

CHEM101 Report for Laboratory Exercise #6

Extraction of caffeine from Tea ¹

Using Microsoft Word, students are to **insert responses in all yellow highlighted areas**. It is recommended that the report be completed without changing font size, column width, row width, margins, and highlights. The completed report must be uploaded to the CHEM 101 lab Brightspace site as a .pdf file by the due date posted on Brightspace. All answers must be the student's own work without assistance from others. Only reports which are completed using the template will be marked.

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Abstract (max. 3 lines. See page 11 of the lab manual on how to write the abstract)

This experiment focused on the extraction of caffeine from tea leaves using liquid-liquid extraction with isopropanol, followed by precipitation with ethanol ^[1]. The obtained caffeine yield was 1.7%, and based on LD50 data for rats, an average 700g rat would need to consume approximately 2 tea bags ^[2] to reach a lethal dose.

Data / Results

Table 1. Experimental data and calculated values

Extraction and isolation of caffeine from green tea	
Mass of tea ² leaves (g)	3.012
Mass of caffeine (g)	0.052
%Mass caffeine in tea	1.7%
Lethal dose 50 for a 700 g rat (g)	0.1
Number of cups of tea lethal dose for a 700 g rat	2

Algebraic Equations

%Mass of caffeine in tea = $[(\text{mass of tea leaves}) / (\text{mass of caffeine})] * 100\%$

LD50 for a 700 g rat = $0.7 \text{ kg} \times 0.192 \text{ g/kg} = 0.1344 \text{ g} \cong 0.1 \text{ g}$ (1 significant number)

Number of cups = $0.1 \text{ g} / 0.052 \text{ g} = 1.923 \cong 2$ (1 significant number)

Discussion Respond to the following:

1) What are the organic functions found in the caffeine molecule? (max. 5 lines)

The caffeine molecule contains several key organic functional groups: amide, amine, and alkene. Specifically, it has two cyclic amide structures (carbonyl groups adjacent to nitrogen atoms), two tertiary amines (nitrogen atoms bonded to three carbon atoms), one alkene group (carbon-carbon double bond), and three methyl (CH₃) substituents. These functional groups contribute to the molecule's biochemical activity and solubility properties.

2) *Considering the chemical characteristics of the three solvents used, briefly discuss, using chemistry concepts learned in CHEM 101 lecture, the pathway that caffeine followed from the tea leaves to the crystals generated. (max. 6 lines)*

The pathway followed from the tea leaves to the crystals generated is as follows: caffeine initially dissolves in hot water due to its polar nature. Adding NaCl increases ionic strength, helping separate caffeine from other compounds. The tea solution is filtered, and isopropanol, a moderately polar solvent, extracts caffeine from the aqueous phase. Caffeine dissolves in the isopropanol layer, which is separated. Ethanol, a polar solvent, is added to precipitate caffeine due to solubility differences. Vacuum filtration then isolates the caffeine crystals.

3) *It is advertised that one bag of tea brewed in 250 mL of water for 3 – 5 minutes would release about 34 mg of caffeine. Based on your results, discuss one shortcoming of this experiment, not a personal error, that could contribute to an inaccurate weight of caffeine extracted than the advertised. (max 3 lines).*

One shortcoming of this experiment is the potential degradation of caffeine due to prolonged boiling, which can result in a lower yield than advertised. Additionally, losses during transfer and filtration steps can reduce the final weight of caffeine extracted.

4) *The lethal dose of caffeine with 50% kill for rats (LD50) is approximately 0.192g/kg. Assuming the lethal dose scales with body weight, what is the equivalent lethal dose 50% (LD50) of caffeine for an average adult human weighing 70 kg?*

Given that, LD50 for rats is 0.192 g/kg and the body weight of an average adult human is 70 kg. $LD50 \text{ (human)} = LD50 \text{ (rat)} \times \text{body weight (human)} = 0.192 \text{ g/kg} \times 70 \text{ kg} = 13.4 \text{ g} \cong 13 \text{ g}$ (2 significant numbers). So, the equivalent lethal dose 50% (LD50) of caffeine for an average adult human weighing 70 kg is 13 grams.

5) *Based on your results, how many cups of tea would an average human weighing 70 kg need to drink to consume a lethal dose?*

Given that, LD50 for an average adult human weighing 70 kg is 13 grams. One cup of tea releases about 0.058 g of caffeine. So, $\text{number of cups} = LD50 \text{ (humans)} / (\text{caffeine per cup}) = (13 \text{ g} / 0.058 \text{ g}) = 224.5 \text{ cups} \cong 220 \text{ cups}$ (2 significant numbers).

Conclusions (max. 3 lines)

The experiment successfully extracted caffeine from tea leaves, yielding a 1.7% mass of caffeine. The process involved liquid-liquid extraction and precipitation techniques. Despite potential caffeine degradation and losses during transfer and filtration, the experiment demonstrated the practical application of solvent extraction methods in isolating bioactive compounds from natural products.

References

1. Reimer, M. et al, Laboratory Manual, Chemistry 101, pp. 39-40. (University of Victoria: Victoria, B.C.) **Summer 2024**
2. Red Rose® Orange Pekoe Tea. Unilever Canada Inc, Toronto, Ontario, M4W 3R2, Canada, Drug Identification Number: 6840044376.

Feedback Summary	max.
Pre-lab quiz: Are all responses correct?	4
Laboratory Notebook: Have ALL data, observations, and procedures been recorded?	1
Report (results and assessment): Are all sections completed accurately? Is the abstract accurate and complete? Are responses in the Discussion, correct? Does the conclusion only include the appropriate information? Are the References correctly formatted and cited?	3
Participation: Did the student come prepared, was the time used well in the lab and was the student engaged in the experiment? Did the student show the email confirmation letter and request the TA to check their drawers for completeness before they left the lab?	1
Performance evaluation: Did the student follow the safe practice guidelines throughout the whole lab period?	1
Total mark	10