Using in situ UV-vis spectroscopy to measure N, C, P and suspended solids at a high frequency in a brackish tidal marsh

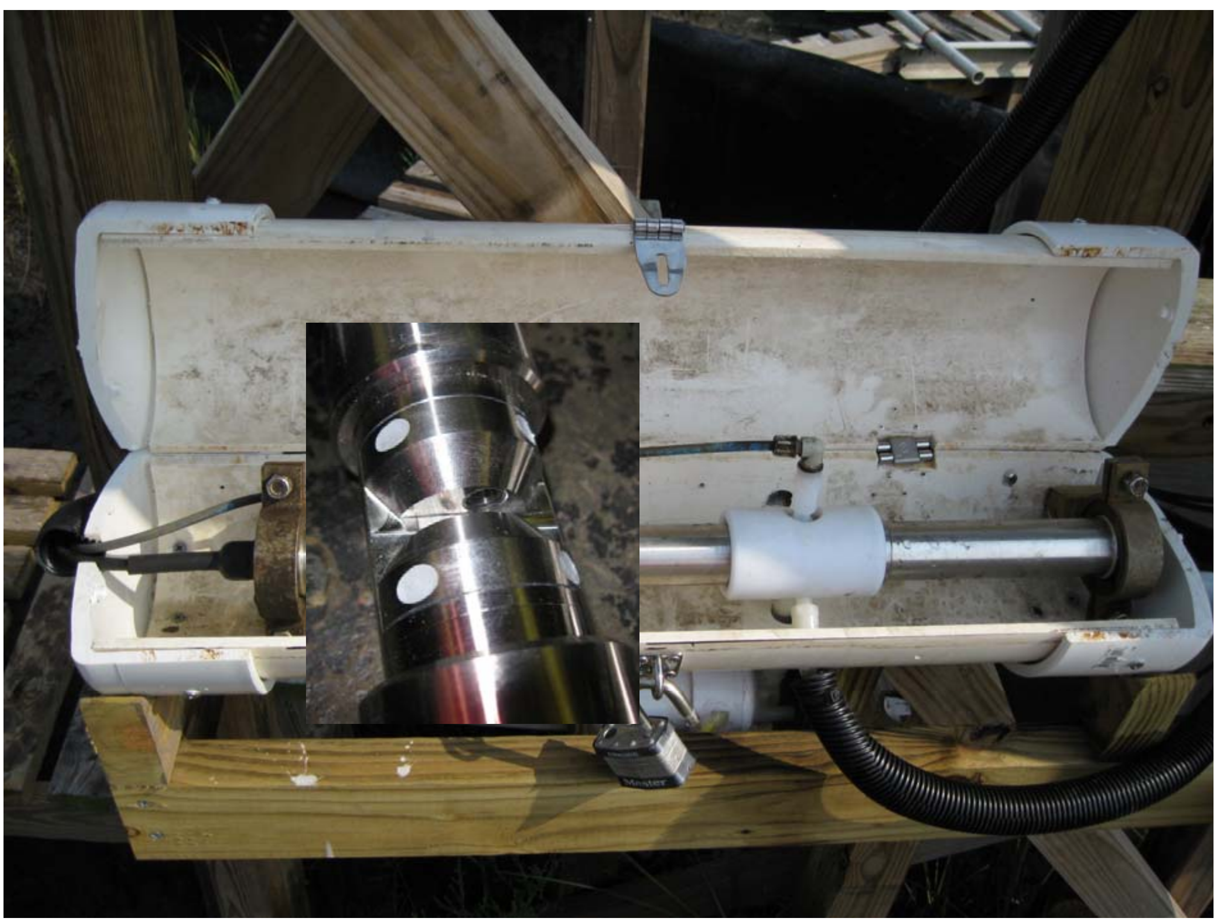
Randall Etheridge, François Birgand, Mike Burchell

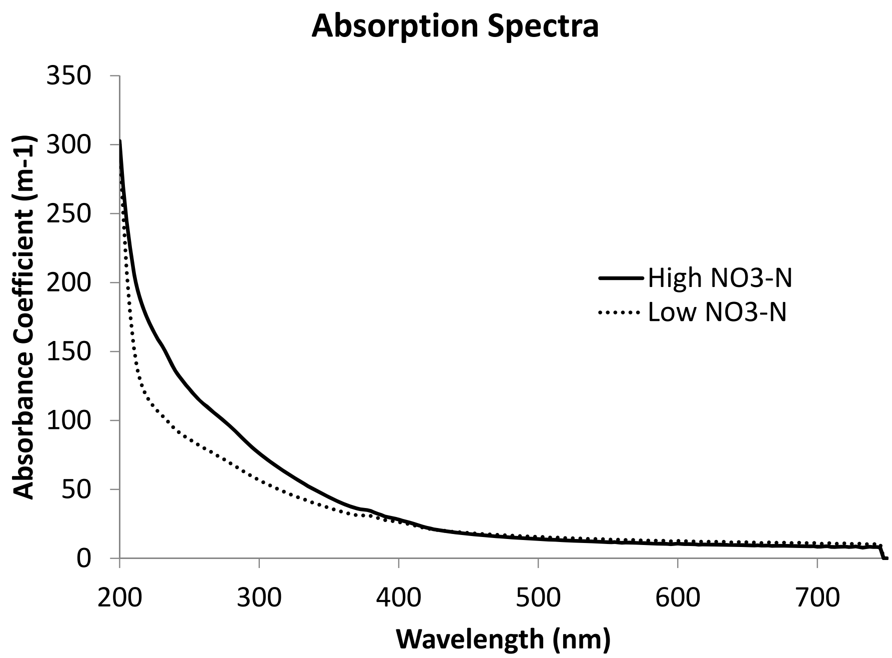
A missing legacy

- Continuous data available
  - For flow: over one century
  - For climate: decades
  - For water quality: just starting …
- Currently water quality data 2-3 orders of magnitude less frequent than e.g. flow data
- Could new sensors be the beginning of a new legacy?

UV-Vis field spectrometers

- Measure absorbance of light in water from the UV to the visible range
- Some constituents like nitrate, Dissolved Organic Carbon (DOC) and particles absorb light





Parameters known to be measurable

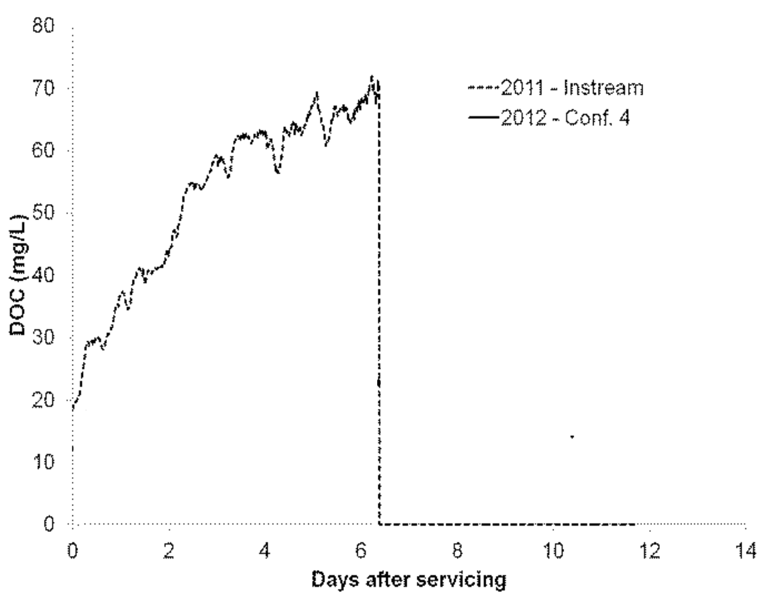
- Nitrate: absorbs light from 190 to 250 nm
- DOC: absorbs light from ~270-295 nm
- Turbidity

- Others parameters of interest:
  - NH4, ON, PO4, TP, salinity, SO4, etc.
- Theoretical reasons why UV-vis spectroscopy would not be able to measure those?

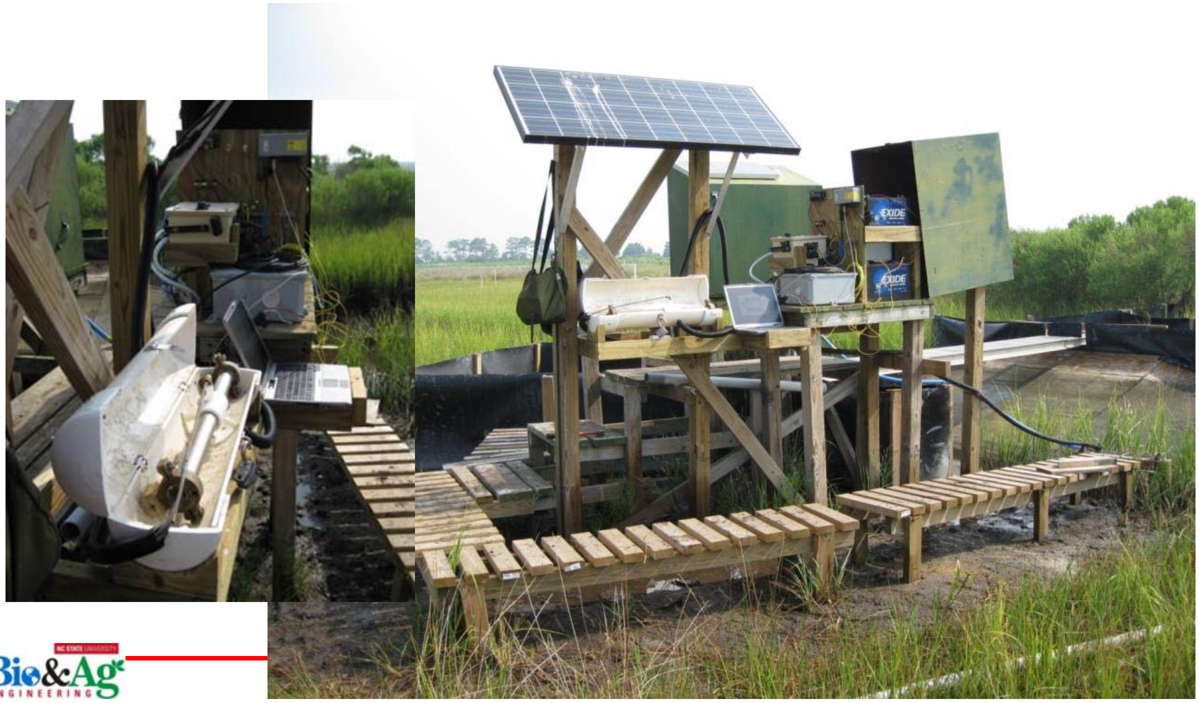
Dirty little secret…

Two Weeks Later

Fouling…



Anti-fouling system



Journal of Environmental Quality SHORT COMMUNICATIONS

Addressing the Fouling of In Situ Ultraviolet-Visual Spectrometers Used to Continuously Monitor Water Quality in Brackish Tidal Marsh Waters

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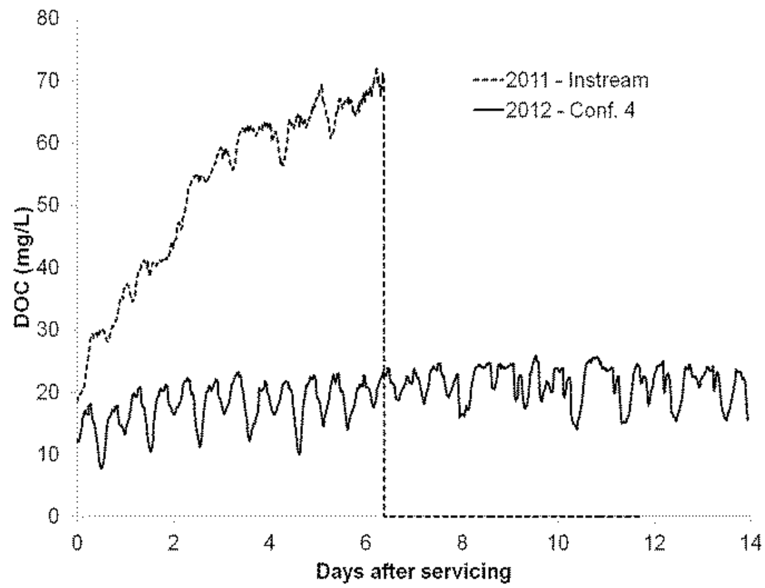
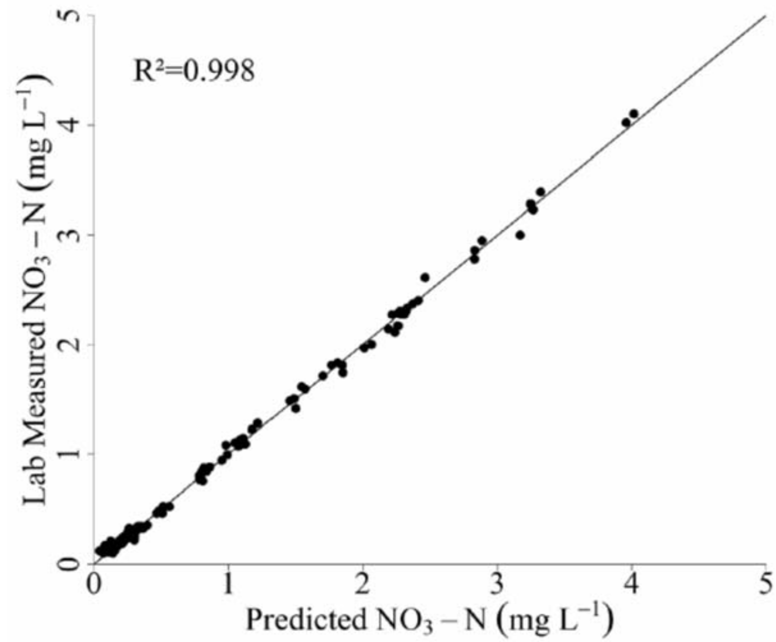
Fouling…



Breaking the manufacturers code

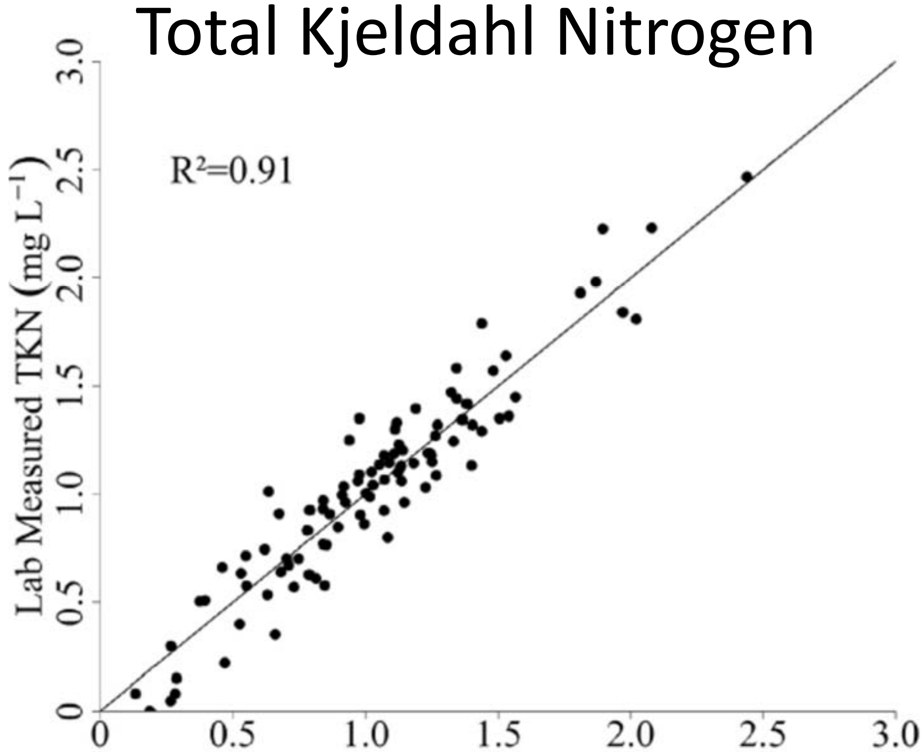
- Manufacturers have created algorithms able to calculate concentrations
- Relatively simple to require affordable computational capabilities
- Use chemometrics to create regressions between absorbance and concentrations
- Main tool: Partial Least Square Regression (PLSR)

Nitrate



F. Birgand

Total Kjeldahl Nitrogen



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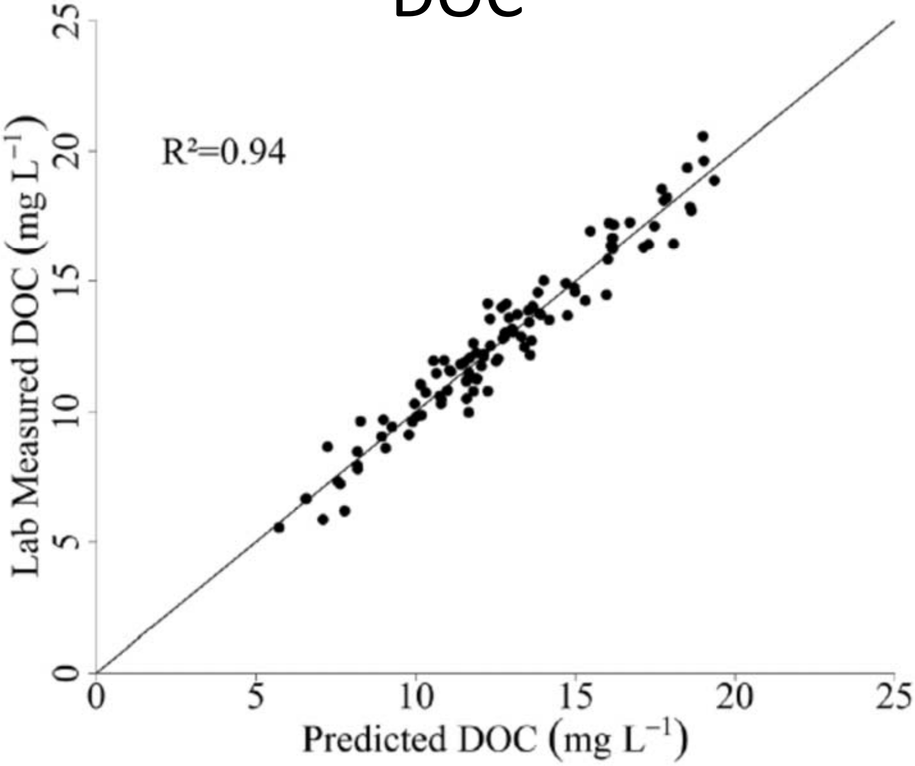
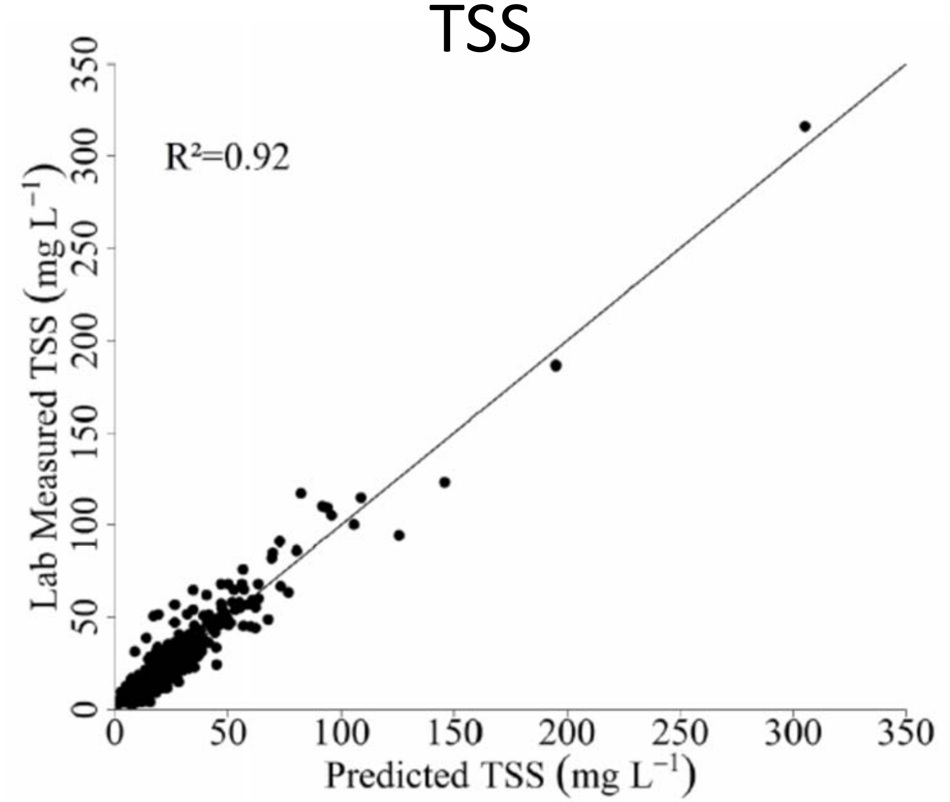
DOC



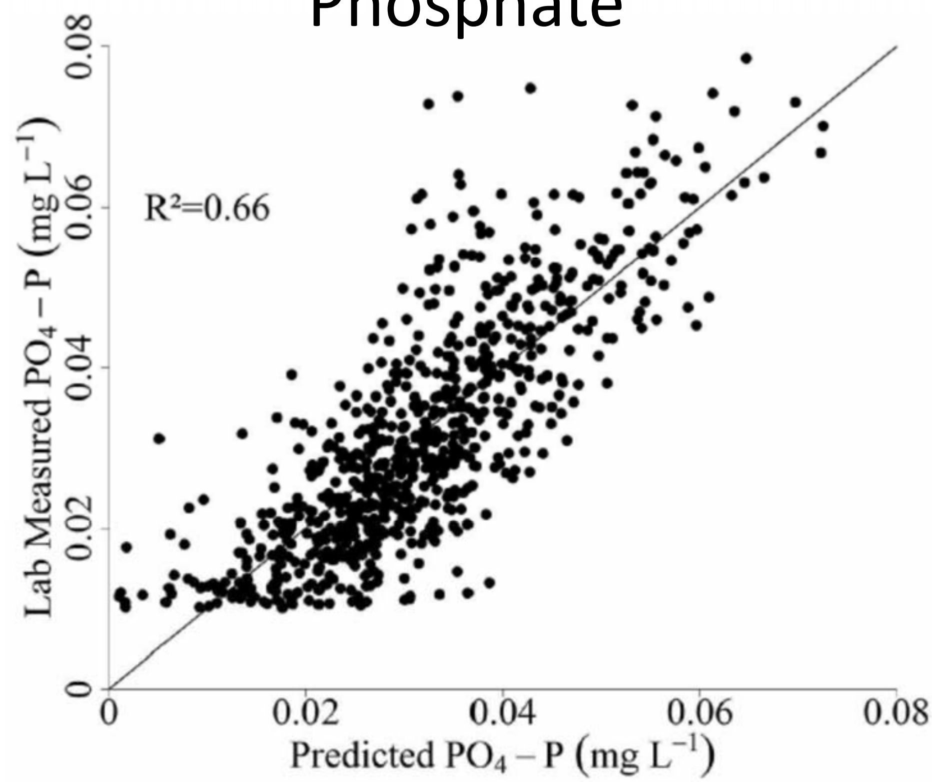
F. Birgand

TSS

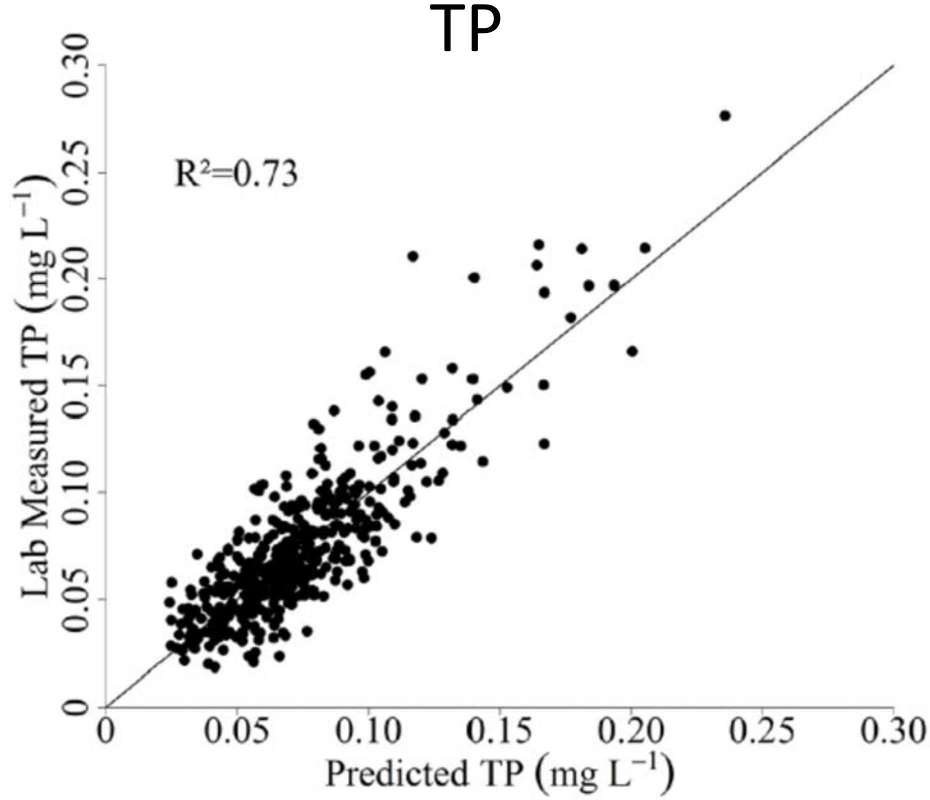


F. Birgand

Phosphate



TP



Parameter	Calibration method	R^2	RMSEP	*Nb Comp*
NO_3-N	PLSR3	0.998	(0.10)	*14*
TKN	PLSR + FDOM3	0.91	(0.27)	*10*
DOC	PLSR + FDOM2	0.94	(1.3)	*13*
TSS	PLSR1	0.92	(7.3)	*6*
PO_4-P	PLSR2	0.66	(0.010)	*18*
TP	PLSR3	0.73	(0.024)	*14*
Salinity	PLSR3	0.97	(1.8)	*12*

What we were able to find

- Absorbance and/or covariability between concentrations and absorbance: more parameters predicted
- The code is available for all to use: create local calibration
- Needs to be tested for many other areas and several path lengths and concentration levels

LIMNOLOGY and OCEANOGRAPHY: METHODS

Limnol. Oceanogr.: Methods 12, 2014, XX–XX

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Questions?