"How Much Caffeine Is in My Soft Drink?" Answers to Calculations and Analysis and Conclusions:

Calculations – show your work:

1. Calculate the mass in μ g of deuterated caffeine you pipetted into your sample in Step 2 of the procedure.

Since density = mass/volume, then mass = density x volume Volume pipetted is 100 μ L = 0.100 mL Mass in mg = 1 mg/mL x 0.100 mL = 0.100 mg deuterated caffeine 0.100 mg x 1000 μ g/1mg = **100 \mug deuterated caffeine**

2. Calculate the mass in μ g of pure caffeine in your sample.

Based on the abundance peaks when the data is returned from the Mass Spectrometry Facility.

In the formula below: Subscript 1 is for pure caffeine; subscript 2 is for deuterated caffeine. R is given on page 1 of the lab protocol as 1.40. C_2 is calculated in the previous calculation (Calculation #1). Solve for C_1 .

Note: in the concentrations, the volumes are identical in the reaction mixture, so they cancel out in the calculation. You may need to direct your students about this.



Sample numbers from data:

If abundance peak areas for pure caffeine is 500,000 and for deuterated caffeine is 250,000, then the calculation would look like this:

 $C_1 / 100 \ \mu g = 1.40 \ x \ (500,000 / 250,0000)$

Solve for C_1 . $C_1 = 280 \ \mu g$ pure caffeine in sample

3. Calculate the mass in mg of pure caffeine in your sample.

Using answer from previous calculation (Calculation #2): 280 μ g x 1 mg/1000 μ g = **0.28 mg pure caffeine in sample**

4. Calculate the mass in mg of pure caffeine if you had 1 fl. oz. of your sample. [Hint: 1 fl. oz. = 29.5735296 mL]

Since the volume of soft drink is 1 mL, the concentration is calculated by dividing the mass by 1 mL volume.

Using answer from previous calculation (Calculation #3): 0.28 mg/mL x 29.5735296 mL/fl. oz. = **8.28 mg pure caffeine per fl. oz.**

5. Calculate the mass in mg of pure caffeine in a 12 fl. oz. can of your sample.

Using answer from previous calculation (Calculation #4): 0.100 mg/fl. oz x 12 fl. oz./can = **99.4 mg pure caffeine per 12 fl. oz. can**

6. Calculate percent error.

Percent error = (actual - expected) / expected x 100%

For example, if calculating percent error of Monster energy drink with 120 mg caffeine/can (assuming a can is 12 fl. oz.):

Using answer from previous calculation (Calculation #5): Percent error = (99.4 - 120 mg) / 120 mg x 100% = 17.2% error

Analysis and Conclusions:

1. Explain in terms of chemistry how density, molecular polarity, and solubility each played a role in this separation experiment.

Density: Density of 2-propanol: 0.785 g/mL at 25°C

Density of water: 1.000 g/mL at 25°C

Isopropanol is less dense than water, so it floats on top. So in the separation process, that is why the top later is extracted.

Molecular Polarity: Sodium carbonate makes sugars and other compounds more soluble in water by making the pH more basic and attracting the water molecules more tightly to itself. Sodium carbonate is an ionic compound, so when it is mixed with water, it separates into ions. The cations and the anions attract to the water very strongly because opposite charges attract. Since caffeine is not as strongly charged as the ionic compound, it does not attract with the water well, so the caffeine migrates to the isopropanol.

Solubility: Caffeine is more soluble in isopropanol than in water because of the molecular polarity explanation above.

2. If you had the opportunity to do this experiment again, how would you change the procedure or your methods to reduce error? Explain why.

Accept reasonable answers. Possible answers include:

- Use a greater volume of reagents to reduce error, like using 10 mL of soft drink instead of 1 mL. Same proportions, just scale larger.
- Try to remove more of the isopropanol layer. Maybe not all of the isopropanol layer was removed. Maybe some of the caffeine was left there.
- Wash with rubbing alcohol more times to collect as much pure caffeine as possible.

3. Research GC-MS. Why is GC-MS a useful tool for distinguishing between pure caffeine and deuterated caffeine in the same sample, like in your experiment?

GC-MS separates compounds by mass over charge. Pure caffeine and deuterated caffeine are structurally similar, but their molar masses are slightly different at 194 and 197, respectively. Similar structures allow for similar chemical behaviors, but the difference in molar masses allow them to be distinguished by GC-MS.