EMPLOYING A LOW-COST CUSTOM SPECTROPHOTOMETER WITH LOCAL CALIBRATION CURVE TO ESTIMATE NITRATE CONCENTRATIONS IN LOCAL STREAMS

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INTRODUCTION

- Understanding nutrient fluctuations in streams is important for analyzing pollutant dynamics, BMPs, and seasonal patterns
- Current methods of grab/composite sampling with laboratory analysis are cumbersome and restricted in quantity of data points[3,7]
- Past field studies have shown the accuracy of UV-VIS spectroscopy to measure water quality parameters using commercial spectrophotometers and a local calibration curve (LCC)[3,4,7]
- High-quality field-deployable UV-VIS spectrophotometers are expensive (~$20k +)
- A low-cost (~$2500) and custom-build spectrophotometer (GatorSpec) accurately predicted nitrate levels in high-nitrate (>3 mg/L) synthetic samples[2]
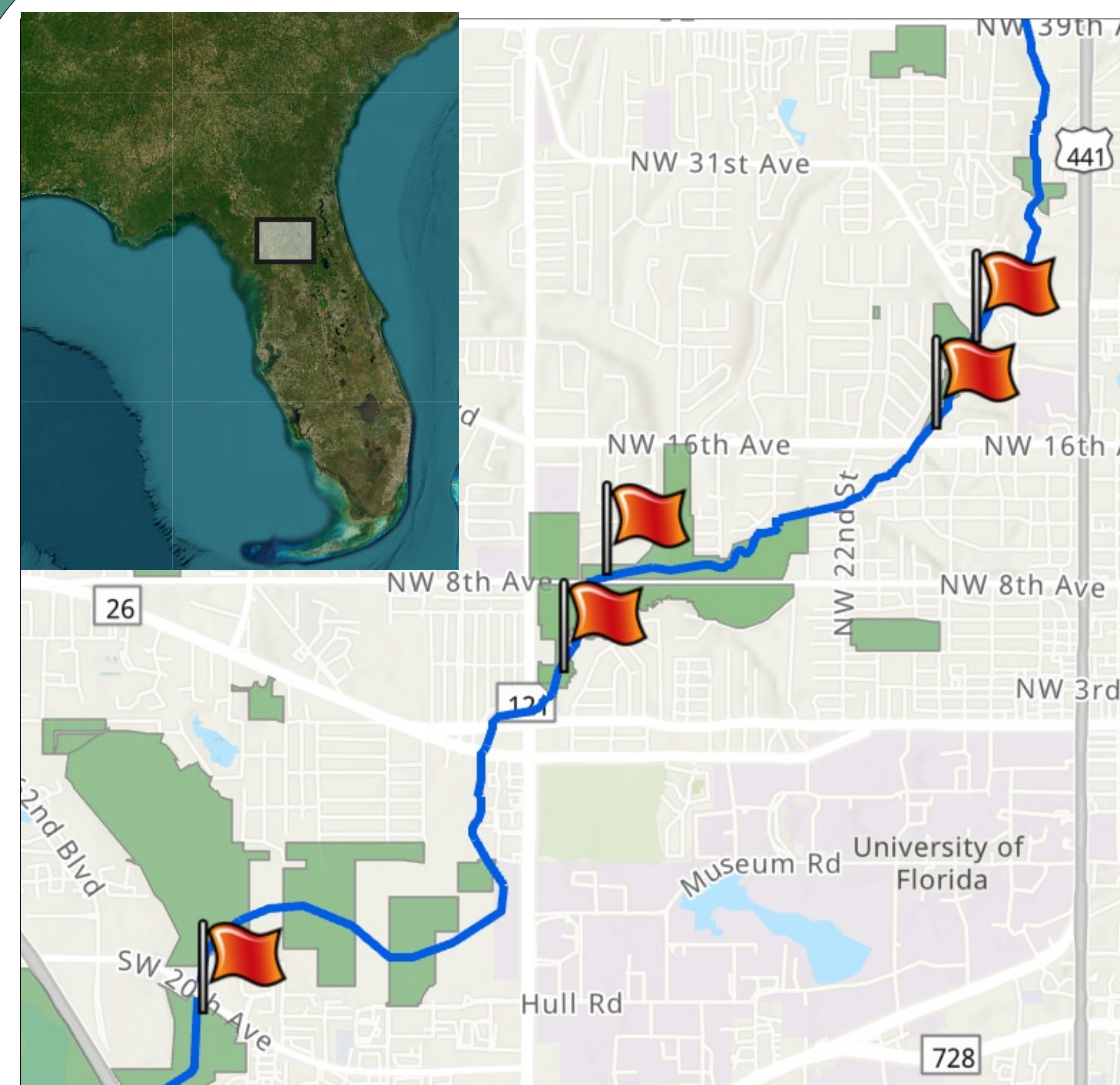
GOAL

Validate the accuracy of GatorSpec to measure nitrate levels in local streams through comparison with EPA analysis procedures

METHODS

- 50 filtered samples were collected from five sites along Hogtown Creek in Gainesville, Florida
- Samples were taken twice per week for five weeks (09/25 to 10/26/2023).
- GatorSpec collected absorption spectra at 1024 wavelengths (spectral range of 184.2 to 663.1 nm with a 0.47 nm resolution)
- LCC was trained on Python using PLSR with a 70/30 train/test split
- Seal AQ400 reported True Analysis Results for Nitrate-N in accordance with EPA Method 353.2
- PLSR model reported Predicted Analysis Results

Figure 1: GatorSpec Schematic[1]

- Xenon flash lamp (Hamatsu)
- 3D-printed enclosure
- Miniature UV-Vis spectrophotometer (Ocean Insights)
- Raspberry Pi (3B+)
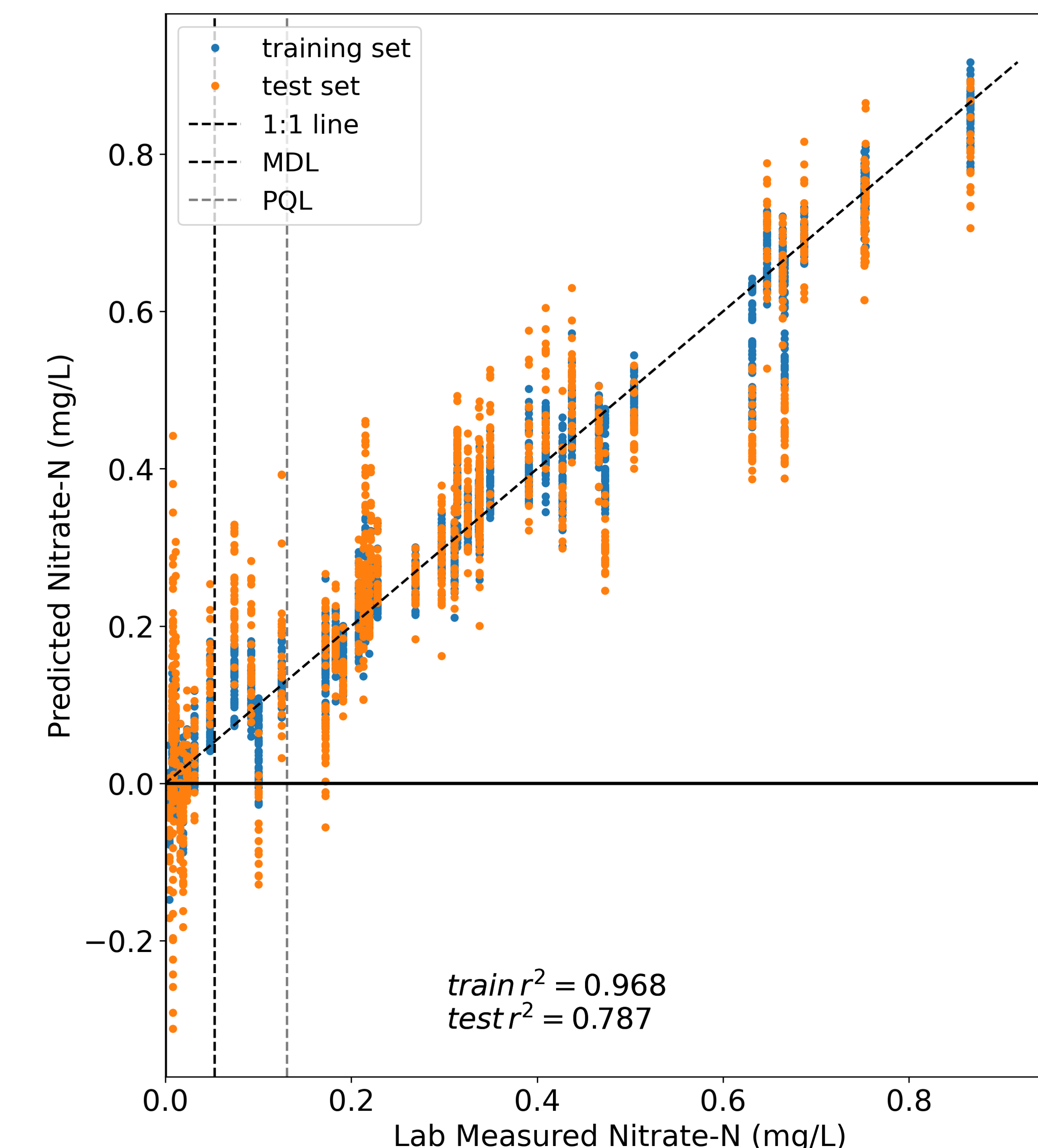
SITE DESCRIPTION

Figure 2: Site Map of Sampling Locations in Gainesville, FL. From left to right, sampling sites are labeled from A to E.
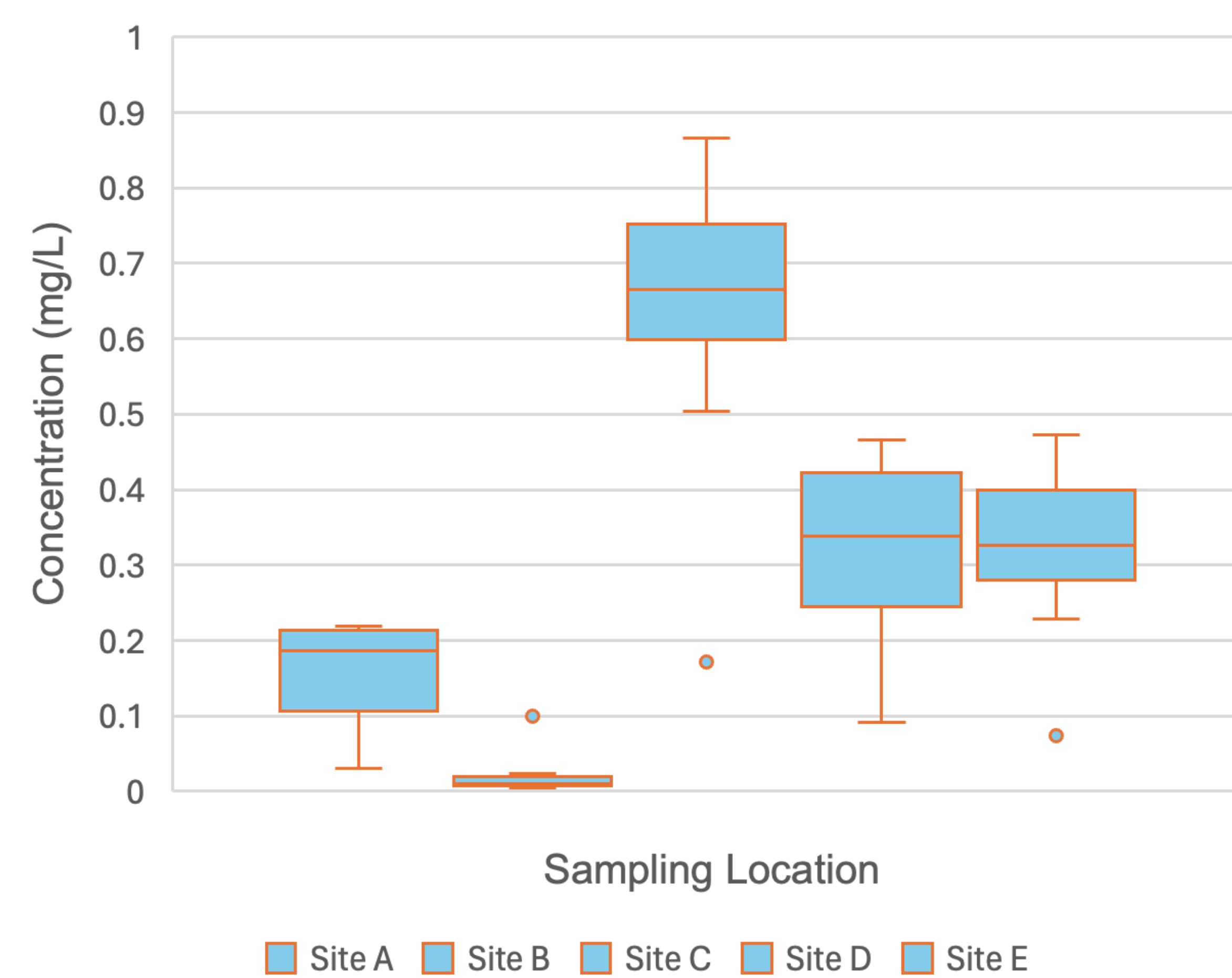
Figure 3: Nitrate levels at the five sampling sites shown in Figure 2.

RESULTS

train r^2 = 0.968
test r^2 = 0.787

Figure 4: Comparison of true and predicted analysis results from PLSR model ran through 80 iterations of train/test subsets.

- Comparison of predicted and lab-measured nitrate values had a coefficient of determination of 0.787
- Minimum Detection Limit (MDL) was 0.053 mg/L
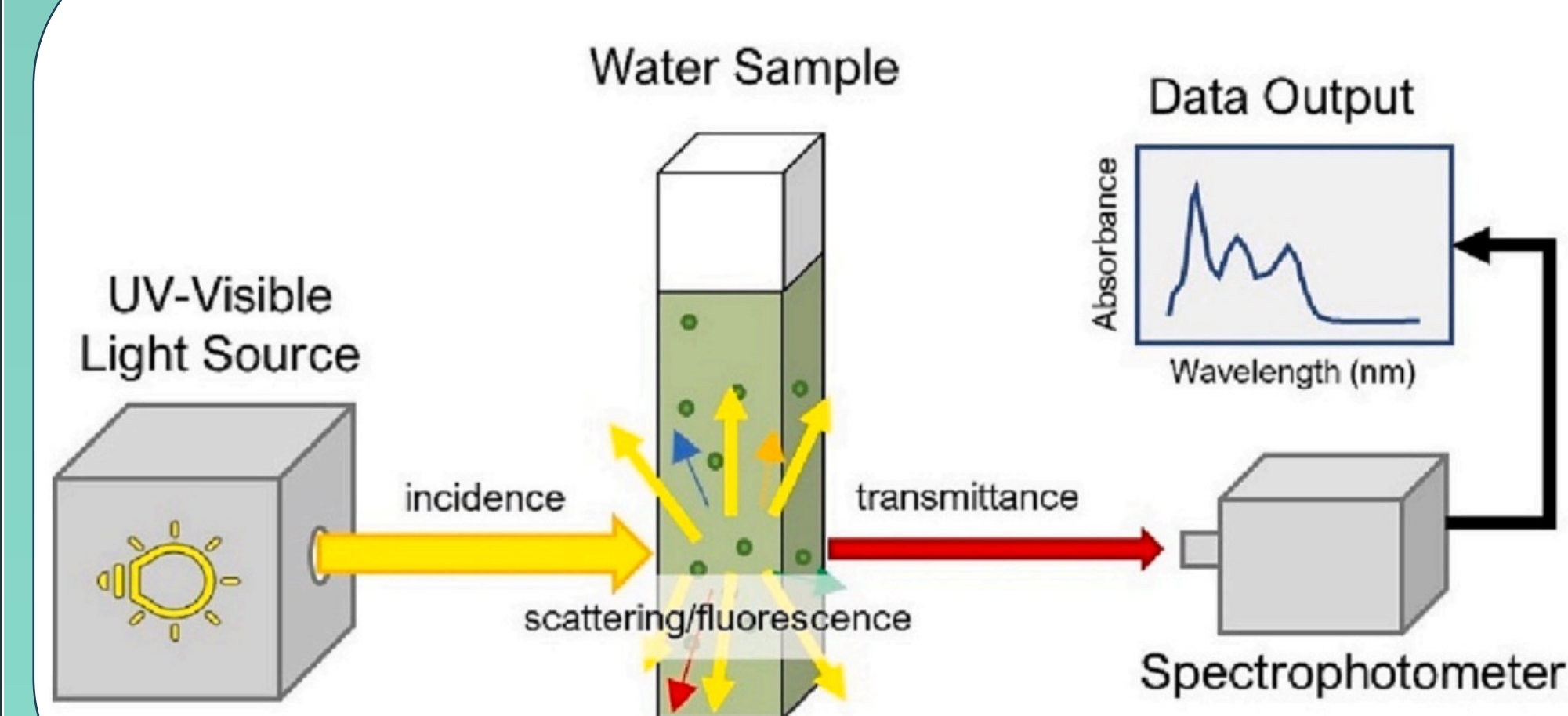- Practical Quantitation Limit (PQL) was 0.131 mg/L

DISCUSSION

- Predictive model was moderately accurate based on a limited number of training samples (R^2 > 0.79)
- In-situ applications could lead to real-time and detailed pollutant information
- Use of advanced machine learning models could improve accuracy

← **REFERENCES**