Determination of Sodium in Tonic Water by Flame Atomic Absorbance (DSF)

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CHEM438 - 021L

I submit this laboratory report as an original document. I assert that all ideas and discussion of data contained herein are my own work, unless otherwise referenced.

ABSTRACT

A standard addition curve was obtained by collecting 5 unknown plus spike solutions absorbance data. The fitted linear trendline has a slope of (4.73 ± 0.26) x 10^{-3} μM^{-1}, y-intercept of (1.019 ± 0.002) x 10^{-1}, and R^2-value of 0.991. Within 95% confidence interval, the final concentration of sodium in the diluted tonic water sample was found to be 21.54 ± 4.81 μM (95% C.I., n = 5). Taking into account all dilutions process made for the purpose of collecting absorbance data, the original concentration of sodium from the tonic water bottle was 0.0431 ± 0.0002 M (95% C.I., n = 5). The calculated concentration was greater by a magnitude of molarity from the labelled concentration of 0.0063 M. This might be due to the error in dilution or when collecting the absorbance data.

INTRODUCTION

Tonic water contains a variety of ingredients, and mainly is quinine. It also contains a preservative sodium benzoate, which also acts as the antibacterial agent.[1] Sodium is a part of daily human diet and tonic water helps to regulate the concentration of sodium in the body. The sodium concentration in tonic water can be determined by using atomic absorbance spectroscopy. Specifically, flame atomic absorbance spectrometry (FAAS) will be used as it is best to detect a single element of interest at a time and sample solution concentration in the range of ppm concentration units with a few number of samples.[2]

Generally, in a sample solution, the sample matrix contains everything other than just the analyte of interest to be measured. Due to this, a simple calibration curve could not be utilized to determine the concentration of analyte in the sample due to the matrix effect. The method of standard addition is usually used as it employs the idea of spiking the sample with a small volume of known concentration standard solution without actually changing the composition of the sample matrix significantly. This method ensures high efficiency of atomization by the FAAS as it is heavily dependent on the sample matrix. Precision and accuracy of the analysis will be impacted as the presence of other ingredients in the sample reduces the probability of the analyte atoms to be atomized and absorbed in the FAAS.

PROCEDURE [3]

Three different concentrations of the stock solutions (NaCl solution) were prepared to obtain spike solutions for standard addition calibration. Firstly, 1 mL of 0.1 M NaCl solution was diluted in a 100-mL volumetric flask, resulting in 0.001 M of stock solution. 25 mL of 0.001 M NaCl solution was then diluted again in a 100-mL volumetric flask to obtain 0.00025 M solution. Lastly, 2-fold dilution was performed by diluting 25 mL of 0.00025 M solution in a 50-mL volumetric flask, resulting in 0.000125 M of solution.

5 sample solutions were prepared by adding 1 mL of 40-fold diluted tonic water, which was the unknown, into 50-mL volumetric flasks each. 5 varying volumes of the spike solutions, with varying concentrations were added next (0 mL of spike, 2 mL of 0.00025 M of spike, and 1, 2, and 3 mL of 0.000125 M of spike) and labelled properly. Each sample was diluted up to the neck of the flask with distilled water.

The absorbance data for each sample was collected by using the flame atomic absorbance spectrometry. For each sample, the absorbance blank was collected first before measuring the sample solutions. Three absorbance values were recorded and averaged for each sample. The absorbance data was limited up to 0.5, hence trial and error of spike and unknown solution volume added into each sample was done beforehand. The finalized volumes of unknown and spikes were as previously stated. All chemicals were disposed of appropriately and glasswares were cleaned and restored to their original place.

RESULTS AND DISCUSSION

Table 1. Absorbance data of 5 sample solutions with spike solutions added.

Sample	[a] $V_{standard}$ (mL)	[b] $[S]_i$ (M)	[c] $[S]_f$ (μM)	Absorbance, A			
				1	2	3	Average
1	0.00	0.00×10^{-0}	0.00	0.102	0.106	0.102	0.103
2	2.00	2.50×10^{-4}	10.00	0.153	0.148	0.148	0.150
3	1.00	1.25×10^{-4}	2.50	0.112	0.111	0.110	0.111
4	2.00	1.25×10^{-4}	5.00	0.129	0.124	0.129	0.127
5	3.00	1.25×10^{-4}	7.50	0.137	0.137	0.136	0.137

[a] Volume of standard added
[b] Initial concentration of standard solution added
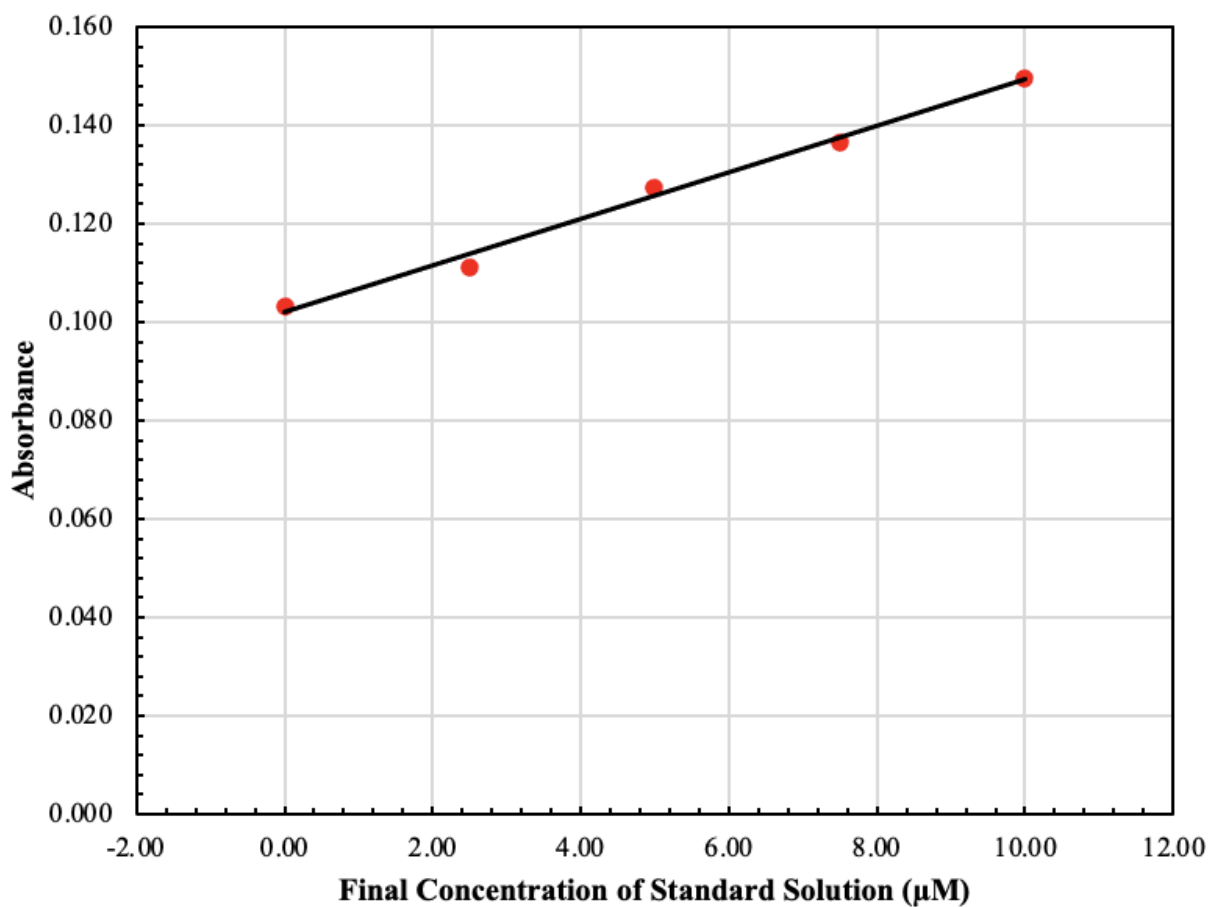[c] Final concentration of standard solution

Figure 1. Standard addition curve for tonic water samples.

The absorbance data against the final concentration of standard solution tabulated in **Table 1** was plotted as shown in **Figure 1**. A linear trendline was fitted against the 5 sample data points and obtained the linear equation as in **Eq. 1**.

$$A = (4.73 \pm 0.27) \times 10^{-3} \mu M^{-1} [S]_f + (1.019 \pm 0.002) \times 10^{-1}$$ **Eq. 1**

The trendline obtained was almost perfectly linear with an R^2-value of 0.991. From **Eq. 1**, the x-intercept of the linear trendline could be determined. The x-intercept reflected the concentration of the sample diluted in the final sample. As the volume of unknown added into each sample was constant, the concentration could be determined easily.

The x-intercept was found to be -21.54 $\pm$ 1.51 µM. Taking the absolute value of the x-intercept and by using 95% confidence interval to estimate the error, the final concentration of sodium in the diluted tonic water sample was 21.54 $\pm$ 4.81 µM (95% C.I., n = 5).

From a dilution of 1-mL sample in a 50-mL volumetric flask, the provided tonic water sample in the lab has a sodium concentration of 0.0011 $\pm$ 0.0002 M (95% C.I., n = 5). Since the provided sample in the lab was diluted 40-fold at the beginning of the lab, the original concentration of sodium from the tonic water bottle was 0.0431 $\pm$ 0.0002 M (95% C.I., n = 5).

The label on the tonic water bottle included a sodium concentration of 0.0063 M. The calculated sodium concentration was greater by a magnitude of molarity. This could be due to the inaccuracy and imprecision when preparing the diluted stock solutions from the provided 0.1 M NaCl solution. It could also be due to the mixing of solutions on the tiny tubing used on the FAAS as it was not cleaned properly each time. Thus, the absorbance readings would not reflect the actual concentration in the sample.

CONCLUSIONS

       Standard calibration curve could not be used to determine the concentration of unknown in a sample due to interfering matrix effect. It will provide inaccurate reflection of the actual concentration of the analyte of interest. Standard addition method is the best approach as the added spike solution does not change the composition of the original matrix significantly. The additional absorbance signal from the added spike is comparable to the matrix alone, thus will be used to determine the concentration associated with the signal collected. Flame atomic absorbance spectrometry was used to determine the concentration of sodium in the sample due to the high accuracy in signal detection for a few samples and detecting a single element at a time. The calculated concentration of sodium in the tonic water from the x-intercept value of the standard addition curve, after taking into account all dilutions made, was a magnitude greater than the concentration indicated on the product's label. This was suspected to be associated with the inaccuracy of preparing diluted stock solutions and improper method of collecting absorbance data.

REFERENCES

[1] Quinine in Tonic Water: Safety, side effects, and possible benefits. https://www.medicalnewstoday.com/articles/323692#_noHeaderPrefixedContent (accessed Oct 8, 2021).

[2] Atomic Spectroscopy: A Guide to Selecting the Appropriate Technique and System.

[3] Cruz, F. *CHEM438 Instrumental Methods Laboratory - Determination of Sodium in Tonic Water by Flame Atomic Absorbance lab*; University of Delaware: Newark, Delaware, 2018; pp 1-3.

APPENDICES

Lab Notebook

Exp. No. 3	Experiment/Subject CHEM 438 (DSP)		Date 9/27/2021	
Name Abdul Fayeed	Lab Partner Thanh, Nguyen		Locker/Desk No.	Course & Section No. 021L

PRE-LAB Questions

1.
$$\frac{35\,mg\ Na}{serving} \times \frac{1\,serving}{240\,mL} \times \frac{1000\,mL}{1L} \times \frac{1g}{1000\,mg} \times \frac{1\,mol}{22.99\,g\,Na} = 6.343 \times 10^{-3}\,M$$

2. Corrected absorbance $= 0.230 - 0.008 = 0.222$

$$A = \varepsilon b c$$

$$0.222 = \varepsilon\,(10\,cm)(2.5 \times 10^{-4}\,M)$$

$$\varepsilon = 88.8\ M^{-1}\,cm^{-1}$$

$$A = 88.8\ M^{-1}\,cm^{-1}\,(10\,cm)(6.343 \times 10^{-3}\,M)$$

$$A = 5.633$$

can be wrong, but at least less than 0.5
⇒ Record the instruments used!

3.

Sample	Conc. Of Standard (M)	V_{tonic} (mL)	$V_{standard}$ (mL)	Expected Absorbance
1	0.00100	5.00	0.00	0.0000
2	0.00100	5.00	4.00	0.1421
3	0.00025	5.00	1.00	0.0089
4	0.00025	5.00	2.00	0.0178
5	0.00025	5.00	3.00	0.0266

4.
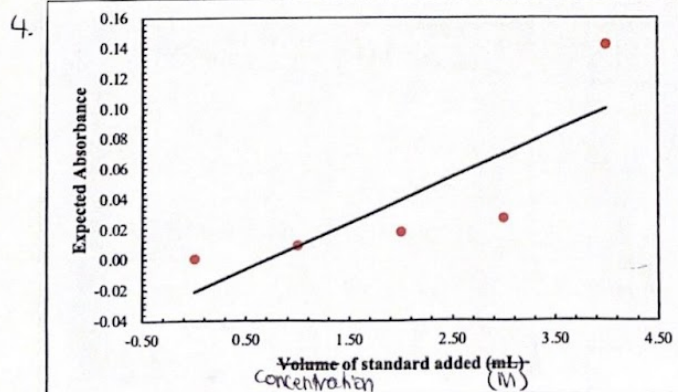
⇒ the x-intercept of the calibration line will indicate the concentration of diluted tonic water solution!

Signature	Date 9/27/2021	Witness/TA		Date

THE HAYDEN-McNEIL STUDENT LAB NOTEBOOK

Note: Insert Divider Under Copy Sheet Before Writing

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Exp. No. 3	Experiment/Subject CHEM 438 (DSF)	Date 9/27/2021	
Name Abdul Fayeed	Lab Partner Thanh, Nguyen	Locker/ Desk No.	Course & Section No. 021 L

Objective

The purpose of this lab is to determine the concentration of sodium in tonic water, by using the standard addition method.

Introduction

Flame atomic absorbance is one of the instruments that can be used to determine the concentration of sodium in tonic water. Standard addition method is used due to the complicated matrix effect from the sample, which will interfere with the results if normal calibration method is used.
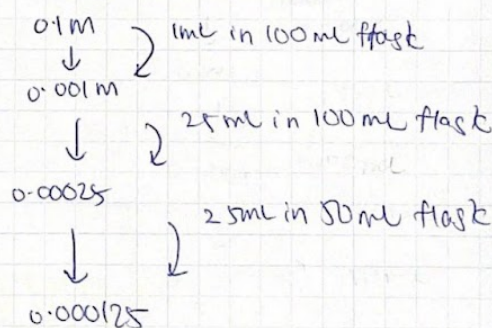
Procedure

1. Prepare 5 sample of varying volume of standard added and a fixed volume of tonic water.

2. Refer to table on page 13 for the specific volume.

3. Dilute the NaCl stock solution given by 100 and 400 -fold.

4. Record the instrument used to measure the volume.

5. Read the manual on the software on how to use it correctly.

6. Regularly zero the instrument prior to absorbance measurement.

7. Repeat at least 3 times when obtaining the absorbance data.

8. Dispose off the Chemicals and clean the glassware. *appropriately.*

Sample	V_{tonic} (mL)	$V_{standard}$ (mL)	Dilution
1	1 mL	0	50mL
2	1	1 (0.00025 M)	50mL
3	1	2 (0.00025 M)	50mL
4	1	1 (0.000125M)	50mL
5	1	2 (0.000125m)	50mL
	1	3 (0.000125m)	50mL

Sample	Abs 1	Abs 2	Abs 3
1	0.1020.106	0.106	0.102
2	0.145	0.145	0.144
3	0.153	0.148	0.148
4	0.112	0.111	0.110
5	0.129	0.124	0.129
6	0.137	0.137	0.136

Sam

stock solution dilution

0.1 M   } 1 mL in 100 mL flask
↓
0.001 m
↓   } 25 mL in 100 mL flask
0.00025
↓   } 25 mL in 50 mL flask
0.000125

Conclusions

Flame atomic absorbance can be used to determine the sodium concentration in tonic water. Standard addition method is used due to the matrix effect of the sample solutions.

Signature	Date 9/27/2021	Witness/TA	Date

THE HAYDEN-McNEIL STUDENT LAB NOTEBOOK   Note: Insert Divider Under Copy Sheet Before Writing