration of caffeine concentration in the brewing coffee.
3. Plot the concentration of coffee as a function of time or aliquot.

**Discussion questions:**

1. Make a figure showing the caffeine elution profile for the brewed pot of coffee. Use this plot to suggest to the overtired coffee drinker how to get the maximum caffeine input per cup of coffee. Compare the maximum concentration of caffeine observed to the concentration of caffeine that would present if all of the fractions were mixed and homogenized.
2. Use the results of the HPLC of triplicate samples to estimate the accuracy and precision of this method.
3. Comment on how you felt the experiment worked overall. Identify what you believe to be the largest source of error in your experiments and discuss how they would have affected your results. Human error is not an acceptable answer.

**Lab write-up:**

1. **Abstract:** In 250 words or less, describe your purpose, what you did, what you found, if that was expected or surprising, and what it all means.
2. **Introduction:** Introduce topic and state why you are performing the experiment.
3. **Materials and Methods:** Prepare a trimmed down procedure in sentence form.
4. **Results:** tabulate your measurements and results; and briefly say what they mean.
5. **Discussion:** respond to the questions above in paragraph form (not Q1: answer, answer). Devote 1-2 paragraphs to discuss each question.
6. **Conclusion:** Write a short paragraph concluding what you learned.
7. **Group dynamics:** let me know how you feel your group worked together.
8. **Appendix 1- Calculations:** You can send me your spreadsheet.