Caffeine Prelab

Instructions: Answer the questions and turn this prelab in to your TA at the beginning of the caffeine lab. You may want to copy some of your answers in your lab notebook for future reference.

1. Find the following information about caffeine (do not forget the units):
   a. Molecular weight:
   b. Solubility in water at 25°C:
   c. Molecular formula:
   d. Structure:

2. Figure 1 shows sample absorption spectra of an aqueous solution of caffeine and of a diluted coffee extract. Both spectra were taken in a 1 cm cell, after appropriately diluting the samples.

![Sample Absorption Spectra of Caffeine and Coffee](image)

The peak absorption wavelength for caffeine is about 273 nm. The extinction coefficient of caffeine is roughly 8800 M⁻¹cm⁻¹ at this wavelength (you will determine a more precise value in this lab). Based on this information, estimate the weight concentration of caffeine (in µg/mL) used to get the absorption spectrum of an aqueous solution of caffeine shown in Figure 1.
3. Solution of caffeine is colorless whereas the coffee extract is brown. Can you see the absorption due to caffeine in the spectrum of the caffeine extract shown in Figure 1? Is caffeine the only compound in coffee that absorbs at 273 nm?

4. Based on the magnitude of the caffeine peak in the spectrum of the diluted caffeine extract shown in Figure 1 estimate the concentration of caffeine in the diluted extract. The diluted extract was obtained by:
   - Dripping 1000 mL of hot water through 50 g of ground coffee
   - Filtering it
   - Taking 1 mL of the filtered extract and diluting it to 100 mL
   - Drinking the rest of the coffee

Based on this information, estimate the mass fraction of caffeine in the coffee beans. Assume that dripping extracted all caffeine from coffee (this is likely not true).

5. The HPLC diode array detector simultaneously measures absorbance of molecules that are being eluted from the HPLC column at 5 fixed wavelengths. This results in 5 separate chromatograms corresponding to these detection wavelengths. Assume that these wavelengths are 240, 255, 270, 285, and 300 nm. You see three peaks in the chromatogram, and you need to find out which one of them corresponds to caffeine.
   - Peak A: signals decrease in the following order: 240 nm > 255 nm > 270 nm > 285 nm > 300 nm
   - Peak B: signals decrease in the following order: 270 nm > 285 nm > 255 nm > 240 nm > 300 nm
   - Peak C: signals decrease in the following order: 285 nm > 300 nm > 270 nm > 255 nm > 240 nm

Which one of these peaks corresponds to caffeine? Explain.