Spectrophotometric Nitrate Measurement in Natural Waters

CONDESA Group 1

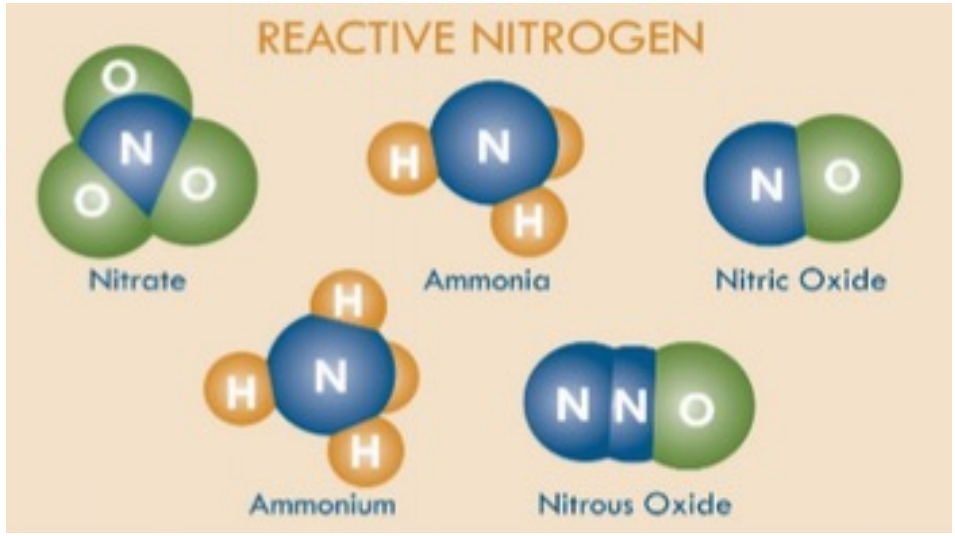
Shelby Defeo, Maria Perez Mendoza, Sam Erickson, Arya Karappilly Rajan

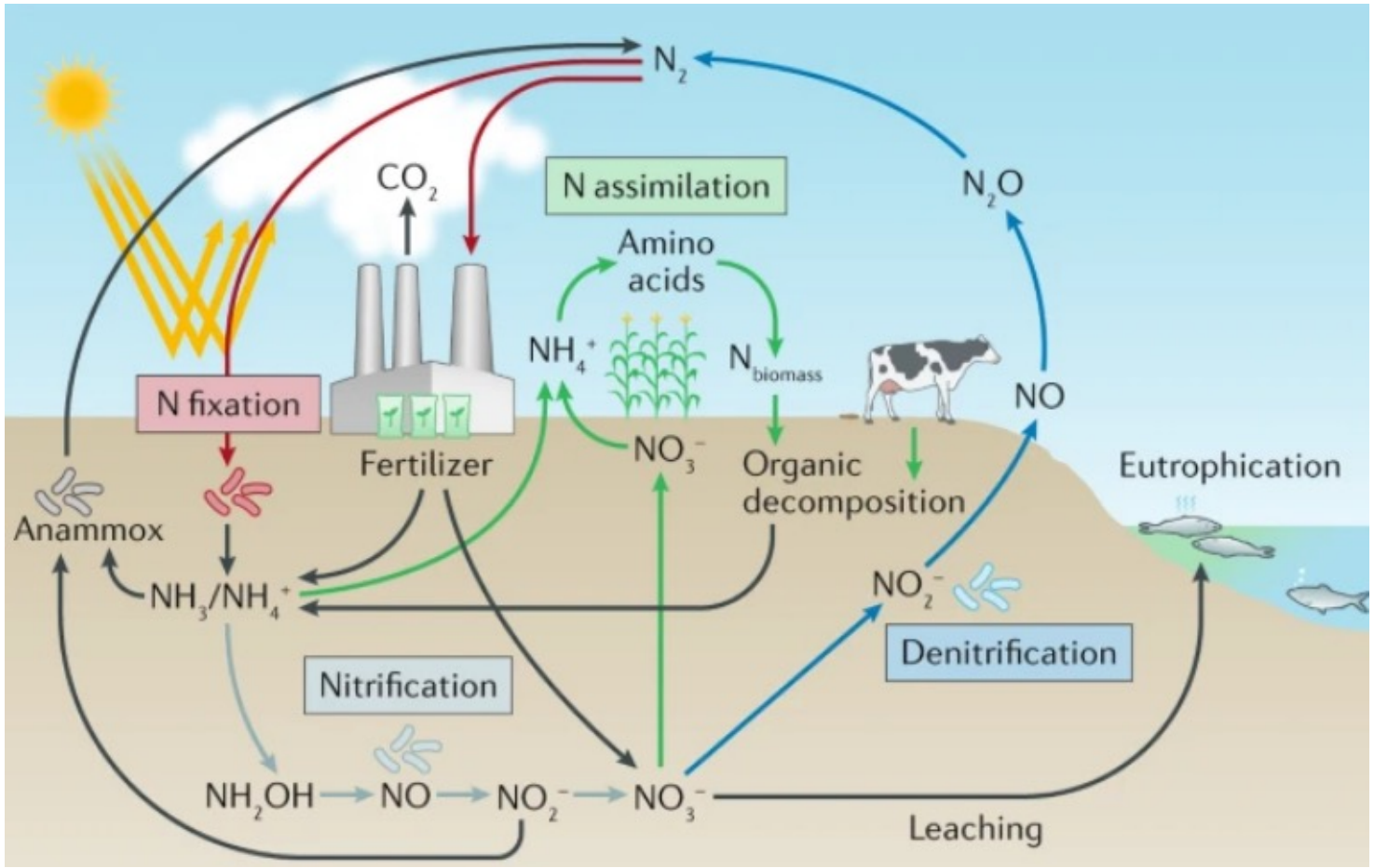
CONDESA
CONVERGENCE OF NANO-ENGINEERED DEVICES FOR ENVIRONMENTAL AND SUSTAINABLE APPLICATIONS

UNIVERSITY OF CALIFORNIA MERCED

NSF

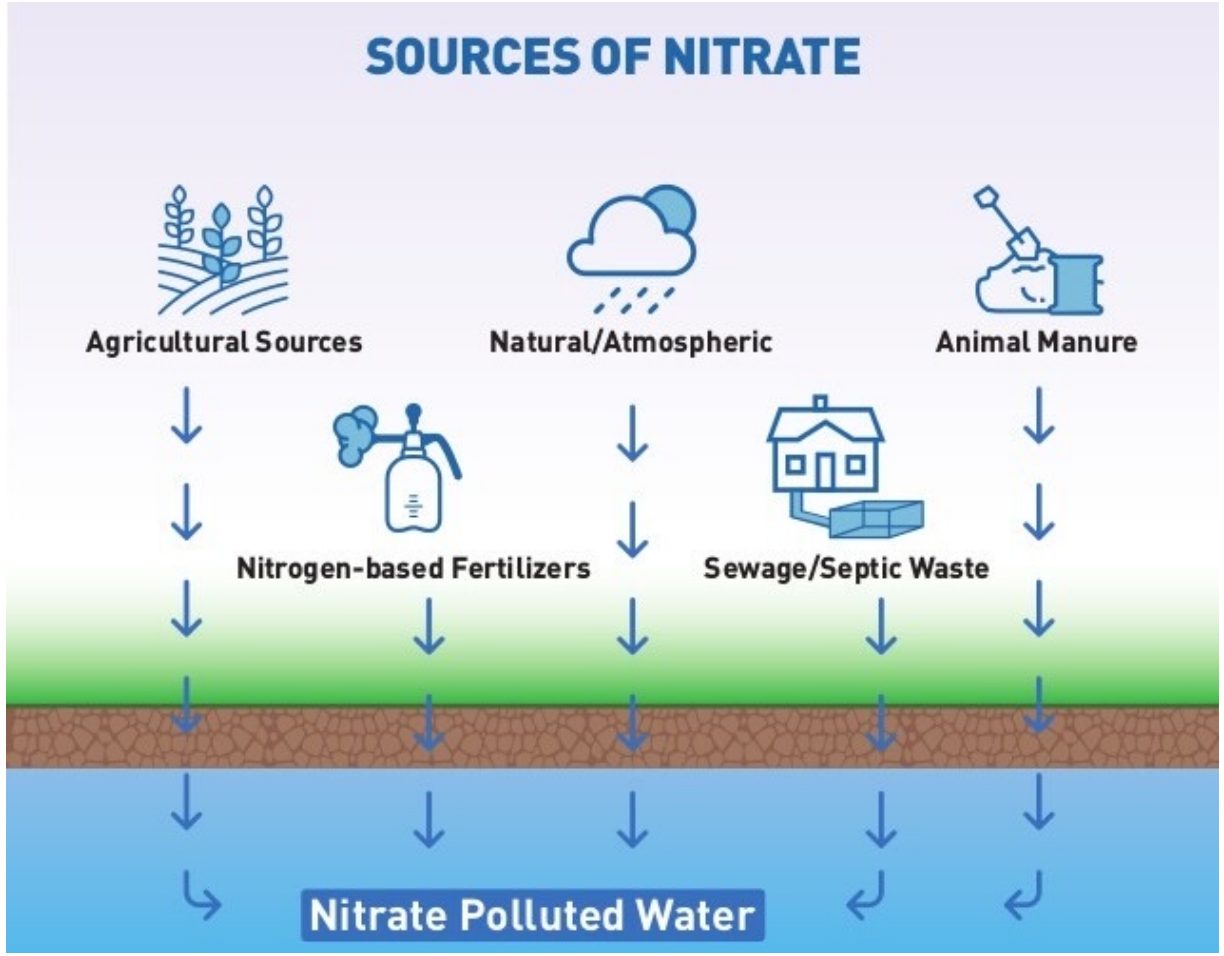
Nitrogen Background

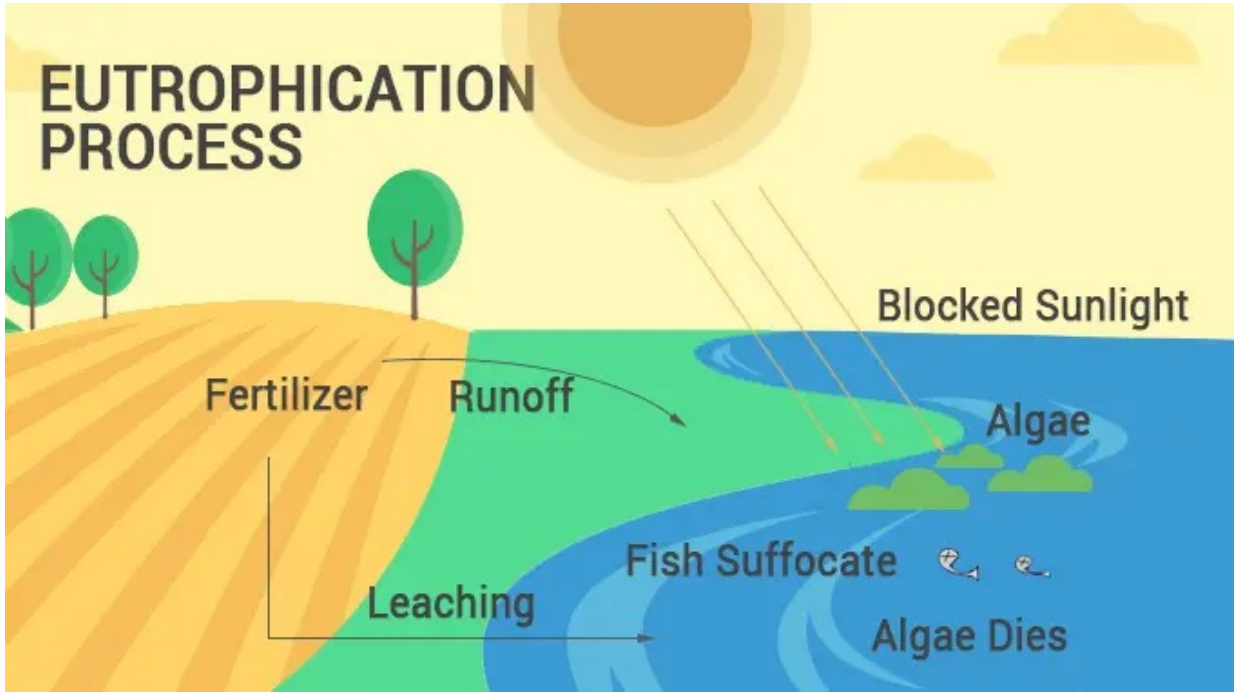




Lehnert, N., Dong, H.T., Harland, J.B. *et al.* Reversing nitrogen fixation. *Nat Rev Chem* **2,** 278–289 (2018). https://doi.org/10.1038/s41570-018-0041-7
http://www.n-print.org/faq

Nitrogen Background



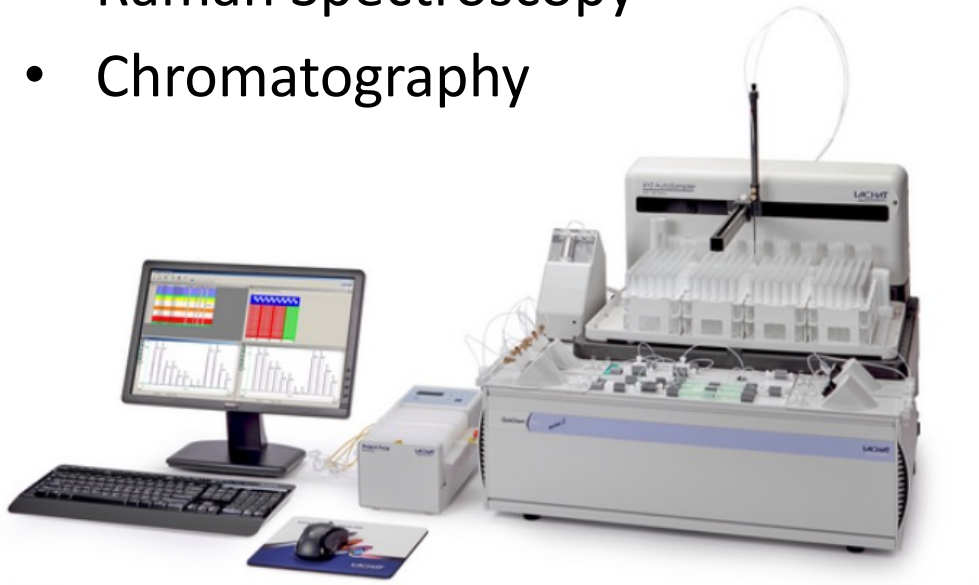


https://kingsbayrestorationproject.com/nitrates-and-ph-in-water-quality/
https://earthhow.com/eutrophication-causes-process-examples/

Methods Background

Lab Methods

- Flow Injection Colorimetry
- Fluorescence
- Raman Spectroscopy
- Chromatography



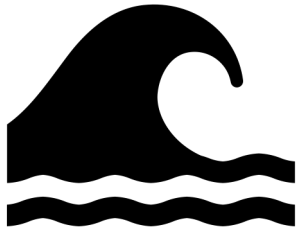
Field Methods

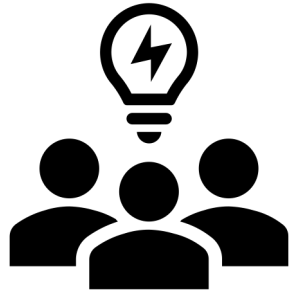
- Nitrate Test Strips
- Field Probes

https://www.hach.com/flow-injection-analysis-fia/lachat-quikchem-flow-injection-analysis-system/family?productCategoryId=35547627752
https://www.preclaboratories.com/product/nitrite-nitrate-test-strip/
https://www.seabird.com/nutrient-sensors/suna-v2-nitrate-sensor/family?productCategoryId=54627869922#

Project Aims

Develop a low cost, portable, and easy to use sensor capable of detecting nitrate in natural waters from 0.2 ppm N – 40 ppm N



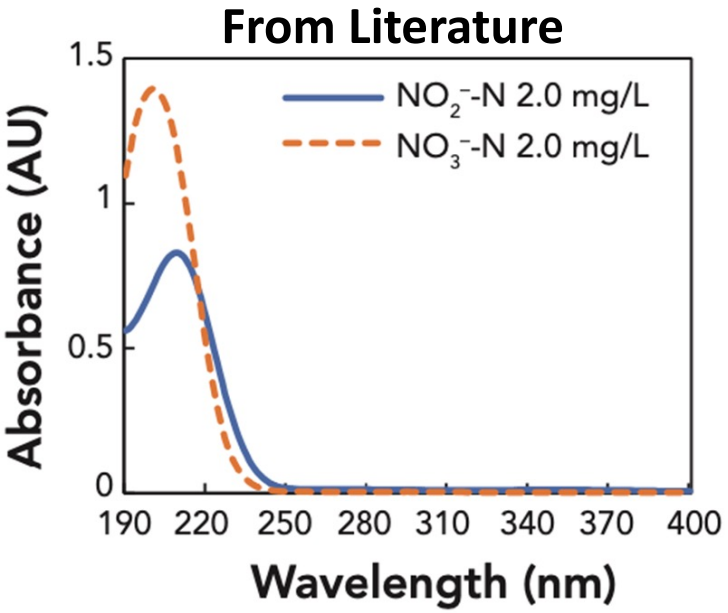


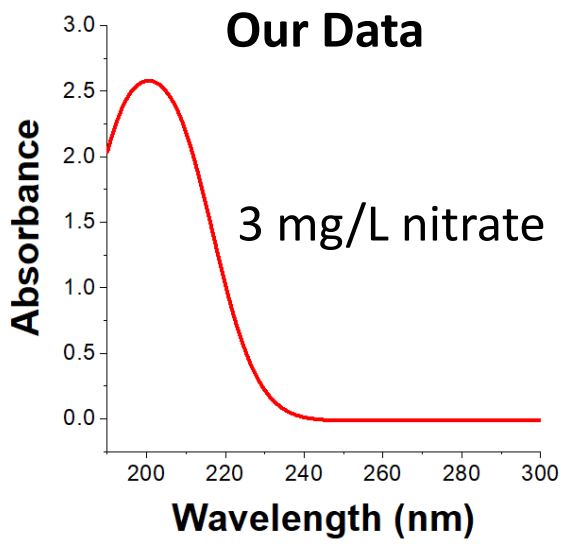
UV Absorption by Nitrate Ions

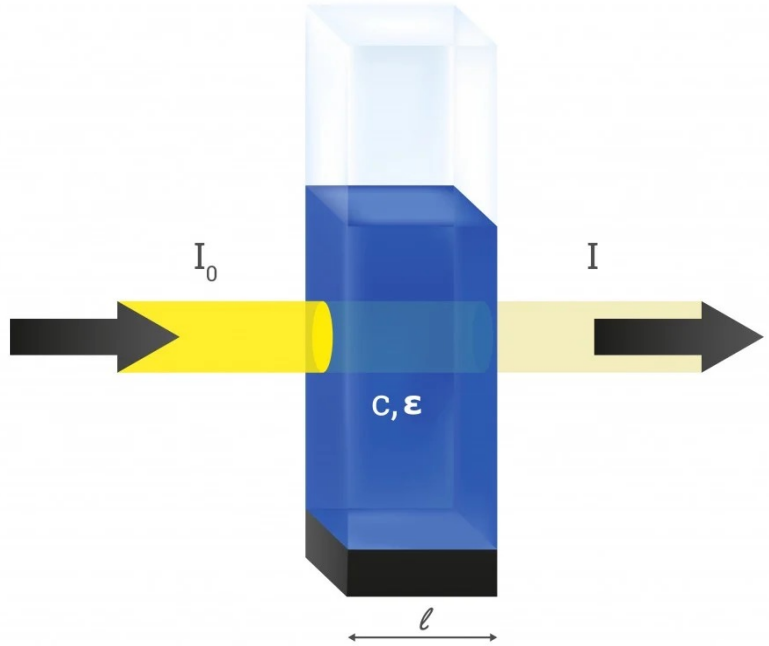
Beer-Lambert's Law

$$A = \log_{10}\left(\frac{I_o}{I}\right) = \epsilon c l$$

A = absorbance
I= intensity
ε = molar absorptivity
L = path length
c = concentration of analyte

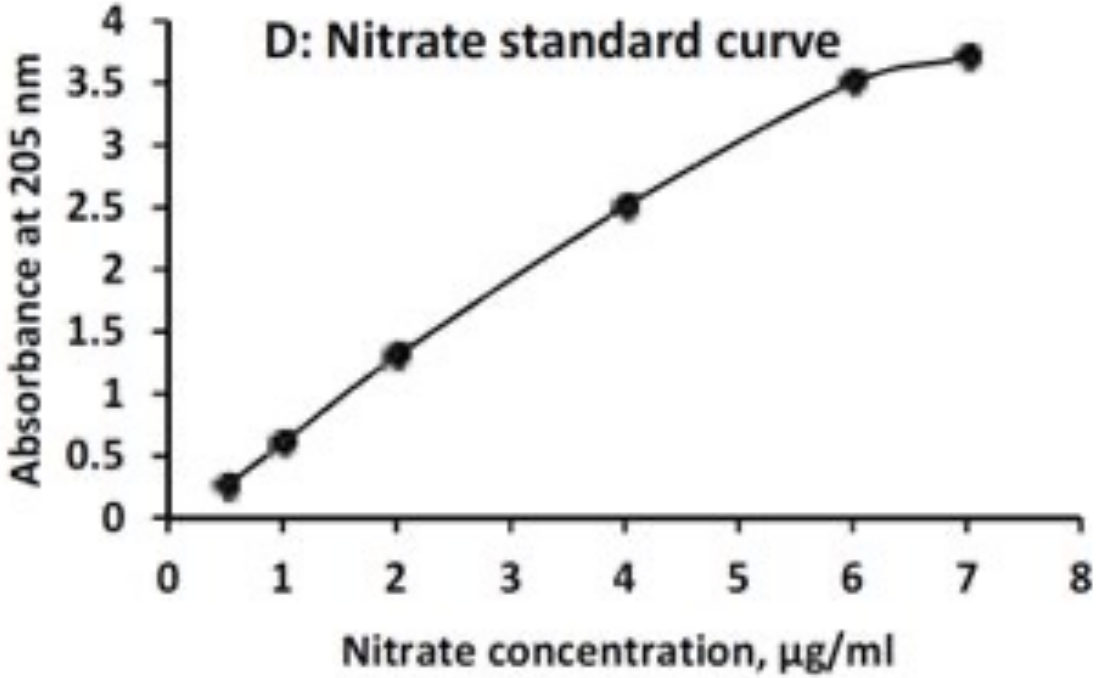


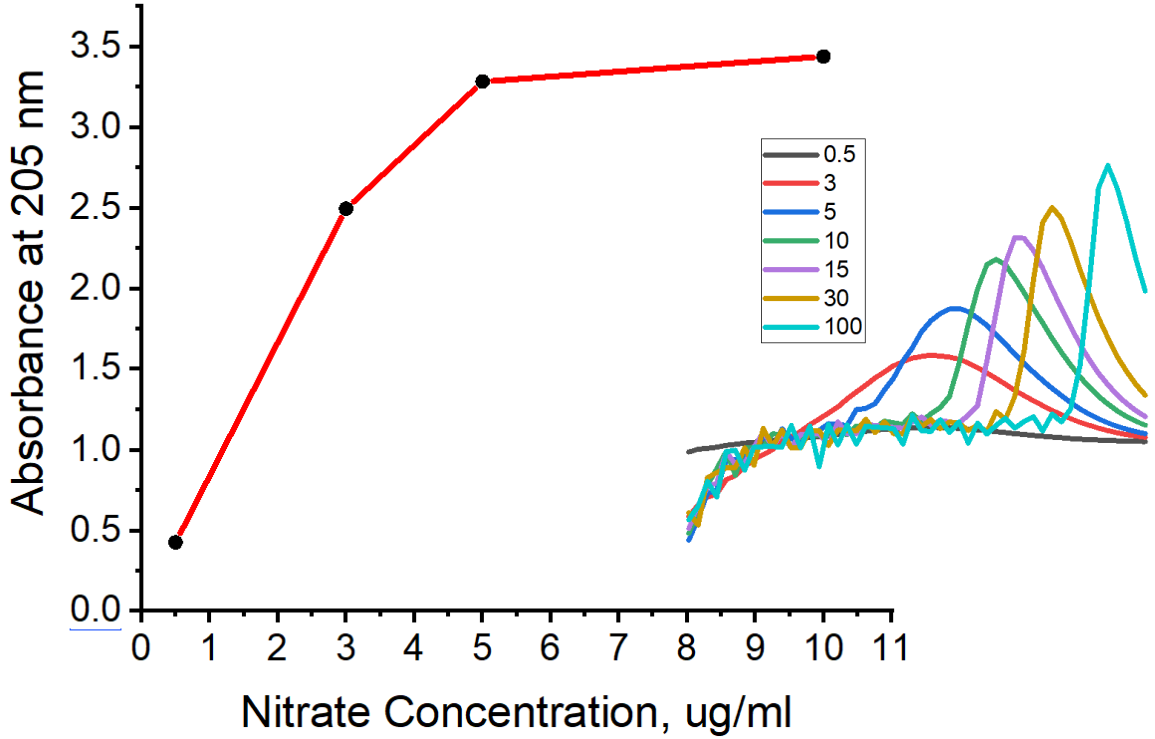




https://www.spectroscopyonline.com/view/simultaneous-detection-of-nitrate-and-nitrite-based-on-uv-absorption-spectroscopy-and-machine-learning
https://www.scienceabc.com/pure-sciences/what-is-beers-law.html
Pellerin, B.A., Bergamaschi, B.A., Downing, B.D., Saraceno, J.F., Garrett, J.A., and Olsen, L.D., 2013, Optical techniques for the determination of nitrate in environmental waters: U.S. Geological Survey Techniques and Methods 1–D5, 37 p.

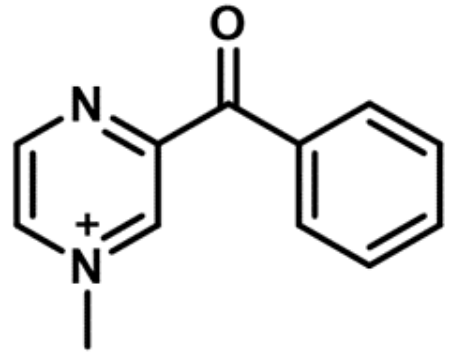
Limitations of Beer-Lambert's Law

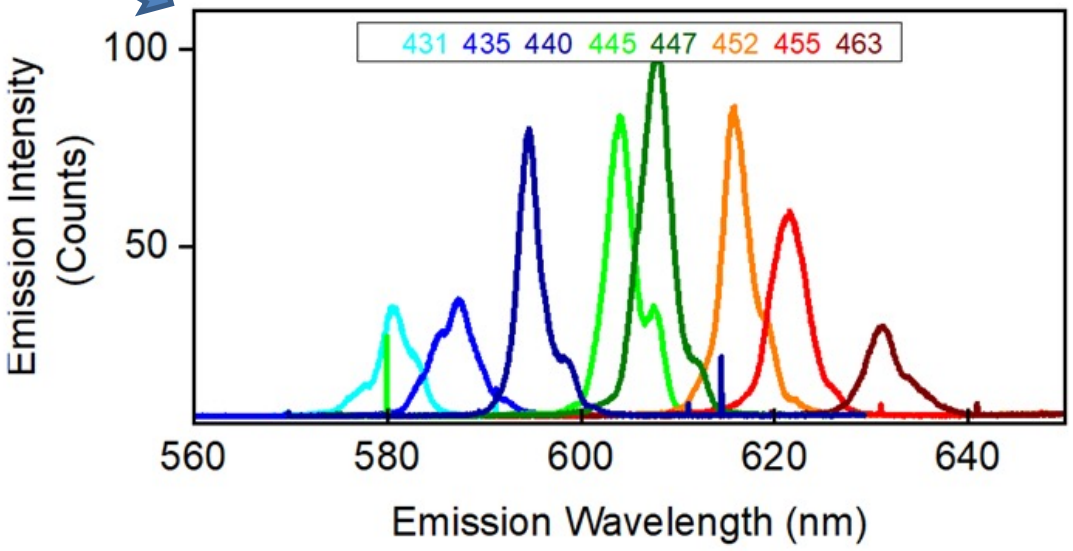


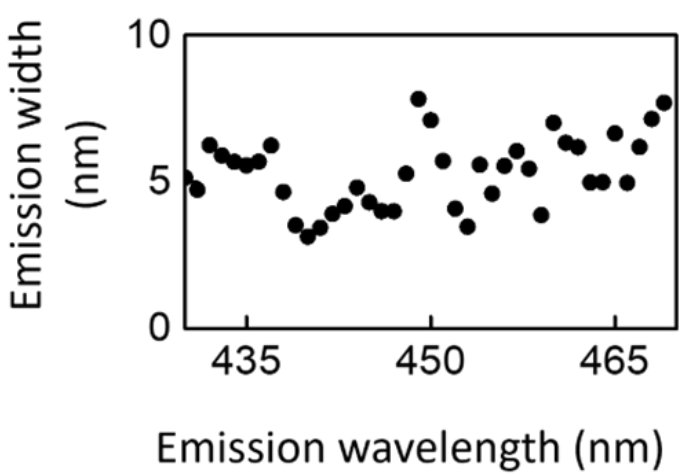


Organic Luminescent Molecules

- Substituted Benzoyl Pyraziniums [synthesized in Baxter Lab] show interesting optical properties in solution and solid state
- Solid state studies show emission **tunability** with excitation wavelength
- Concentration-dependent **tunable** emission
- Significantly narrowed emission, with a FWHM of 4 nm





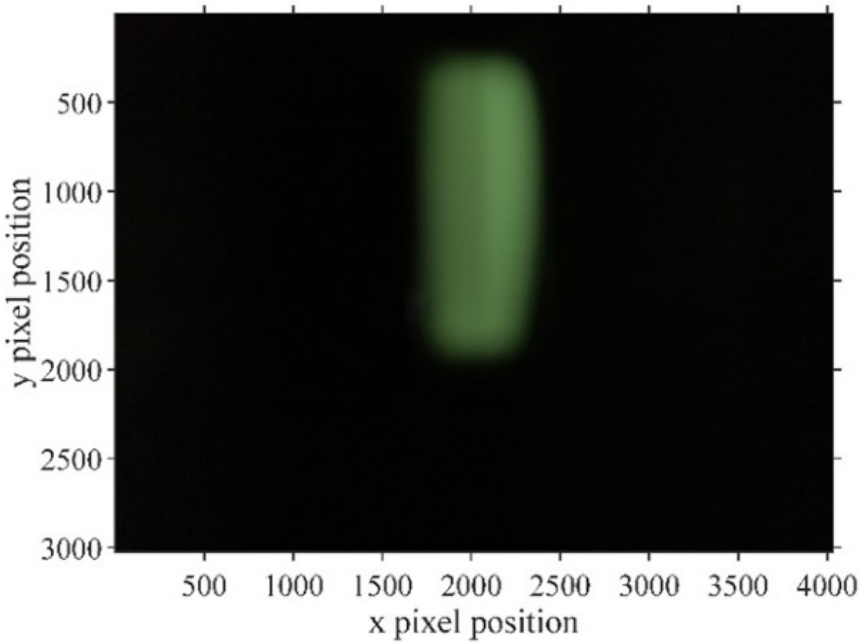


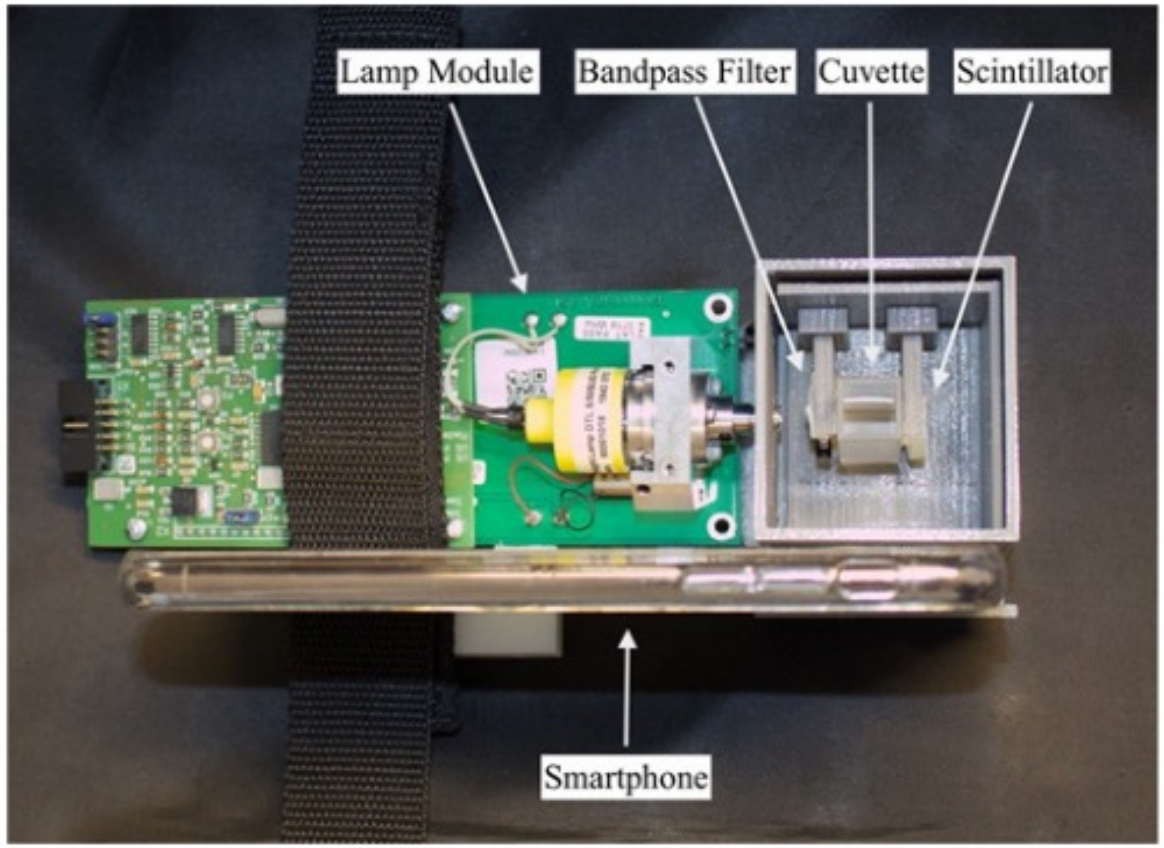
Prototype Spectrophotometer

Water quality assessment using a portable UV optical absorbance nitrate sensor with a scintillator and smartphone camera

JMDFP Ingles[1], TM Louw[2] and MJ Booysen[1]

[1]*Department of E&E Engineering, Stellenbosch University, Stellenbosch, South Africa*
[2]*Department of Process Engineering, Stellenbosch University, Stellenbosch, South Africa*

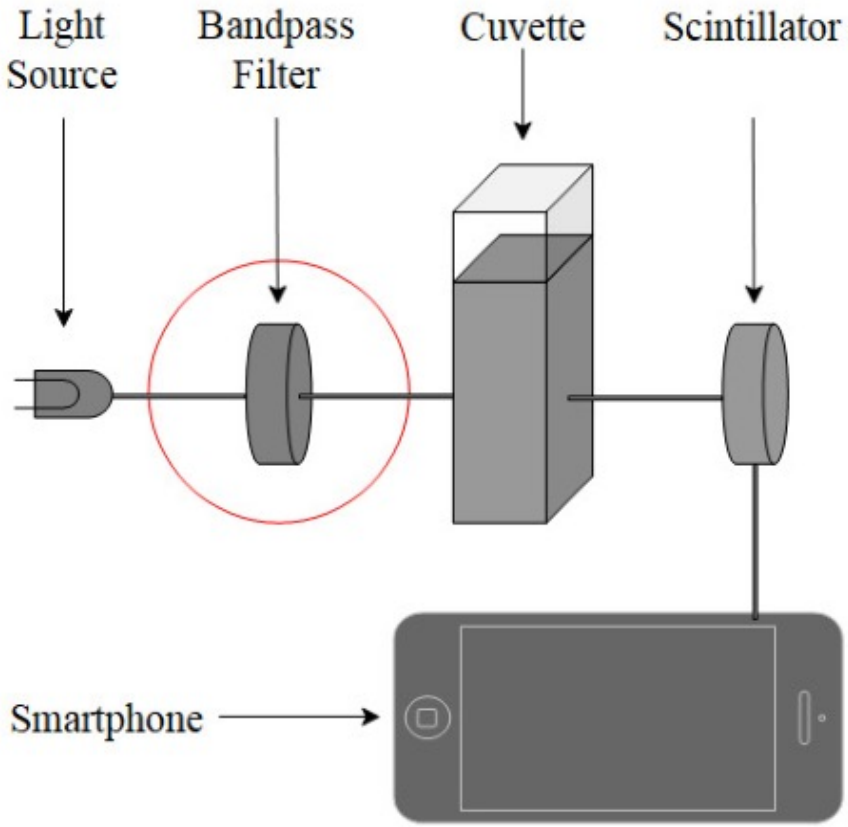




Ingles, J. M. D. F. P., Louw, T. M. & Booysen, M. J. Water quality assessment using a portable UV optical absorbance nitrate sensor with a scintillator and smartphone camera. *Water SA* **47**, 135–140 (2021).

Proposed Optical Sensor

Original	Improvements
Deuterium lamp $525	UV-C LED < $300 Lower power, longer lasting
Quartz cuvette $75	$15 on Amazon
200 nm bandpass $75	Possibly not needed
Green glass scintillator $75	No improvements found
Total: $750	Total: $300-$500



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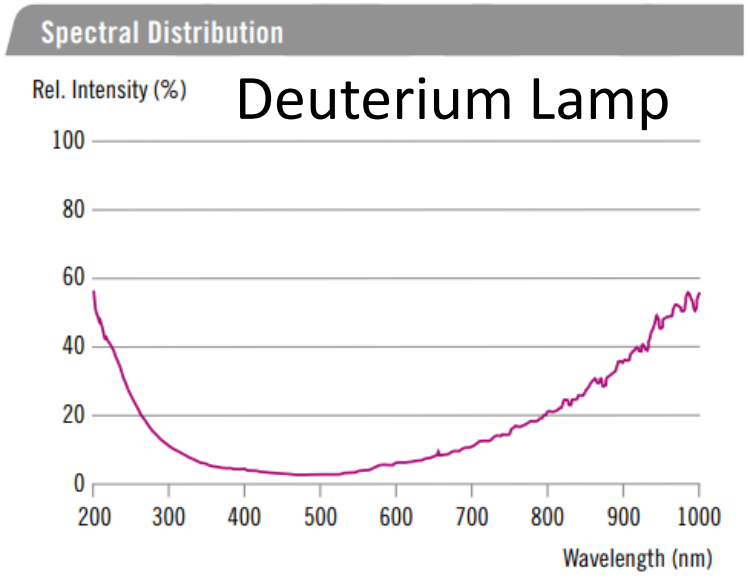
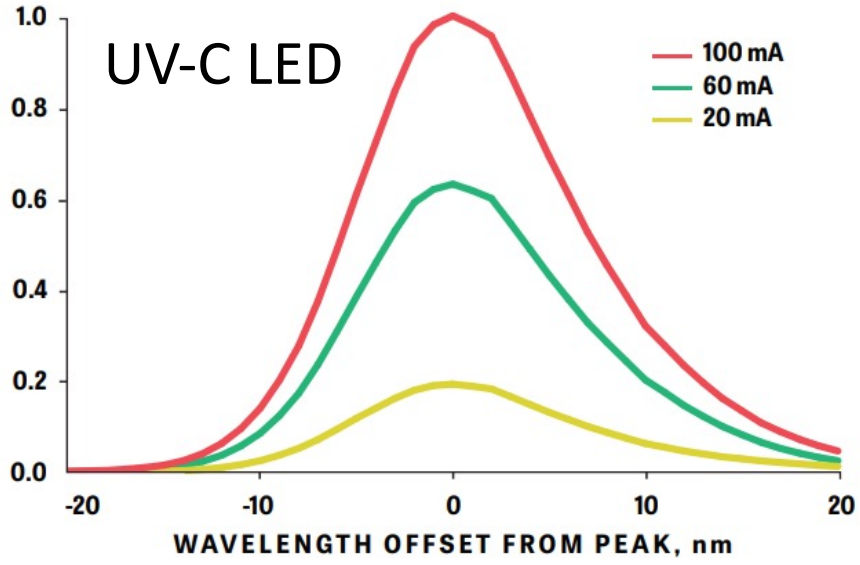
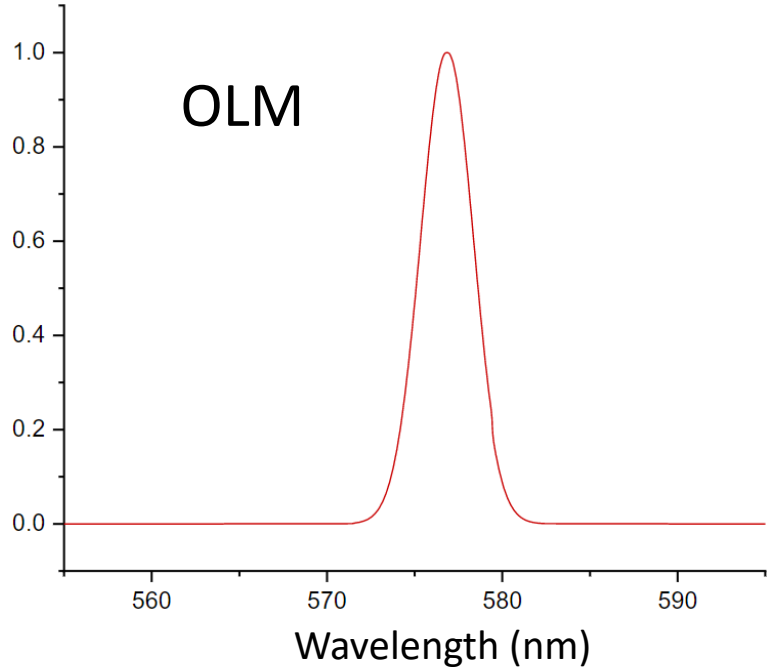
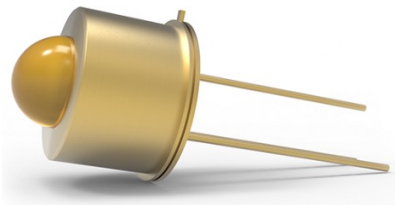
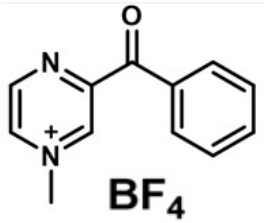
Comparing Light Sources

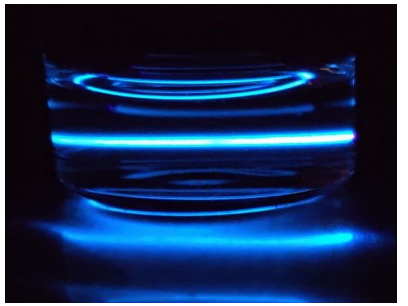








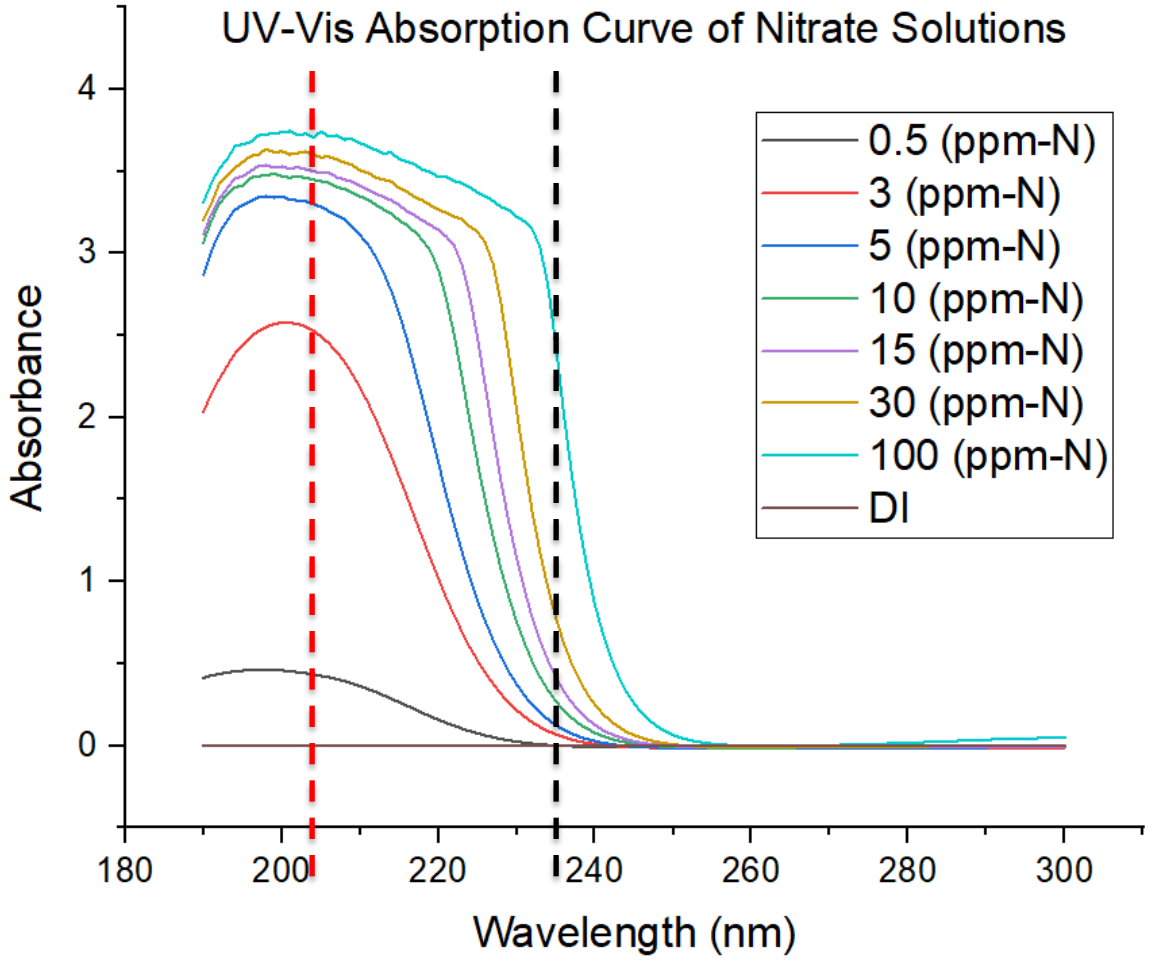


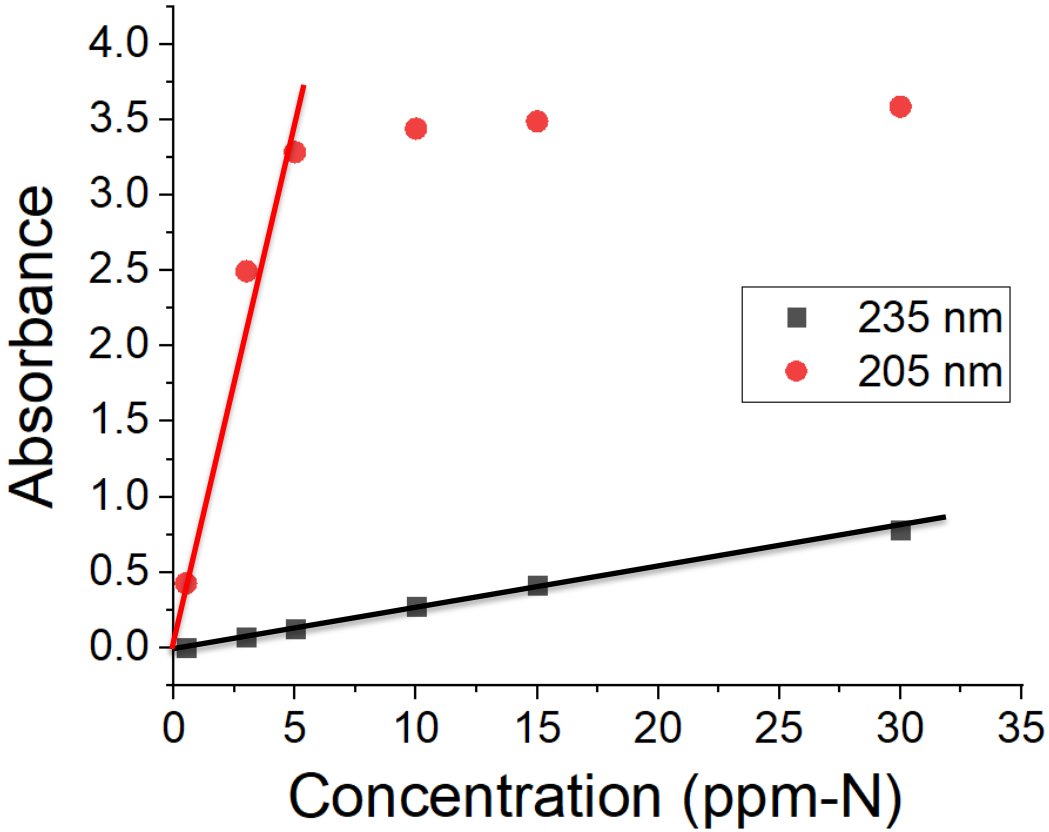


LEDs and OLMs = low power consumption and narrow spectral emission

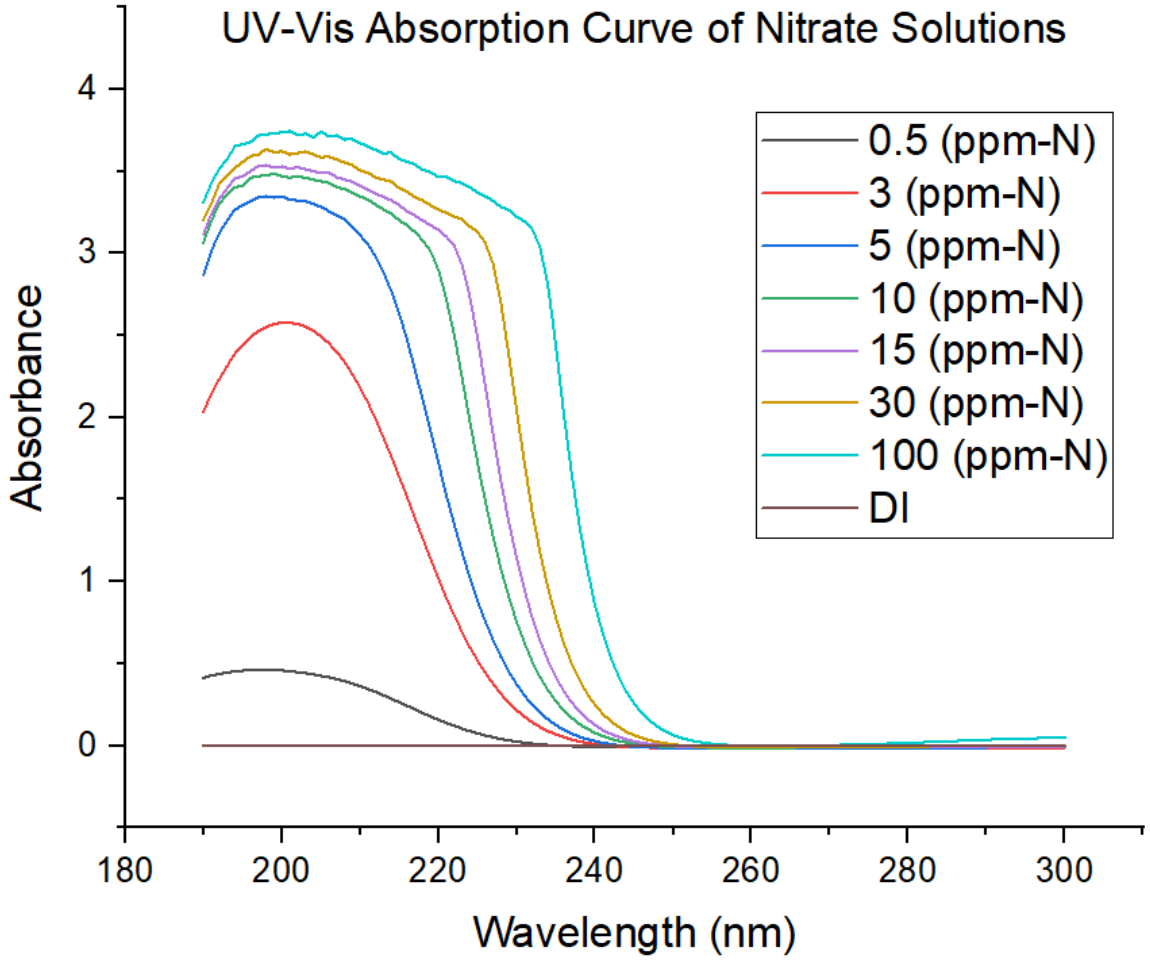
https://cisuvc.com/images/cis/optan/optan_ball_lens_090921f.pdf
https://www.heraeus.com/en/hng/products_and_solutions/lamps_for_optics_and_analytics/fiberlight/fiberlight_d2/fiberlight.html

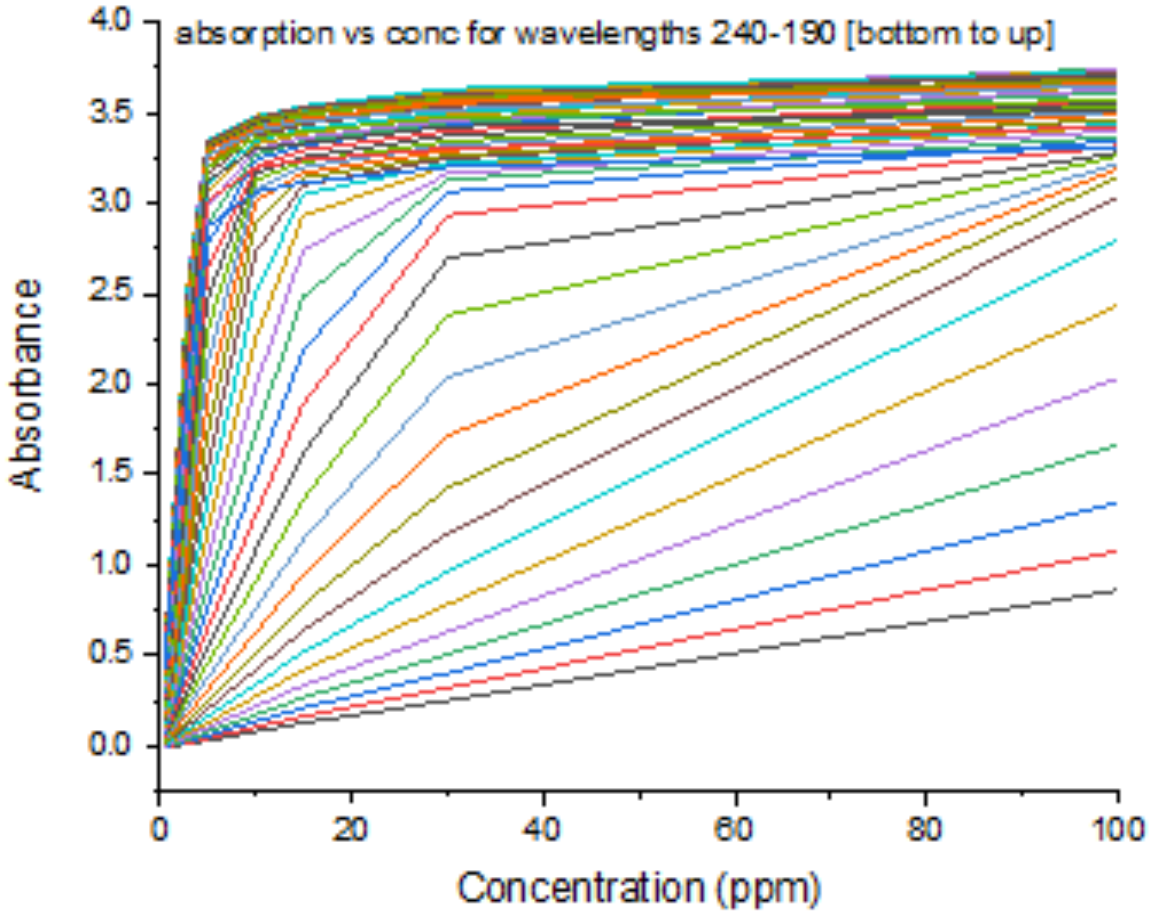
Nitrate Absorption Test





Determining Concentration





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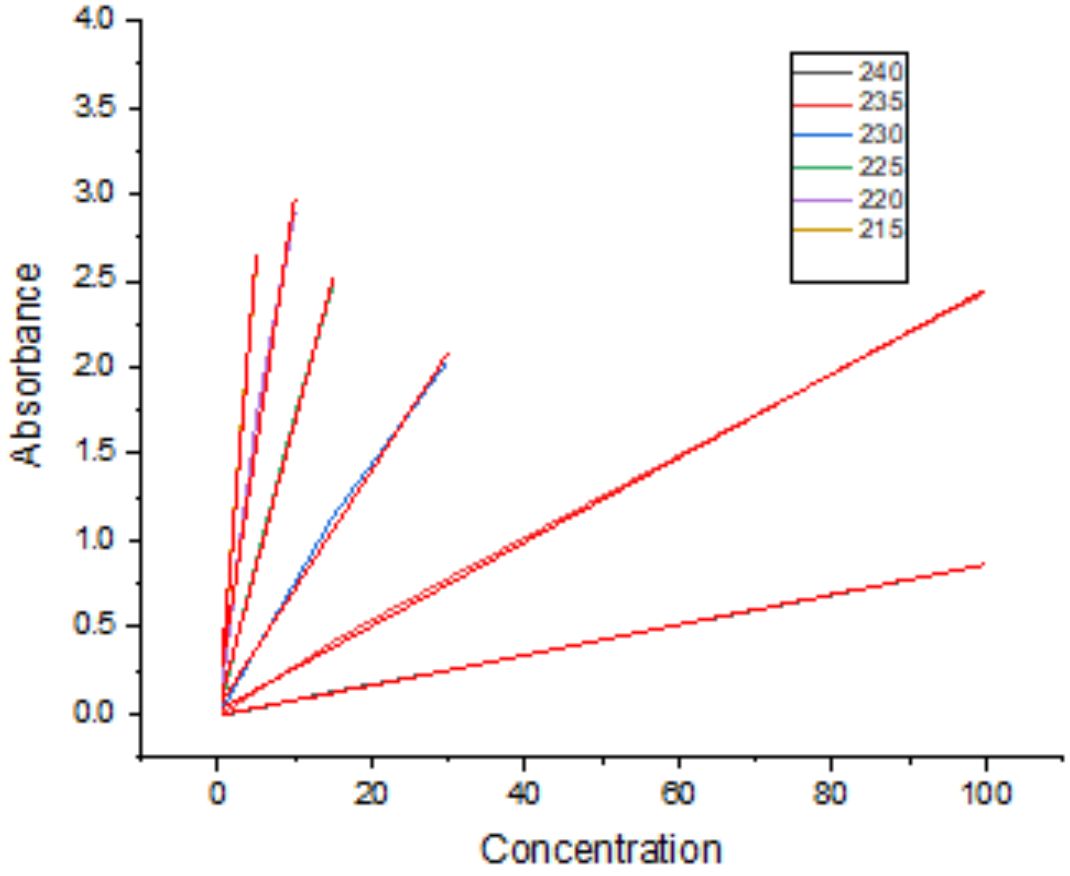
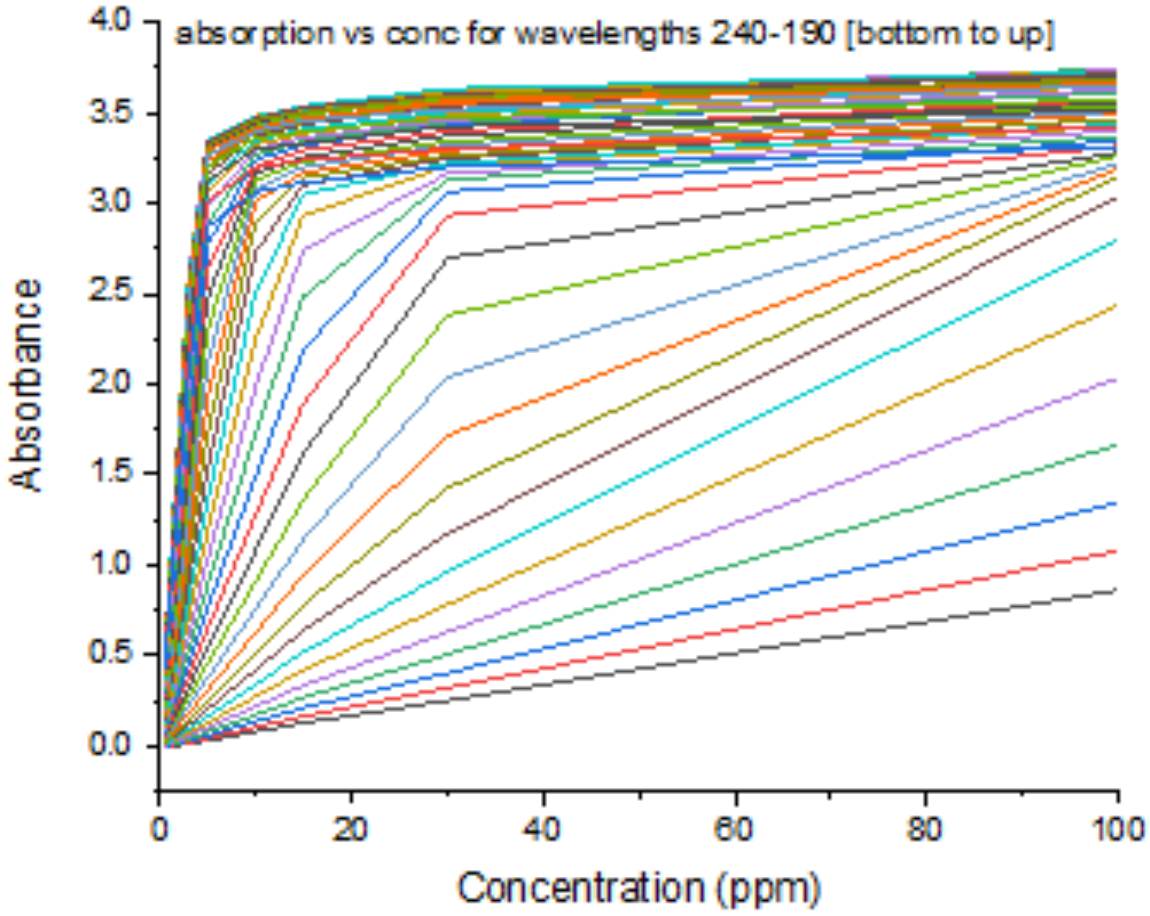
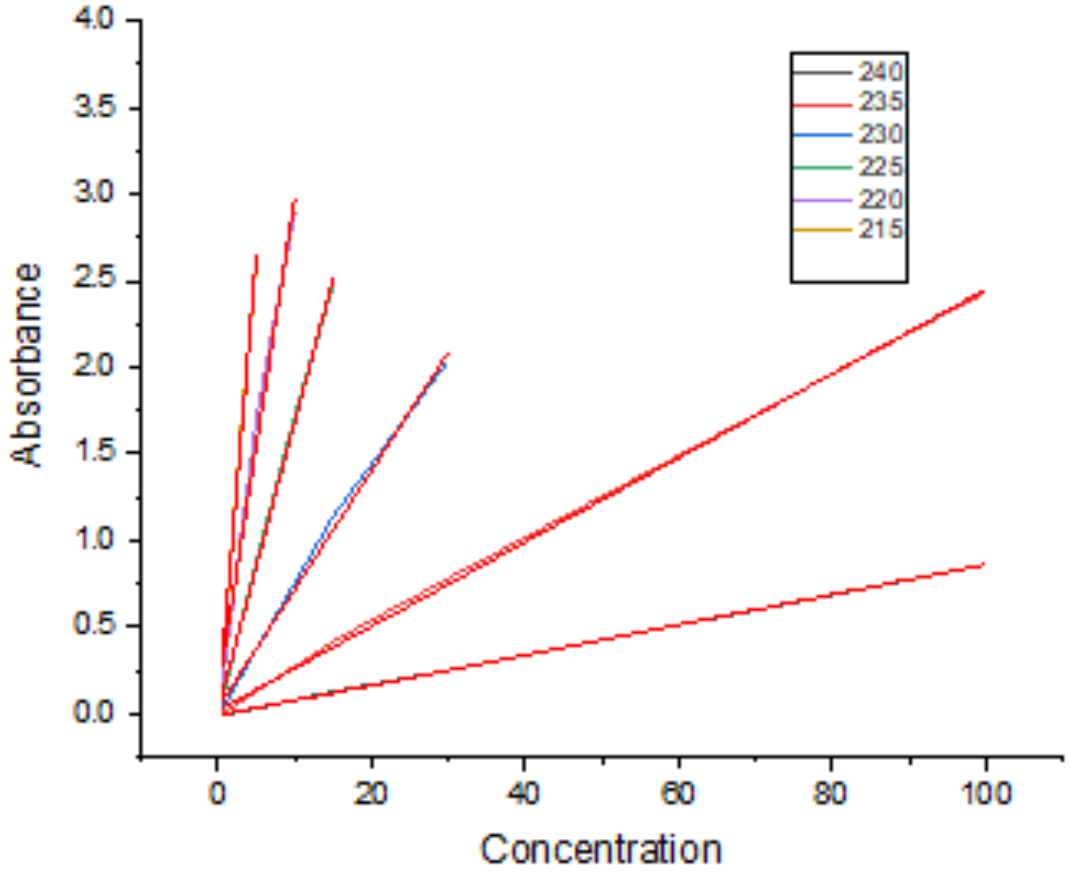




Determining Concentration

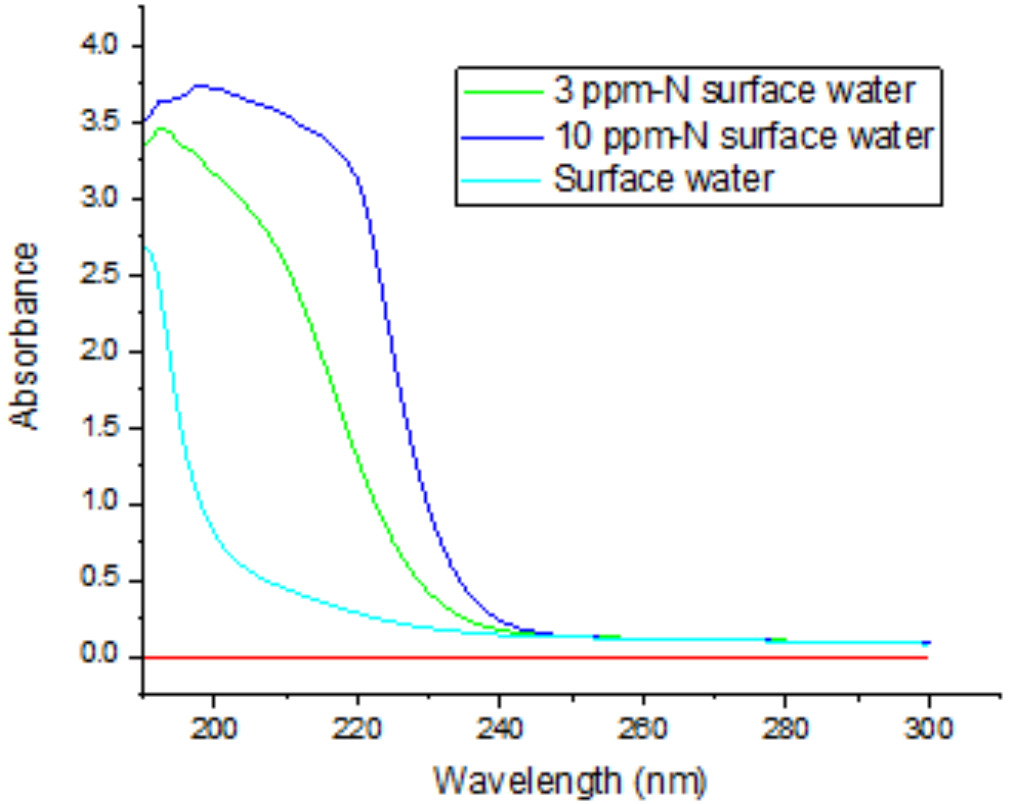


wavelength	slope
240	0.00873
235	0.02432
230	0.06849
225	0.16638
220	0.28577
215	0.52674

$$A = \epsilon C$$

Wavelength	predicted concentration
215	0.503
215	3.111
215	4.995
220	10.145
225	14.937
230	29.793
235	100.156

Determining Concentration



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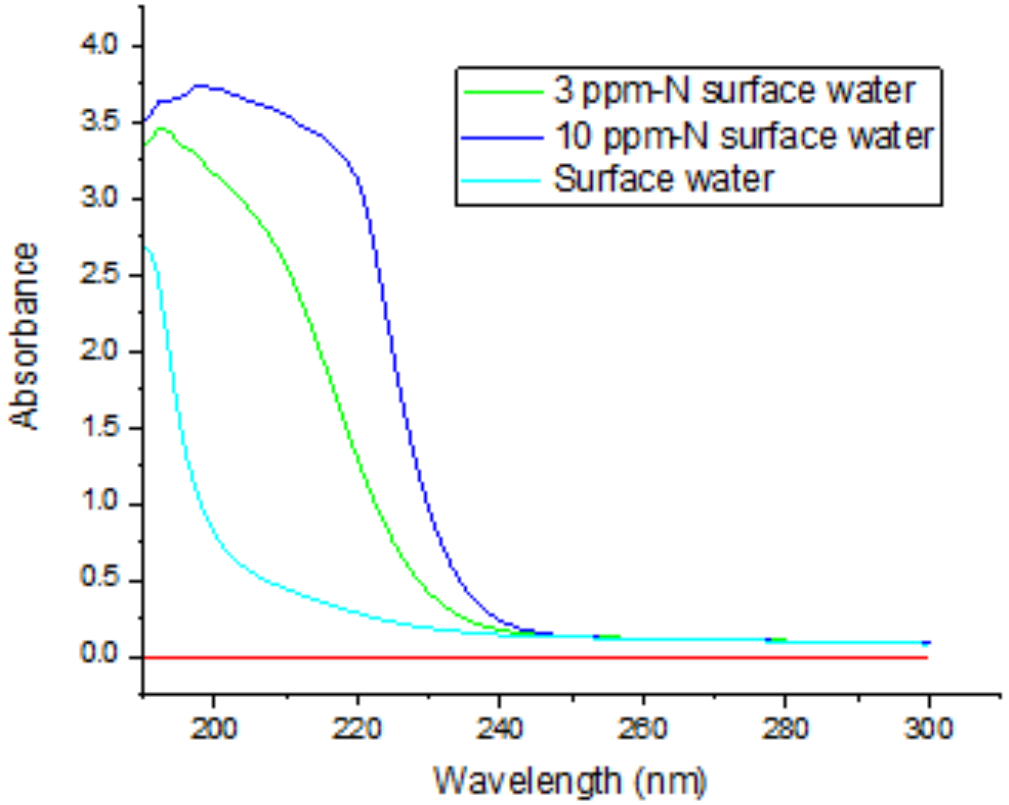


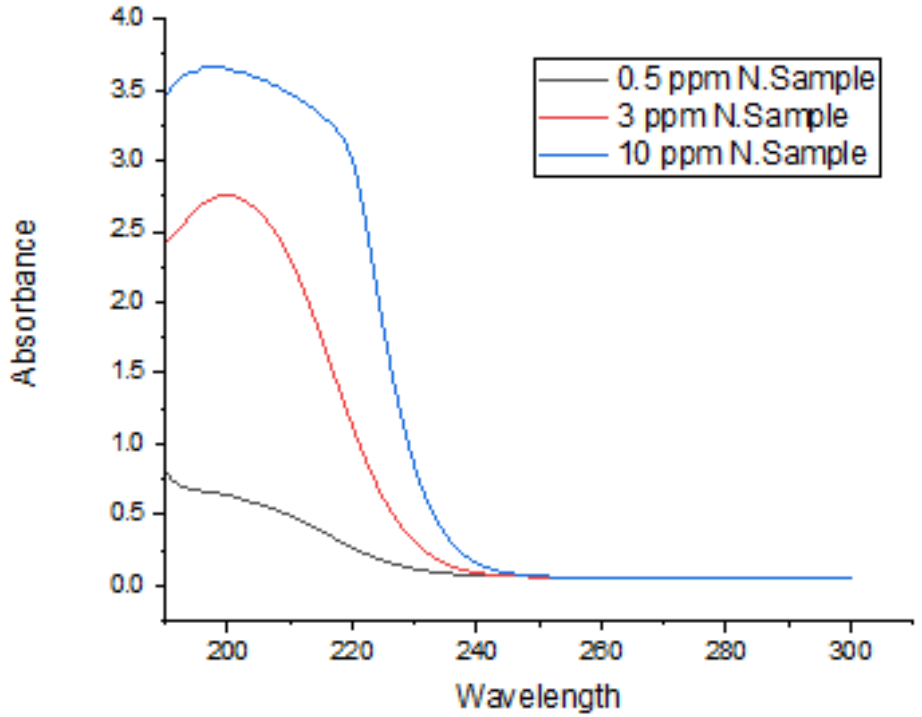
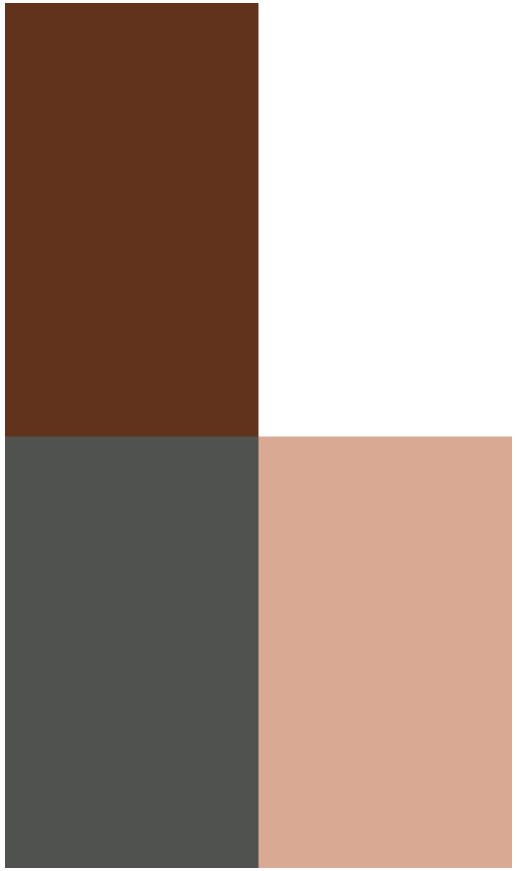
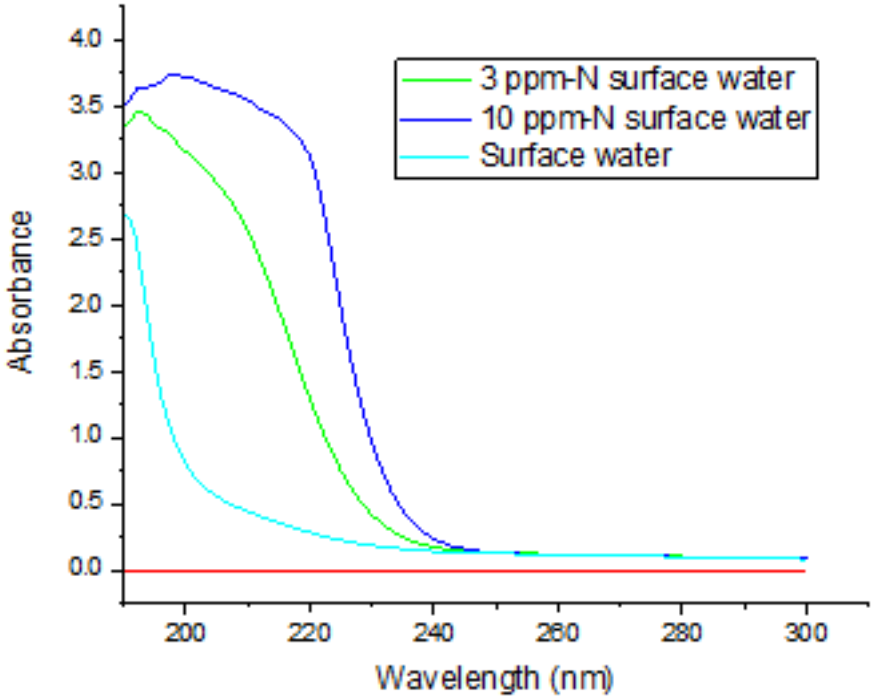


Image Analysis

Deconvolution algorithms



Pixel intensity
↳ absorbance



Other solutions: utilize a photodiode to capture light signal from sample

Interface

Nitrate Testing

Tuesday June 21, 2022

How much nitrate is in the water? Let's find out!

0-5 ppm-N 5-10 ppm-N 10-15 ppm-N 15-30 ppm-N 30-50 ppm-N

Concentration Output

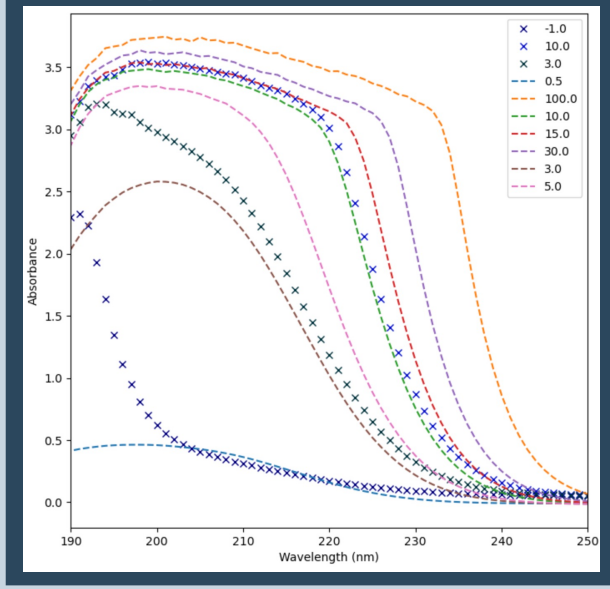
```
calculated concentration @ 205.0:
  sample 1: 0.6344831456088803 ± 0.3013497413212077
  sample 2: 5.427491429970619 ± 0.0352283065333071
  sample 3: 4.31862400016324 ± 0.044273669528691315
calculated concentration @ 235.0:
  sample 1: 2.765503833483671 ± 0.00845769675248732
  sample 2: 13.688113660825854 ± 0.0017087666986858499
  sample 3: 6.092397409731739 ± 0.0038391771282162593
```

Control Panel

Click 'Go' to sample more water.

Go Exit

Plotting



Acknowledgements

- Thank you to our group advisors and the CONDESA team
- We are incredibly grateful for the funding and opportunity provided by NRT CONDESA, funded by National Science Foundation grant no. 2125510

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