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Section: 01

TA: Supriya

Ion Chromatography – Cations in Seawater

	GRADING	Max	Points
1	Abstract		
2	Table with names and contribution of each of your partners		
3	Table summarizing important instrumental parameters such as flow rate, approximate pump pressure, eluent with instrumental set-up		
4	Calibration factor for pipet		
5	Table presenting retention times and instrumental sensitivity for single cation with ordered list of sensitivity for different cations		
6	Calibration curves from cations		
7	Table presenting best fit of the calibration curves		
8	Chromatogram of sea-water sample		
9	Calculation of the concentration of each identified cation in seawater		
10	Chromatogram of Unknown, No. 2		
11	Calculation of the concentration of cations in Unknown No, 2		
12	Table of comparison with complexometric analysis		
13	Comparison with LEO-15		
14	Answer to questions		

Abstract:

From the lab, the concentration of Sodium was 10066.5 ppm and 10.069 ppt. The Calcium concentration was 374.8 ppm and 374.6 ppt. For Magnesium it was 1666ppm and 1.6663 ppt.

Introduction:

This lab looks at the concentrations of each cation within seawater. With these cations, Sodium, Calcium, and Magnesium, they can determine the hardness of the water. To create softer water, water softener is used which replaces the Magnesium, Calcium and Iron cations within the water with more Sodium cations. This creates water that is able to be used within households. Having hard water is not bad per se, but can create a lot of nuisances within the mechanical aspects of the household. Clogging the pipes due to high mineral content is one thing that can be avoided.

Experimental Methods:

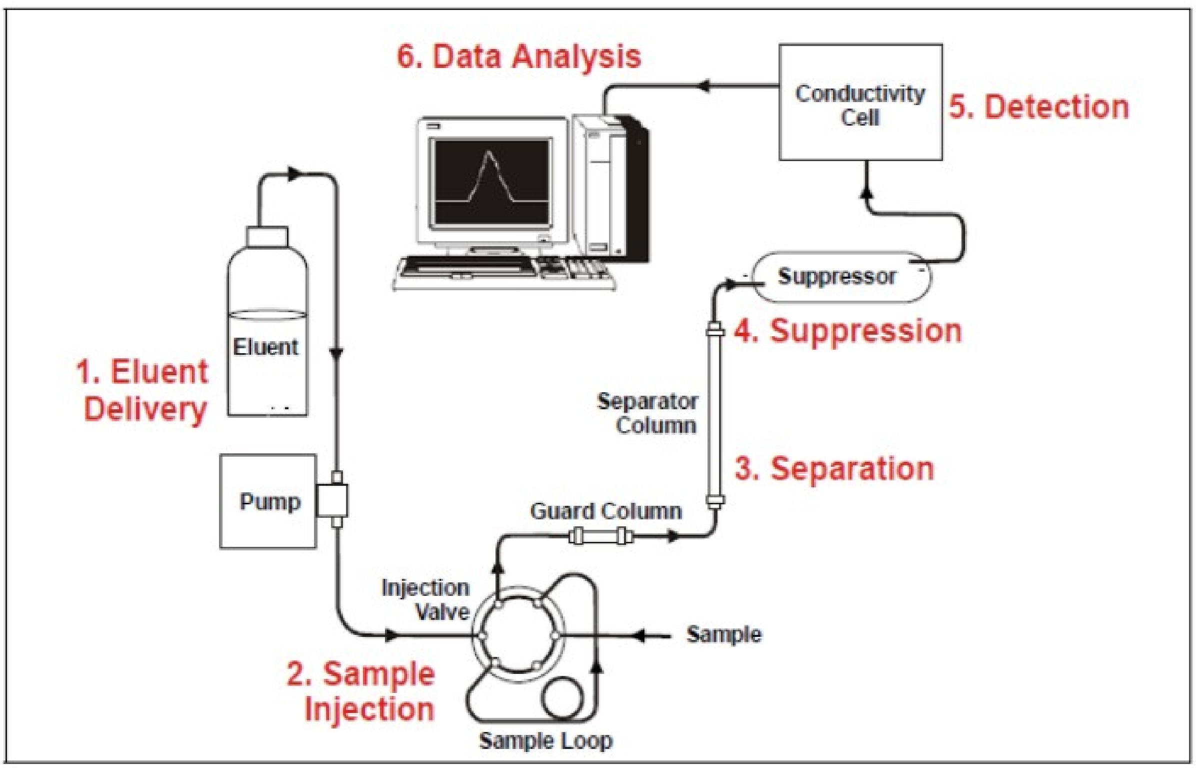

Table I: Various numerical components of Schroeder 2 Machine:

Flow Rate	1.00 microL/min
Pump Pressure	~1111PSI
Eluent	MSA
GroupMates	
Tim	Solution Dilution

1 https://marine.rutgers.edu/nurp/leo-15.html

Leah	Solution Dilution
Tara	Solution Dilution

Table I contains numerical values for machine flow rate, pump pressure, and the eluent as well as group members and their tasks.

Results and Discussion:

Table II: Raw Collected Data

CaCO3 mass:	.9984g
MgCl2 * 6H2O mass:	1.6726g
NaCl mass:	.6357g
Pipette Calibration:	4.9995mL per 5mL
CCPS Prepared Solution	
CaCO3 mass:	.9988g
MgCl2 * 6H2O mass:	1.6734g
NaCl mass:	.6356g

Table II contains the data for the stock room solutions that were prepared and the pipette calibration.

Table III: Prepared Standards' Calculated Data

	Area (microS*min)	Concentration (ppm)	Sensitivity (microS*min/ppm)	Retention Time (min)
Sodium	113.00604	250.0811	.45188	3.973
Calcium	199.367	399.79	.4987	6.743
Magnesium	147.6156	200.700	.7355	5.787

Table III includes the area, concentration, sensitivity and retention times with the sensitivities increasing from top to bottom.

Calculations:

Sodium: Area: 403.593 microS * .280min = 113.00604 microS*min

Concentration: .6357g x 1mol NaCl / 58.44g NaCl x 1 mol Na+ / 1 mol NaCl x 22.99g Na+ x 1000mg / 1g = 250.0811 ppm

Sensitivity: 113.00604 / 250.0811 = .45188 microS*min/ppm

Calcium: Area: 295.358 microS * .675min = 199.367 microS*min

Concentration: .9984g x 1mol CaCO3 / 100.0869g x 1mol Ca2+ / 1mol CaCO3 x 40.078g Ca2+ x 1000mg / 1g = 399.79 ppm

Sensitivity: 199.367 / 399.79 = .4987 microS*min/ppm

Magnesium: Area: 292.888 microS * .504min = 147.6156 microS*min

Concentration: 1.6762g x 1mol MgCl2*6H2O / 203g x 1mol Mg2+ / 1mol MgCl2*6H2O x 24.305g Mg2+ x 1000mg / 1g = 200.700 ppm

1 https://marine.rutgers.edu/nurp/leo-15.html

Sensitivity: 147.6156 / 200.700= .7355 microS*min/ppm

Table IV: CCPS, Unknown and Seawater Samples

Sodium	Concentration (ppm)	Height(µS)	Width(min)	Area (µS*min)	Retention Time (min)
CCPS 2mL	5.00084	9.297	0.248	2.3056	3.883
CCPS 4mL	10.00168	18.293	0.249	4.555	3.887
CCPS 6mL	15.00252	27.253	0.248	6.754	3.887
Calcium	Concentration (ppm)	Height(µS)	Width(min)	Area (µS*min)	Retention Time (min)
CCPS 2mL	7.999	7.336	0.576	4.226	7.317
CCPS 4mL	15.998	14.706	0.568	8.353	7.287
CCPS 6mL	23.997	21.907	0.564	12.356	7.253
Magnesium	Concentration (ppm)	Height(µS)	Width(min)	Area (µS*min)	Retention Time (min)
CCPS 2mL	4.007	7.637	0.474	3.62	6.007
CCPS 4mL	8.014	10.05	0.468	4.7034	6.003
CCPS 6mL	12.021	15.06	0.461	6.943	5.99
Unknown Sample 2	Concentration (ppm)	Height(µS)	Width(min)	Area (µS*min)	Retention Time (min)
Sodium	16.672	30.418	0.248	7.544	3.887
Calcium	16.32	15.012	0.563	8.452	7.283
Magnesium	7.944	10.157	0.472	4.794	6
Seawater	Concentration (ppm)	Height(µS)	Width(min)	Area (µS*min)	Retention Time (min)
Sodium	10066.5	181.48	0.251	45.551	3.92
Calcium	374.8	3.364	0.577	1.941	7.333
Magnesium	1666	21.621	0.465	10.054	5.983

This table includes the concentrations in ppm, height in microSiemens, width in minutes, the area calculated and the retention times of each ion within the respective solutions.

Table V: Best fit

Sodium	Y = .4525x
Calcium	Y = .5179x
Magnesium	Y = .6035x

This table includes the best fit lines for each ion.

Calculations:

Pipette Calibration:

4.9995mL / 5mL = .9998 calibrated factor

1 https://marine.rutgers.edu/nurp/leo-15.html

CCPS Calibrations:

NaCl: .6356g NaCl x 1mol NaCl / 58.44g NaCl x 1mol Na+ / 1mol NaCl x 22.99g Na+ x 1000mg / 1g = 250.042ppm

2mL: 250.042 ppm x 2mL = 100mL x M = 5.00084 ppm

4mL: 250.042 ppm x 4mL = 100mL x M = 10.00168 ppm

6mL: 250.042ppm x 6mL = 100mL x M = 15.00252 ppm

4mL Area: 18.293 x .249 = 4.555 µS*min

6mL Area: 27.253 x .248 = 6.754 µS*min

CaCO3: .9988g x 1mol CaCO3 / 100.0869g x 1mol Ca2+ / 1mol CaCO3 x 40.078g Ca2+ x 1000mg / 1g = 399.95 ppm

2mL: 399.95 ppm x 2mL = 100mL x M = 7.999 ppm

4mL: 399.95 ppm x 4mL = 100mL x M = 15.998 ppm

6mL: 399.95 ppm x 6mL = 100mL x M = 23.997 ppm

2mL Area: 7.336 x .576 = 4.226 µS*min

4mL Area: 14.706 x .568 = 8.353 µS*min

6mL Area: 21.907 x .564 = 12.356 µS*min

MgCl2*6H2O: 1.6734g x 1mol MgCl2*6H2O / 203g x 1mol Mg2+ / 1mol MgCl2*6H2O x 24.305g Mg2+ x 1000mg / 1g = 200.35 ppm

2mL: 200.35 ppm x 2mL = 100mL x M = 4.007 ppm

4mL: 200.35 ppm x 4mL = 100mL x M = 8.014 ppm

6mL: 200.35 ppm x 6mL = 100mL x M = 12.021 ppm

2mL Area: 7.637 x .474 = 3.620 µS*min

4mL Area: 10.05 x .468 = 4.7034 µS*min

6mL Area: 15.05 x .461 = 6.943 µS*min

Unknown Solution #2:

Na+: Area = 30.418 x .248 = 7.544 µS*min

Best fit: y=.4525x; x = concentration

7.544 / .4525 = 16.672 ppm

1 https://marine.rutgers.edu/nurp/leo-15.html

Ca^{2+}: Area = 15.012 x .563 = 8.452 µS*min

Best fit: y = .5179x; x = concentration

8.452 / .5179 = 16.320 ppm

Mg^{2+}: Area = 10.157 x .472 = 4.794 µS*min

Best fit: y = .6035x; x = concentration

4.794 / .6035 = 7.944 ppm

Seawater:

Na^+: Area = 181.48 x .251 = 45.551 µS*min

Concentration: 45.551 / .4525 = 100.665 ppm x 100 dilution factor = 10066.5 ppm

Concentration after correction: (10066.5 / .9998) = 10068.51 ppm / 1000 = 10.069 ppt

Ca^{2+}: Area = 3.364 x .577 = 1.941 µS*min

Concentration: 1.941 / .5179 = 3.748 ppm x 100 dilution factor = 374.8 ppm

Concentration after correction: 374.8 / .9998 = 374.57 ppm / 1000 = .3746 ppt

Mg^{2+}: Area = 21.621 x .465 = 10.054 µS*min

Concentration: 10.054 / .6035 = 16.660 ppm x 100 dilution factor = 1666 ppm

Concentration after correction: 1666 / .9998 = 1666.33 ppm / 1000 = 1.6663 ppt

Table VI: Complexometric and LEO-15 Comparison

Cation	Cation Chromatography	Complexometric	LEO-15
Sodium	10.069 ppt	N/A	10.560 ppt
Calcium	.3746 ppt	.348 ppt	.4 ppt
Magnesium	1.6663 ppt	1.144 ppt	1.272 ppt

This table compares the values of this lab to complexometric titration and the LEO-15.

Comparing the values from this lab to the complexometric lab, the Calcium values were about the same but the Magnesium values had a huge gap between 1.6663 ppt and 1.144 ppt. Comparing this lab to the LEO-15[1], the sodium value was about .5 ppt off from 10.069 ppt to 10.560 ppt. For Calcium, it was roughly on point between .3746 ppt and .4 ppt. For Magnesium, there was a gap again between 1.6663 ppt and 1.272 ppt. This error can be due to the machine or even the seawater from the location just having a high amount of Sodium and Magnesium concentrations.

1 https://marine.rutgers.edu/nurp/leo-15.html

Chromatograms and Graphs:

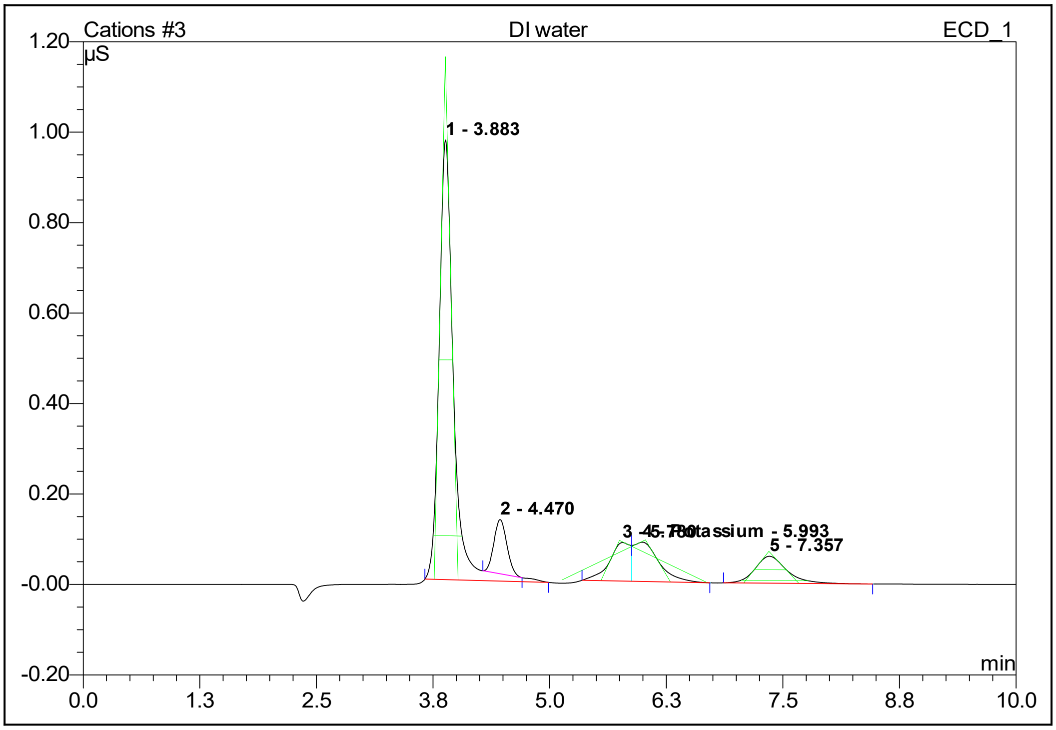

Figure 1. DI water run 1 Chromatogram

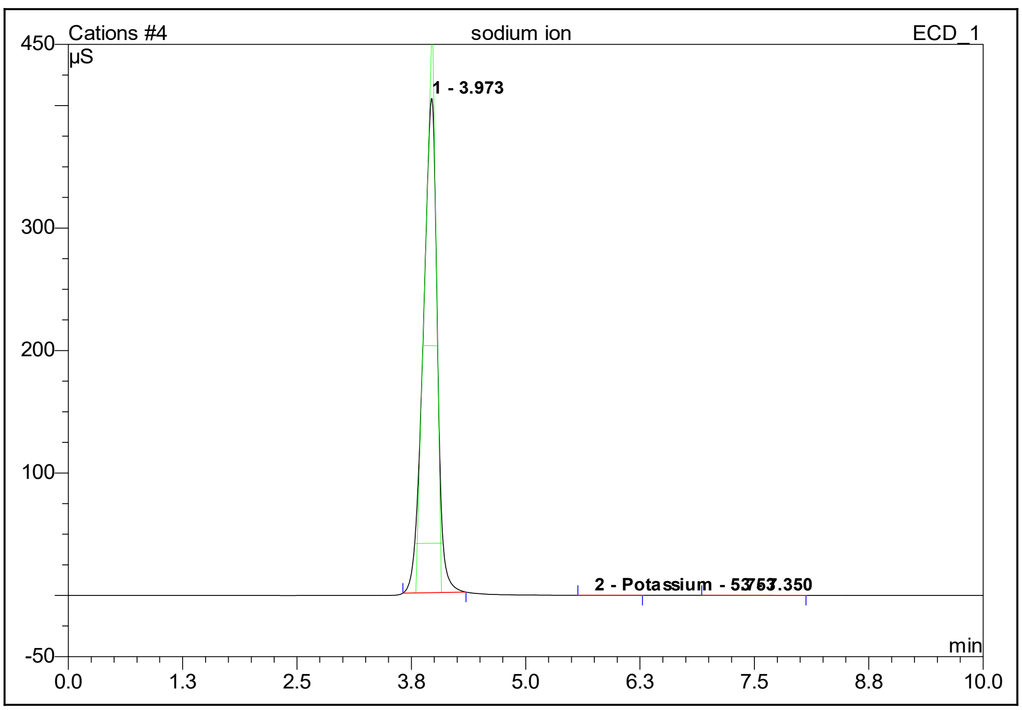

Figure 2. Sodium Chromatogram

1 https://marine.rutgers.edu/nurp/leo-15.html

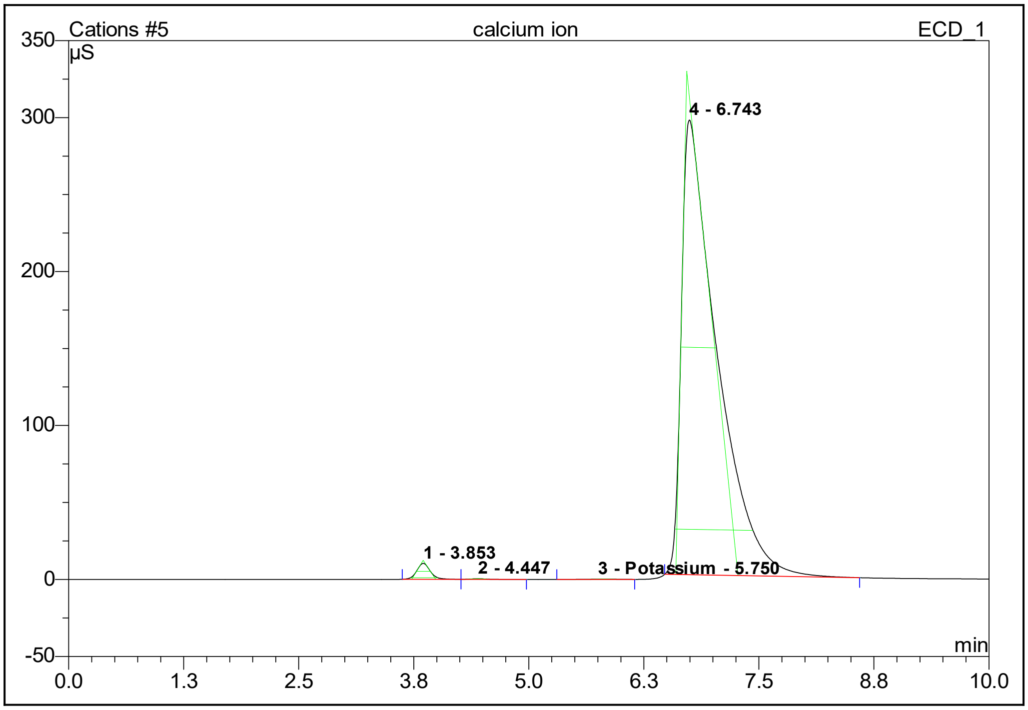

Figure 3. Calcium Chromatogram

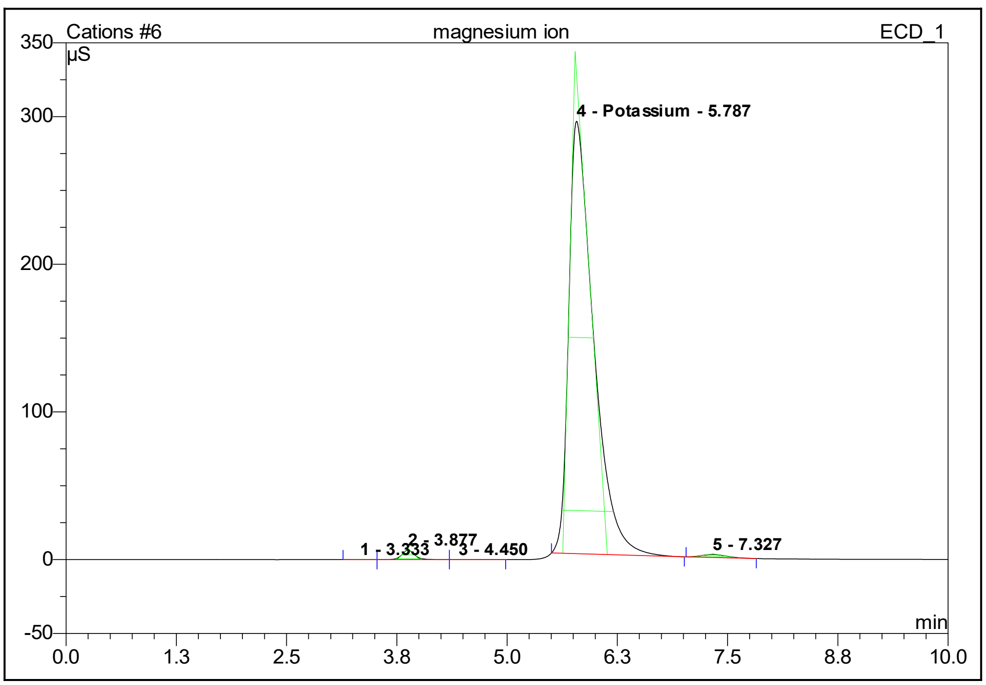

Figure 4. Magnesium Chromatogram

1 https://marine.rutgers.edu/nurp/leo-15.html

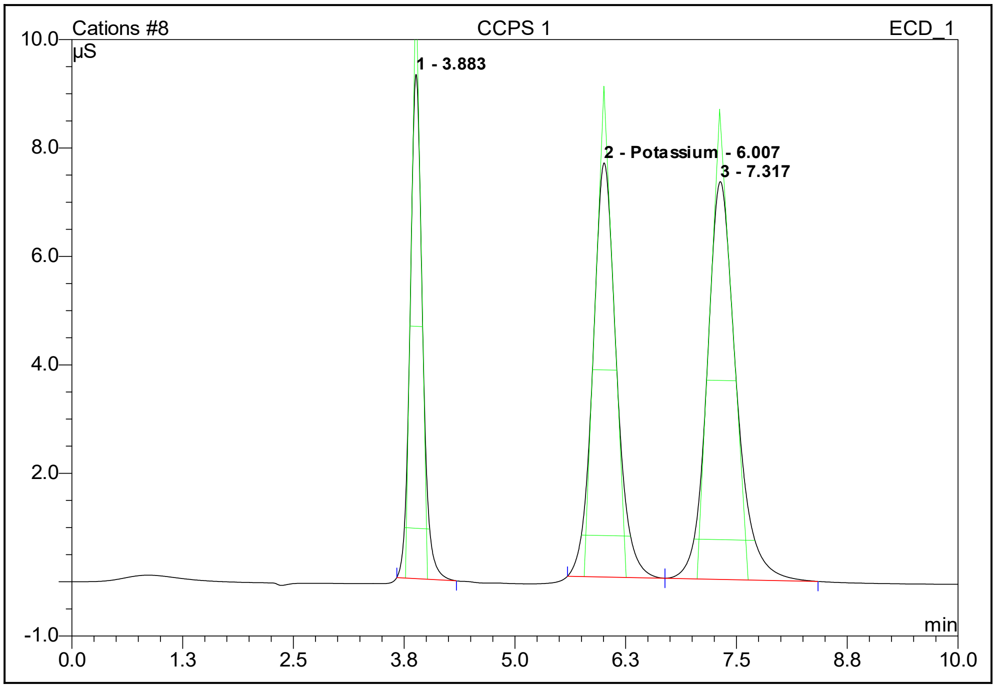

Figure 5. CCPS 2mL dilution Chromatogram

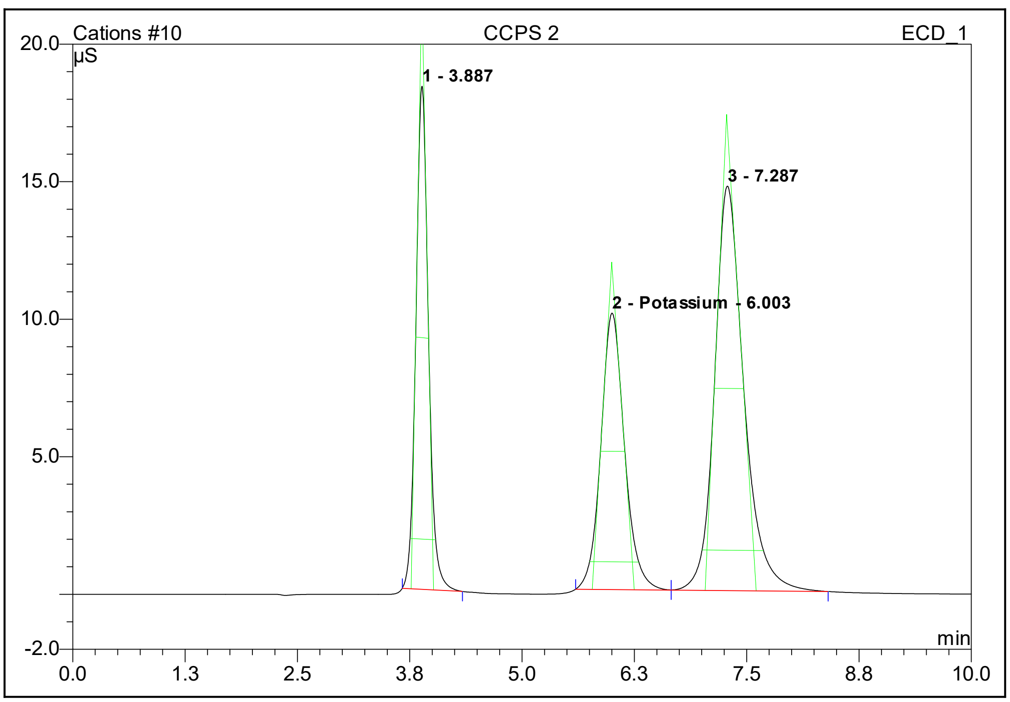

Figure 6. CCPS 4mL dilution Chromatogram

1 https://marine.rutgers.edu/nurp/leo-15.html

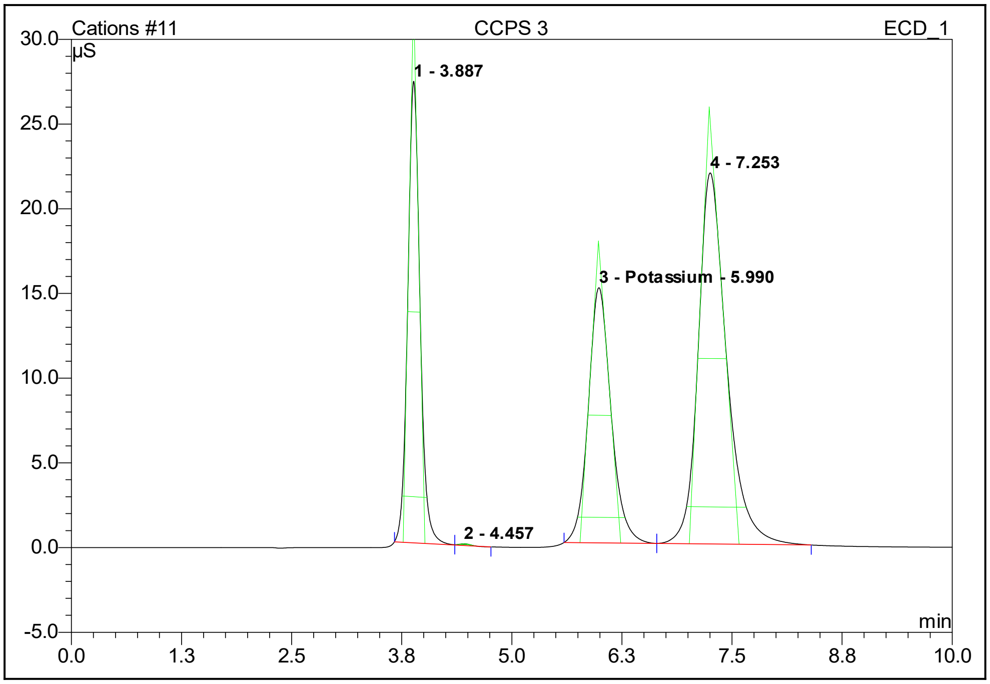

Figure 7. CCPS 6mL dilution Chromatogram

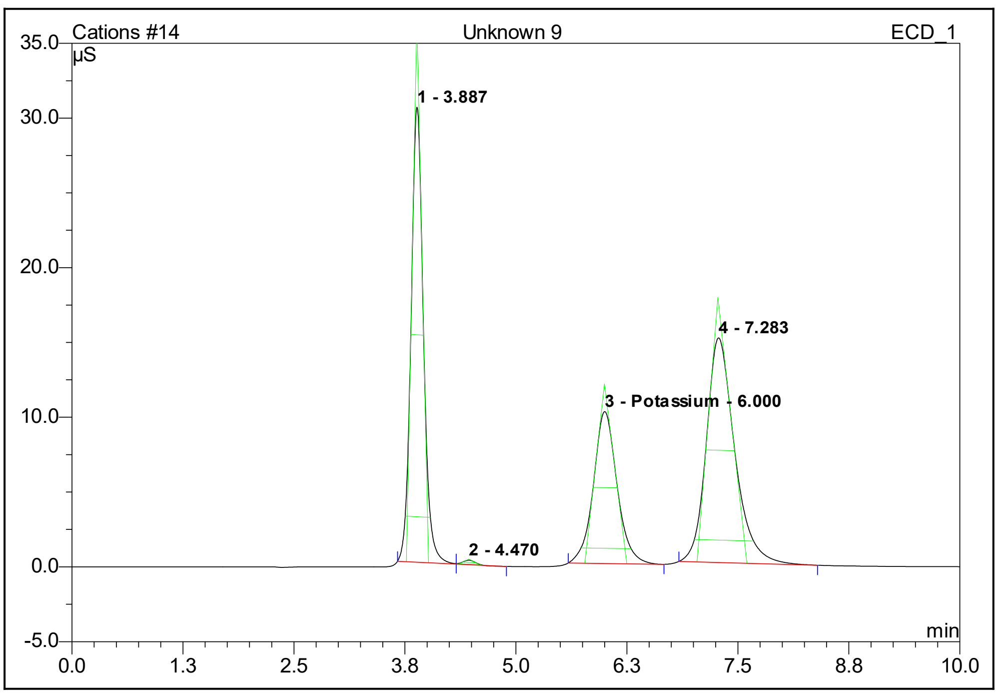

Figure 8. Unknown Solution 2 Chromatogram

1 https://marine.rutgers.edu/nurp/leo-15.html

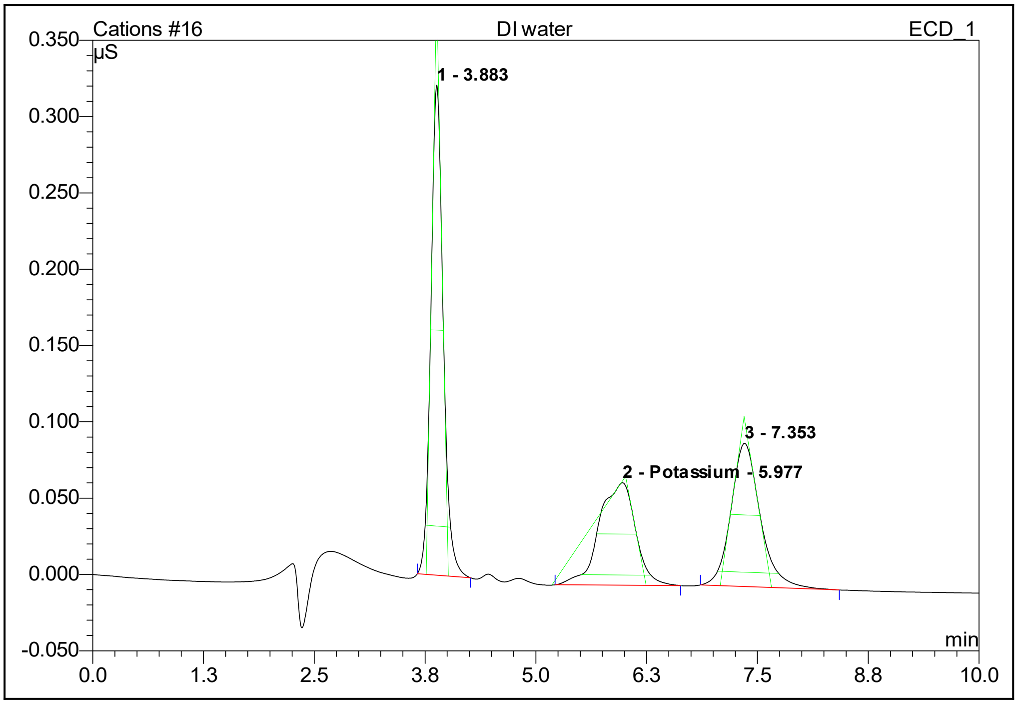

Figure 9. DI water Run 2 Chromatogram

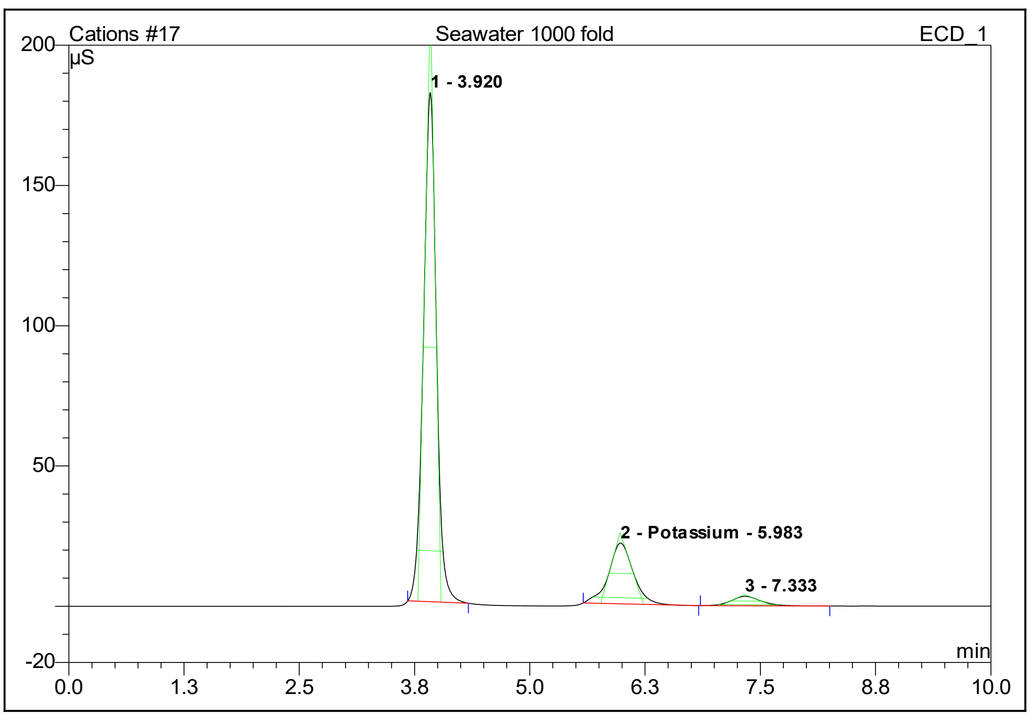

Figure 10. Seawater Chromatogram, first peak is sodium, second is magnesium, third is calcium

1 https://marine.rutgers.edu/nurp/leo-15.html

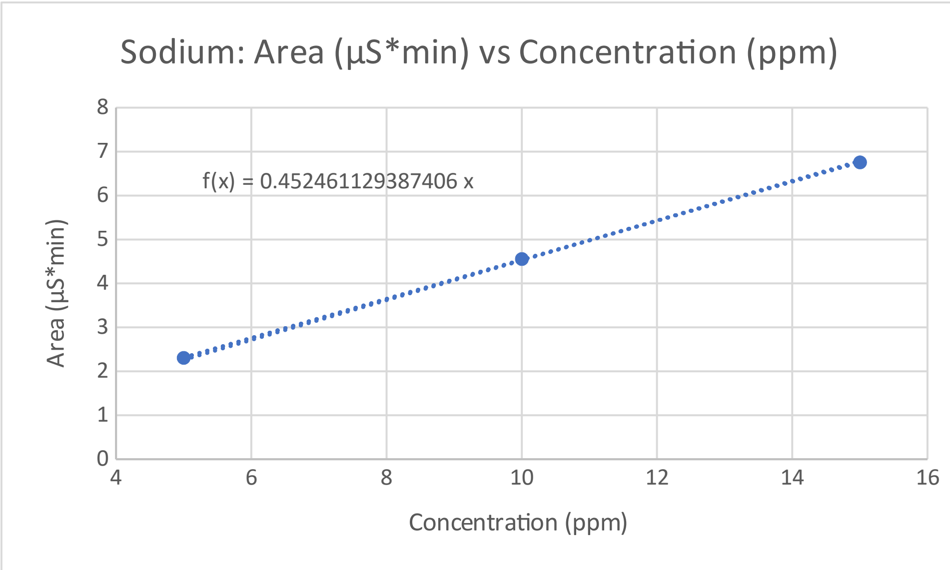

Figure 11. Sodium Calibration Curve

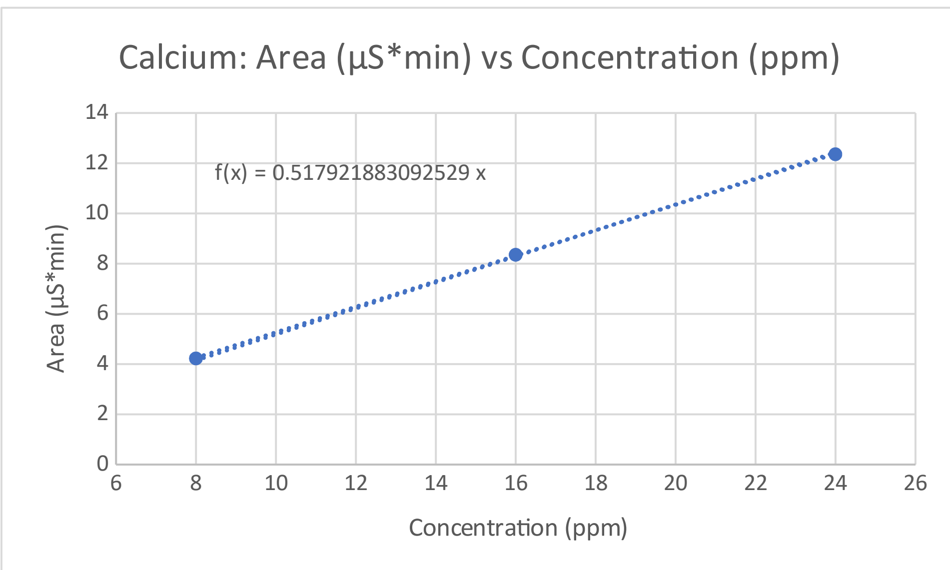

Figure 12. Calcium Calibration Curve

1 https://marine.rutgers.edu/nurp/leo-15.html

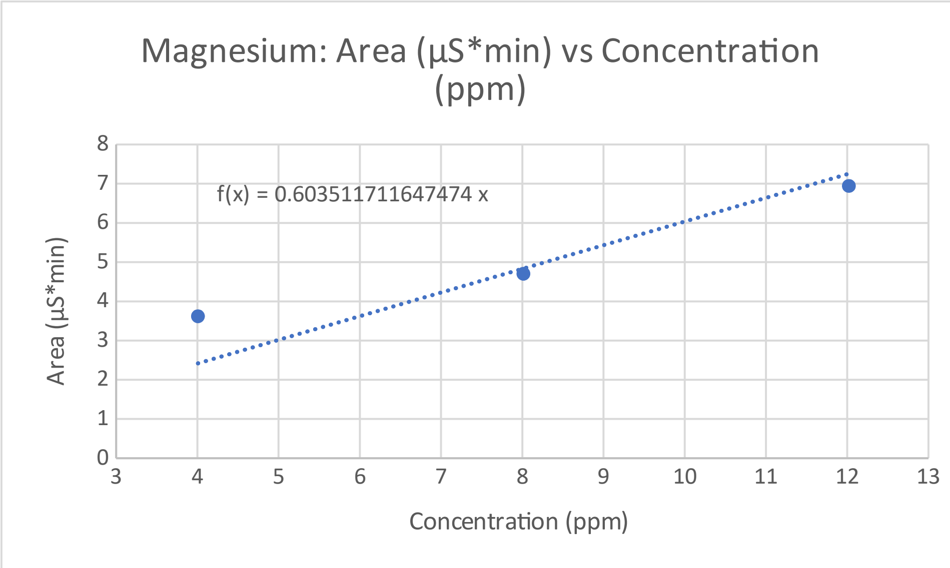

Figure 13. Magnesium Calibration Curves

Lab Questions:

1. To how many units on the syringe does 100 microliters correspond?
    a. 10 units, 10microL = 1 unit
2. Why is it good practice to run the most dilute sample first?
    a. Running the most dilute allows for the lessening of sticking to the machine when the solutions are pumped afterwards.
3. By what factor have you diluted the seawater? Is diluting 4mL of seawater to 100mL reasonable?
    a. It was diluted by a factor of 100x and diluting 4mL to 100mL is just a dilution factor of 25x.

1 https://marine.rutgers.edu/nurp/leo-15.html