Hyperspectral Visible Derivative Spectroscopy for compositional analysis of CPAs in aquatic systems

Dr. Joseph Ortiz (jortiz@kent.edu), Kent State University

Department of Geology

Algal bloom on Lake Erie September 3, 2011

(AGU Blogopshere)

Thanks to…

Funding :

- Old Woman Creek NERR, Ohio Sea Grant, NASA Glenn

Research Access:

- USGS, Ohio EPA, NOAA, ODNR Watercraft Division, Cleveland Water

Collaborators:

- NASA Glenn, OhioView Institutions
- Donna Witter, Sapphire Geoscience Informatics
- Khalid Adem Ali, College of Charleston
- Sushma Parab, KSU Postdoc
- Nick Tufillaro and Curtis Davis
  - Hyperspectral Imager for Coastal Oceanography (HICO) Oregon State University
- Mandy Razzano, Ohio EPA
- Students: N. Bonini, R. Craine, J. Sadallah, N. Wijikoon, D. Fuecht and others

Growing Water Quality Concerns in Lake Erie

- Lake Erie is once more increasingly plagued by toxic algal blooms (CyanoHABs)
- Reduce oxygen levels and cause unwanted taste, color, and odor
- Researchers are looking for ways to monitor, assess, and predict algal blooms

August, 2014

Grand Lake St Marys (photo J. Ortiz)

Photo: J. Ortiz

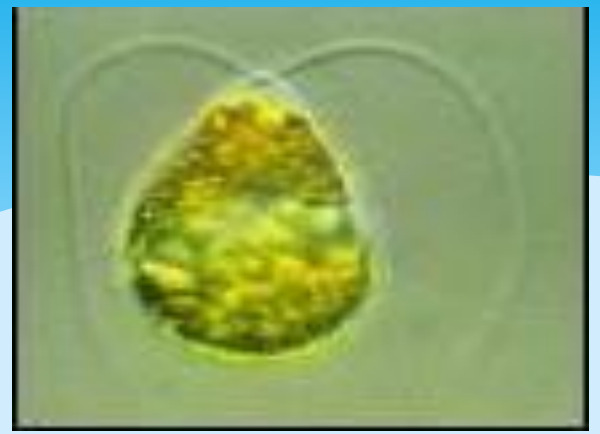
The problem…

- Remote sensing of lake color gives information on plant biomass, but…

- Lake water is a complex "organic soup"
  - Various types of phytoplankton
  - Colored dissolved organic matter
  - Suspended sediment

All natural samples are mixtures!

Spectral identification of phytoplankton from space

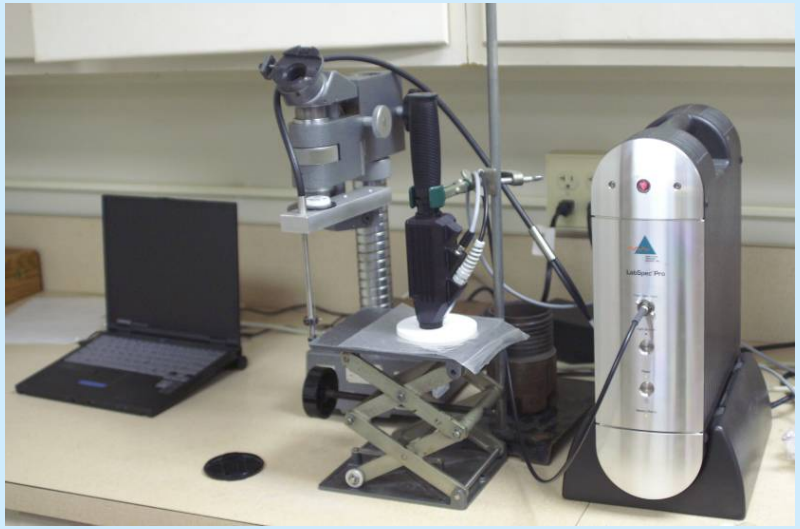


- Different types of phytoplankton have different pigments.
- Pigments have specific absorption and reflectance patterns
- Spectral shapes can be used to identify different algal phyla
- Capitalizes on all information available in hyperspectral-resolution spectra
- But, must <u>unmix</u> reflectance spectra

Graphics: Courtesy of NASA/GSFC.

Our Approach

- Goal: Quantify the relationship between phytoplankton pigments and phytoplankton assemblages from Field Samples, Field Spectroradiometers, Remote Sensing data
- Objectives –
  - Measure water samples by Visible Near-infrared (VNIR) derivative spectroscopy
  - Match spectral pigment assemblages to known signatures for classes of phytoplankton
  - Compare pigment assemblages to measures of concentration in the lake (chl a, degradation products of chl a and other pigments).



Varimax-rotated Principal Component Analysis (VPCA)

- VPCA is a multivariate statistical technique for extracting important information regarding the dataset.
- This method lets us "***unmix***" the data!
- We can use VPCA to determine in-water constituents (pigments, clays, iron oxides, etc.) using the visible part of the spectrum.

Case Study 1: Akron Water supply

Collaboration with M. Razzano (OEPA) and D. Witter

Lab-based measurements

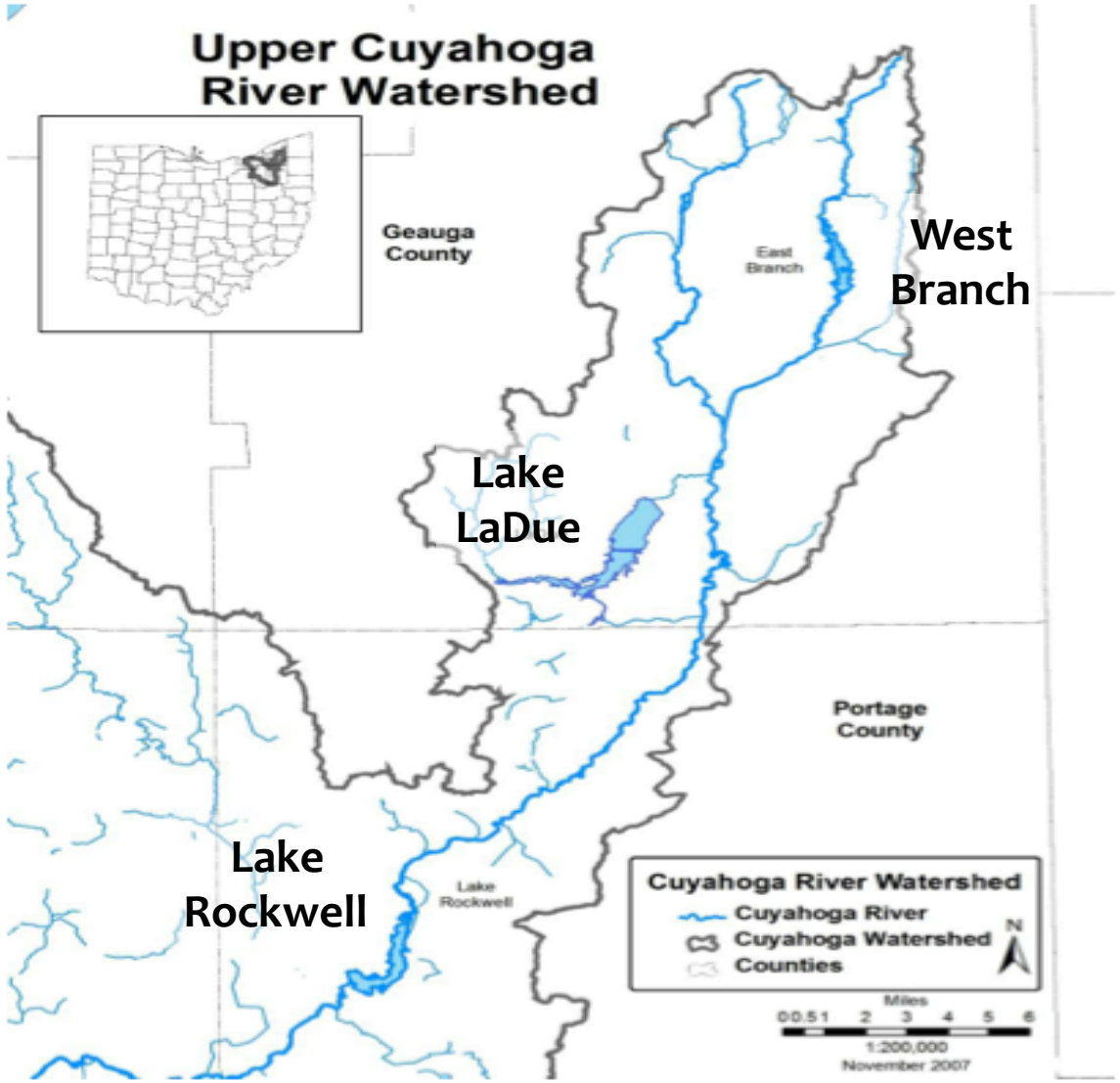
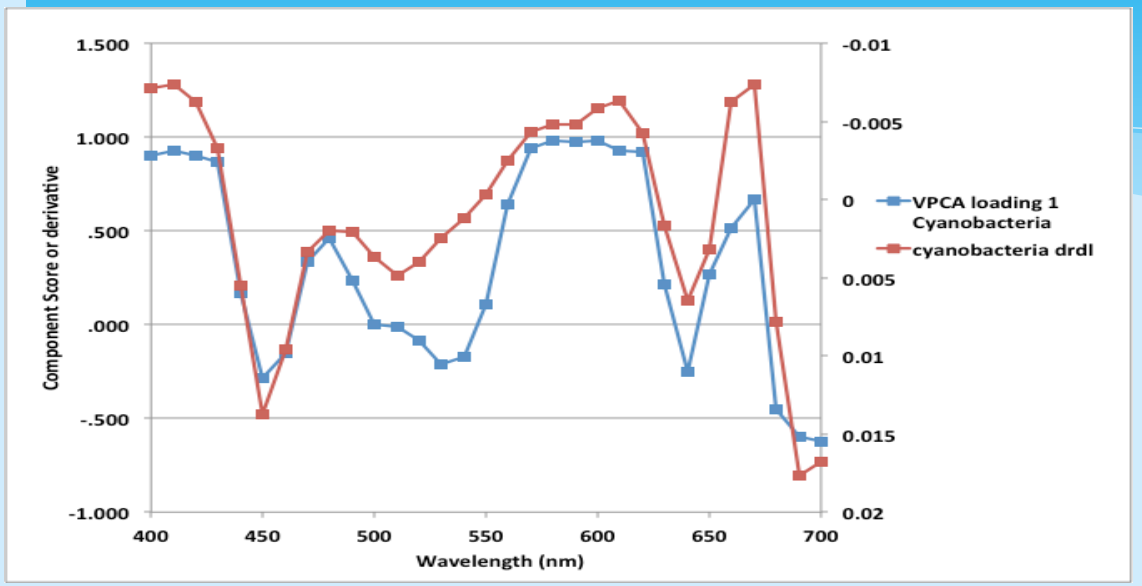
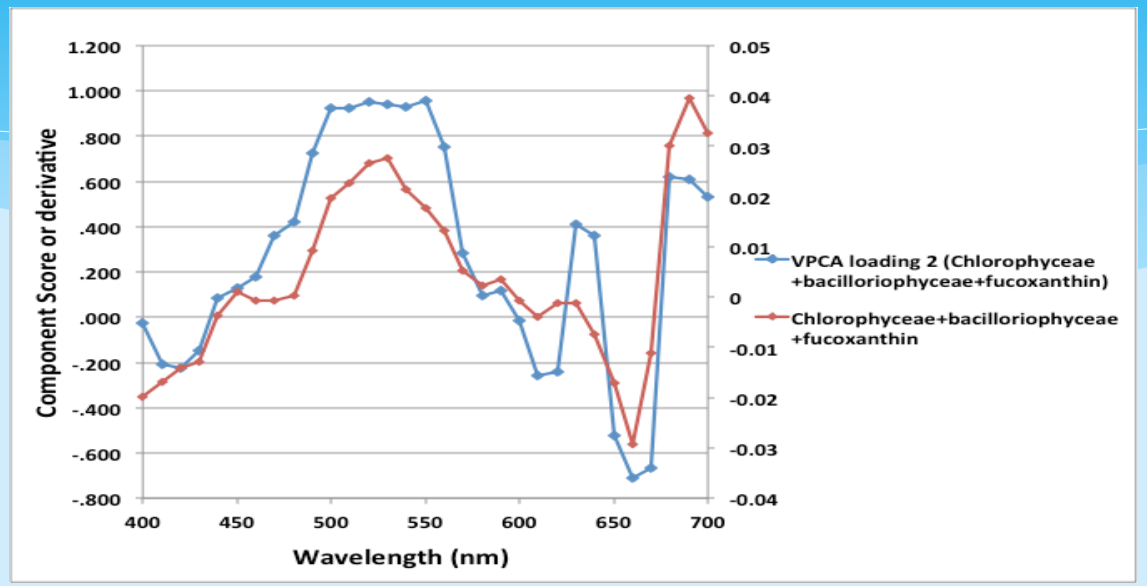
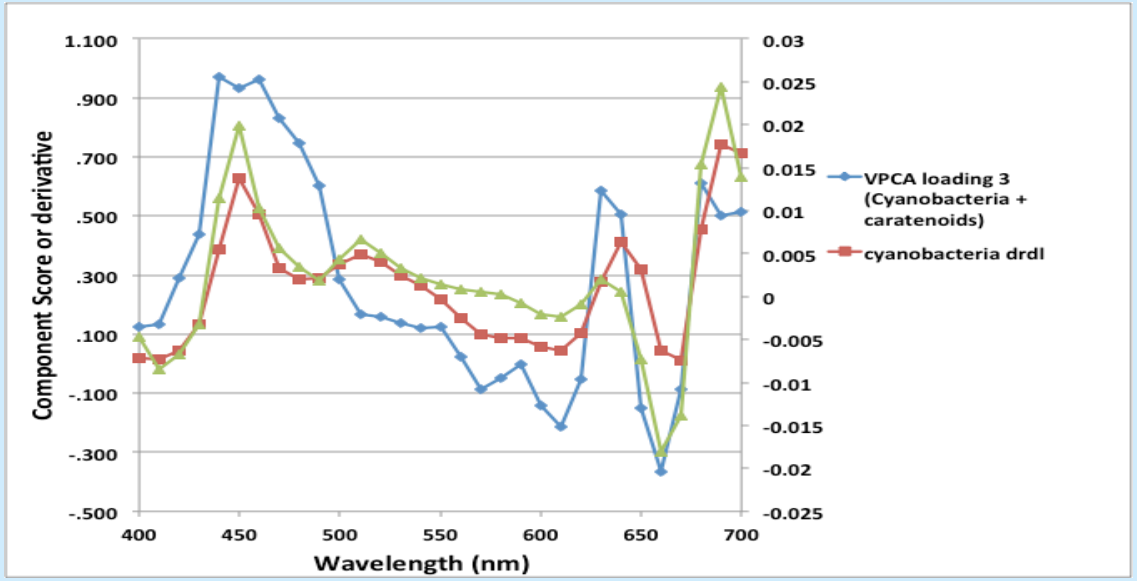


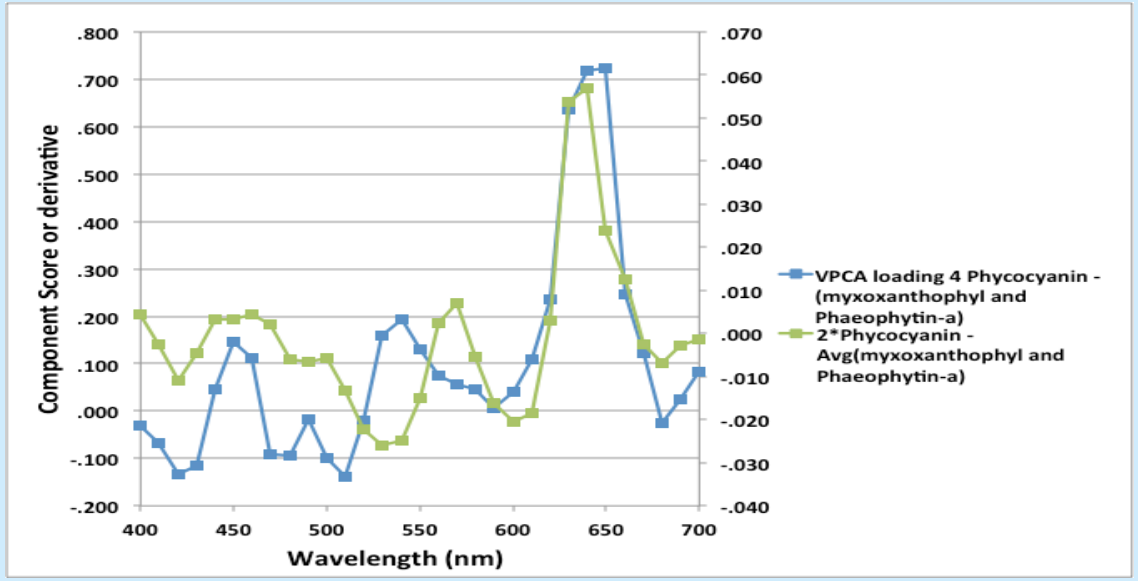
Figure1. Upper Cuyahoga River Watershed.

Pigment components in Lake Rockland, West Branch and La Due Reservoir









We can identify which types of phytoplankton are present in the pigment assemblages.

- For each sample we have:
  - Pigment assemblage information
  - Cell count assemblages

- We can "***unmix***" both of these data and compare them to see how they relate…

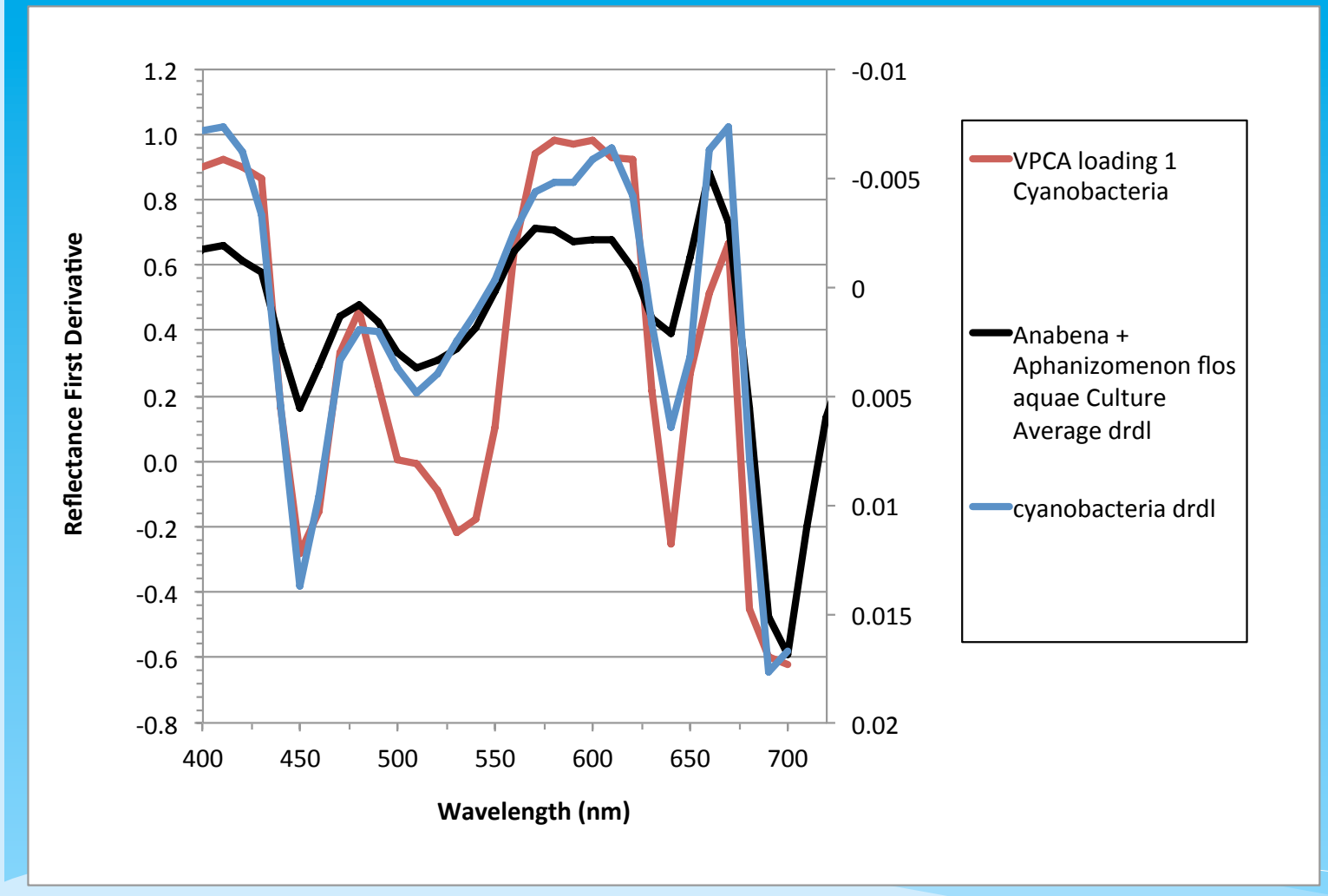
VPCA of algal data indicates Four Algal Cell Assemblages are present

Cell Grouping	Communality	Algal Component 1 (Cyanophytes)	Algal Component 2 (CyanoHAB)	Algal Component 3 (Heterokonts /Cryptophytes)	Algal Component 4 (Dinos/Flagellates)	Comments
Synedra	0.86	0.90	0.04	0.00	-0.23	Diatom blooms
Chlorophyta	0.79	-0.83	0.15	-0.03	-0.26	Green Algae
Cryptophyta	0.90	-0.25	0.36	-0.84	0.05	
Other Cyanophyta	0.97	0.73	0.64	0.15	-0.01	Other B-G algae
Dinophyta	0.73	-0.21	-0.55	0.14	0.60	
Euglenophyta	0.76	0.26	0.52	0.59	0.27	
Flagellates	0.97	0.08	0.12	-0.06	0.98	
Other Heterokonts	0.66	-0.17	0.18	0.77	-0.04	Non-bloom diatoms
Aphanizomenon&Anabaena	0.79	0.14	-0.88	-0.02	-0.01	CyanoHABs

Compare the Pigments and Cell Assemblages

Pigment Component	Cell Component	Multiple Linear Correlation	Significance level (P-value, df=1,10)
VPCA 1	Algal Component 2 (CyanoHAB)	0.83	**0.001**
VPCA 2	Algal Component 1 (Cyanophytes)	0.71	**0.010**
VPCA 3	Algal Component 4 (Dinos/Flagellates)	0.70	**0.011**
VPCA 4	Detritus	N/A	No significant correlation @ 0.050
VPCA 1-3	Algal Component 2 (CyanoHAB), Algal Component 3 (Heterokonts/Cryptophytes), Algal Component 4 (Dinos/Flagellates)	0.96	**0.022**

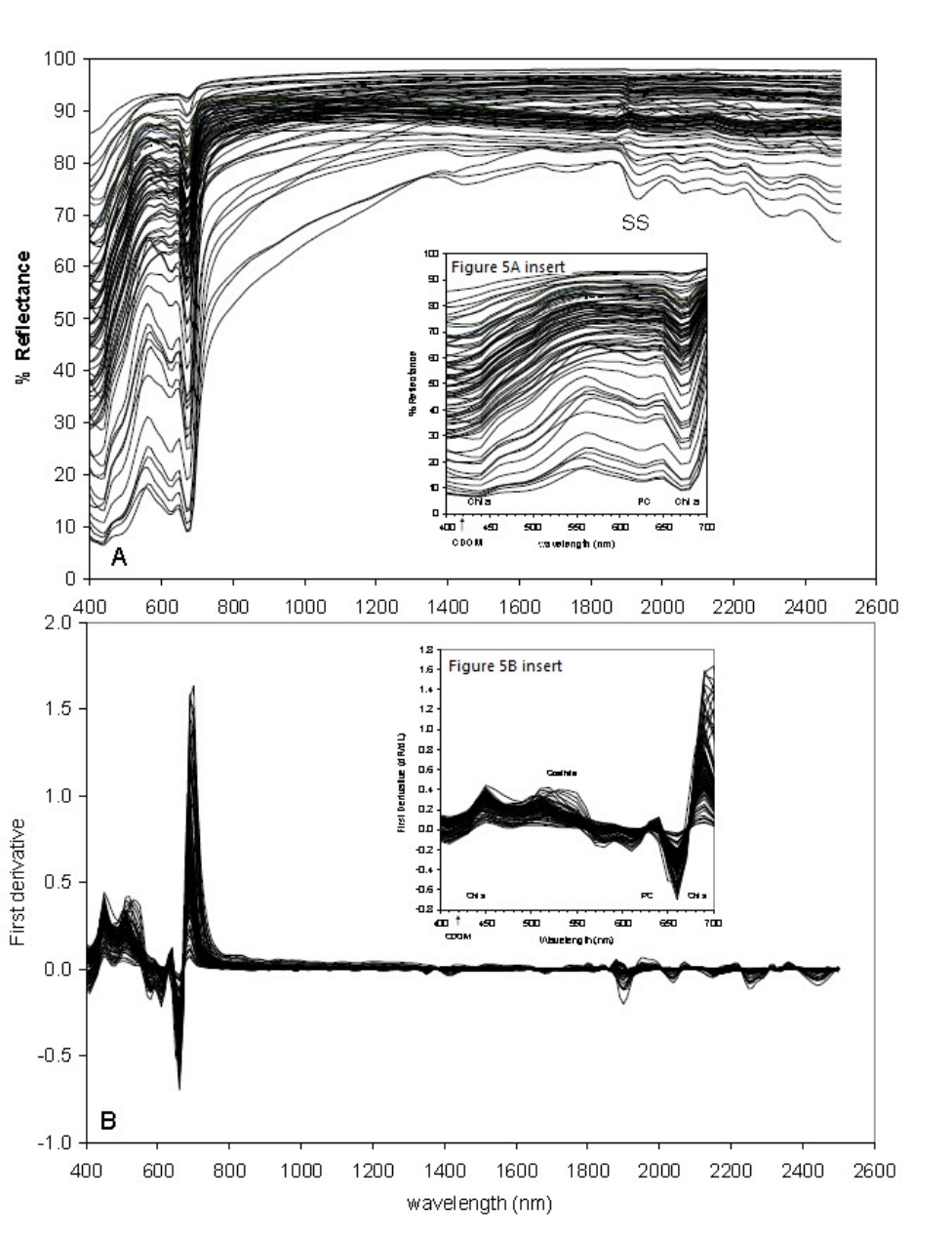
Independent corroboration



Leading component matches derivative spectrum for cultures of HAB forming *Aphanizomenon sp. and Anabena sp and a published cyanophyta spectrum*

Parab et al, unpublished data

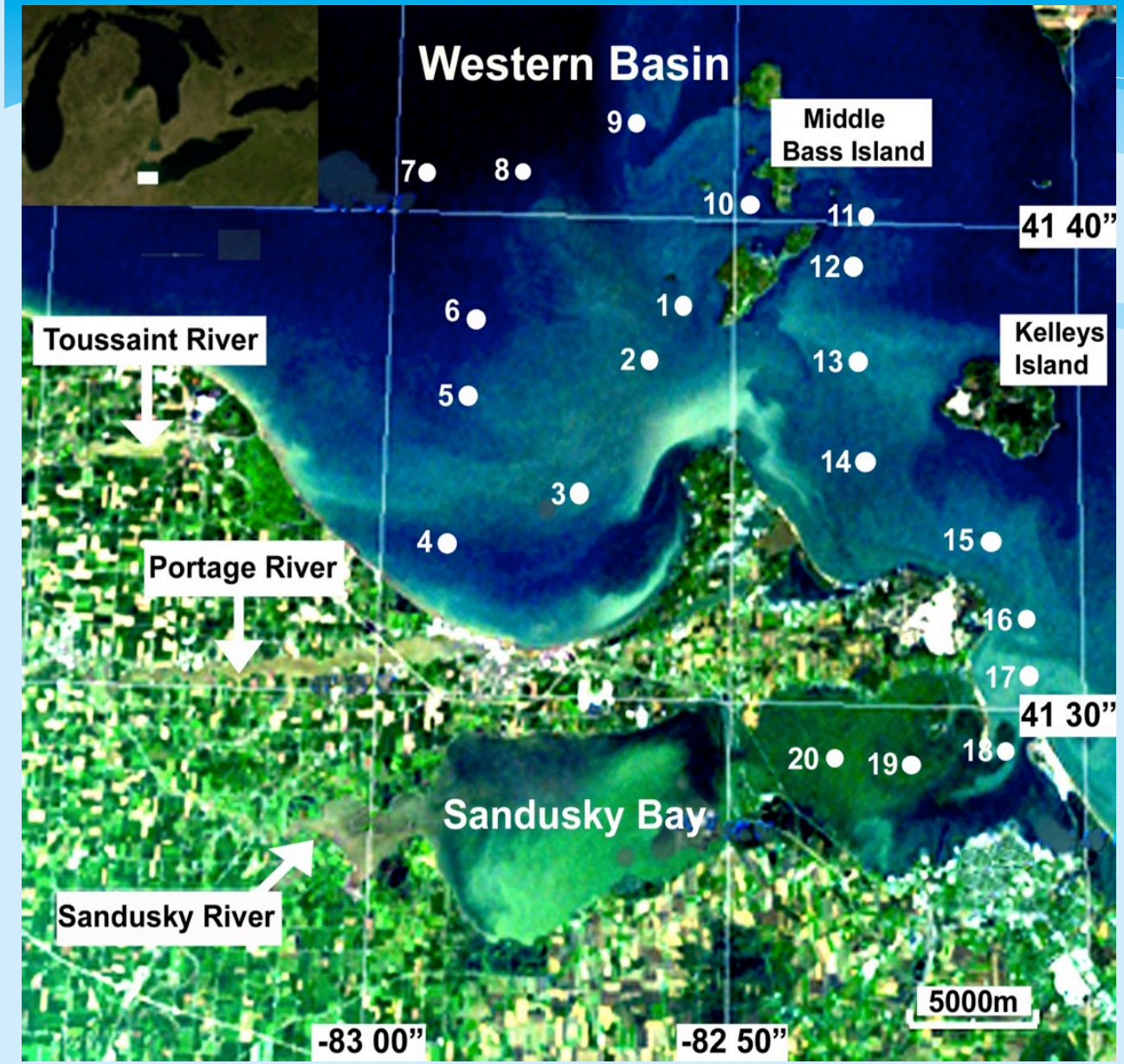
Case Study 2: 2007 and 2011 Western Basin of Lake Erie



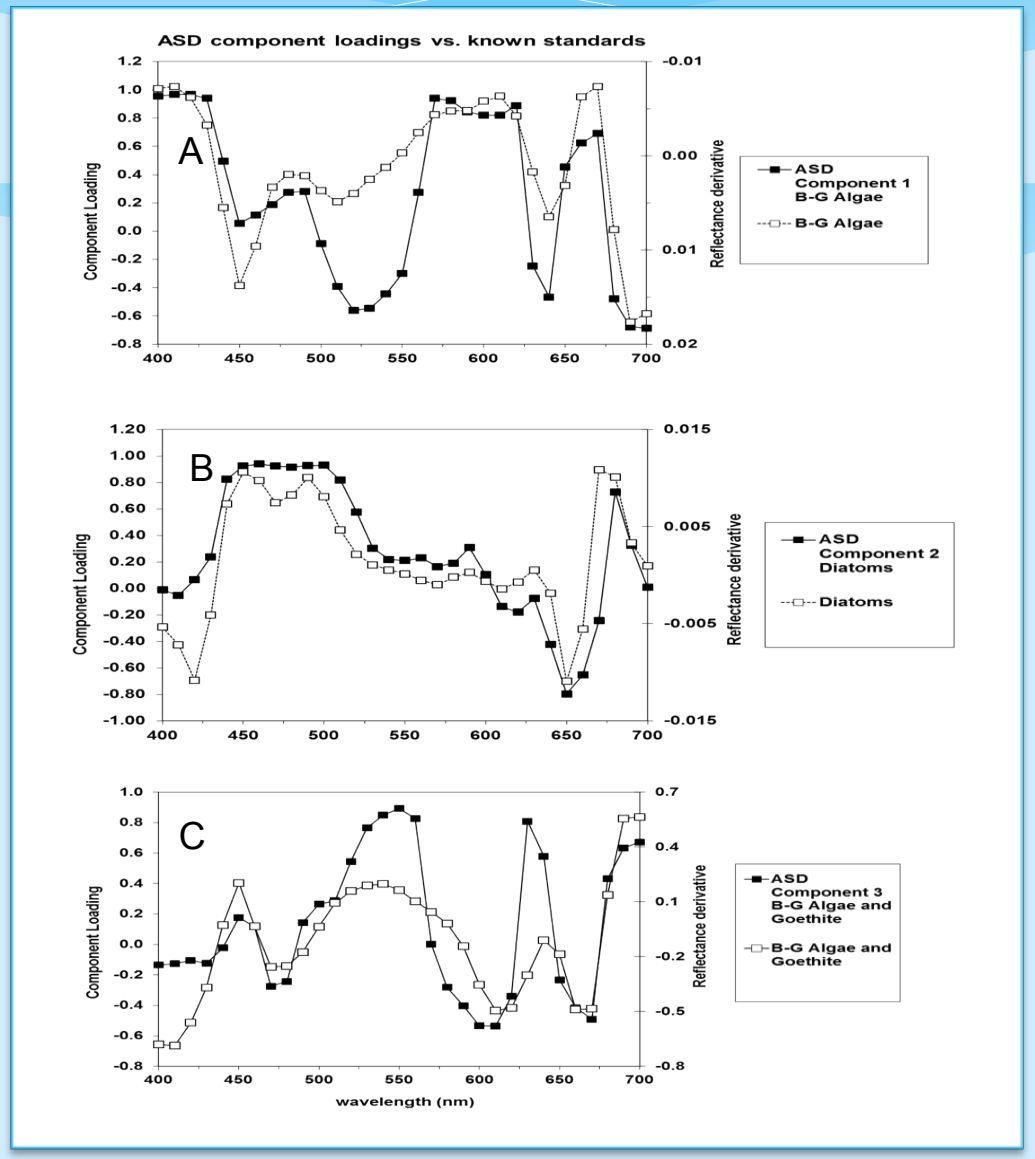
- Samples are ***mixtures*** of different color producing agents (e.g. pigments, CDOM, sediment).
- Peaks and troughs in the Reflectance data relate to different Color Producing Agents
- Derivative-transformed data accounts for scattering and particle size effects
- Still need to ***"unmix"*** or partition the data
- Compare Components from Field samples with HICO components

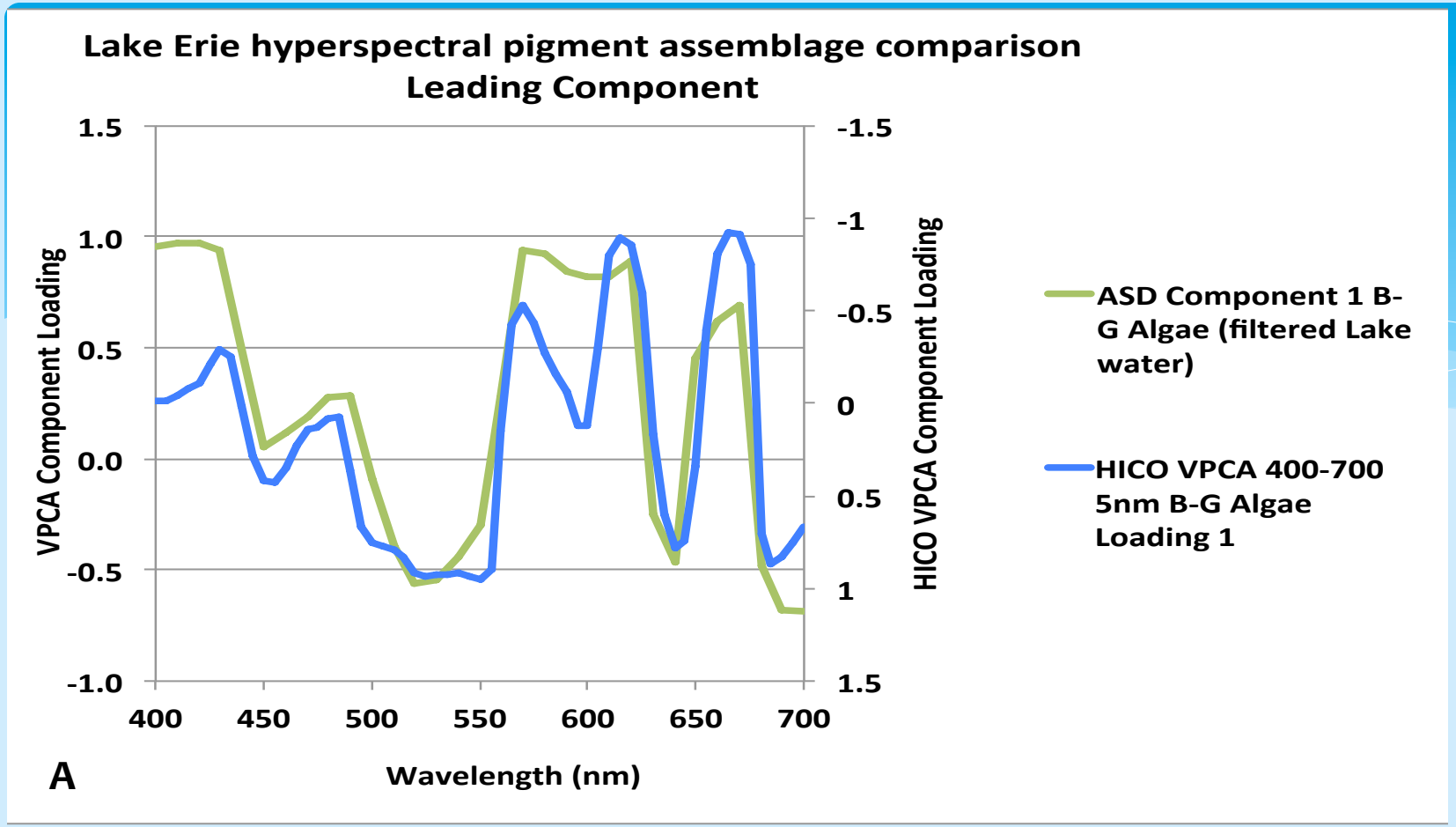
Ortiz et al. (2013)

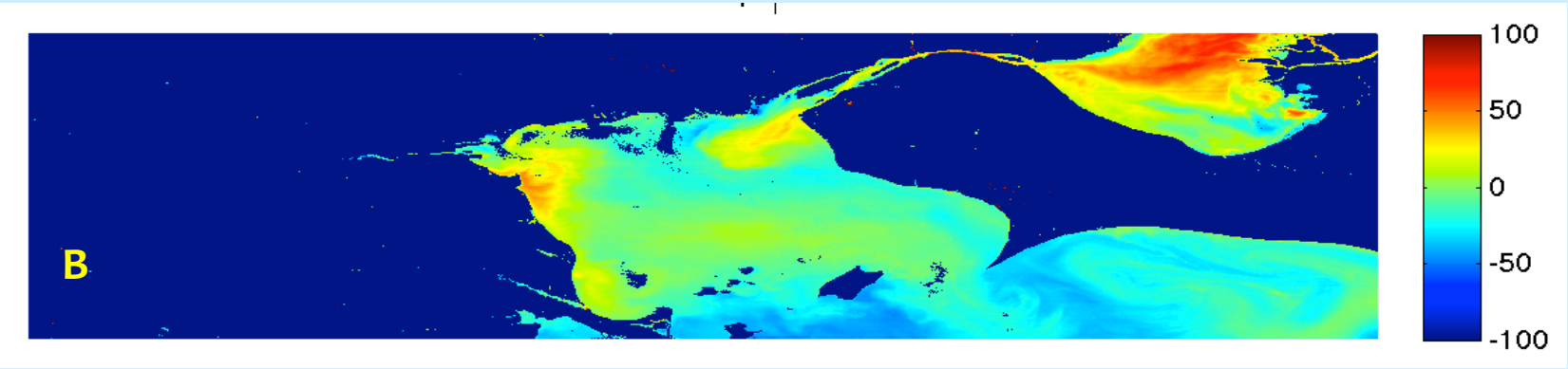
Lab Measurements from 2007 Field Samples



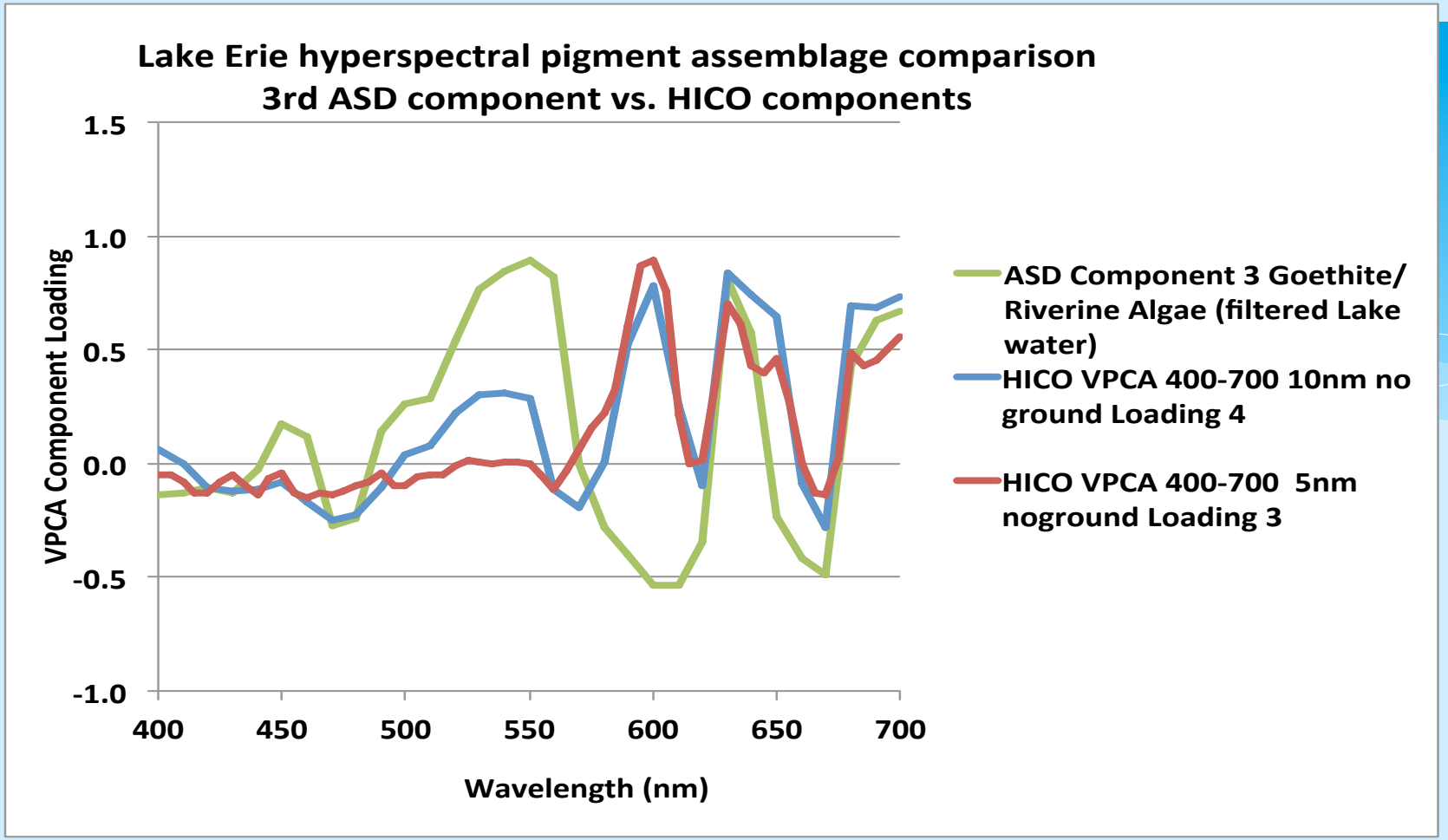
Ortiz et al. 2013



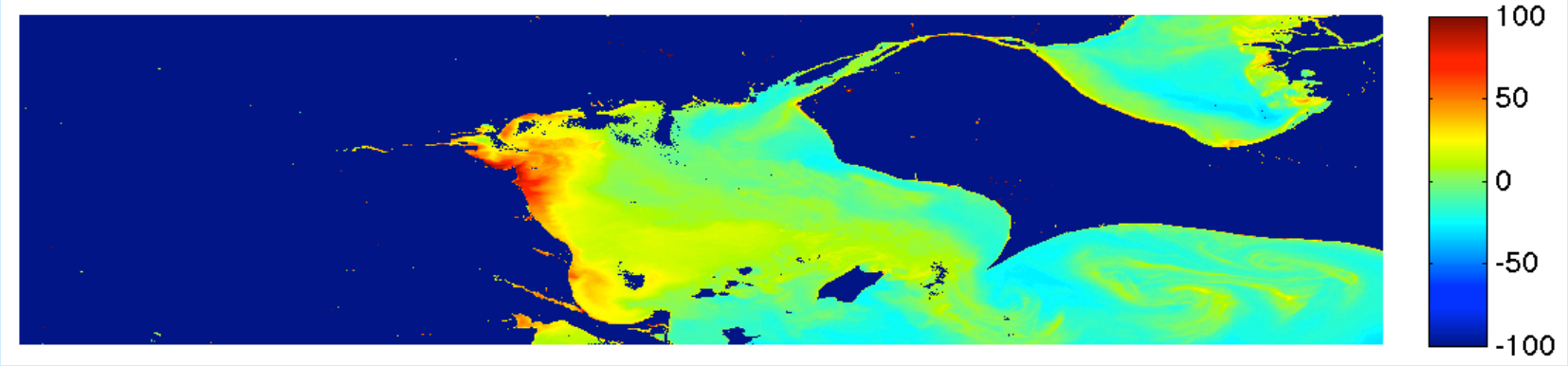




2007 field results (green) vs. HAB-forming Blue-Green Algae Component extracted from HICO image 9-3-11

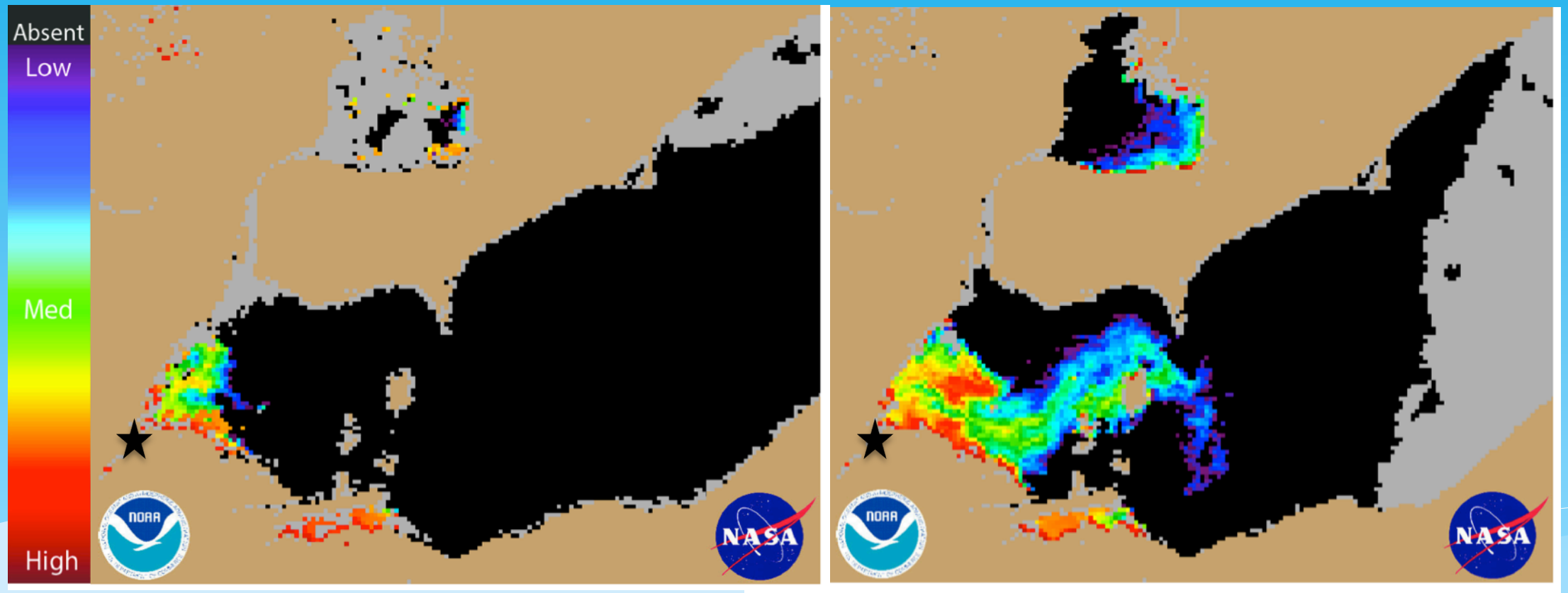


2007 field results (green) vs. Non-HAB Blue-Green Algae Component extracted from HICO image 9-3-11



Case study 3: Western Basin CyanoHAB during the 2014 Toledo Water Shutdown (1 Aug 2014)

31 July 2014 **3 August 2014**



Source: NOAA Experimental Lake HAB Bulletin
(http://www.glerl.noaa.gov/res/Centers/HABS/lake_erie_hab/lake_erie_hab.html)

Field sampling from many lakes and different vessels


ODNR watercraft


Pontoon boat

RV Bowfin: USGS-LEBS

Commercial Fishing boat

RV Muskie: USGS-LEBS

Photos: J. Ortiz

Measuring with the ASD FieldSpec HH Spectroradiometer


Photo: L. Liou


Photo:
L. Liou


Photo: L. Liou

Collecting water samples at Grand Lake St. Marys

- Field and Remote Sensing radiometric data is compared with water samples
- Determine how much algae, sediment and dissolved material is in the water
- Measure chemical properties

Photos: J. Ortiz

NASA Glenn S3 Viking Research Aircraft

- Converted US Navy Submarine chaser aircraft
- Equipped with a high resolution, imaging radiometer (NASA Glenn HSI) similar to satellite-based instruments
- Quantifies the color of the surfaces that the sensor images

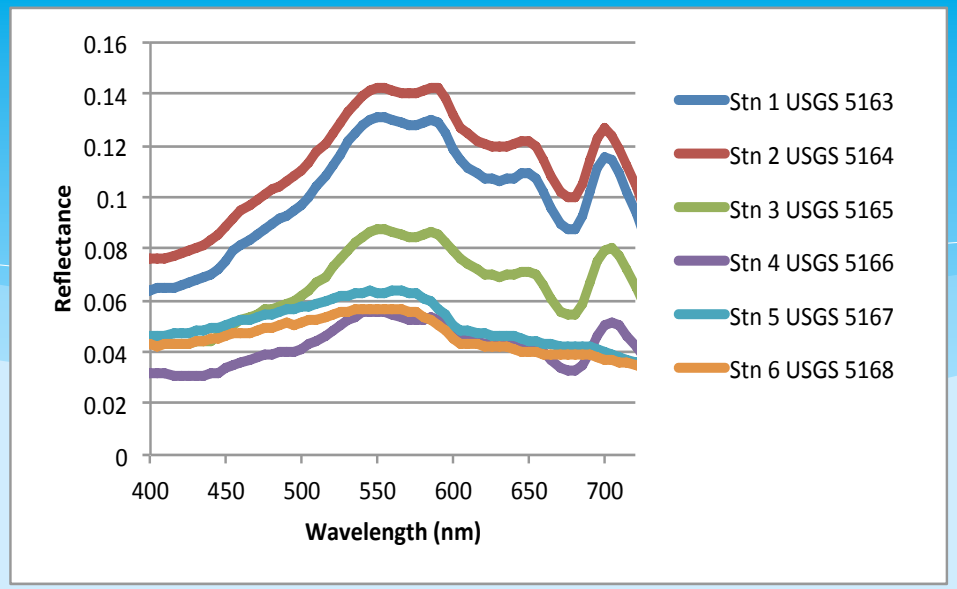

Source: NASA Glenn

Photos: J. Ortiz

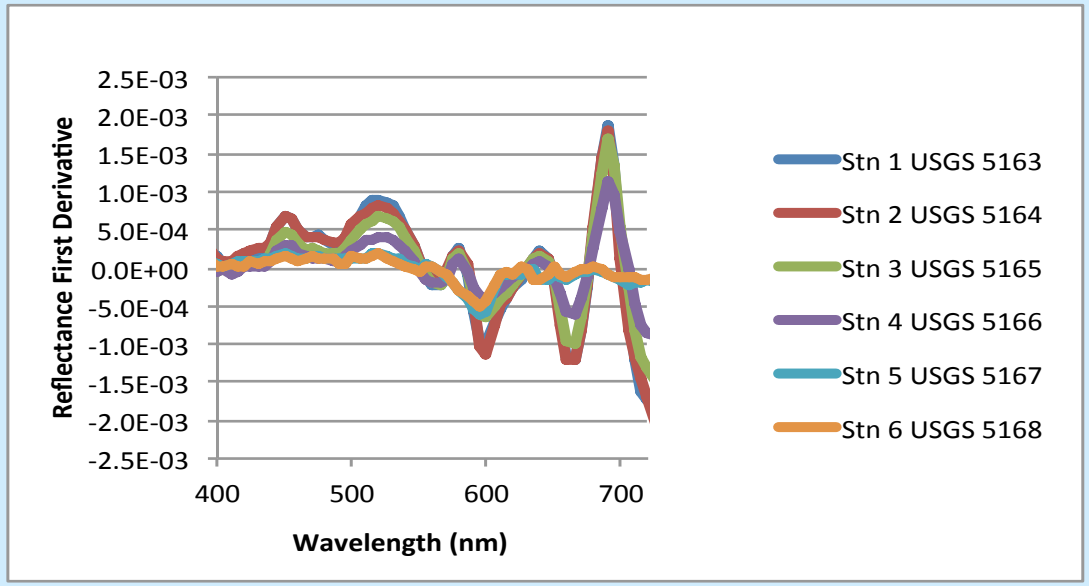
Example data: 8-12-14 USGS CSMI sampling

- Samples collected from 24’ Boston Whaler
- Winds 10-15 NW, overcast with scattered rain showers
- Samples collected at three paired stations in Maumee Bay

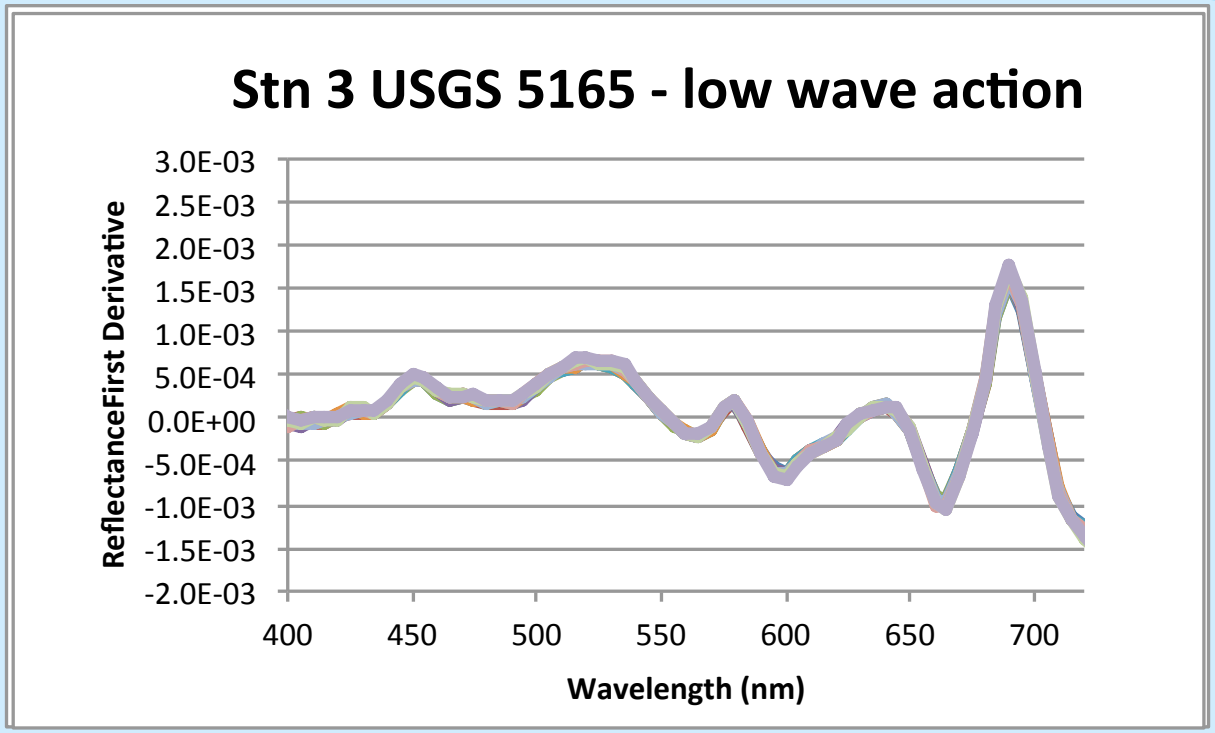
Reflectance vs. First Derivative spectra

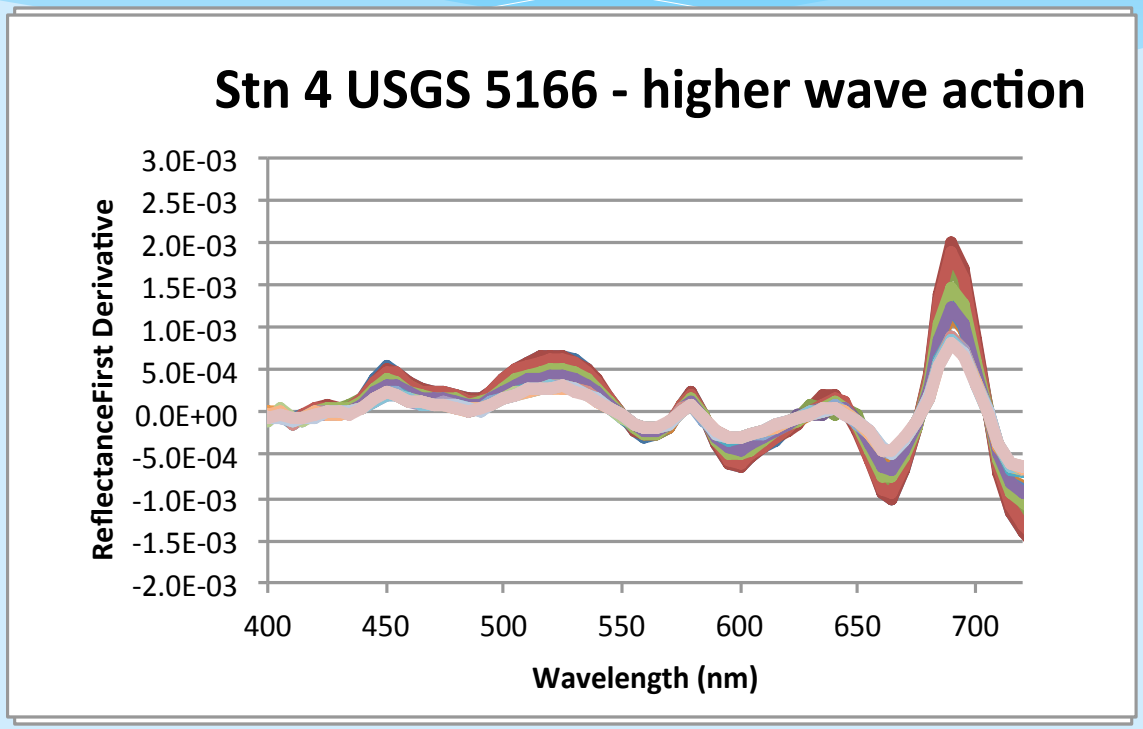


- Reflectance spectra are sensitive to directional quality of the light affected by
  - Solar viewing angle
  - Sun glint
- Problem is accentuated for non-Lambertian surfaces
- Derivative spectra are less sensitive to these problems.



Influence of wave action on reflectance and first derivative spectra

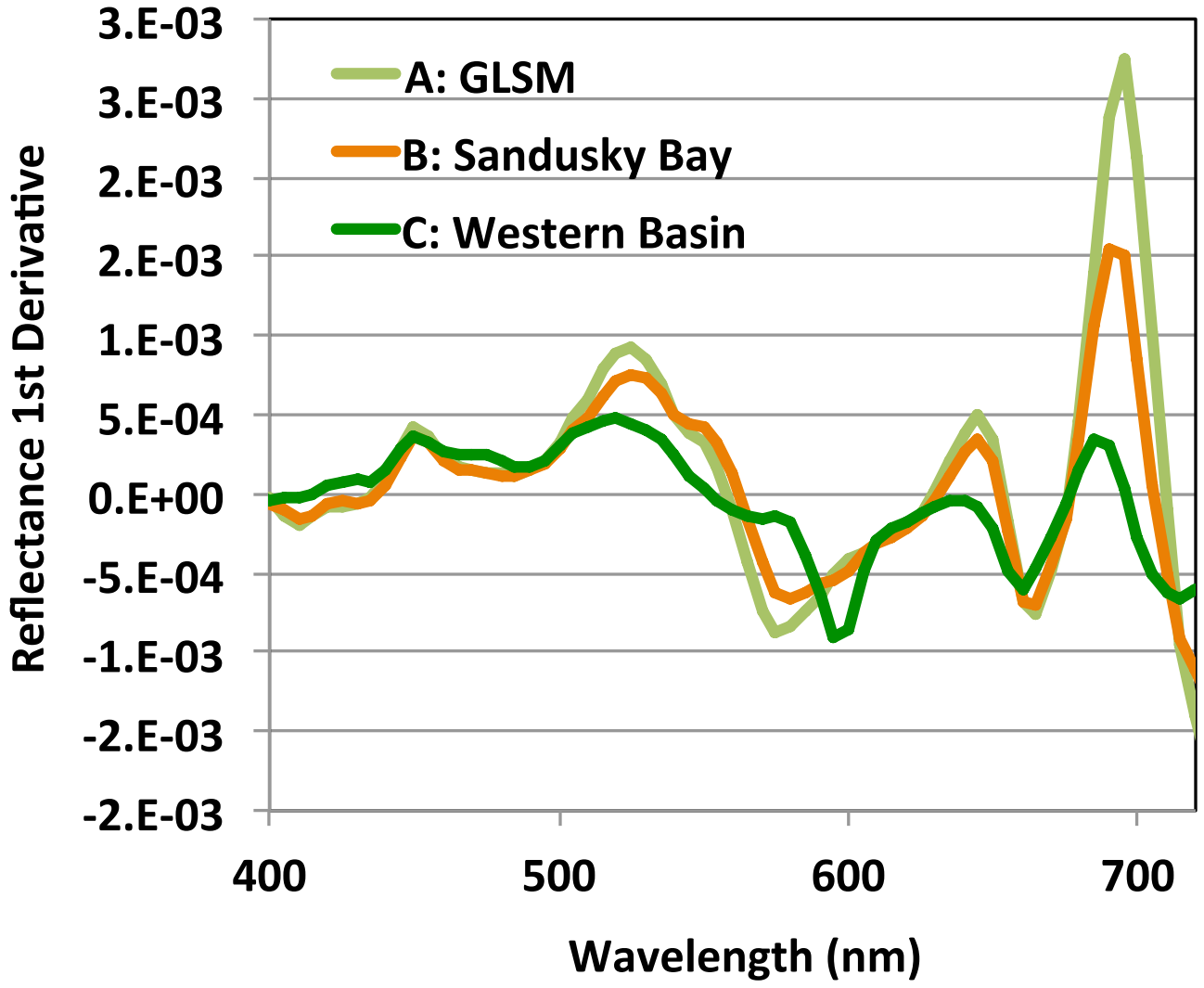




At each site averaged 2-3 sets of 10 replicates with 30 spectra per replicate
Integration time at 10's of milliseconds

Spectral derivative signatures of different lakes

A:



rtiz

Summary

- VNIR derivative spectroscopy quantifies plant pigment assemblages in Case 2 aquatic systems (Akron Reservoirs, Lake Erie, OWC)
- VNIR derivative spectroscopy helps address non-Lambertian scattering effects
- Ties optical assemblages to phytoplankton phyla
- Developing a new means of tracking phytoplankton impacts on eutrophication, with implications for anoxia and harmful algal blooms
- Method can be applied to lab samples, field-based spectroradiometers, Remote Sensing data
- Well suited for application to HyspIRI: Makes use of all information present in hyperspectral spectra

Recent Publications

- See Water quality webpage at: http://www.personal.kent.edu/~jortiz/home/wqr.html

- Ali, K.A., and **J.D. Ortiz**, Multivariate approach for chlorophyll-a and suspended matter retrievals in Case II waters using hyperspectral data, Hydrological Sciences Journal, 2014. DOI 10.1080/02626667.2014.964242.
- **Ortiz, J.D.,** Witter, D.L., Ali, K.A., Fela, N., Duff, M., and Mills, L., Evaluating multiple color producing agents in Case II waters from Lake Erie, International Journal of Remote Sensing, 34 (24), 8854-8880, 2013.
- Mou, X, Jacob, J., Lu, X., Robbins, S., Sun S., **J.D. Ortiz.** Diversity and distribution of free-living and particle associated bacterioplankton in Sandusky Bay and adjacent waters of Lake Erie Western Basin, Journal of Great Lakes Research 2013.
- Ali, K.A., Witter, D.L., and **J.D. Ortiz**, Application of empirical and semi-analytical algorithms to MERIS data for estimating chlorophyll a in Case waters of Lake Erie, Environmental Earth Sciences; DOI 10.1007/s12665-013-2814-0, published Oct 1, 2013.
- Ali, K.A., Witter, D.L., and **J.D. Ortiz**, 2012, Multivariate approach to estimate color producing agents in Case 2 waters using first-derivative spectrophotometer data, Geocarto International, Early online release: 10/30/2012 DOI:10.1080/10106049.2012.743601.
- Witter, D., **Ortiz, J.D.**, Palm, S. Heath, R., Budd, J., Assessing the Application of SeaWiFS Ocean Color Algorithms to Lake Erie, Journal of Great Lakes Research, 35, 361-370, 2009.