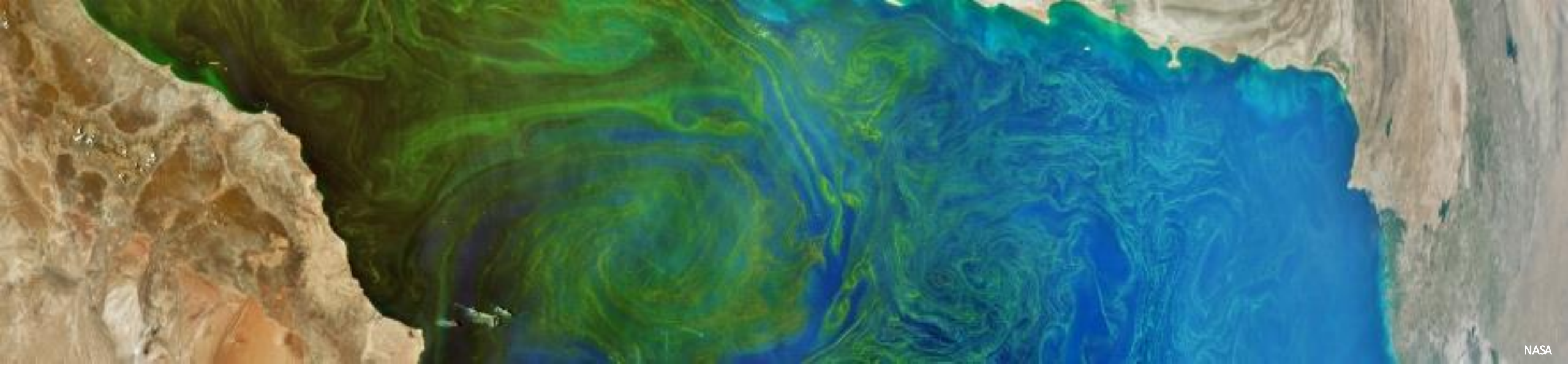


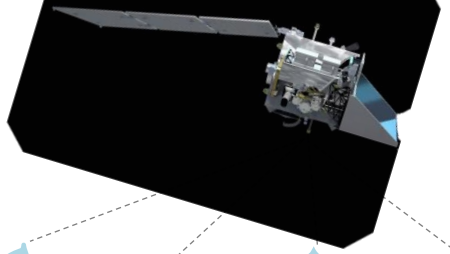
Global phytoplankton community composition from hyperspectral ocean color

Sasha J. Kramer

sjkramer@bu.edu

SEPTEMBER 24, 2025

Goals for today



1) Model surface ocean phytoplankton pigments from hyperspectral $R_{rs}(\lambda)$

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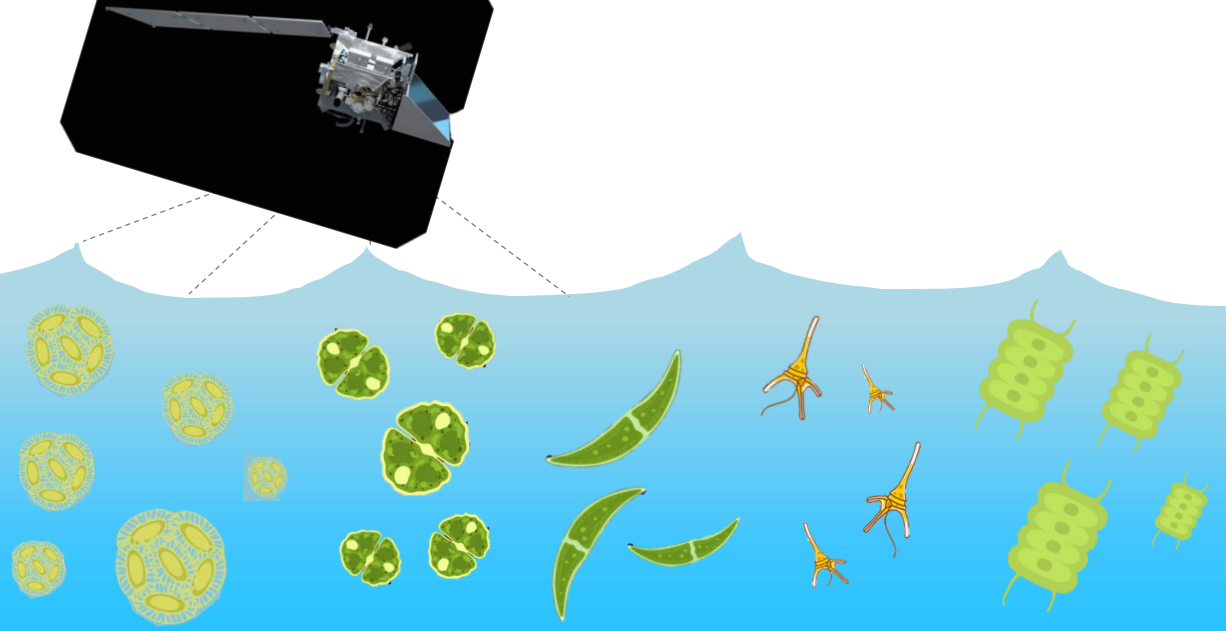
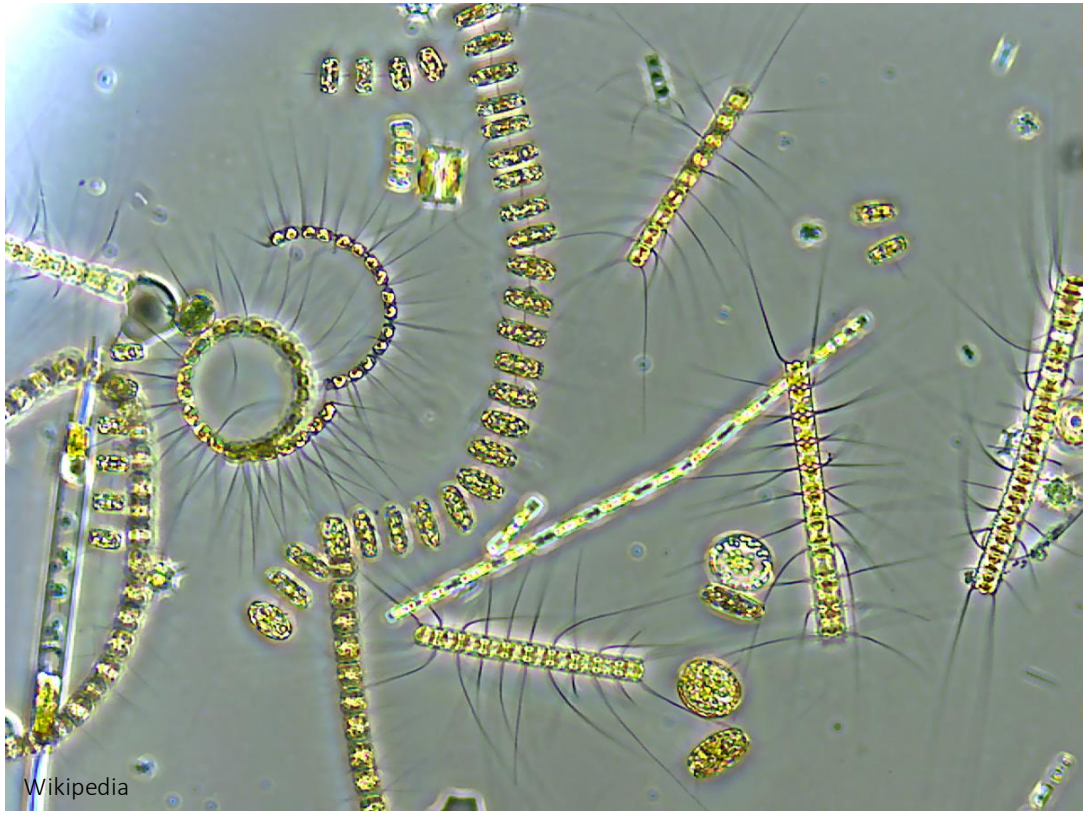


1) Model surface ocean phytoplankton pigments from hyperspectral $R_{rs}(\lambda)$

2) Compare the composition and distribution of communities derived from phytoplankton pigments and from hyperspectral $R_{rs}(\lambda)$

A fundamental challenge when describing phytoplankton communities

Phytoplankton are microscopic…



Wikipedia

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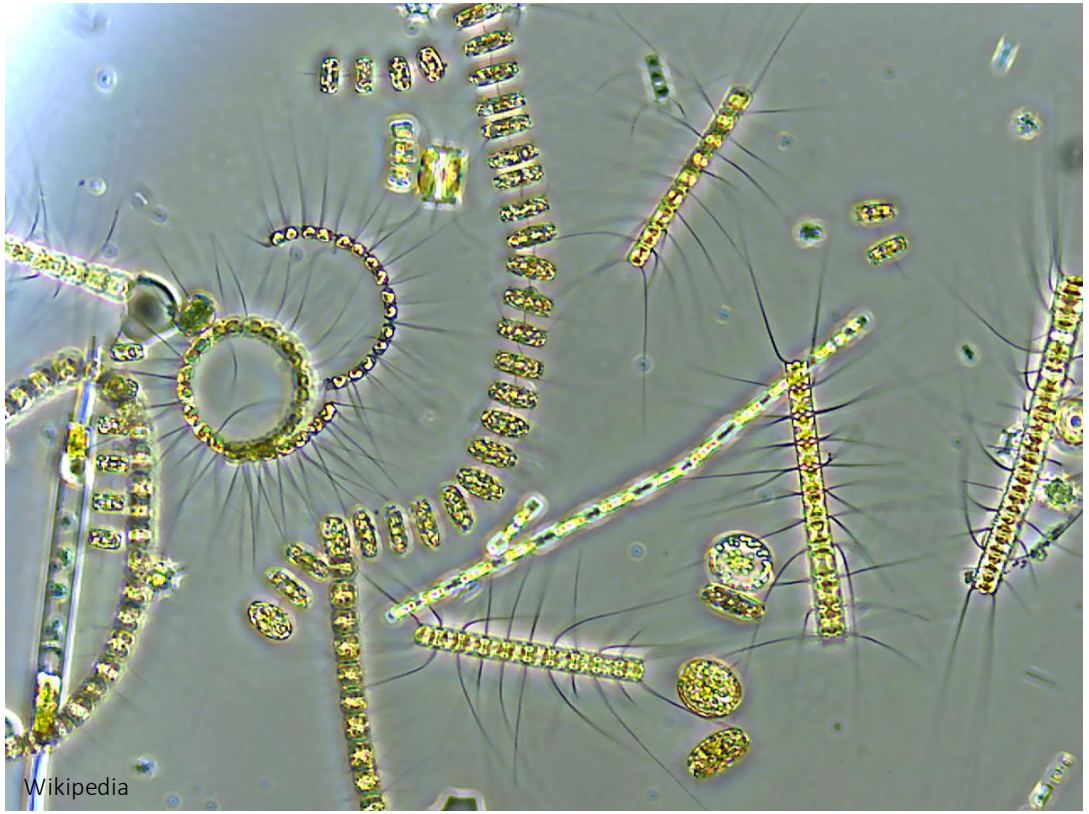


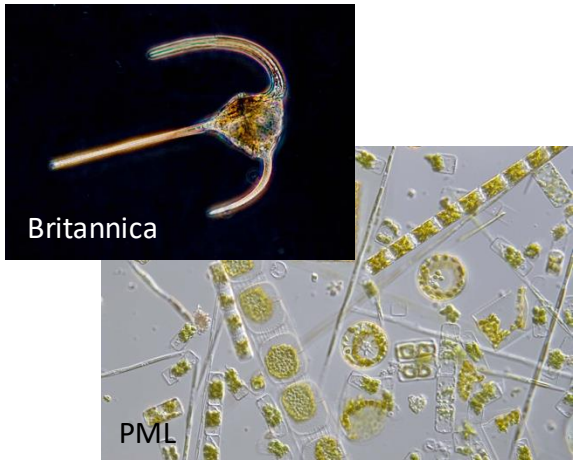
Wikipedia

but can be seen from space

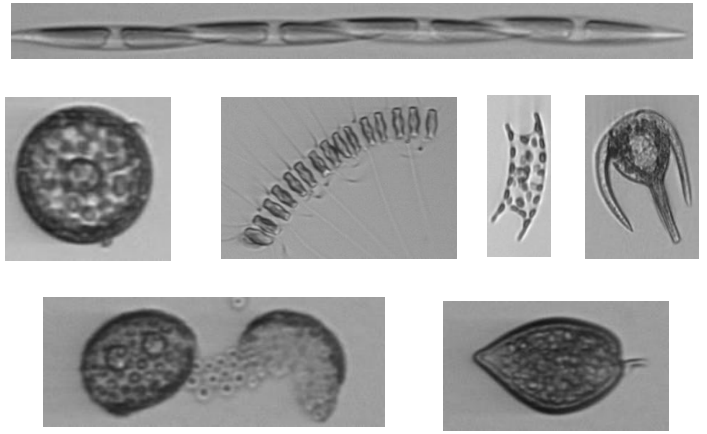
NASA

How do we measure phytoplankton community composition?

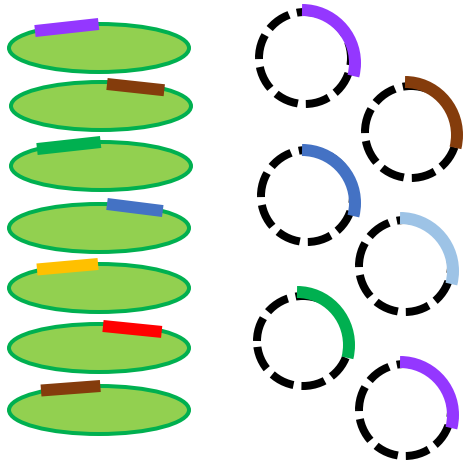
The “ideal” method is the one that is most effective for your system and question – understand the strengths and limitations.



microscopy



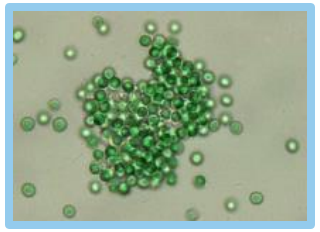
(imaging-in-) flow cytometry

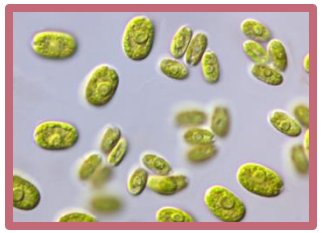


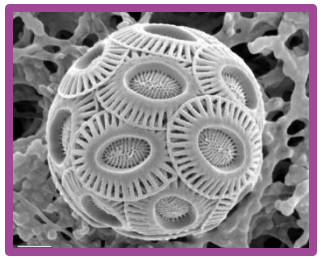
amplicon sequencing

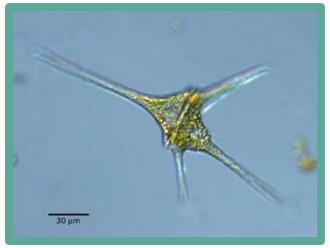
High Performance Liquid Chromatography pigments

Phytoplankton have different pigments; some can be used as biomarkers to separate certain groups.









Phytoplankton pigments affect absorption

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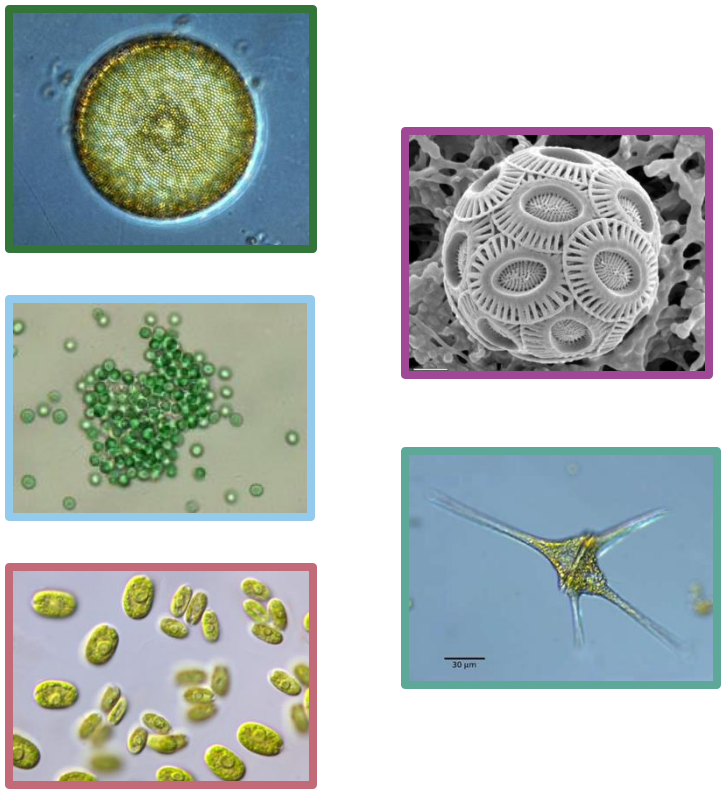
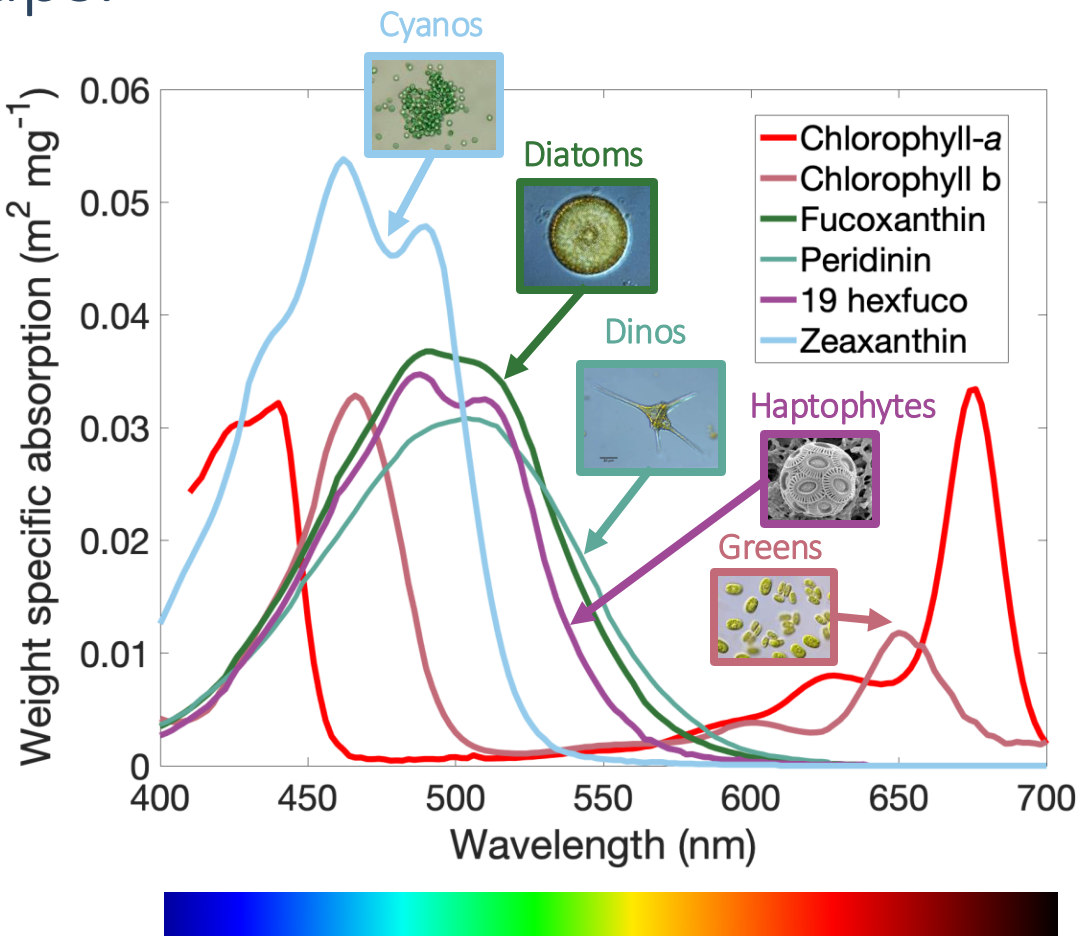
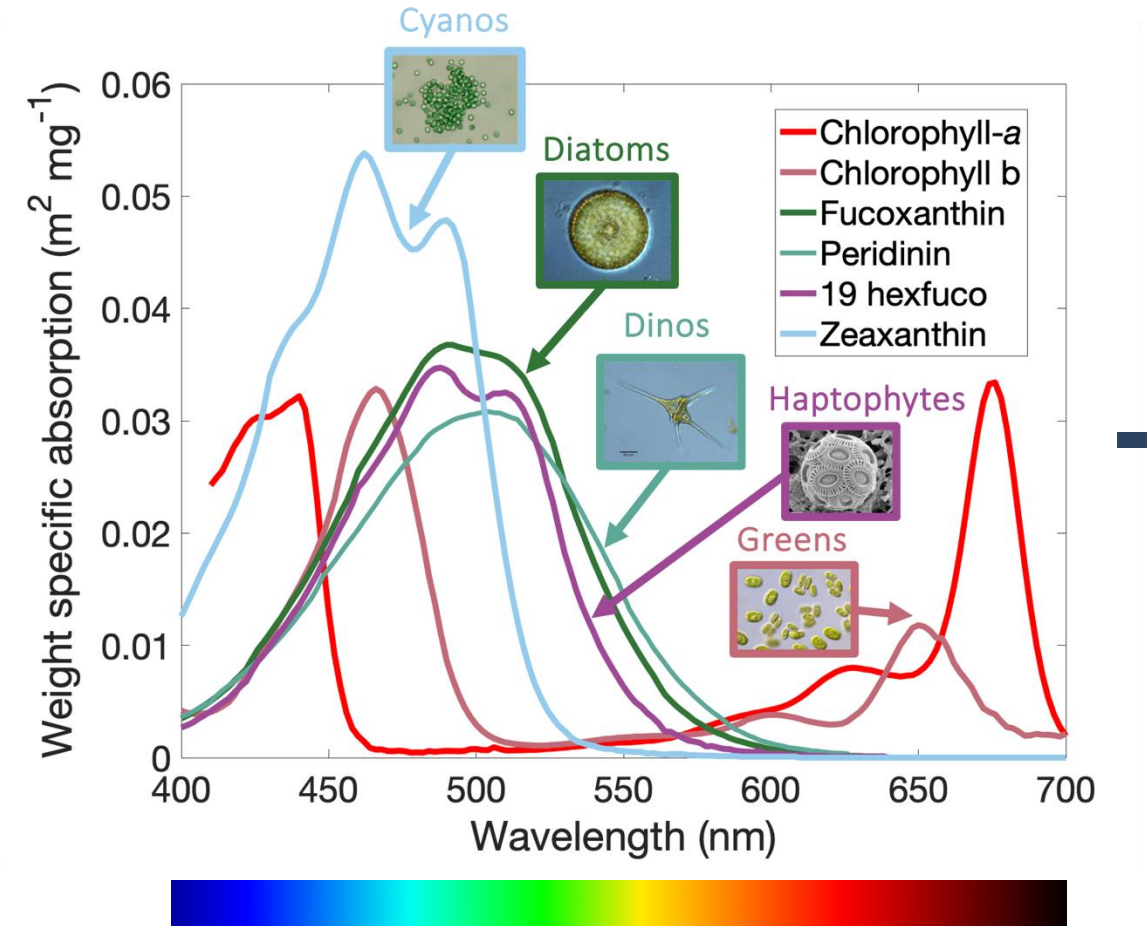
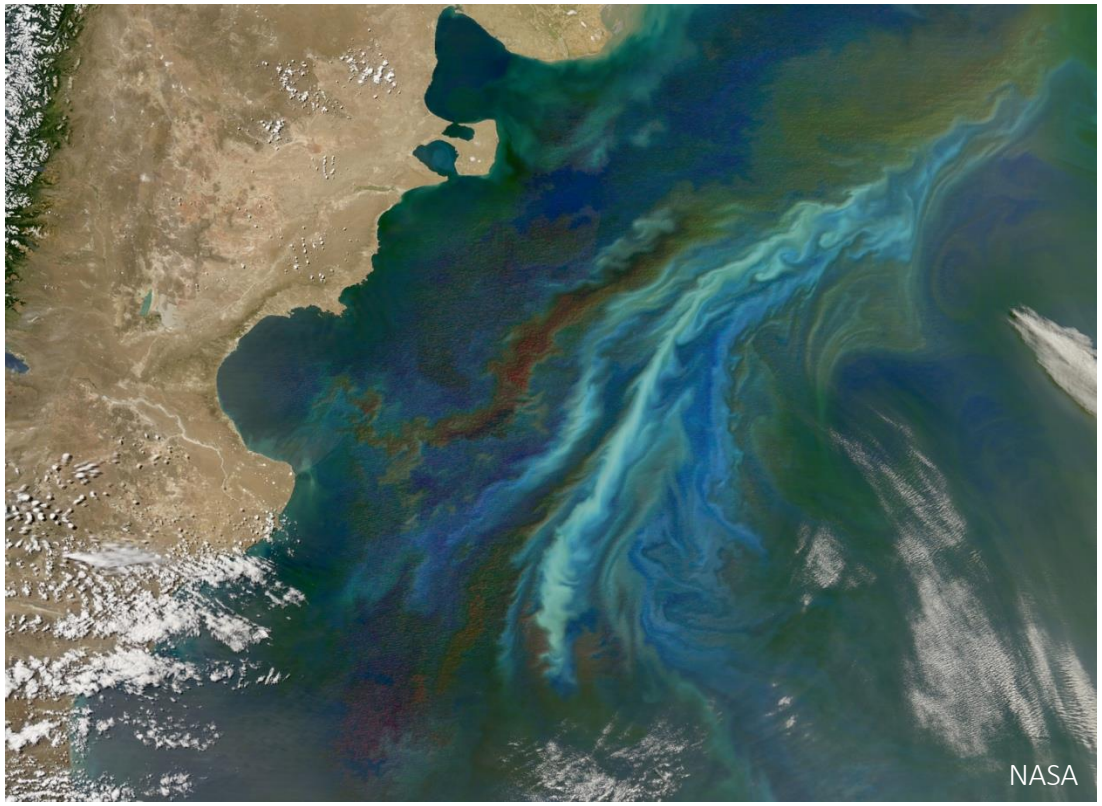
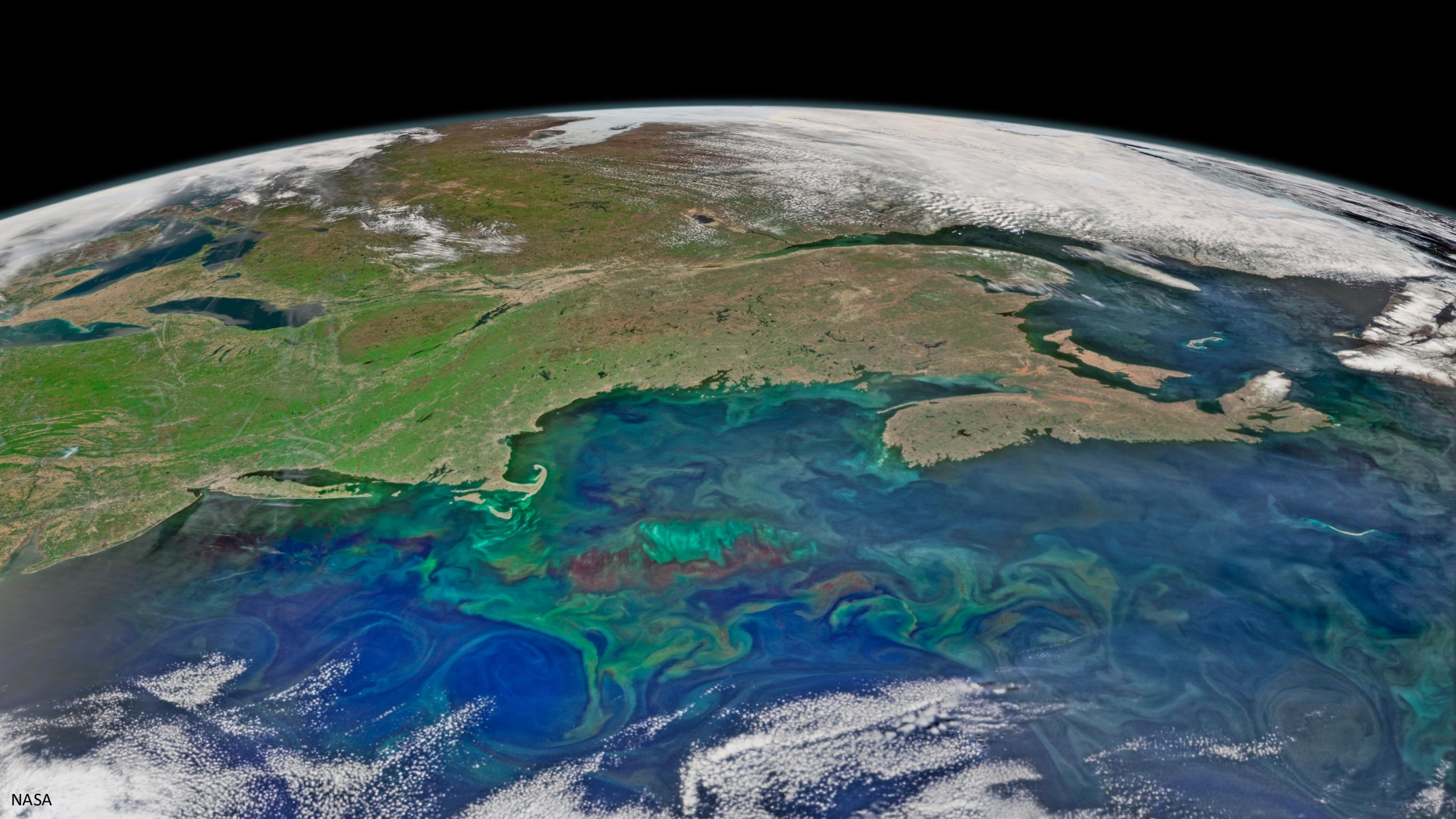


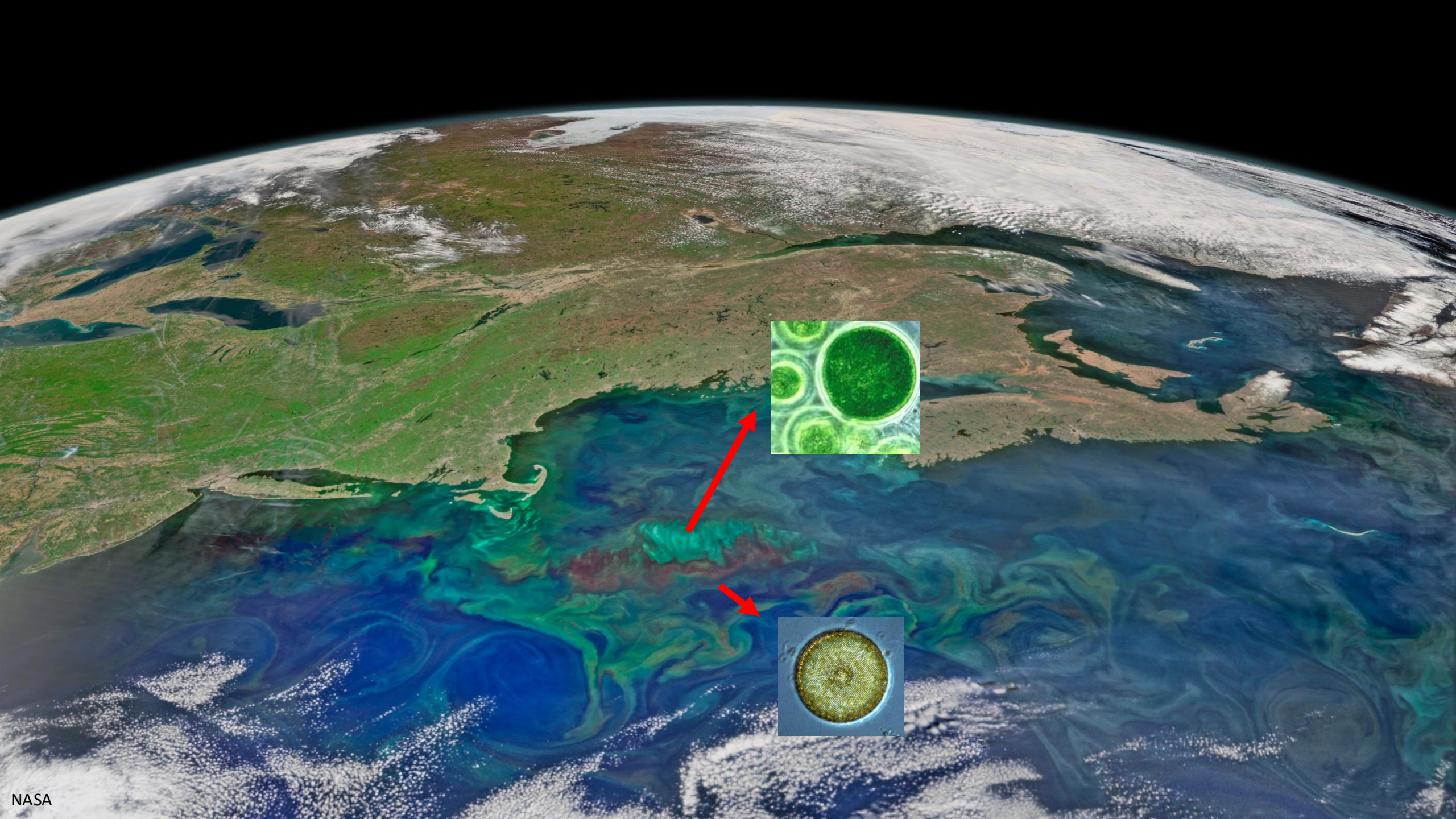


Pigments link phytoplankton and ocean color






NASA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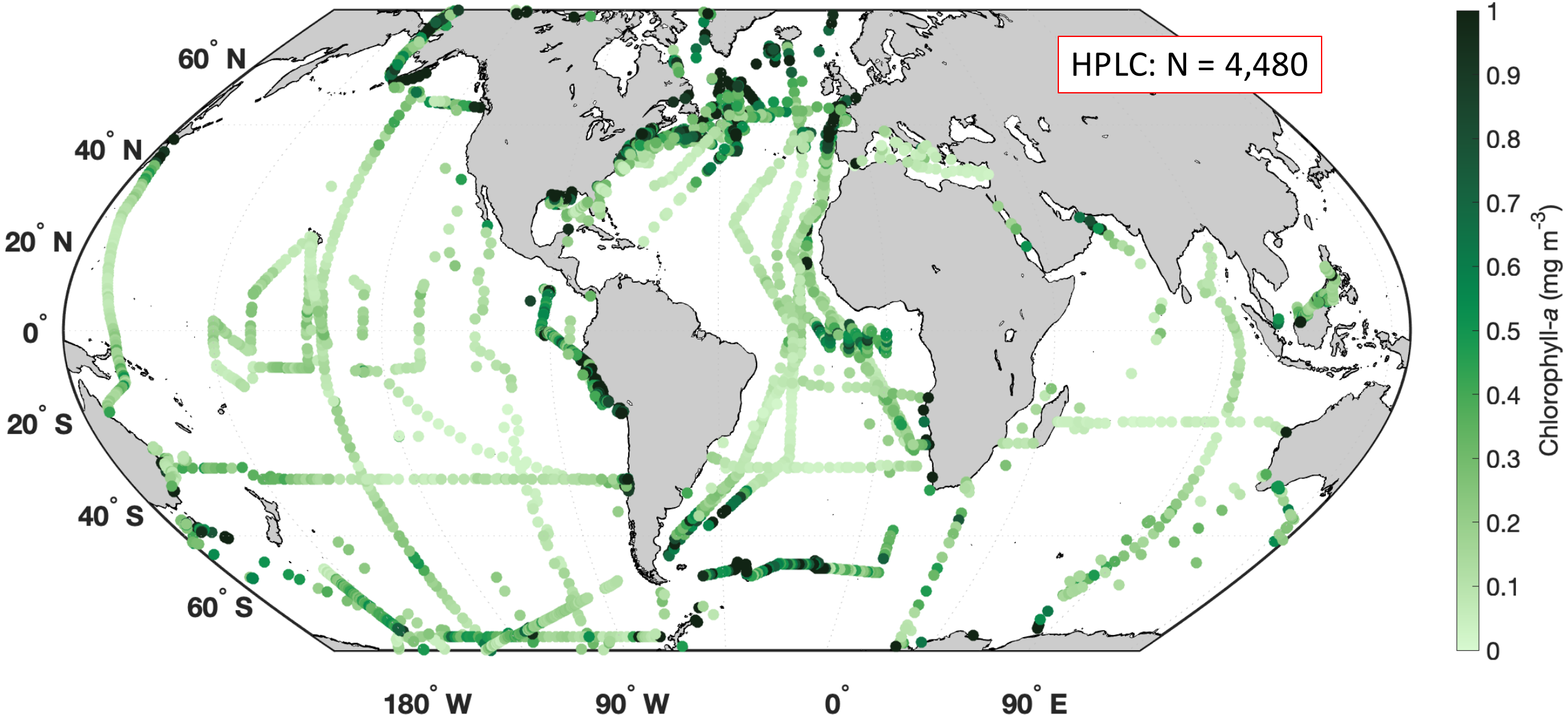
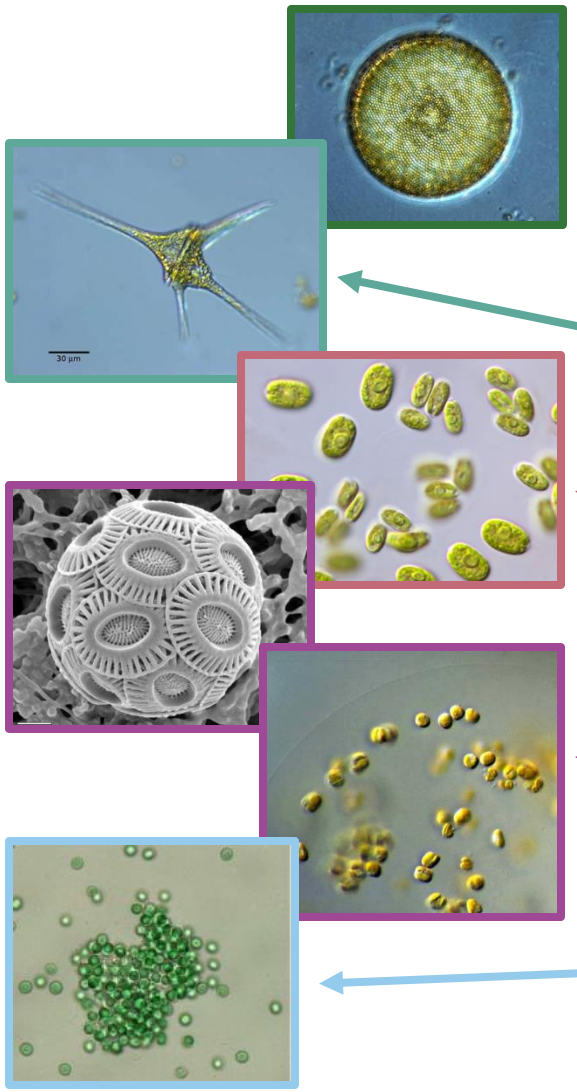
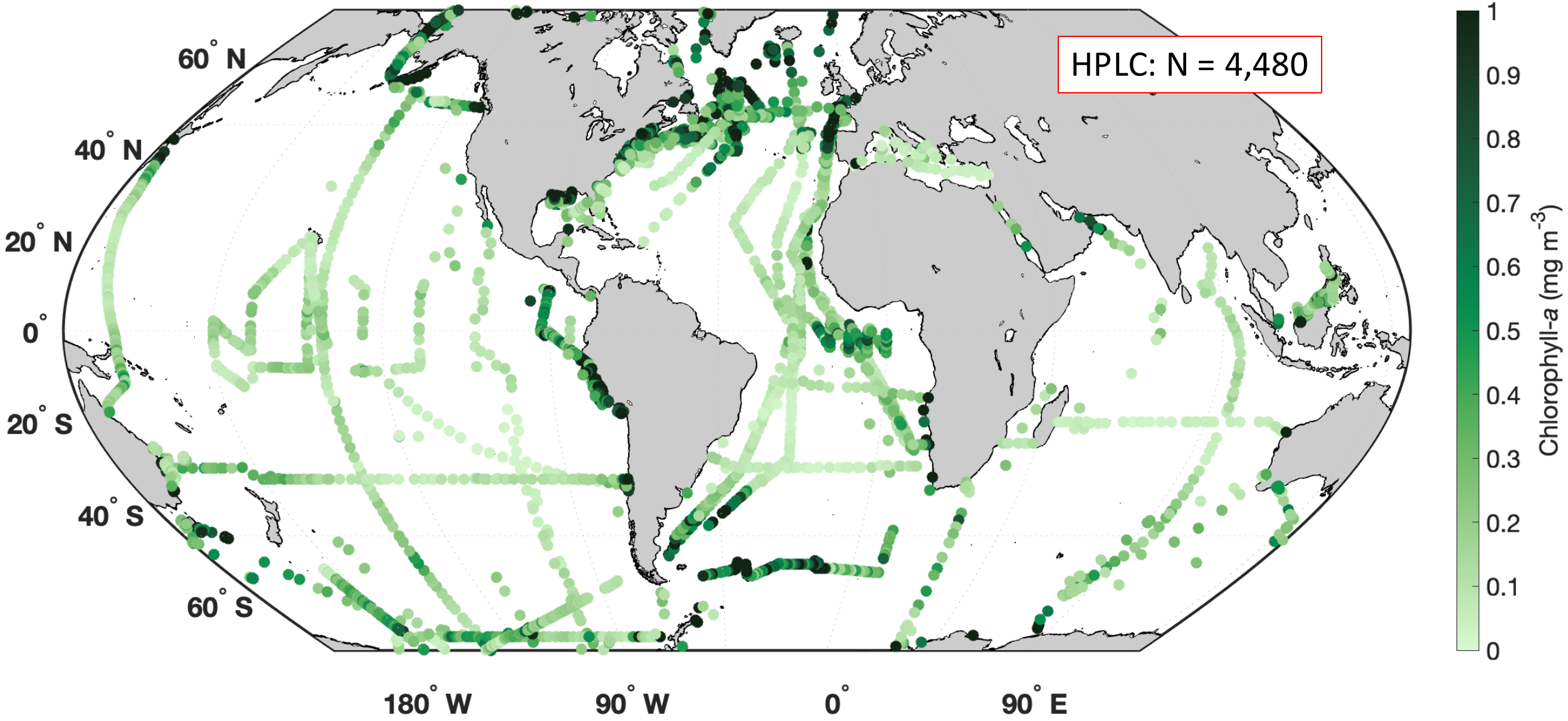


Kramer and Siegel, 2019 *JGR Oceans*

Phytoplankton pigments and taxonomy



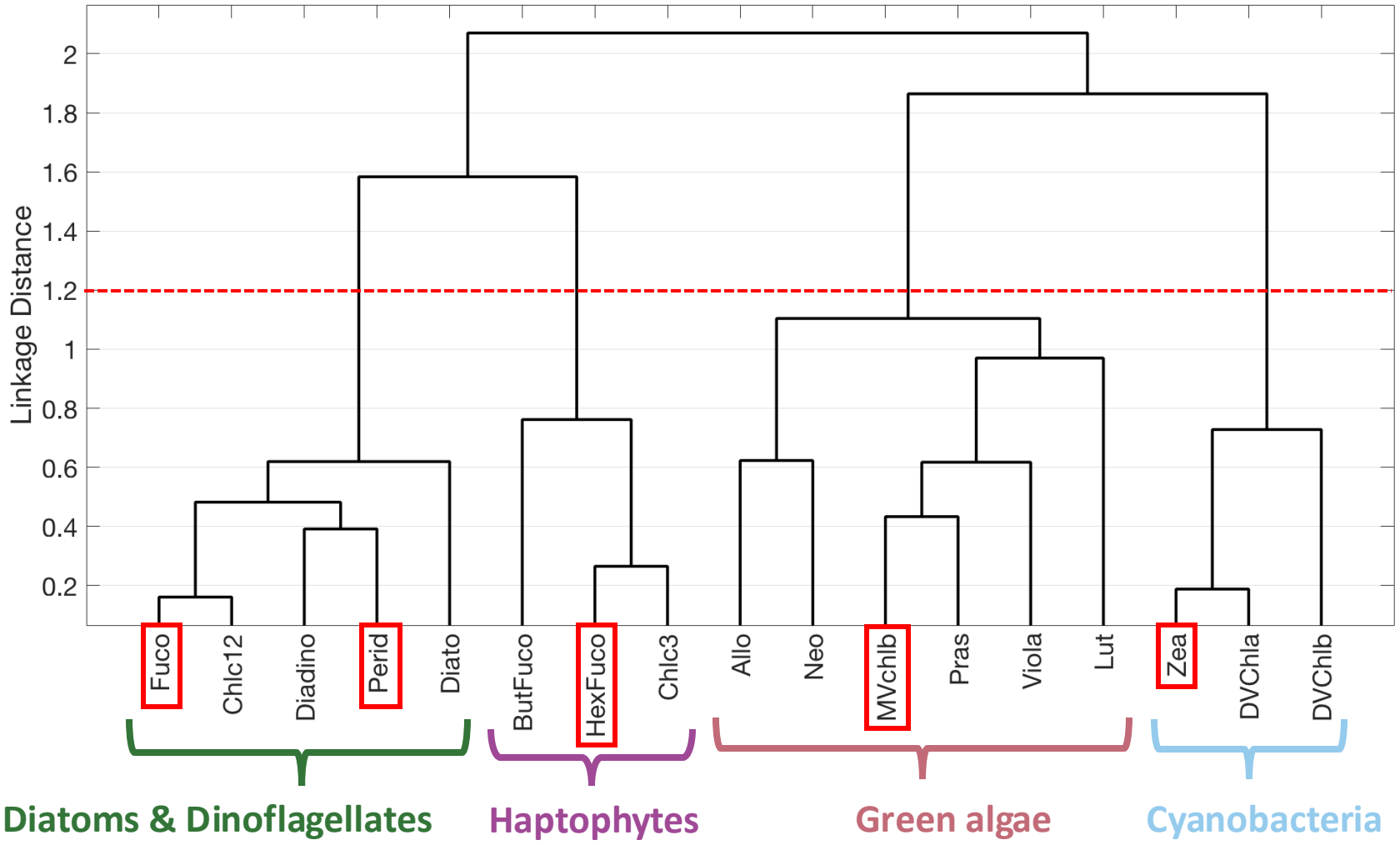
Phytoplankton group	Associated marker pigment(s)
Diatoms	Fucoxanthin
Dinoflagellates	Peridinin
Green algae	MV chlorophyll b
Haptophytes	19’-hexanoyloxyfucoxanthin
Cyanobacteria	Zeaxanthin, DV chlorophyll-*a*



Kramer and Siegel, 2019 *JGR Oceans*

Only 4 pigment-based groups can be separated globally

Using hierarchical cluster analysis to divide pigments based on the strength of correlations.

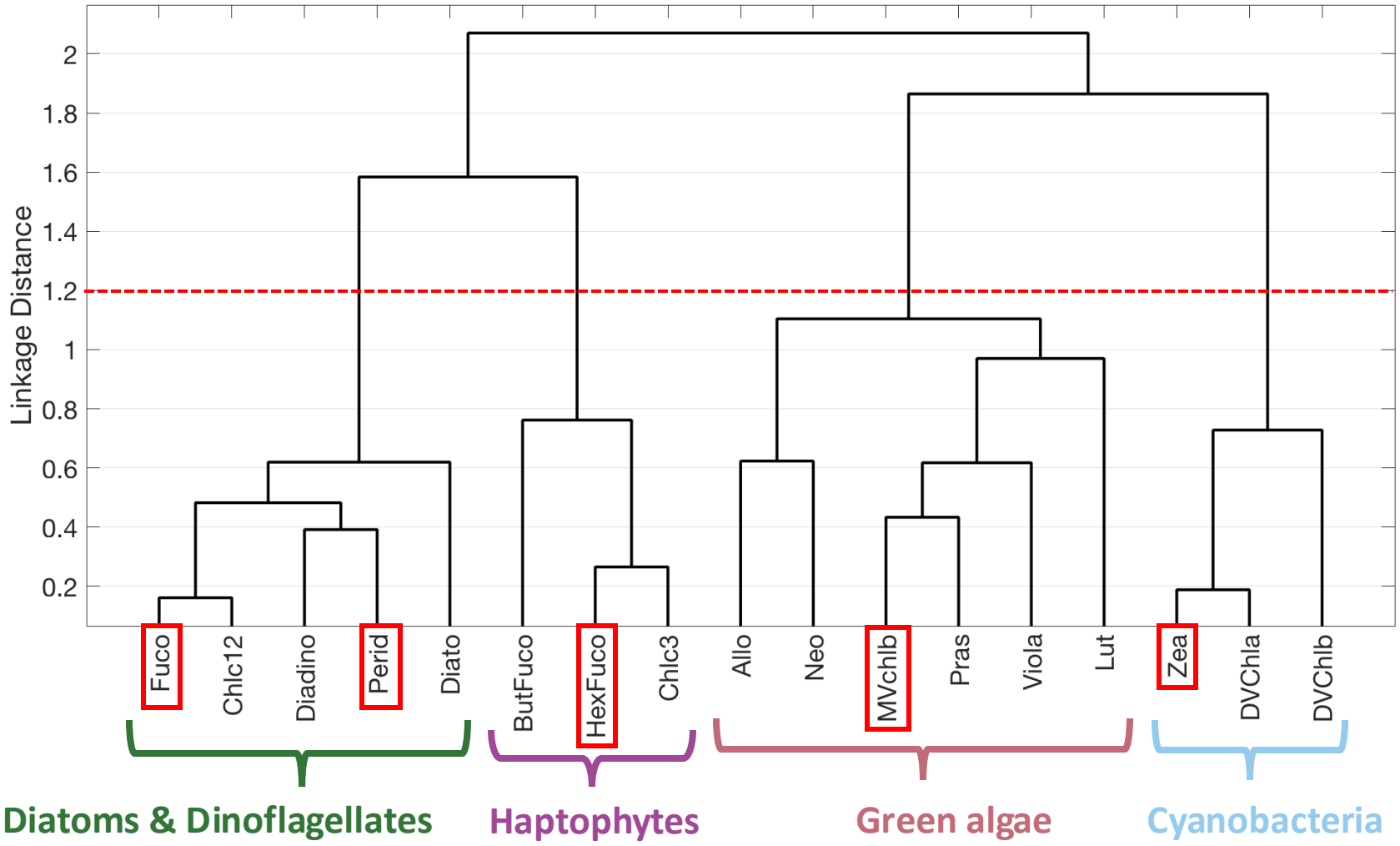


Kramer and Siegel, 2019 *JGR Oceans*

Only 4 pigment-based groups can be separated globally

Using hierarchical cluster analysis to divide pigments based on the strength of correlations.

Pigments are limited in the number of groups they can separate.

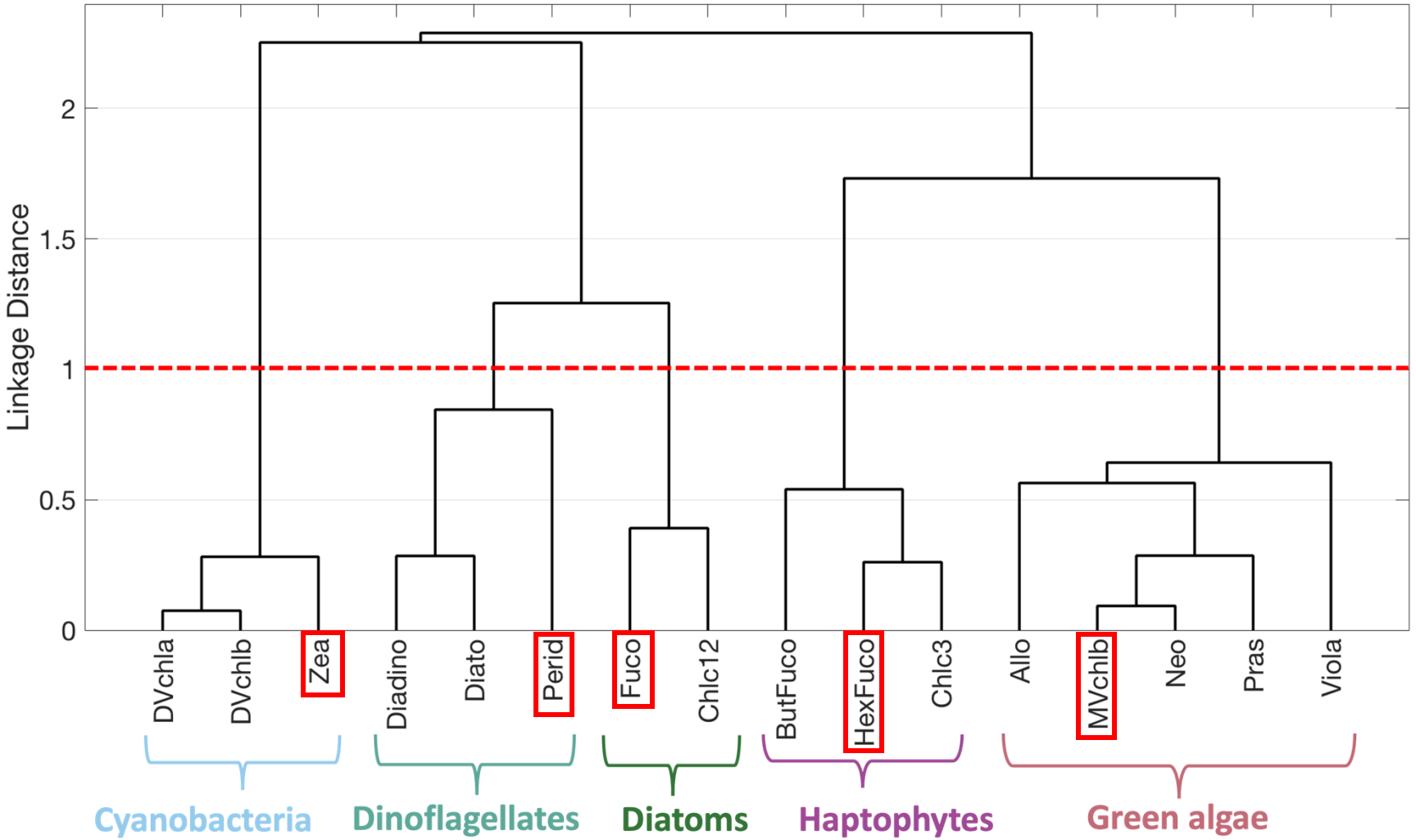


Kramer and Siegel, 2019 *JGR Oceans*

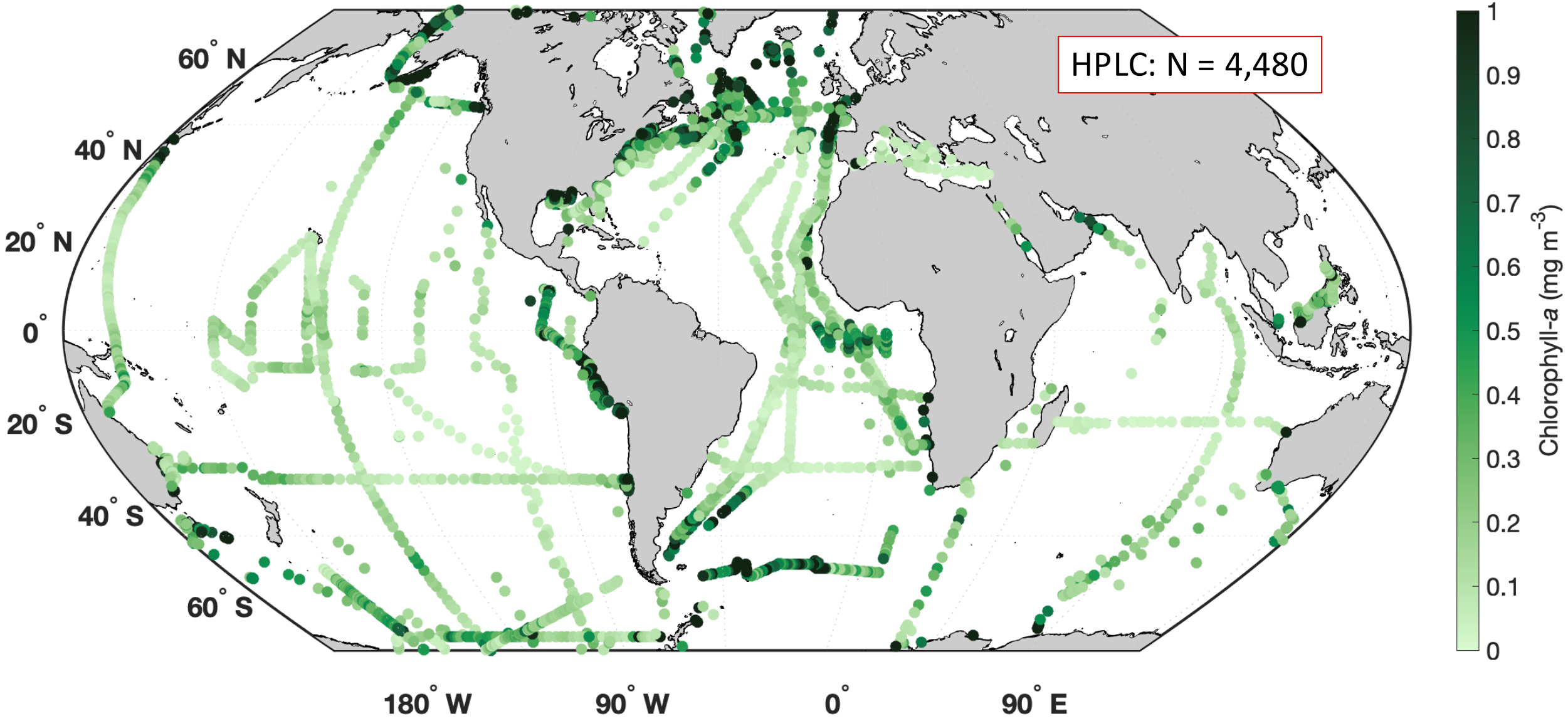
But 5 groups are separated in the western North Atlantic

Comparing global pigment clusters to a dataset collected over a seasonal cycle in the North Atlantic…

Five pigment-based groups separate from hierarchical cluster analysis on a regional scale.



Kramer et al., 2020 *Frontiers in Marine Science*



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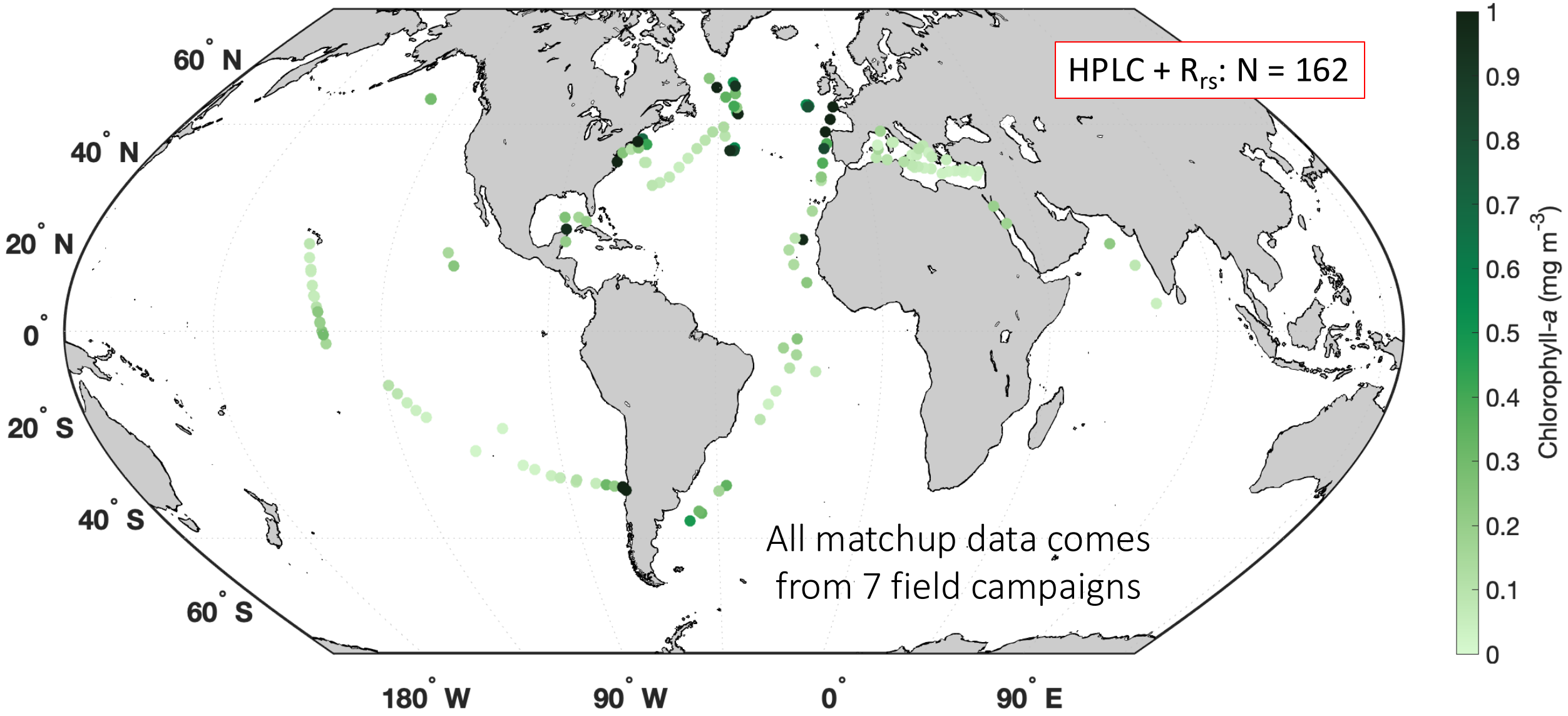
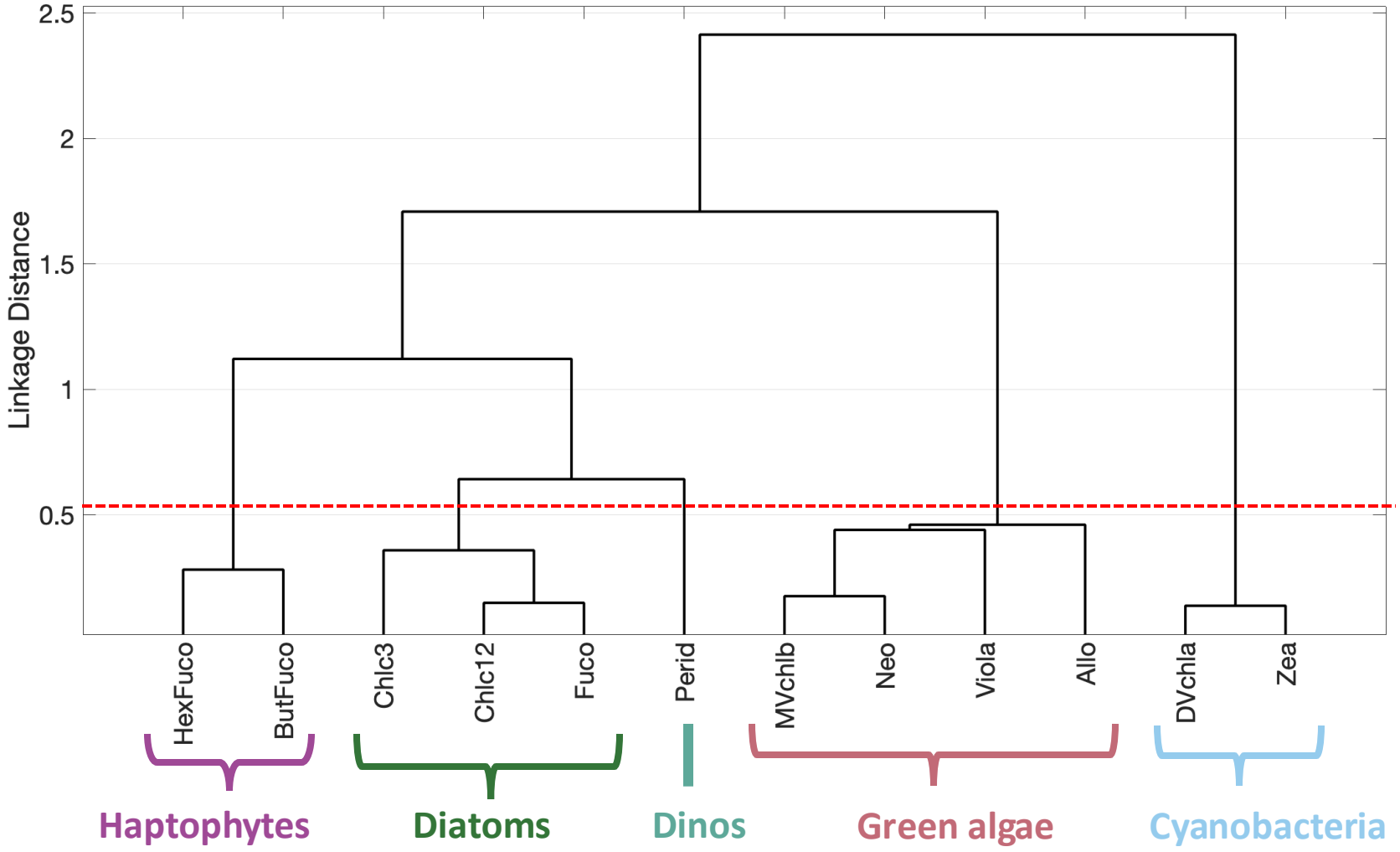


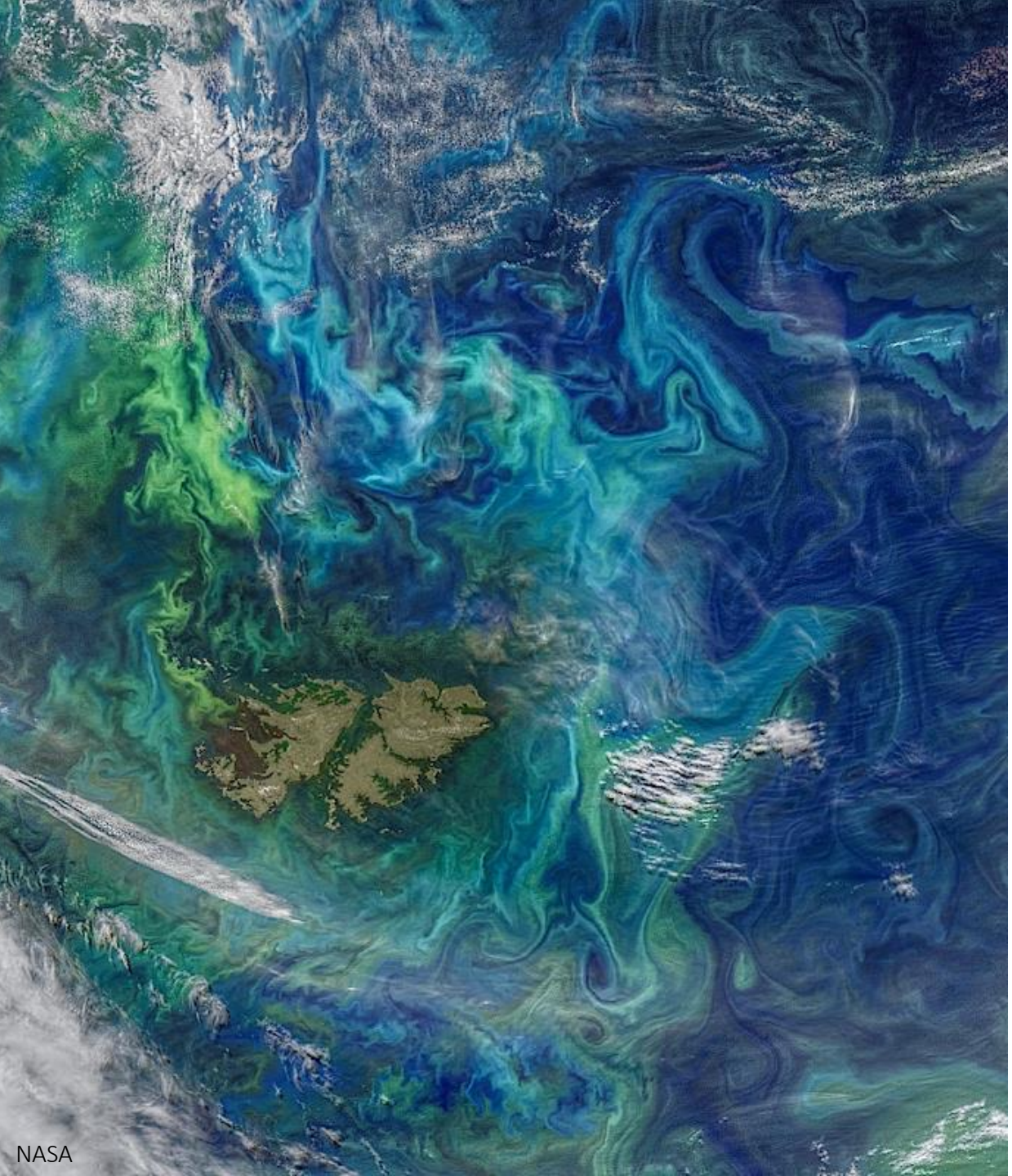
Adapted from Kramer et al., 2022 *Remote Sensing of Environment*

Max *five* pigment-based groups separate in this dataset

Paired global dataset of hyperspectral $R_{rs}(\lambda)$ and HPLC pigments can be separated into more groups than the global HPLC dataset.



Kramer et al., 2024 *Optics Express*

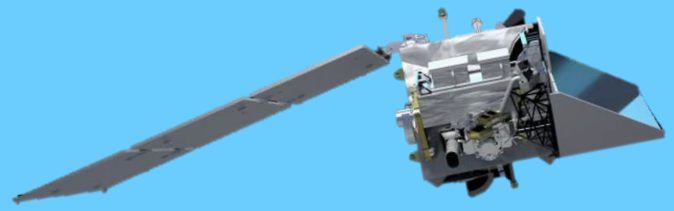

NASA

In-water data provide a baseline for ocean color modeling

Pigments can be used to separate a limited number of phytoplankton groups, depending on the dataset / ecosystem.

But need to test if the relationships between pigments and optics are as strong as we expect…

Ocean color satellite

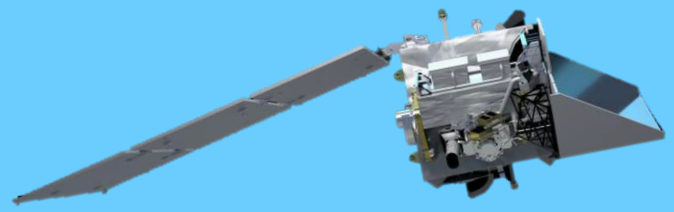


Non algal particles (NAP)

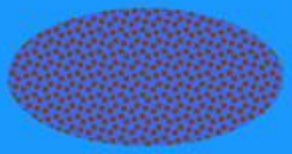
Colored dissolved organic matter (CDOM)

Phytoplankton

Ocean color satellite



$$R_{rs} \propto \frac{\text{Backscattering } (b_b)}{\text{Absorption } (a)}$$



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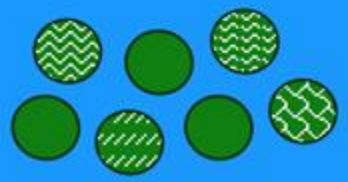
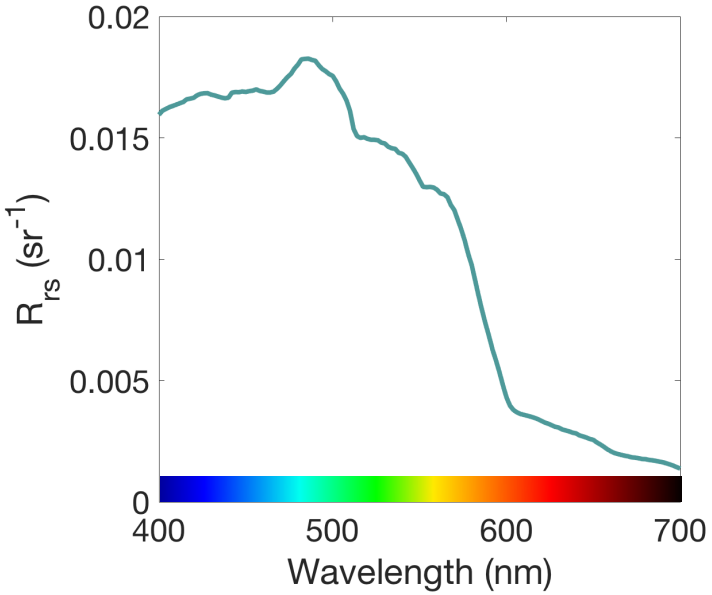


Phytoplankton

The Spectral Derivative Pigments (SDP) model

$$R_{rs}(\lambda) \approx \frac{b_b(\lambda)}{a(\lambda) + b_b(\lambda)}$$



AOP and IOP spectra from Roesler and Perry 1995

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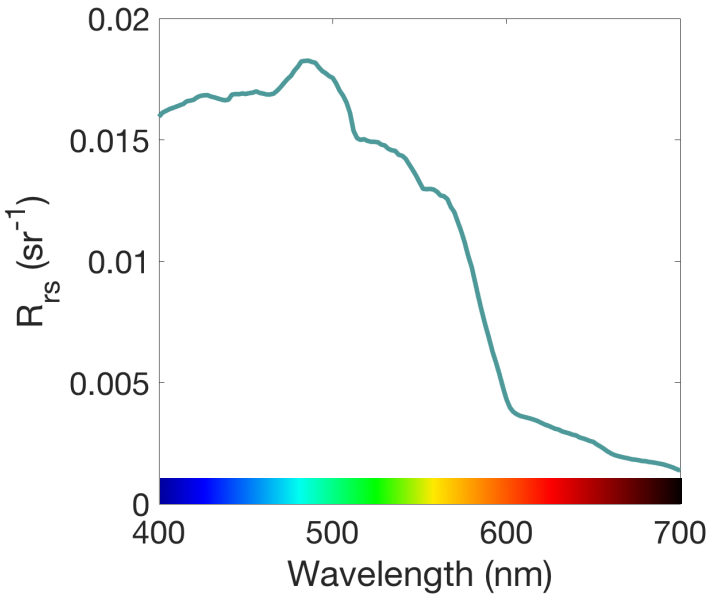

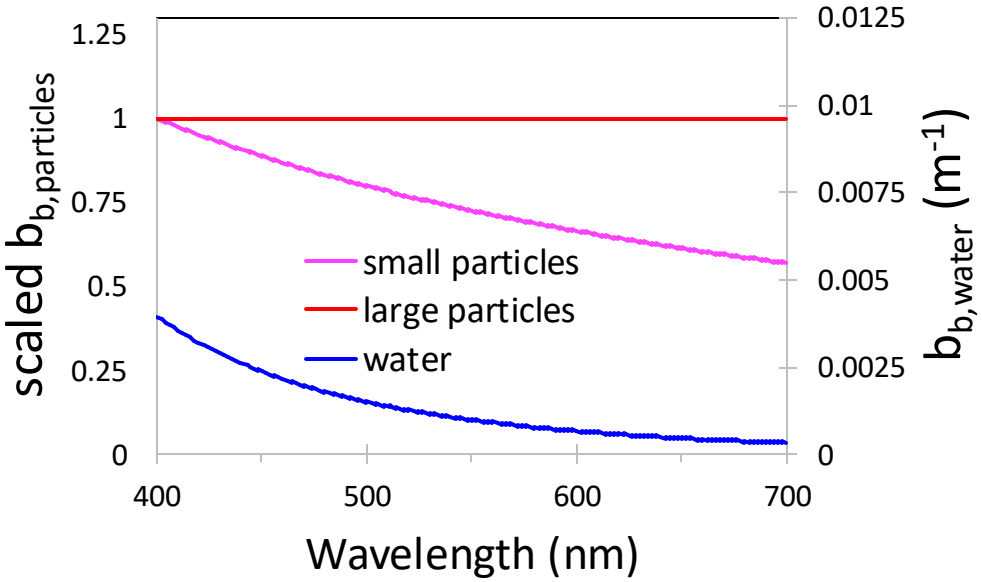

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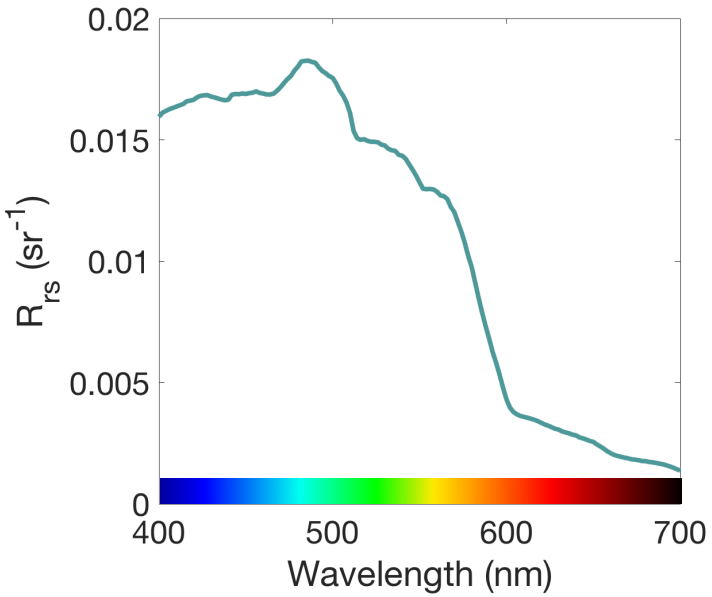

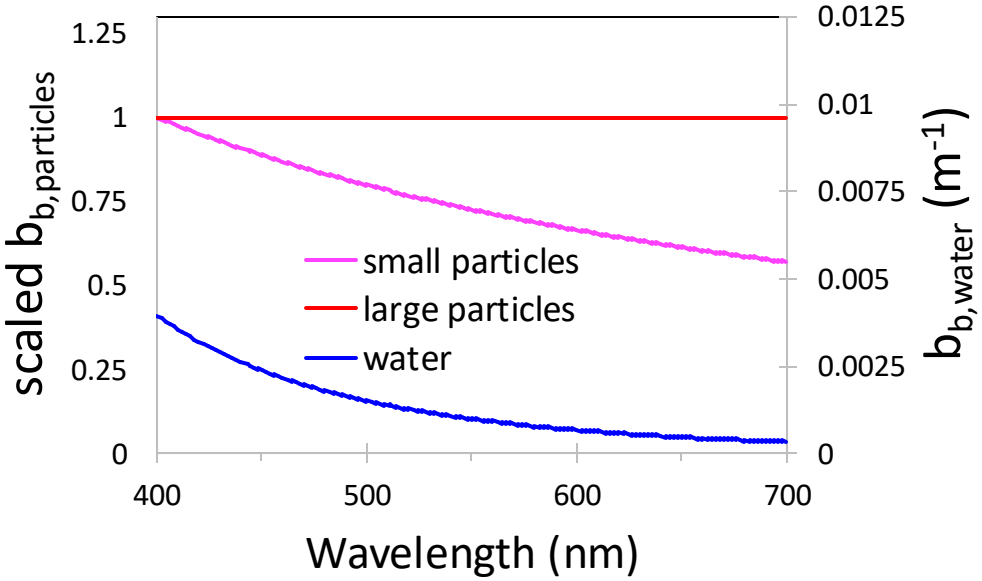

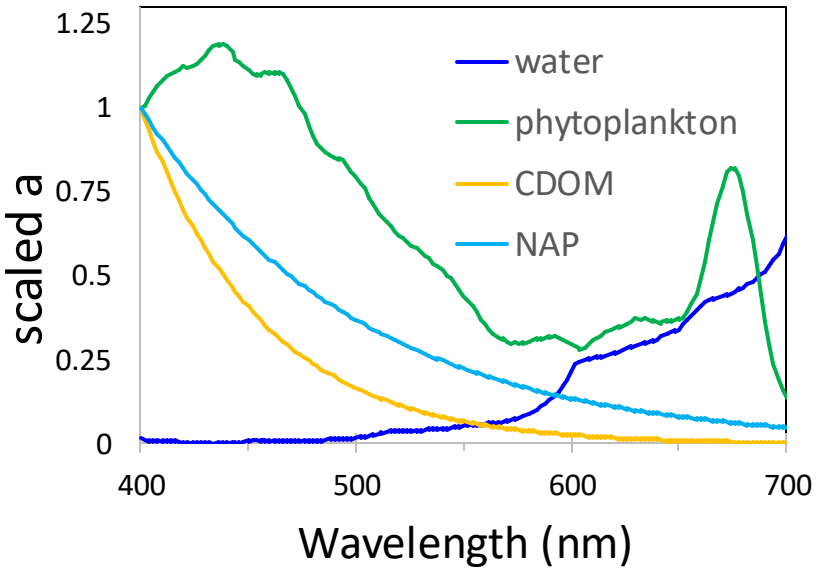

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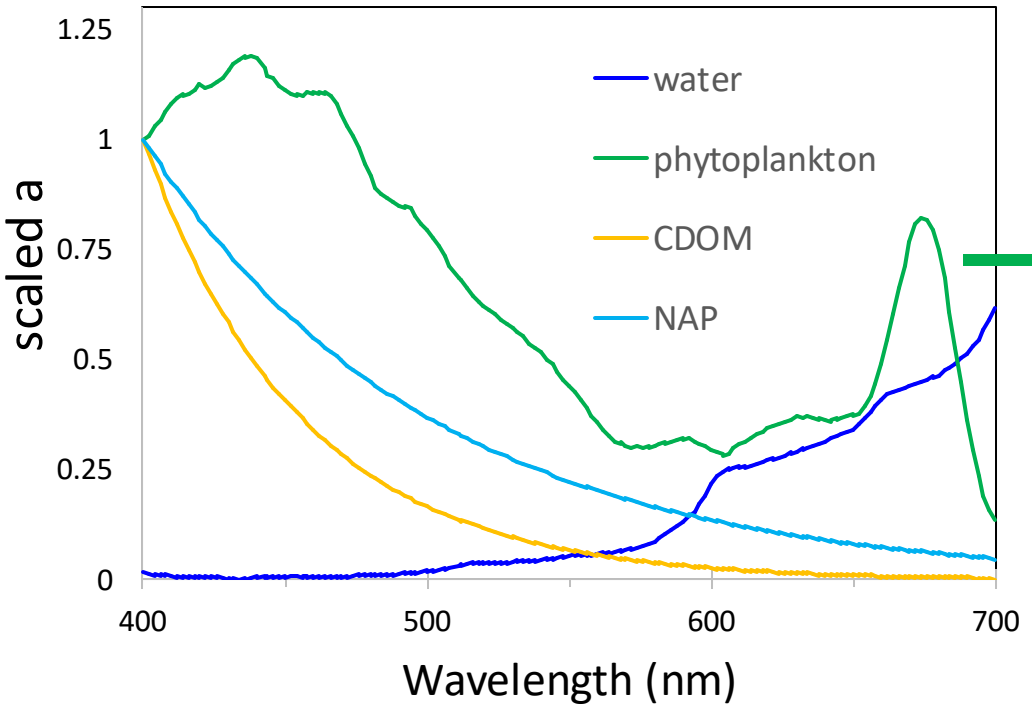

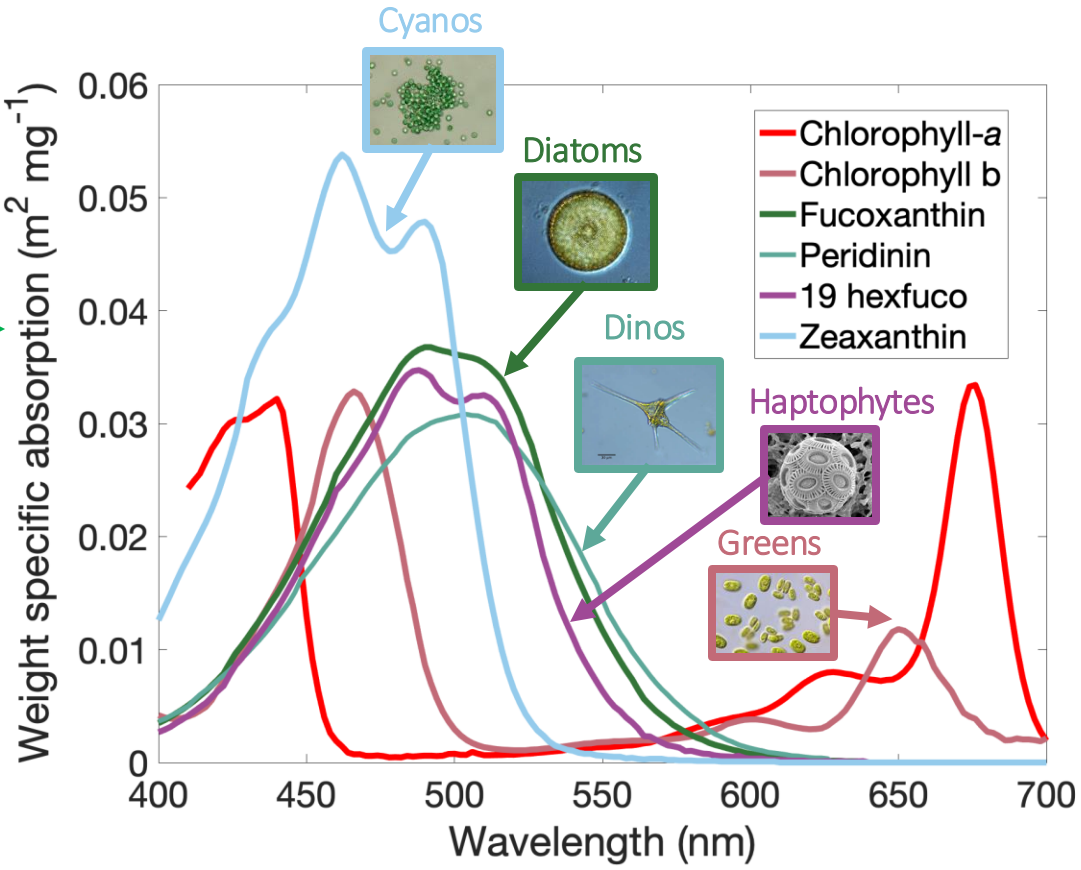

IOP spectra from Roesler and Perry 1995

From reflectance to pigments via absorption

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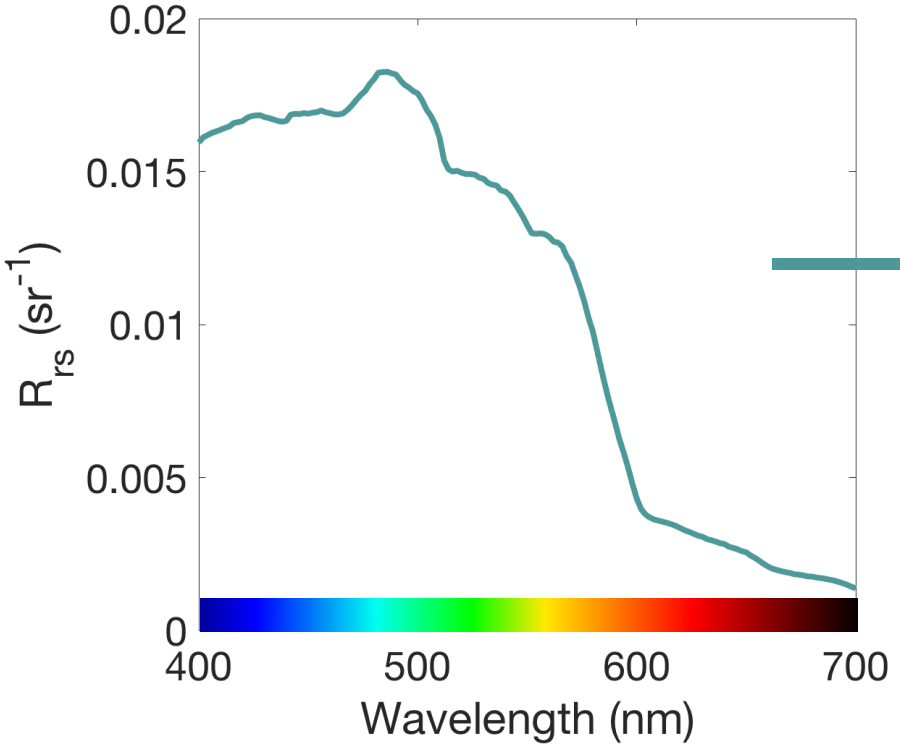

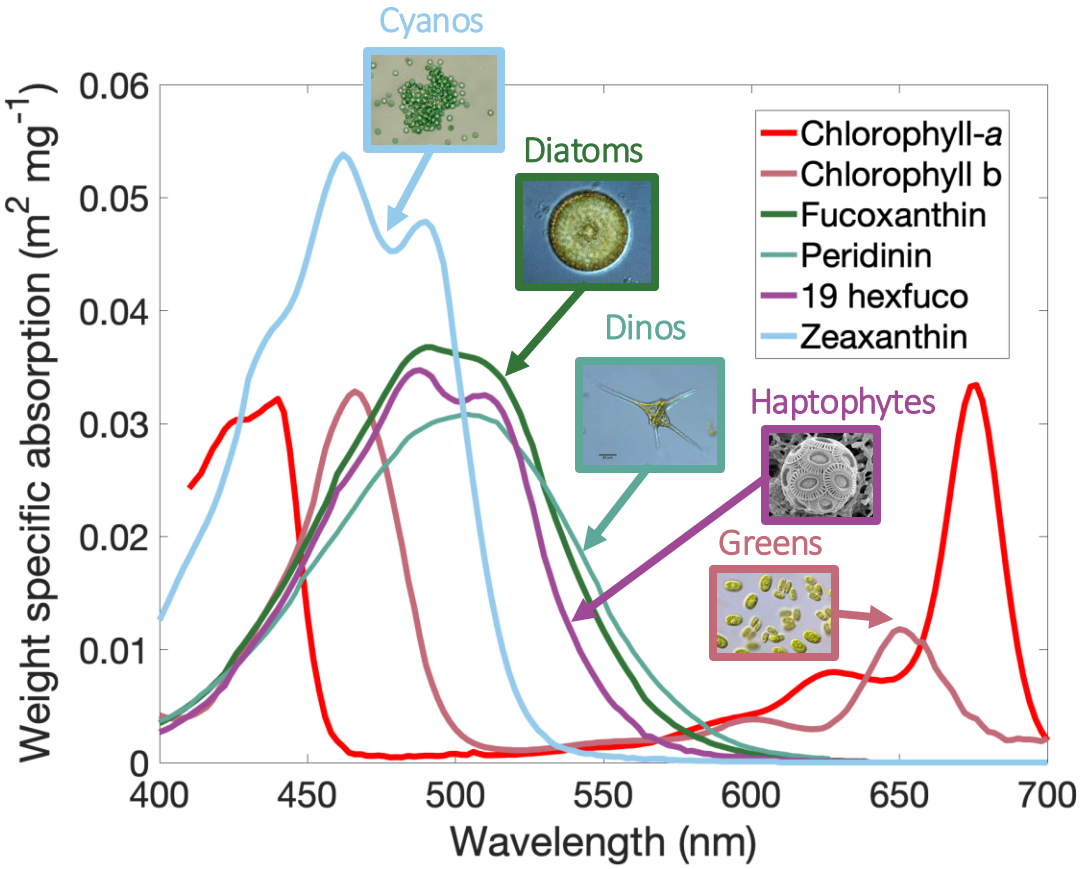

AOP spectra from Roesler and Perry 1995

Maximize short (<50nm) spectral scale variability

$$R_{rs}(\lambda) \approx \frac{b_b(\lambda)}{a(\lambda) + b_b(\lambda)}$$

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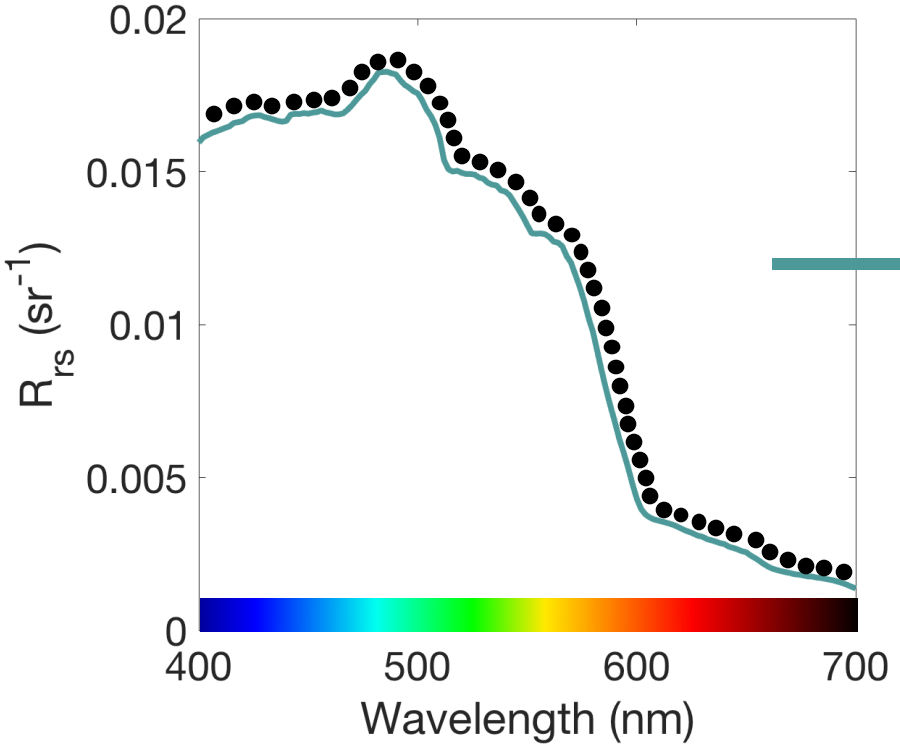

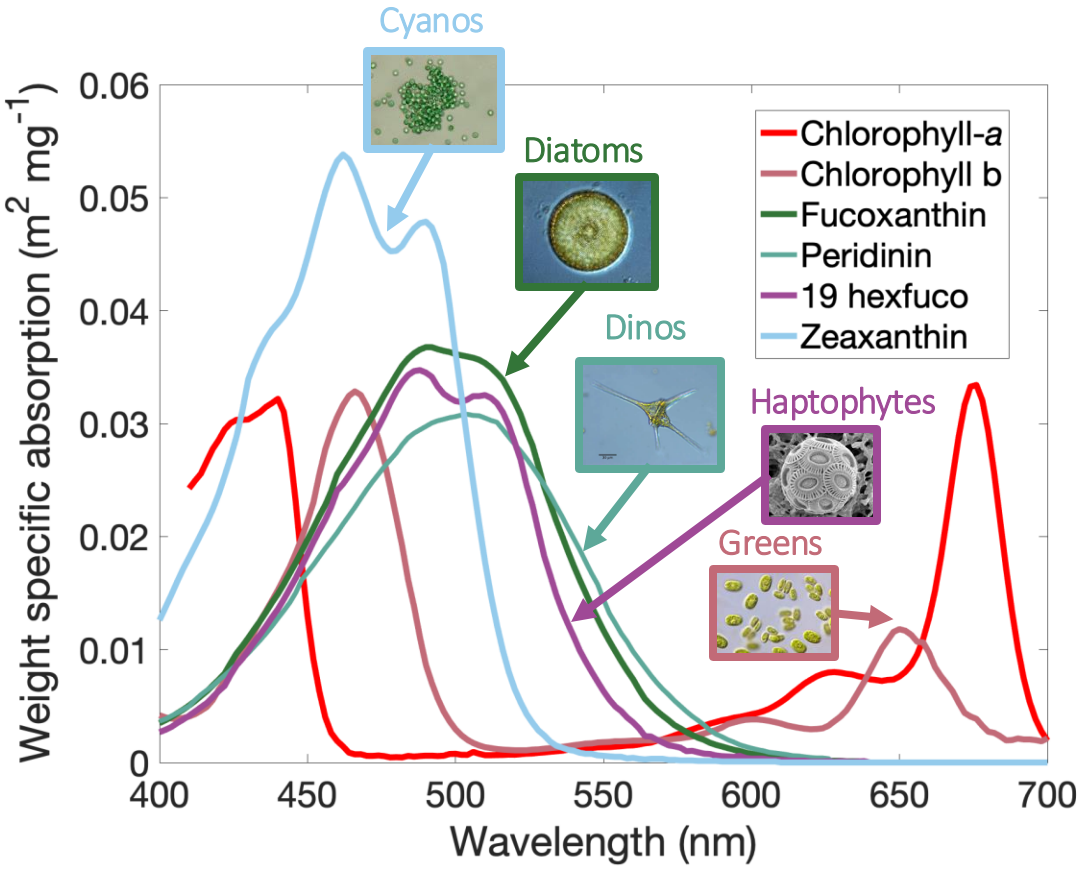

AOP spectra from Roesler and Perry 1995

Past satellite resolution was insufficient…

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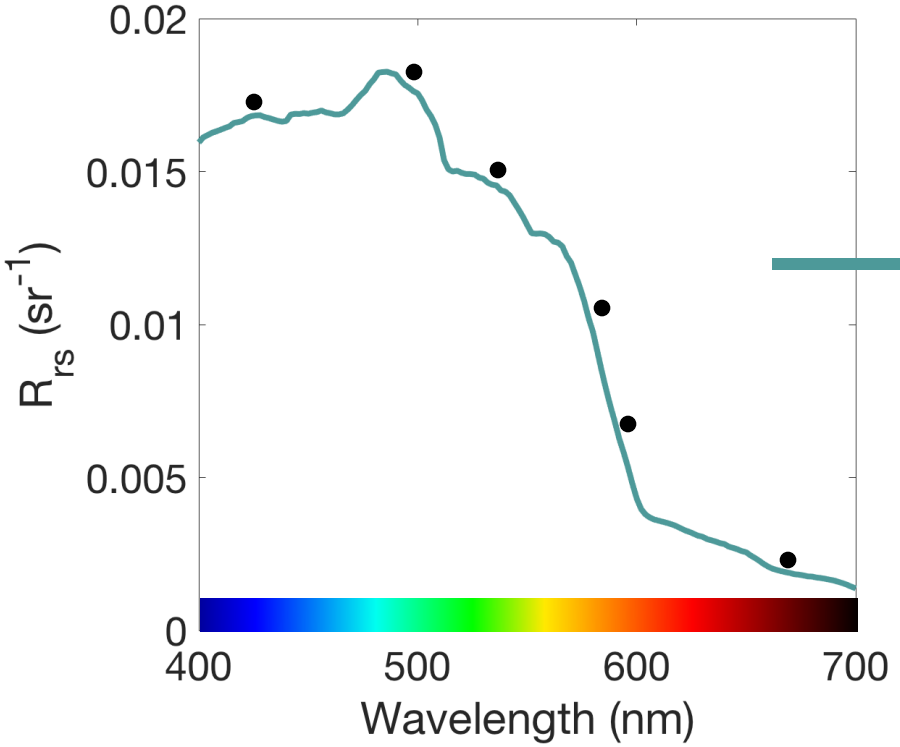

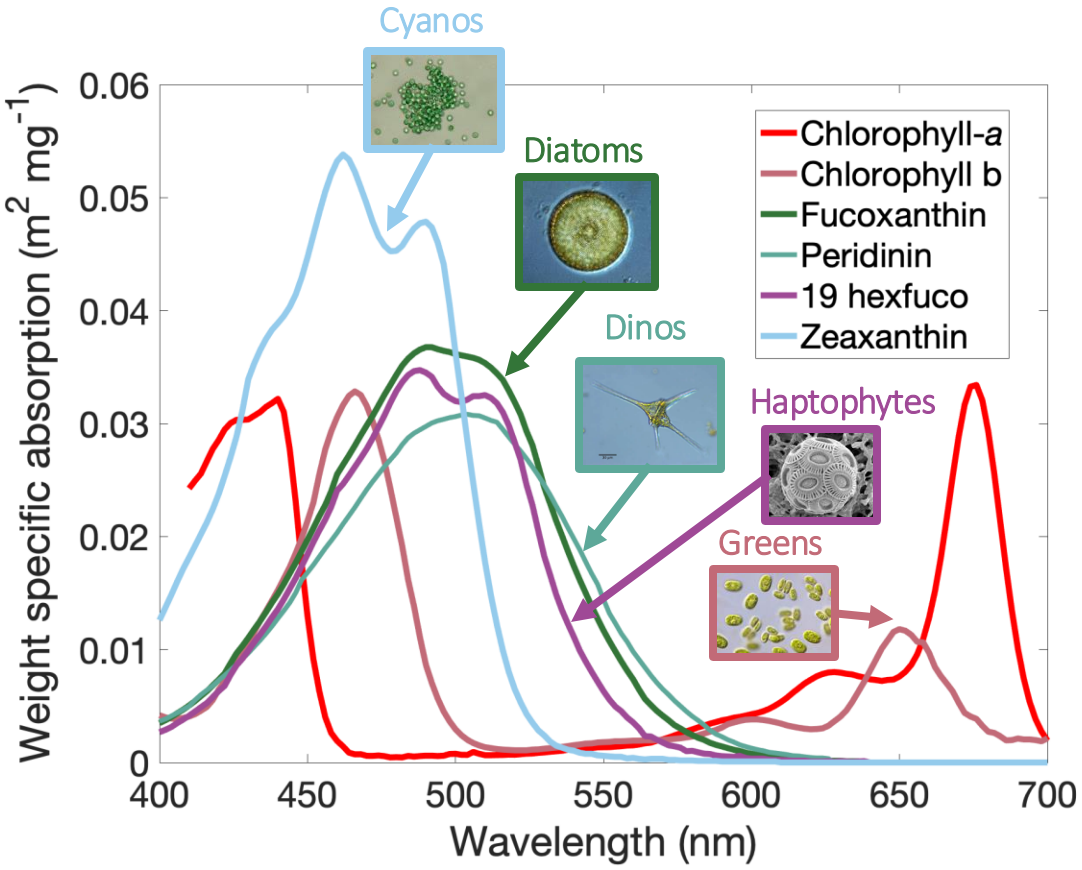

AOP spectra from Roesler and Perry 1995

But PACE provides unprecedented resolution

$$R_{rs}(\lambda) \approx \frac{b_b(\lambda)}{a(\lambda) + b_b(\lambda)}$$

$$b_b = b_{b,water} + b_{b,large\ part.} + b_{b,small\ part.}$$

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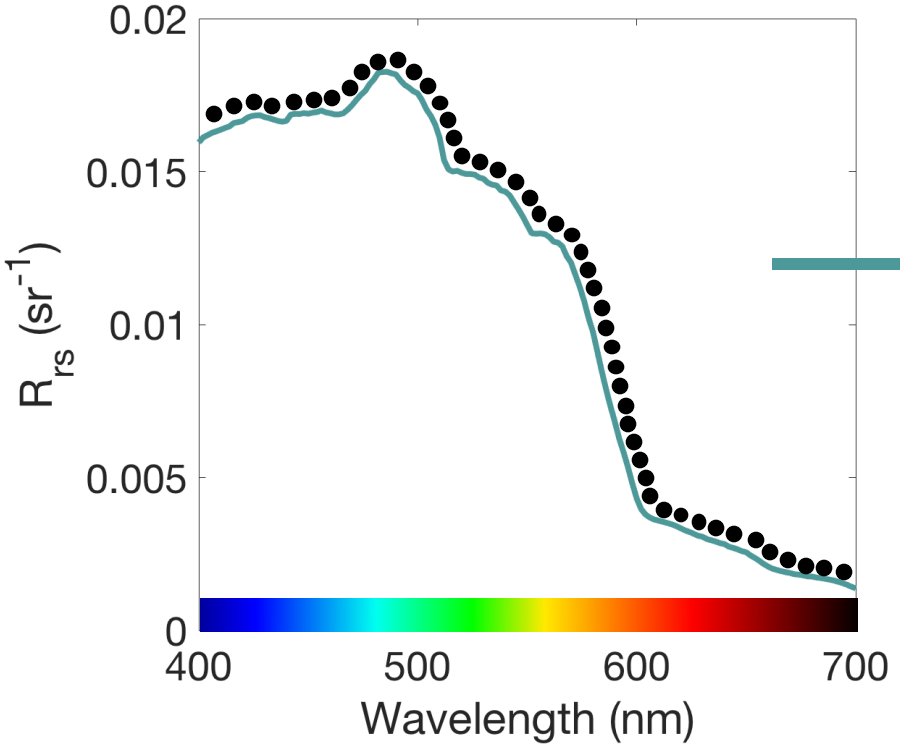
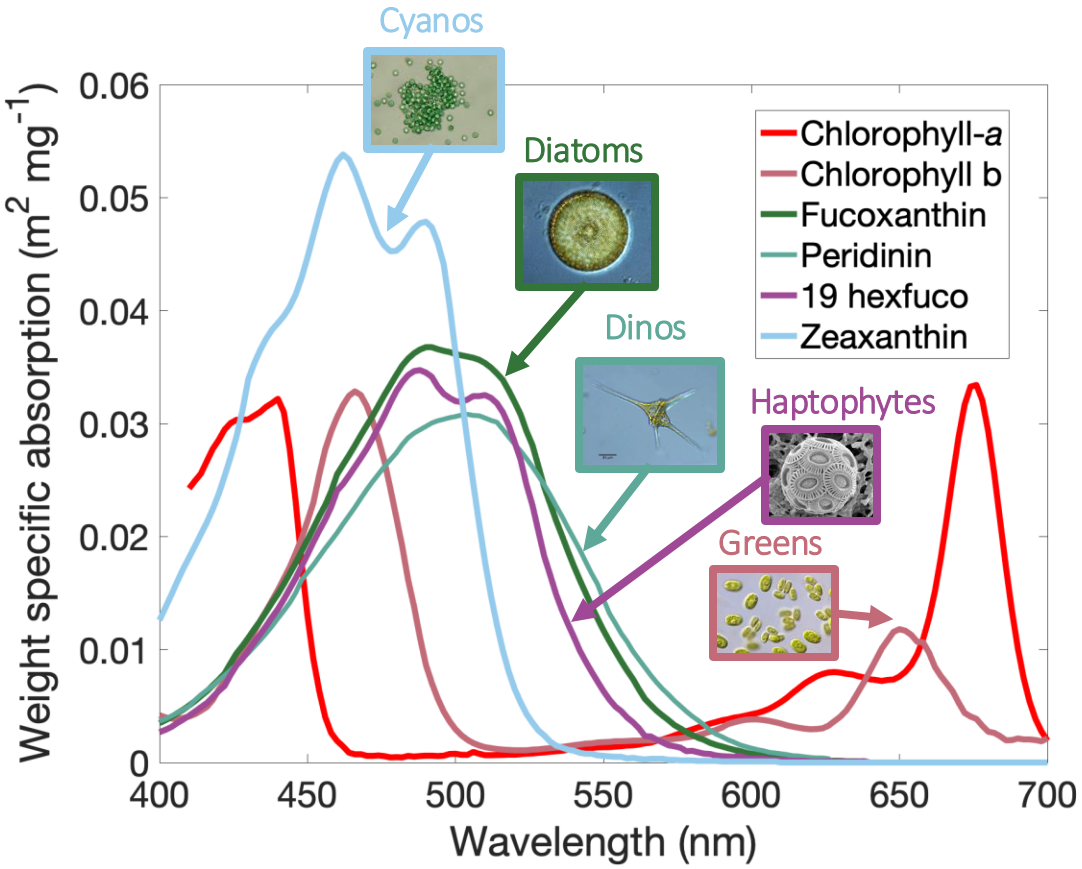
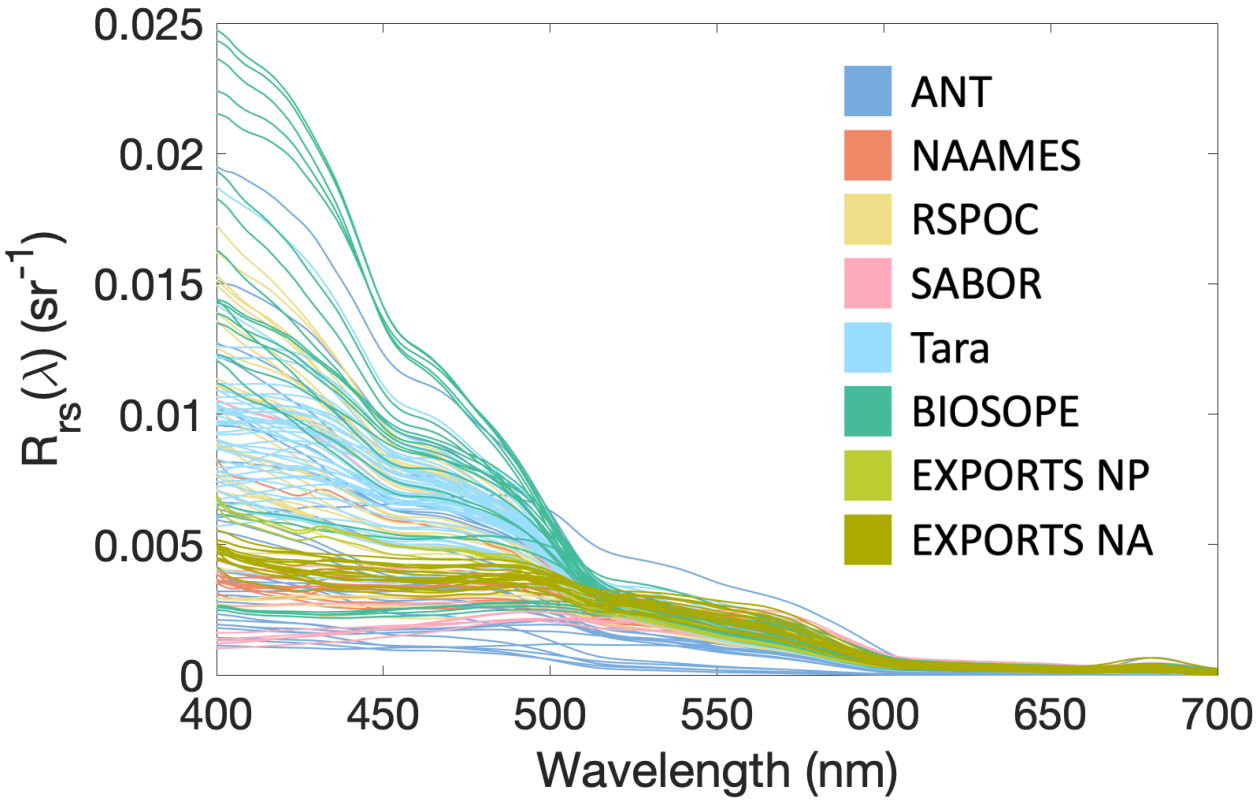




AOP spectra from Roesler and Perry 1995

Implementing the SDP model

Measured spectra



Adapted from Kramer et al., 2022 *Remote Sensing of Environment*

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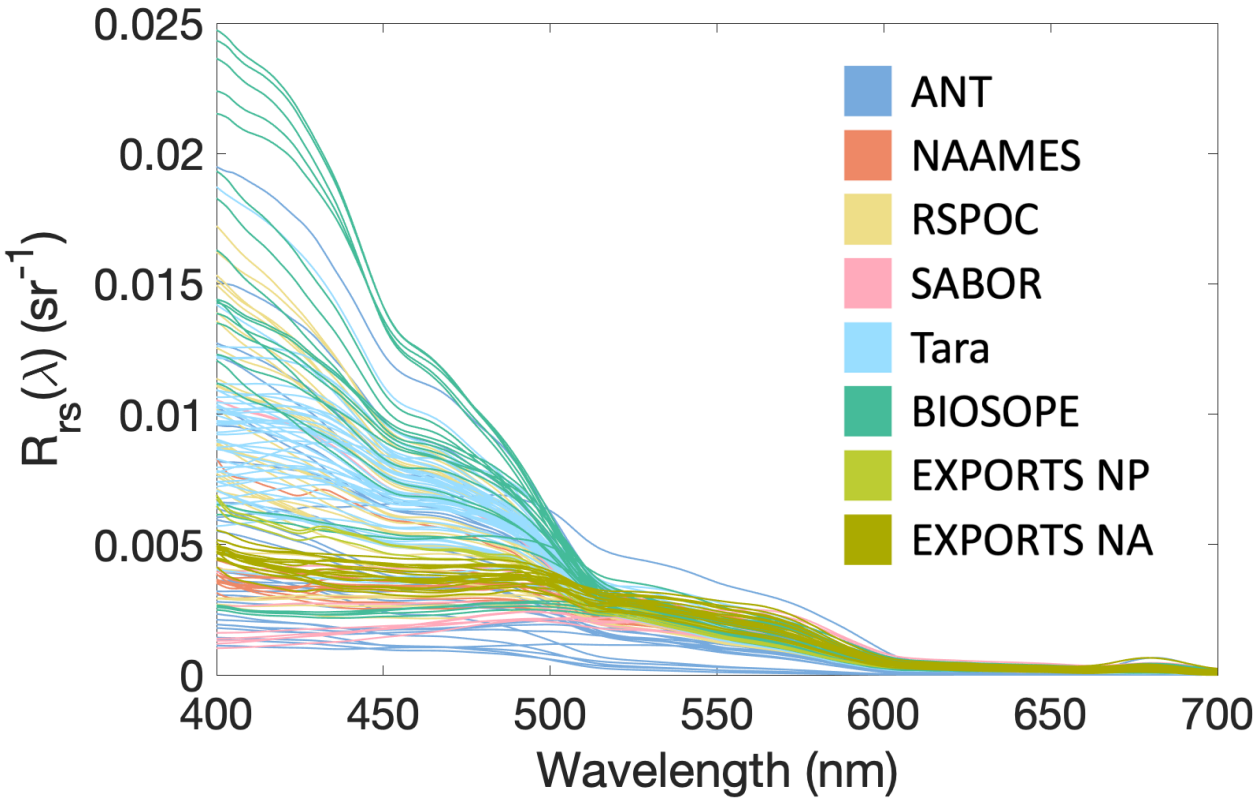


Construct a generic hyperspectral model to reconstruct remote sensing reflectance:

$$R_{rs,mod}(\lambda) = f(a, b_b) \text{ where}$$

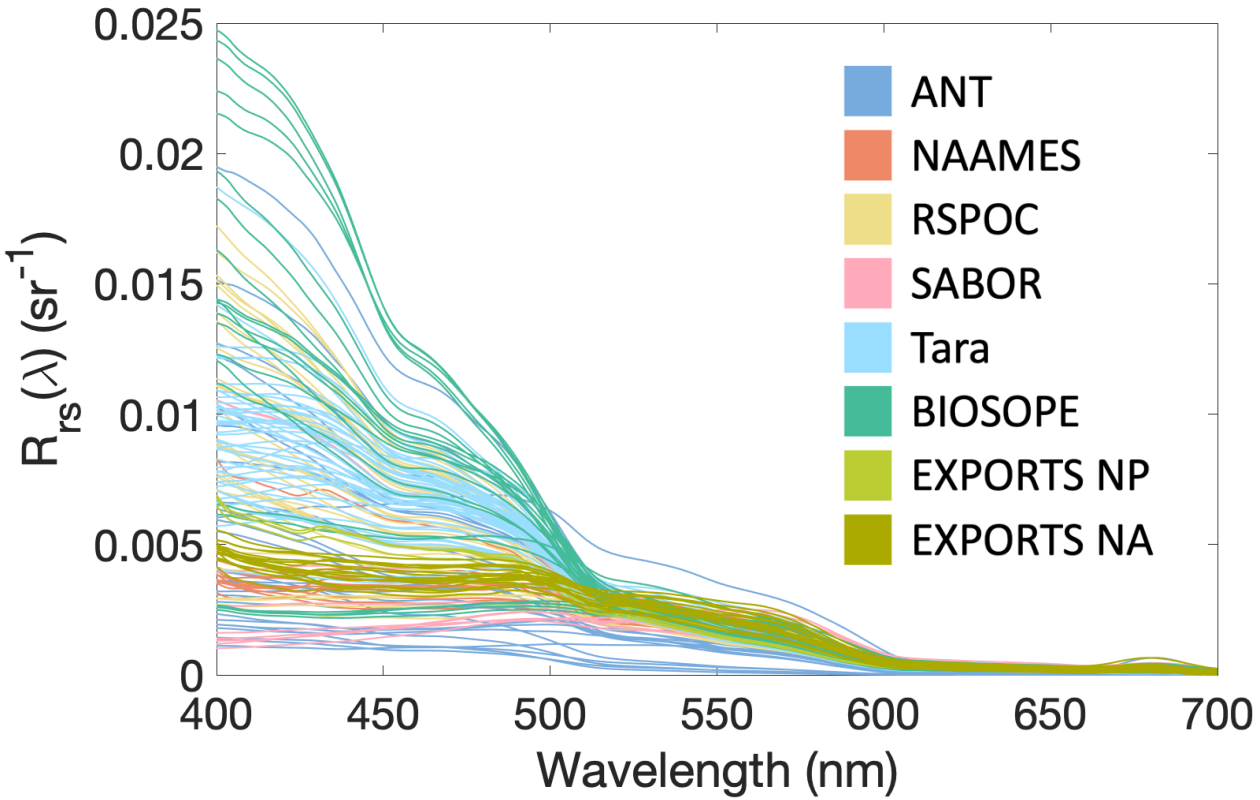
$$a = a_{ph} + a_{dg} + a_{water} \text{ and}$$

$$b = b_{bp} + b_{bwater}$$

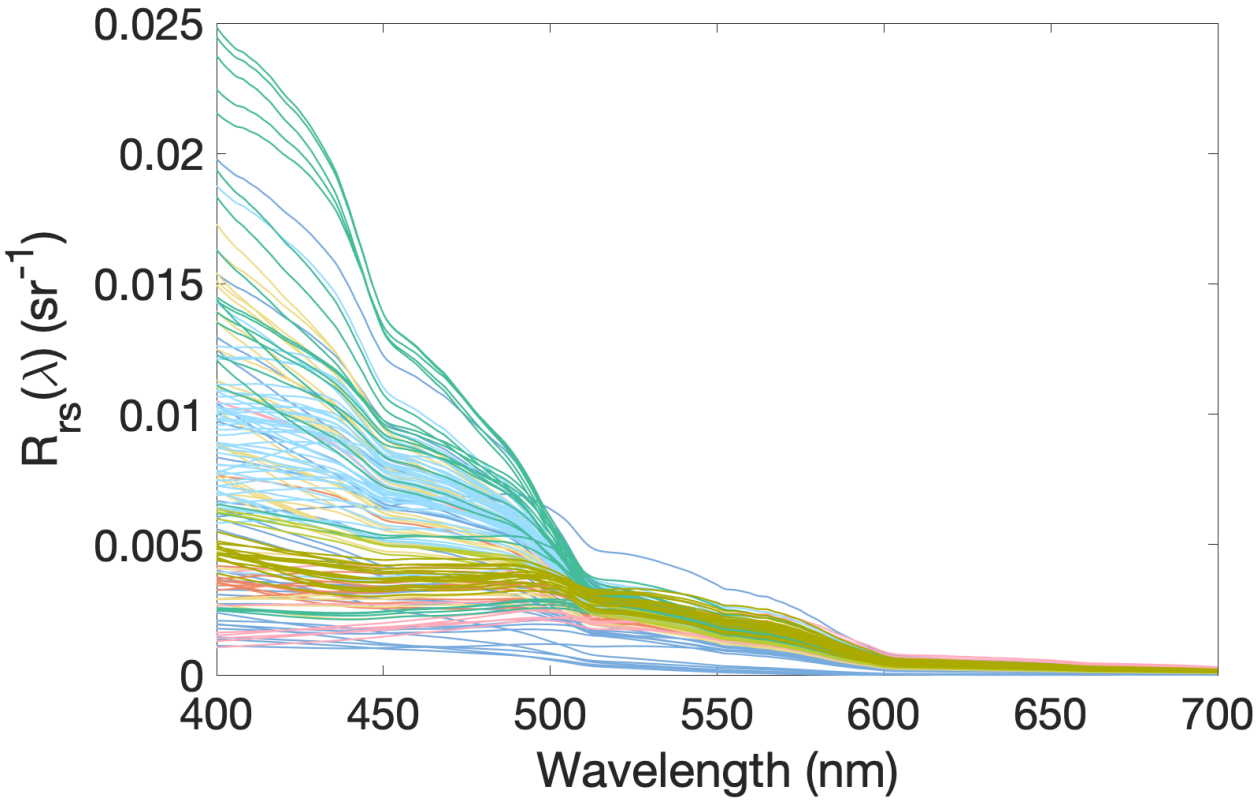
Adapted from Kramer et al., 2022 *Remote Sensing of Environment*

Implementing the SDP model

Measured spectra



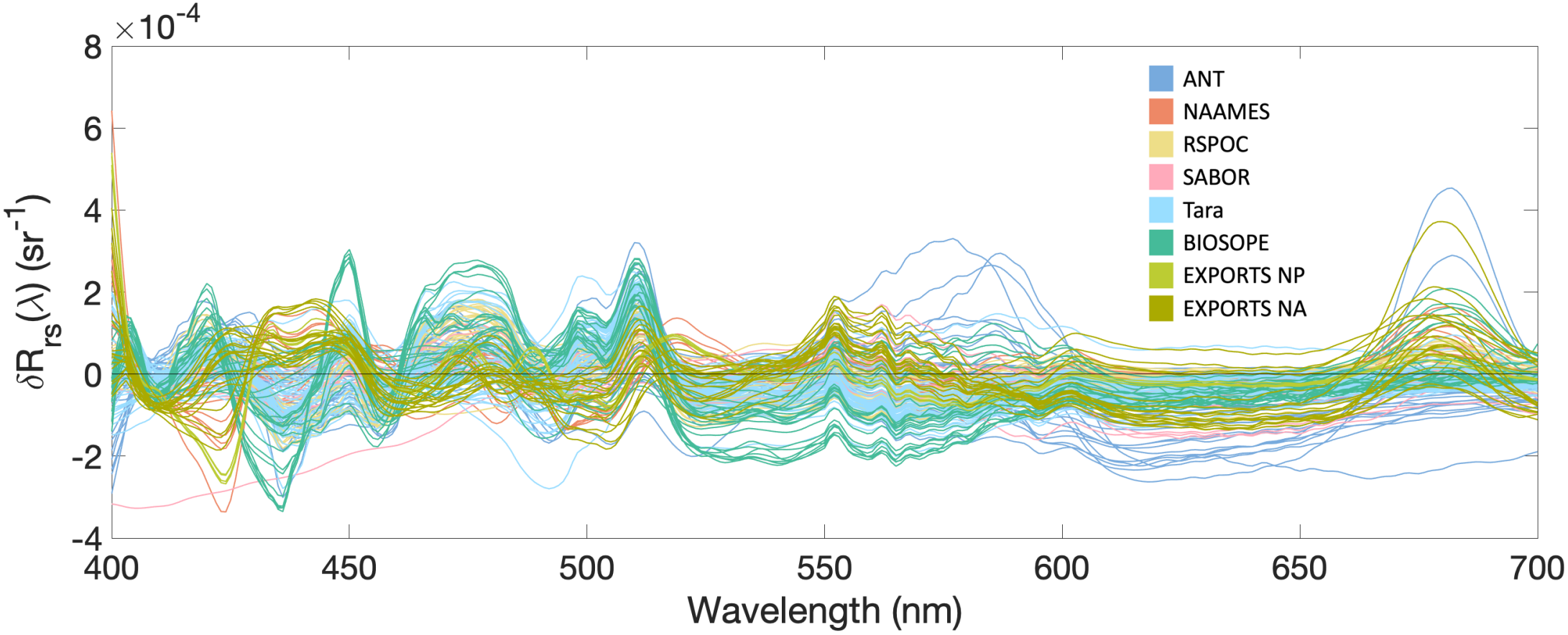
Modeled spectra



They should look identical if our assumptions were correct

Adapted from Kramer et al., 2022 *Remote Sensing of Environment*

R_{rs} residual (δR_{rs}) = $R_{rs,meas}(\lambda) - R_{rs,mod}(\lambda)$

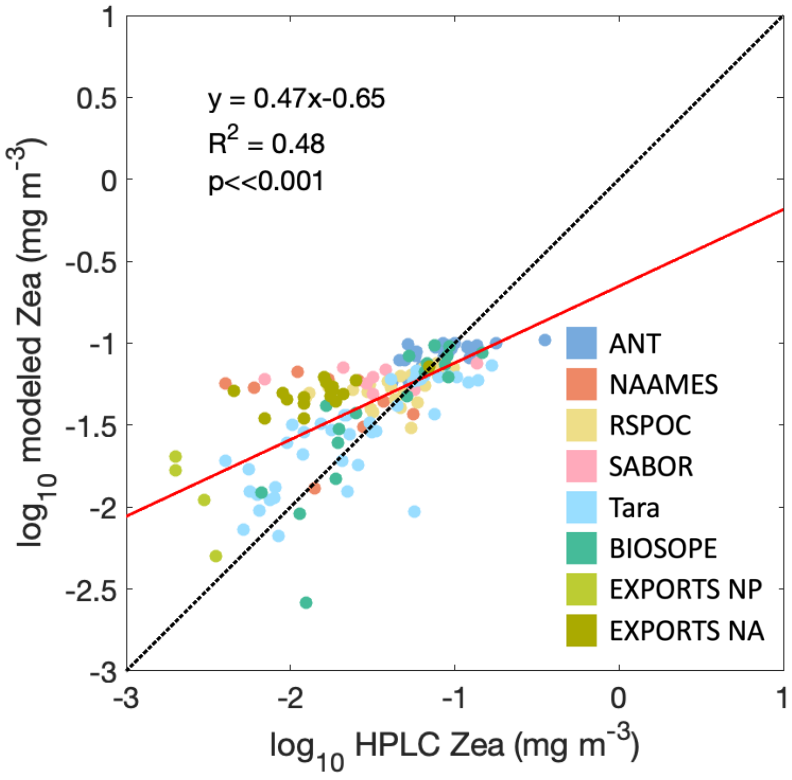


Use the reflectance residual (δR_{rs}) for further modeling…

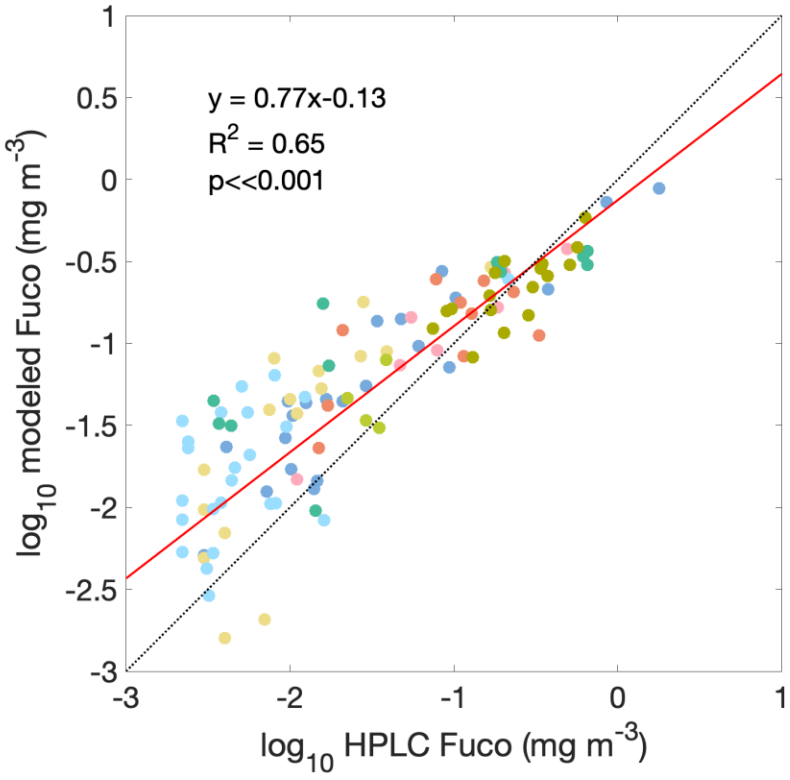
Adapted from Kramer et al., 2022 *Remote Sensing of Environment*

Modeled vs. measured pigments

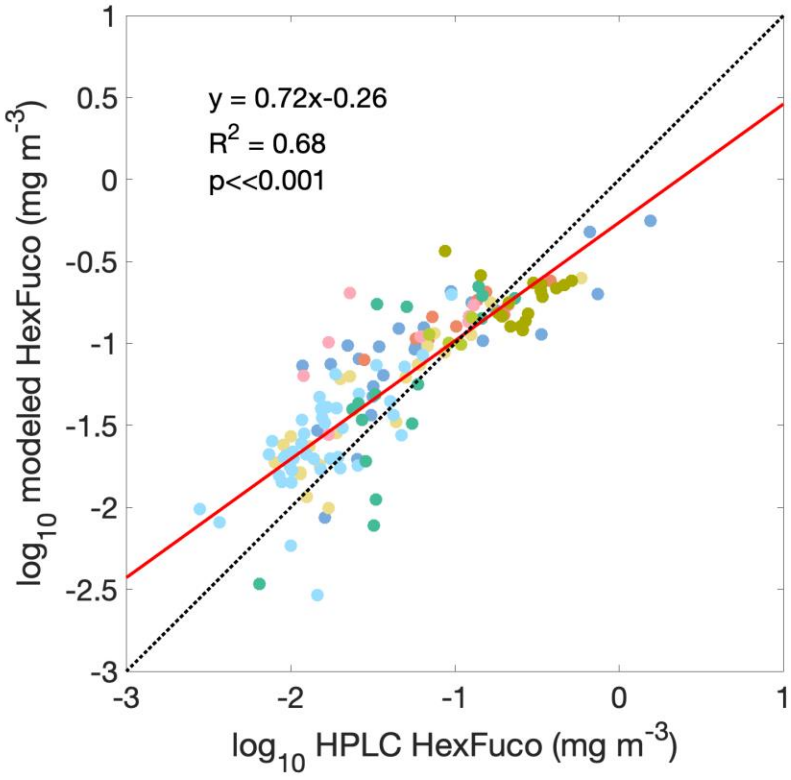
Zeaxanthin (cyanos)



Fucoxanthin (diatoms)



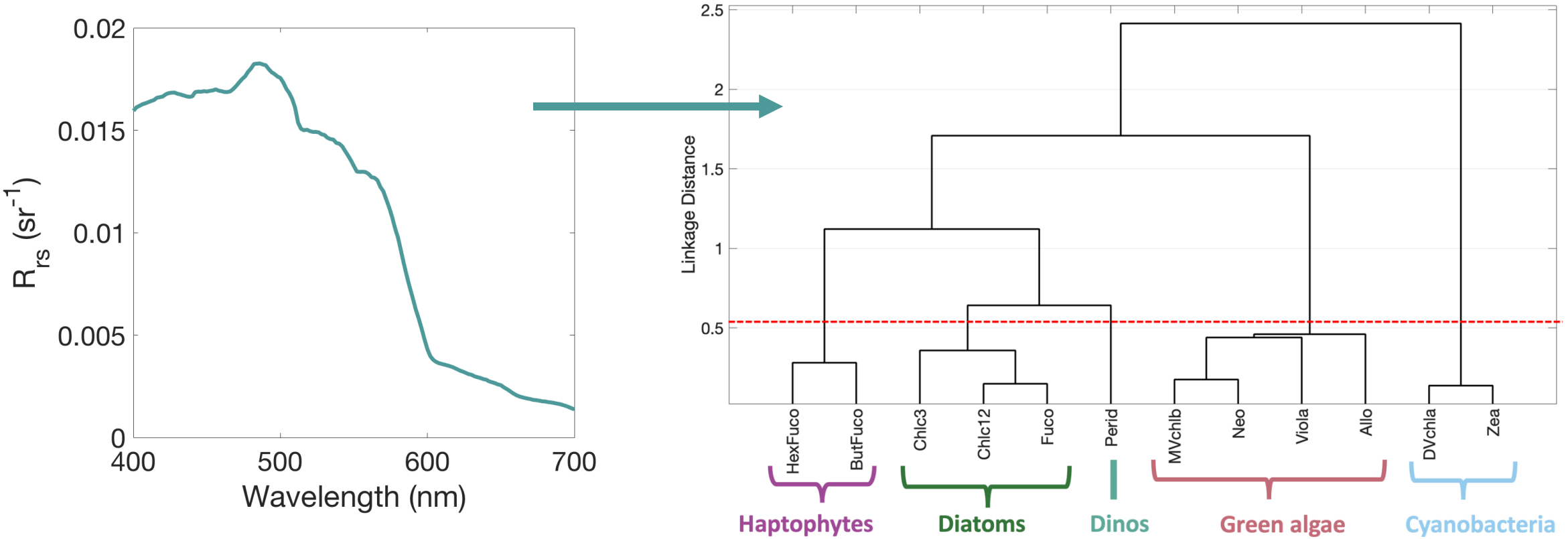
HexFuco (haptophytes)



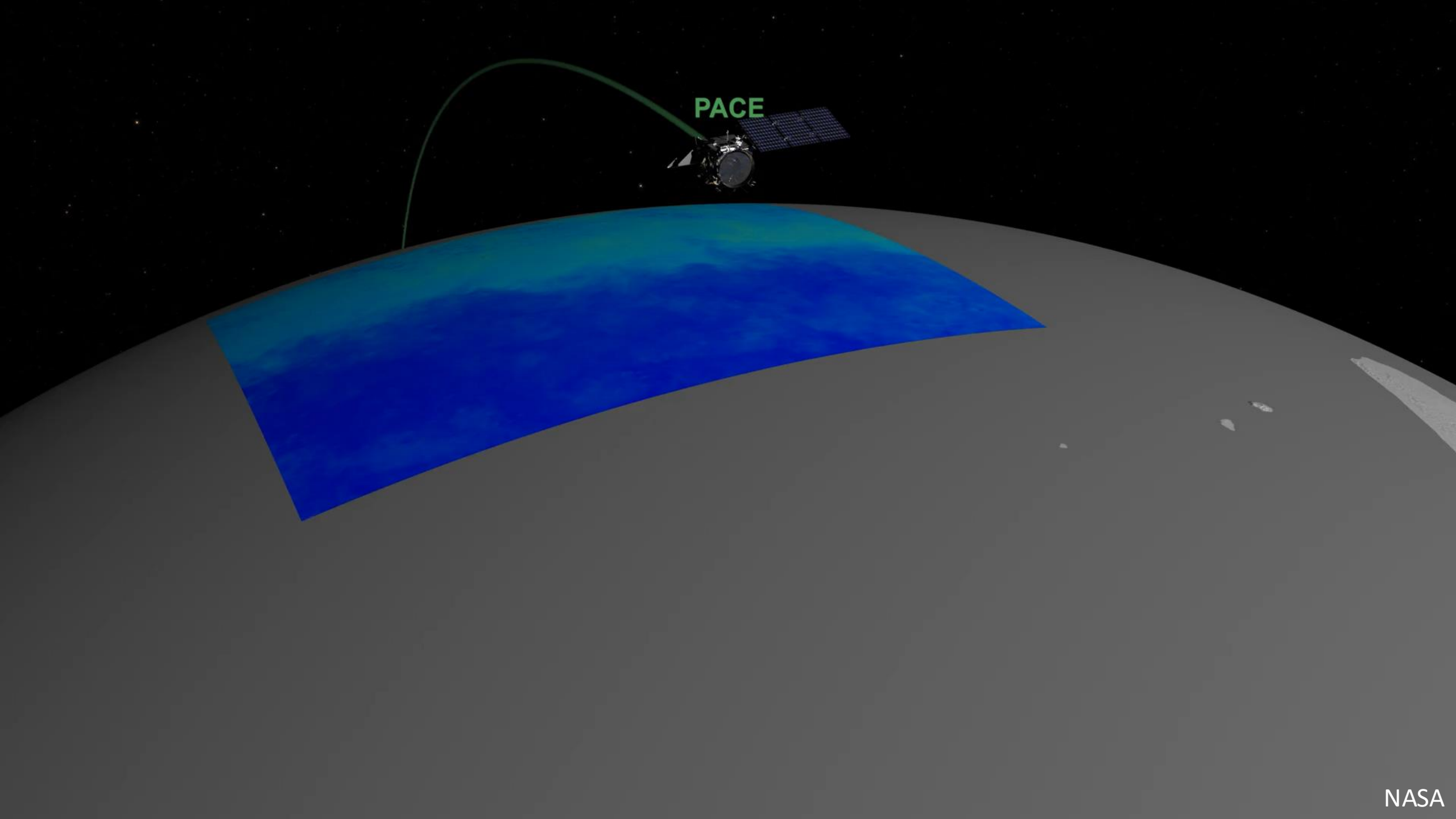
Adapted from Kramer et al., 2022 *Remote Sensing of Environment*
with new data included in Kramer et al., 2024 *Optics Express*

Going from ocean color to phytoplankton with PACE

Using the hyperspectral δR_{rs} data, we can model 13 phytoplankton pigment concentrations and distinct 5 phytoplankton groups.

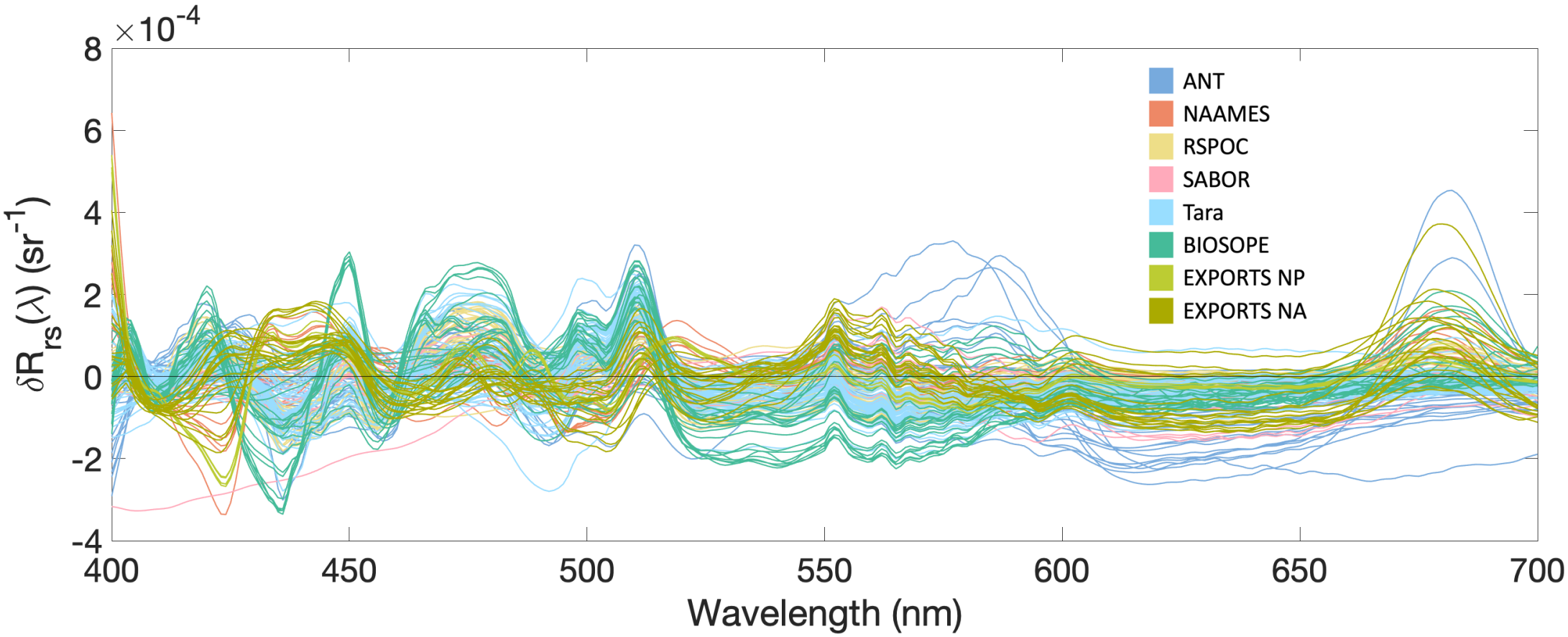


Kramer et al., 2022 *Remote Sensing of Environment*



NASA

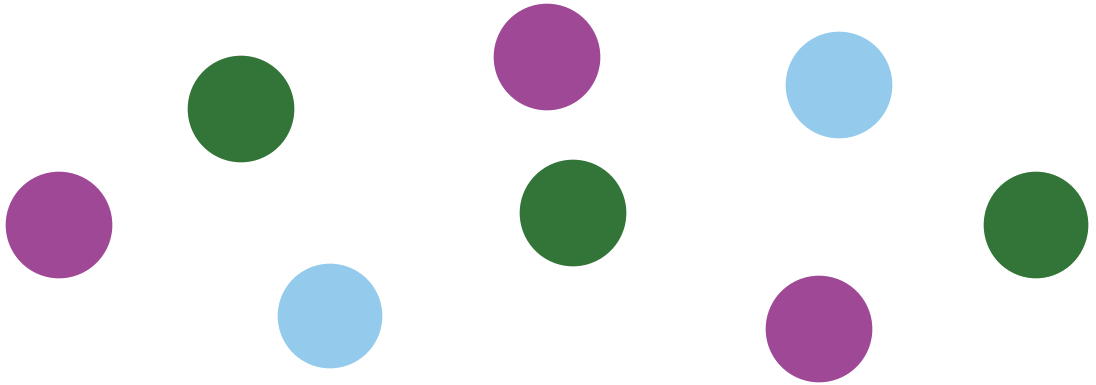
What else can we do with the R_{rs} residual (δR_{rs})?



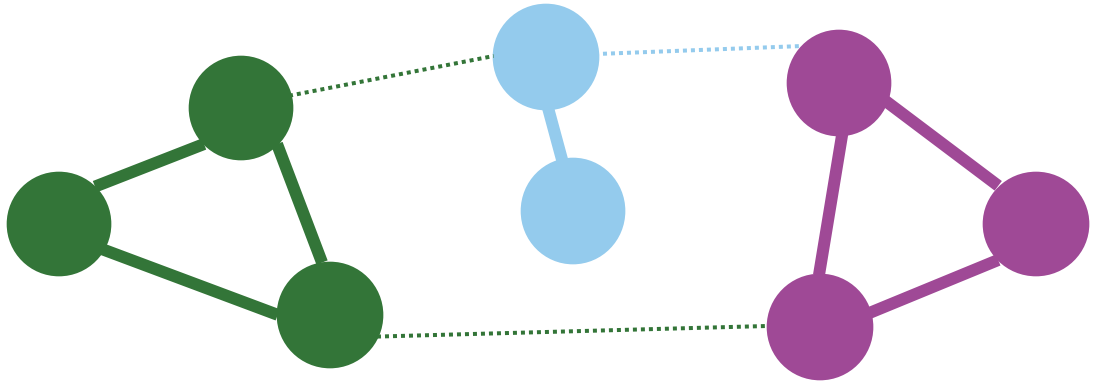
Adapted from Kramer et al., 2022 *Remote Sensing of Environment*

Network-based community detection analysis

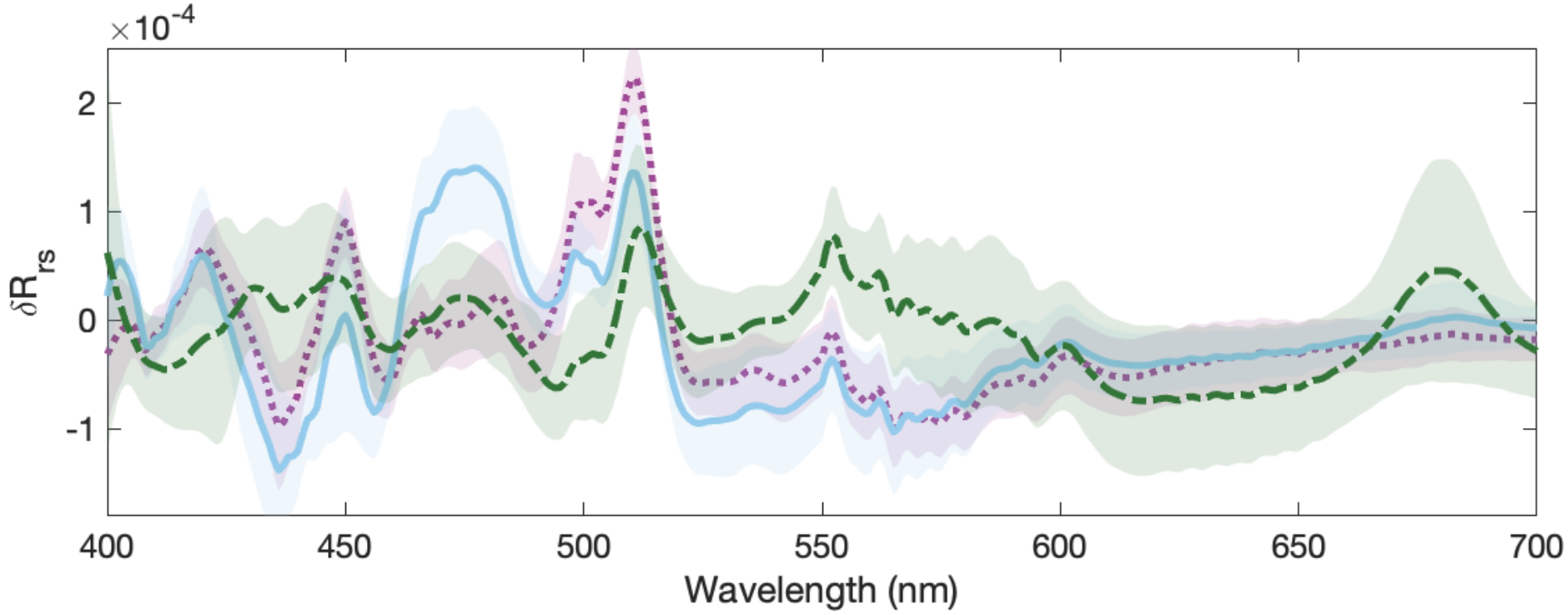
Assign each sample to a community based on its associated characteristics.



Form communities that maximize within-group connections and weaken between-group connections.

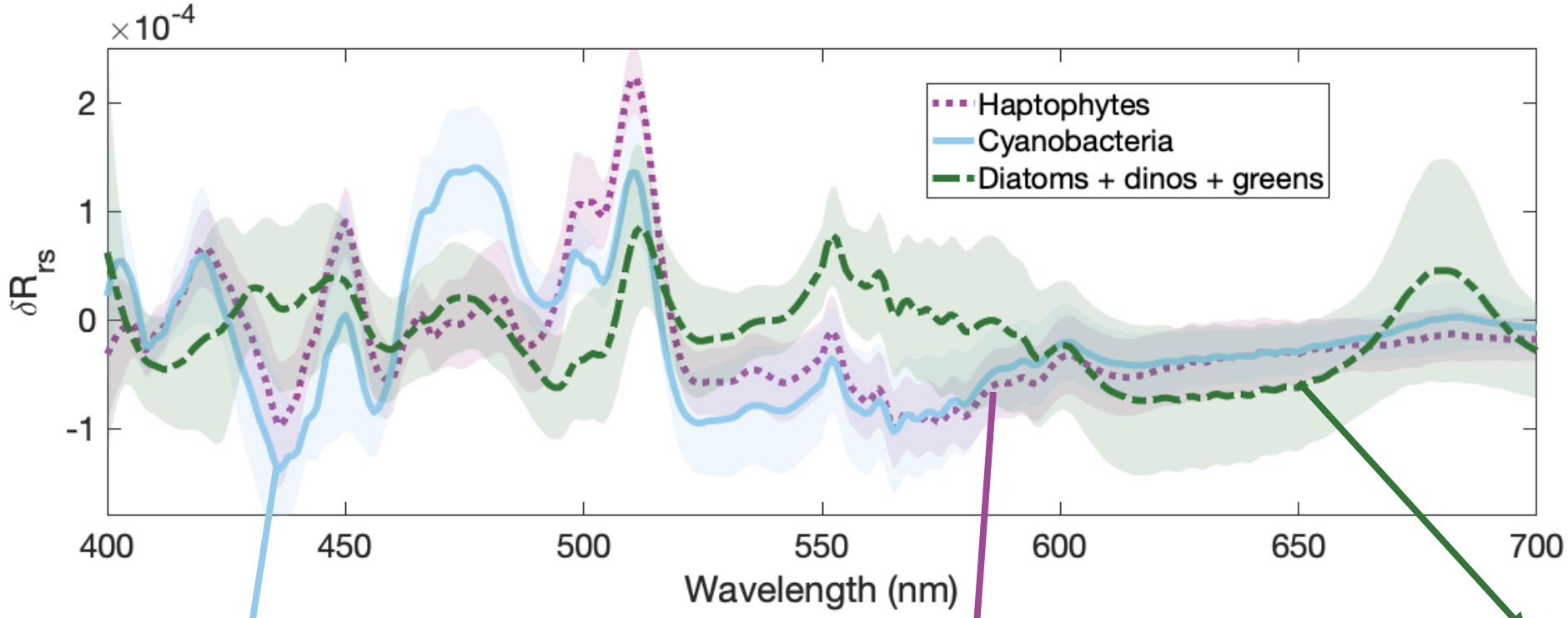


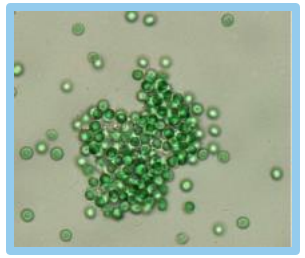
Community detection analysis: 3 δR_{rs} communities

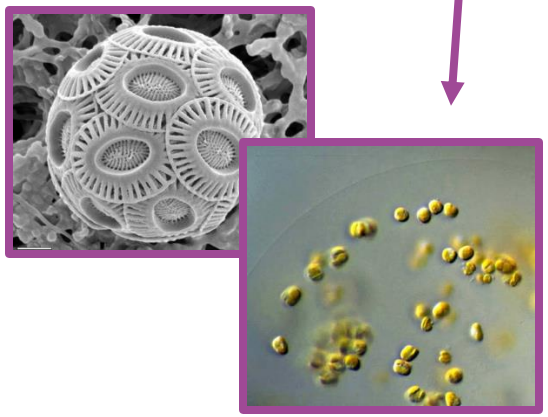


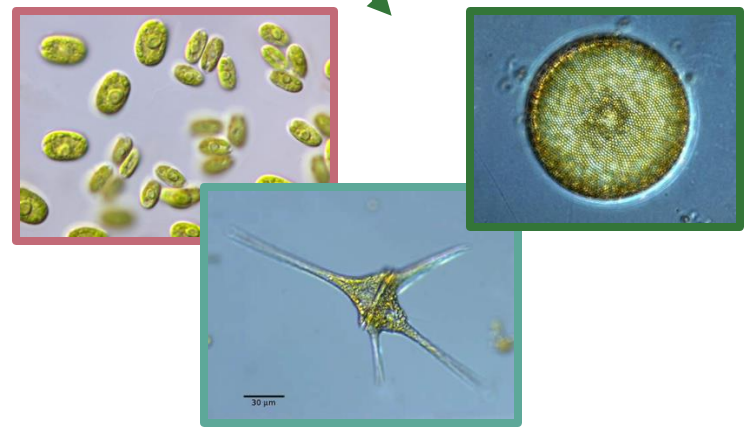
Kramer et al., 2024 *Optics Express*

Community detection analysis: 3 δR_{rs} communities



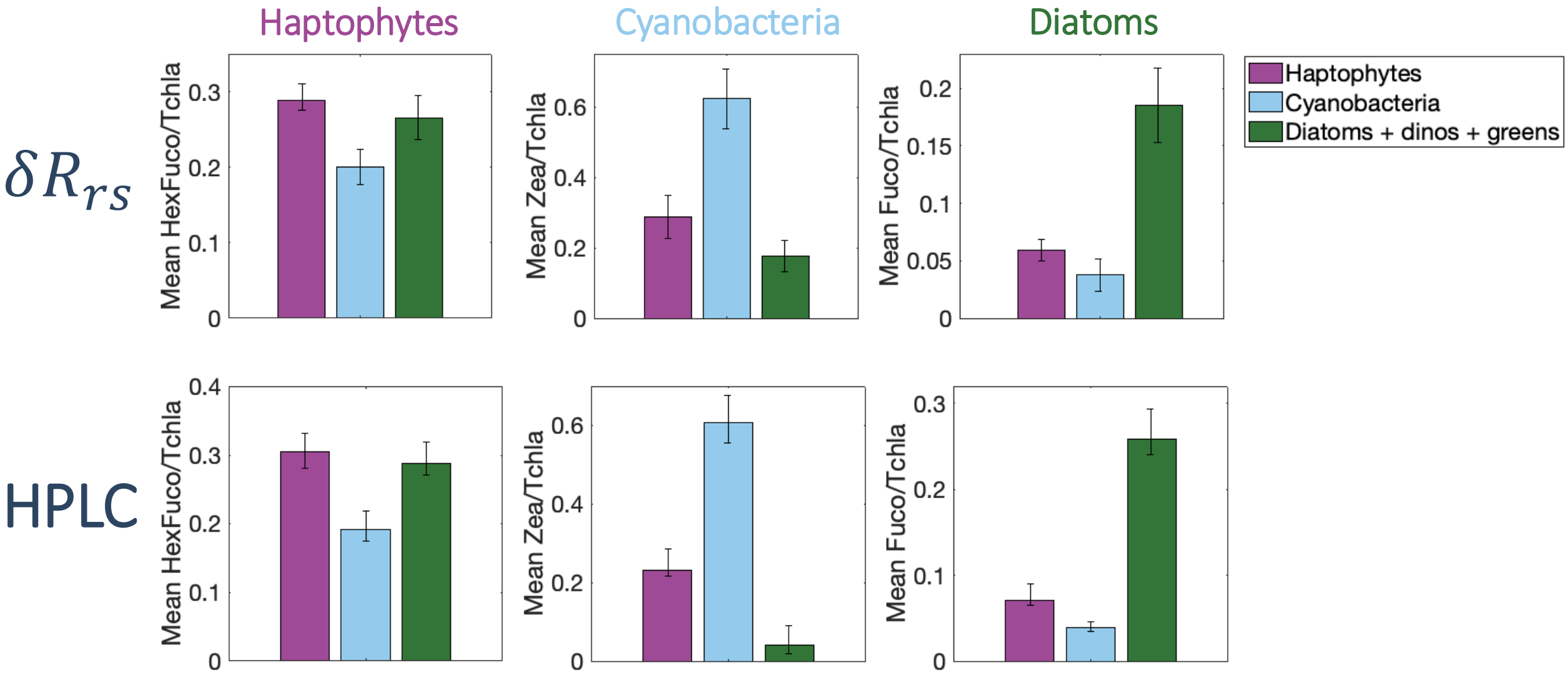






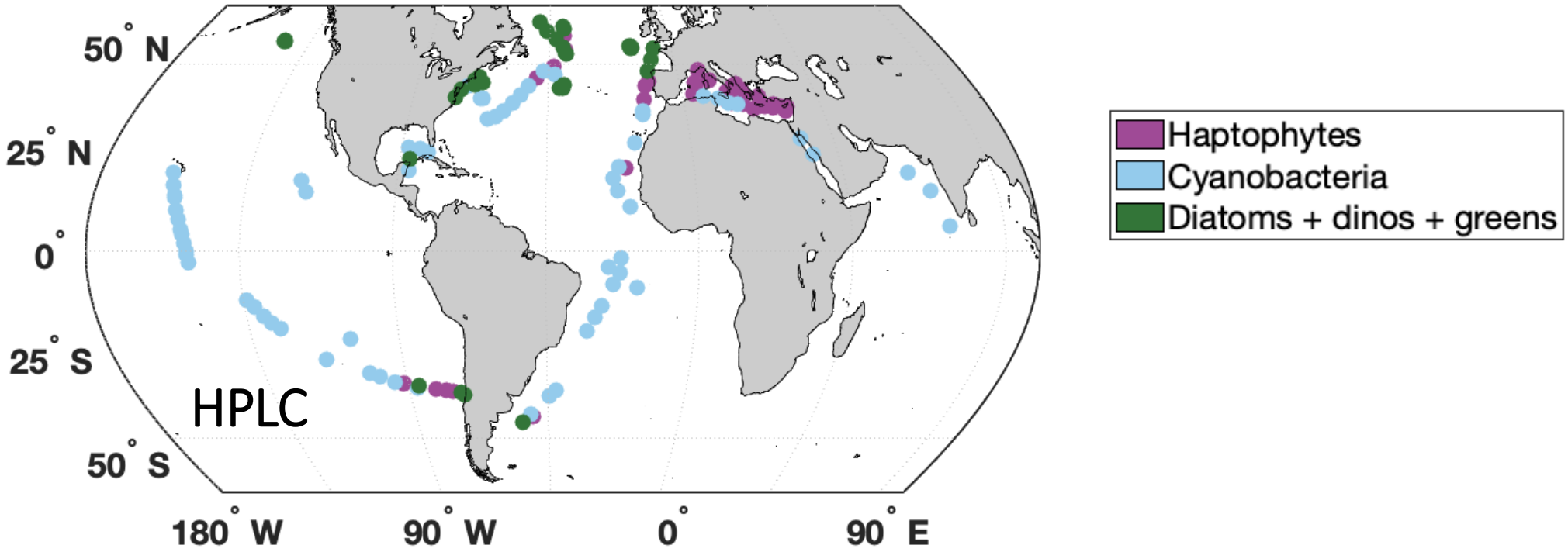
Kramer et al., 2024 *Optics Express*

Three communities also separate from HPLC pigments



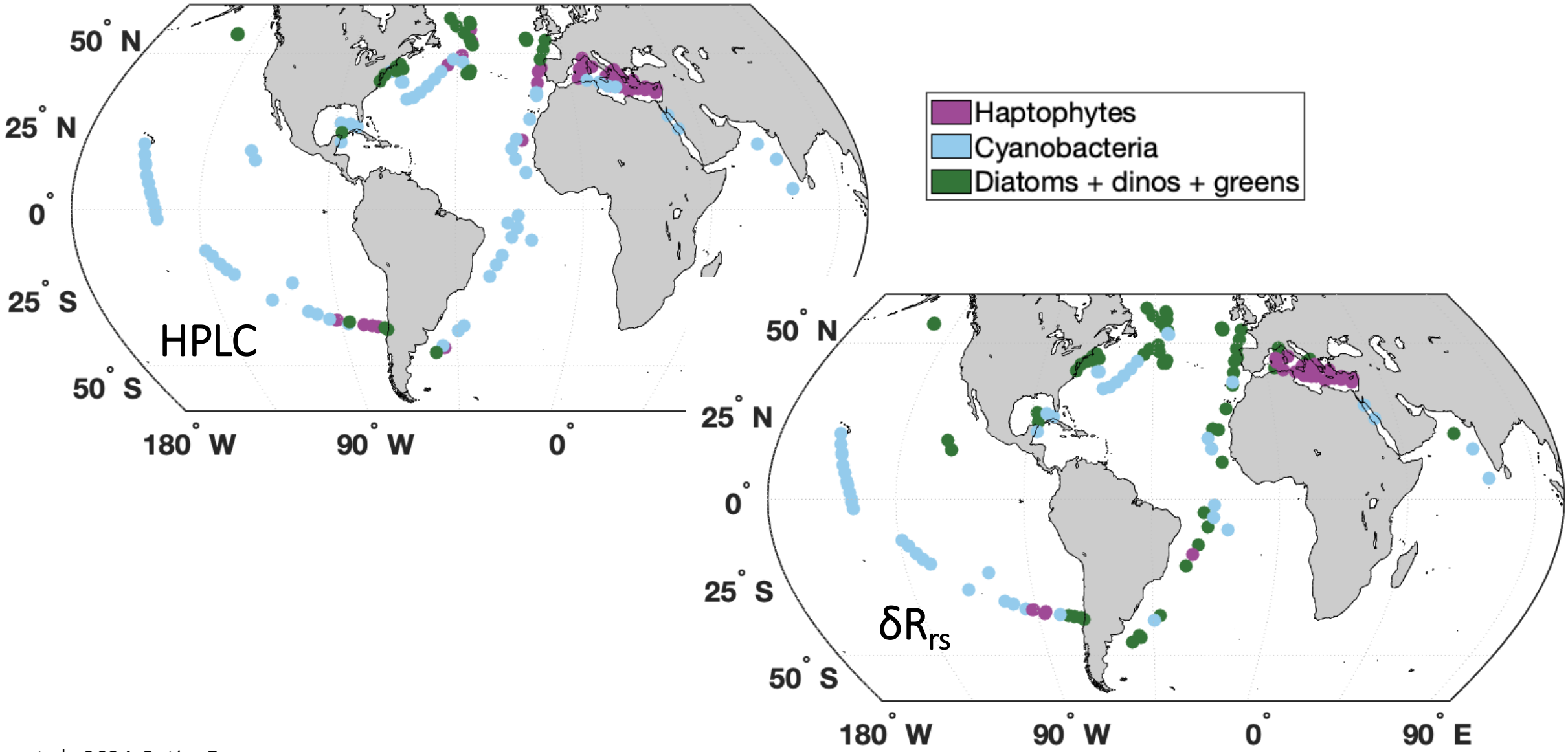
Kramer et al., 2024 *Optics Express*

Global distribution of the three communities



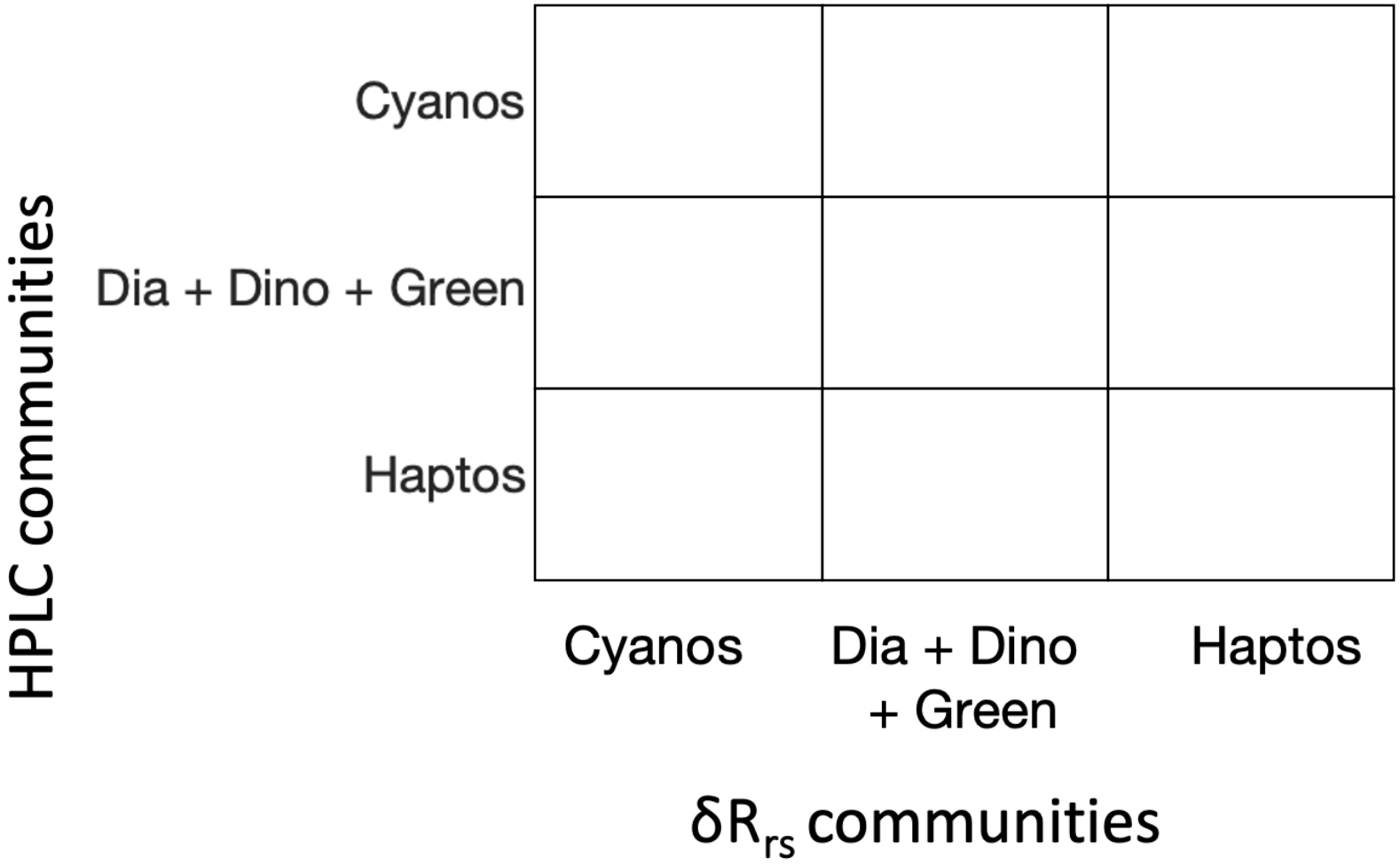
Kramer et al., 2024 *Optics Express*

Global distribution of the three communities

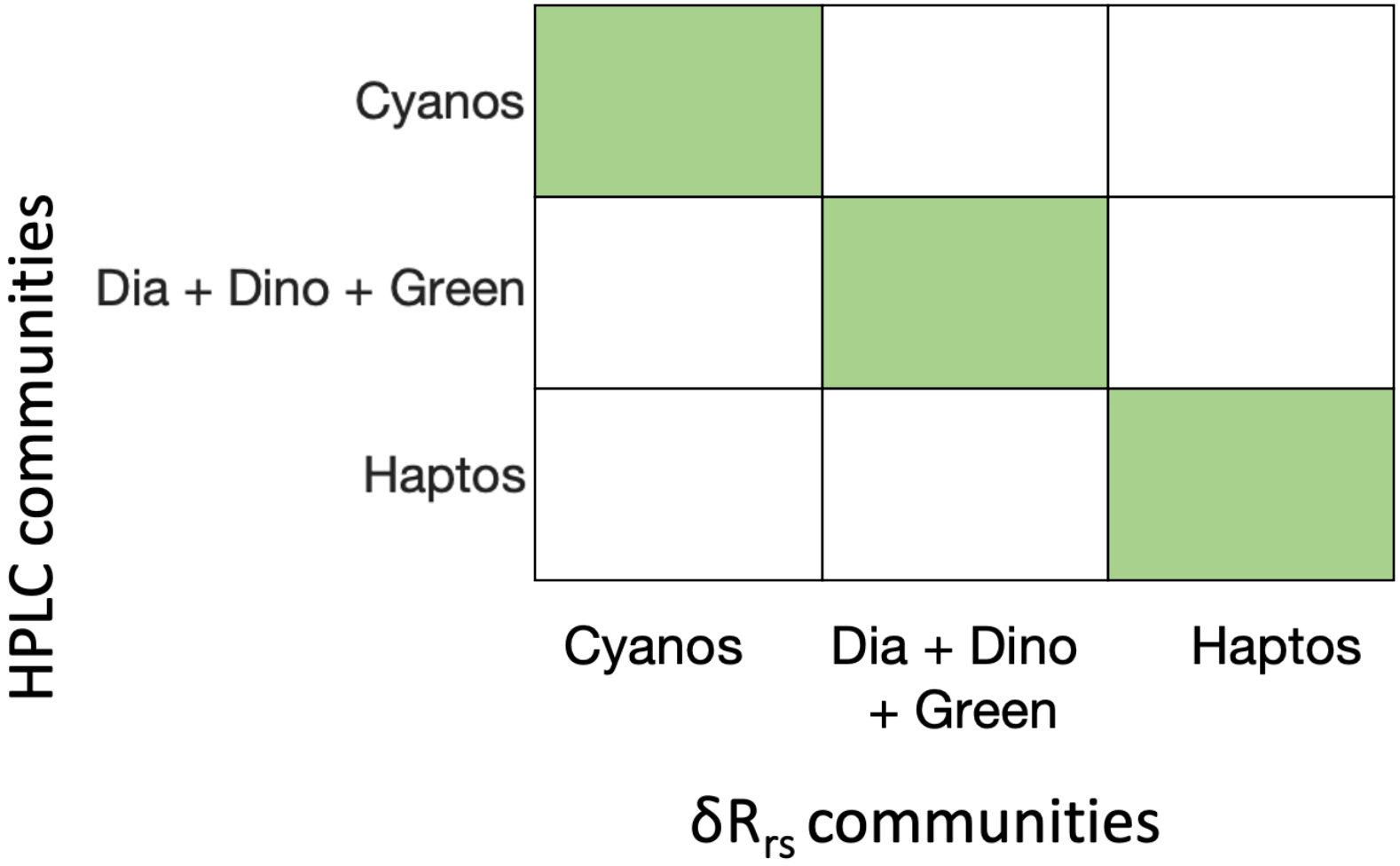


Kramer et al., 2024 *Optics Express*

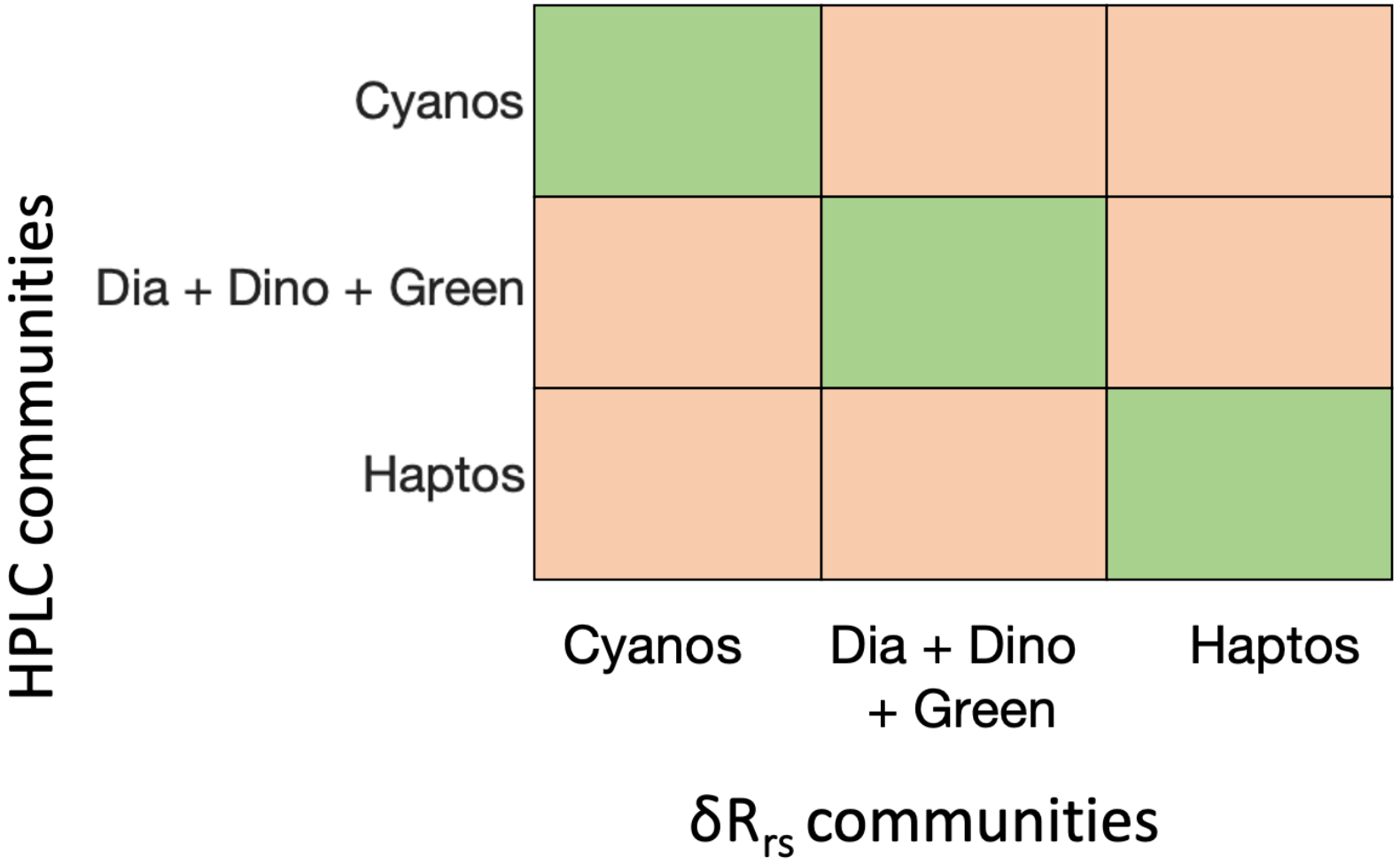
How well do δR_{rs} communities match HPLC communities?



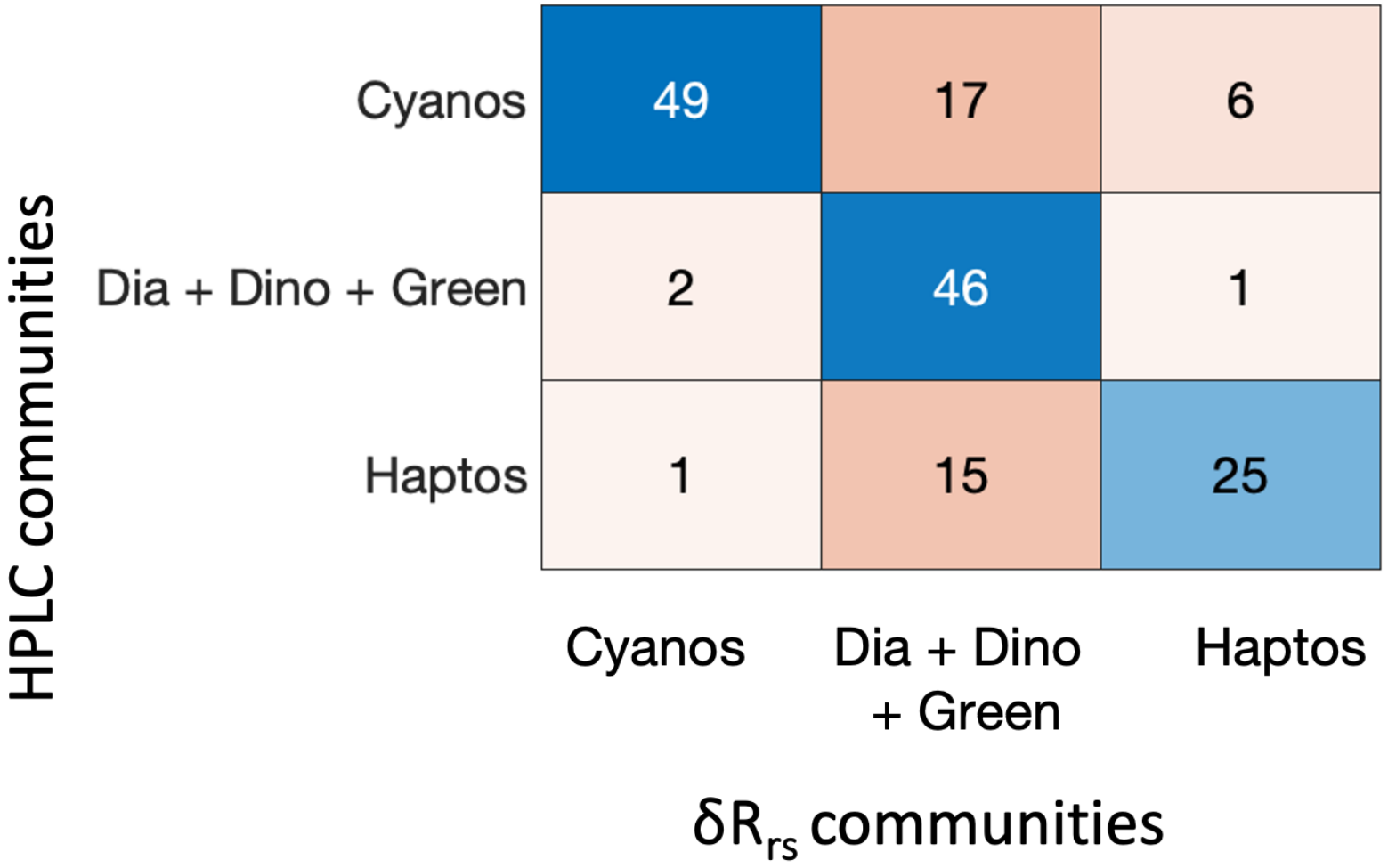
How well do δR_{rs} communities match HPLC communities?



How well do δR_{rs} communities match HPLC communities?



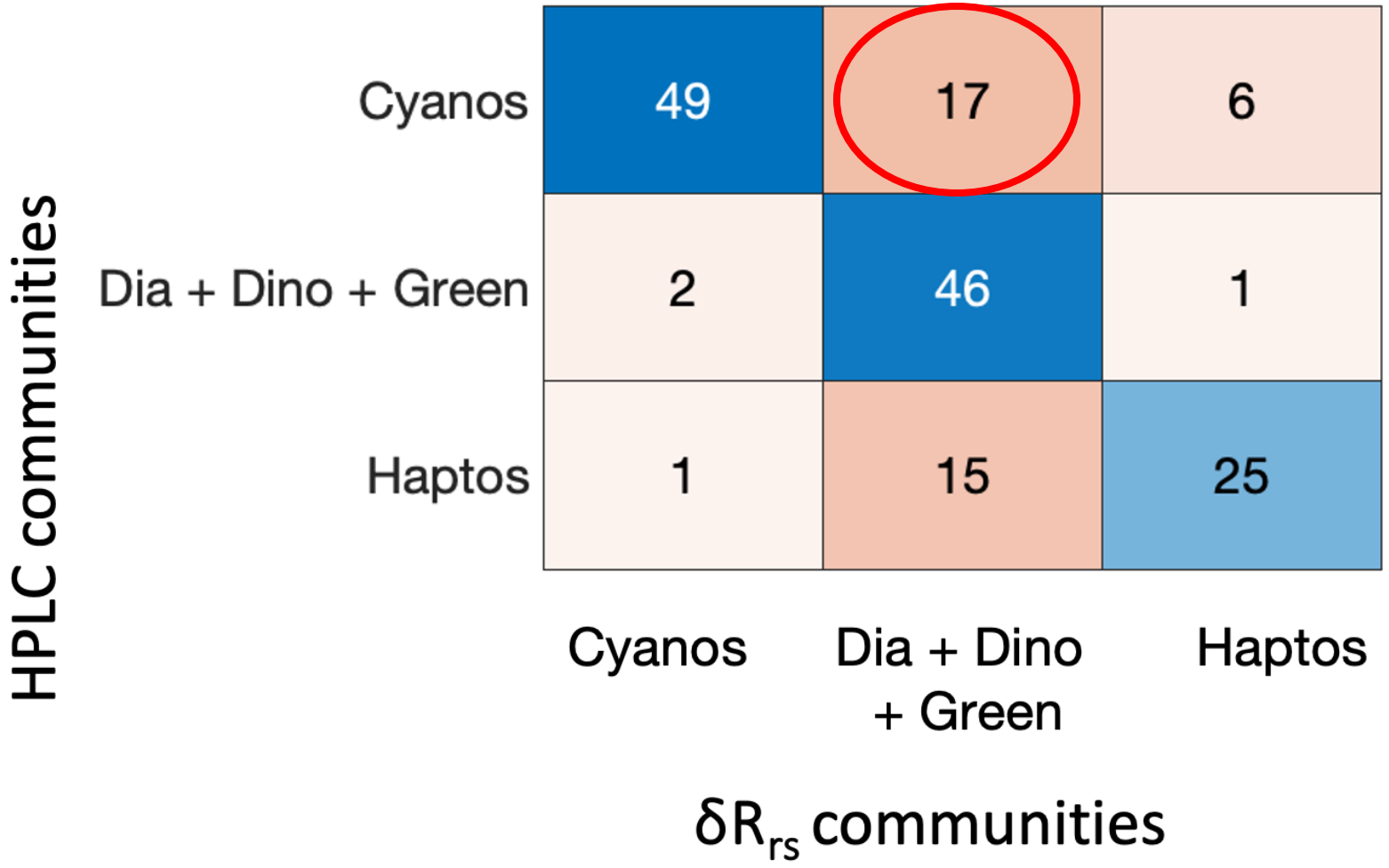
How well do δR_{rs} communities match HPLC communities?



74% of samples correctly assigned (120 of 162)

Kramer et al., 2024 *Optics Express*

Can we use other methods to investigate “confused” samples?



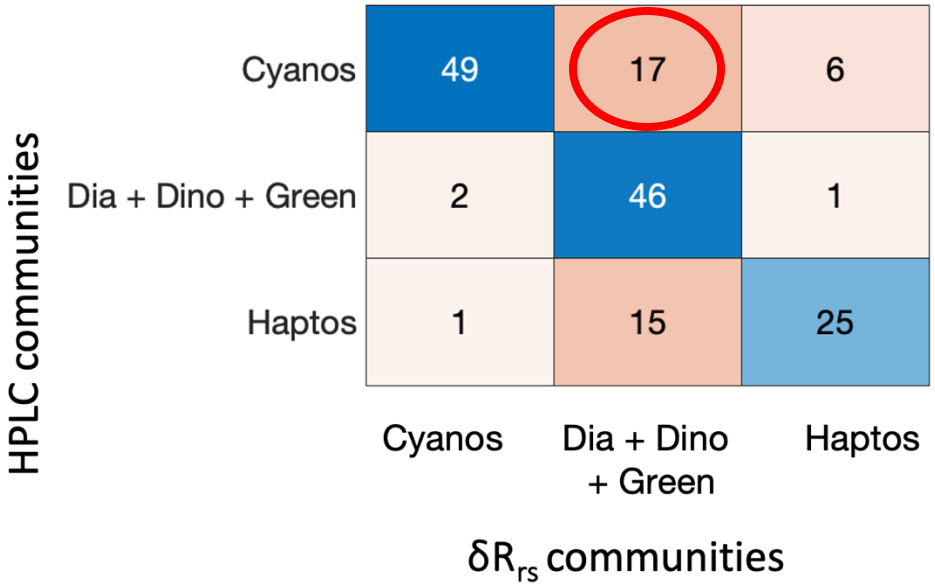
Kramer et al., 2024 *Optics Express*

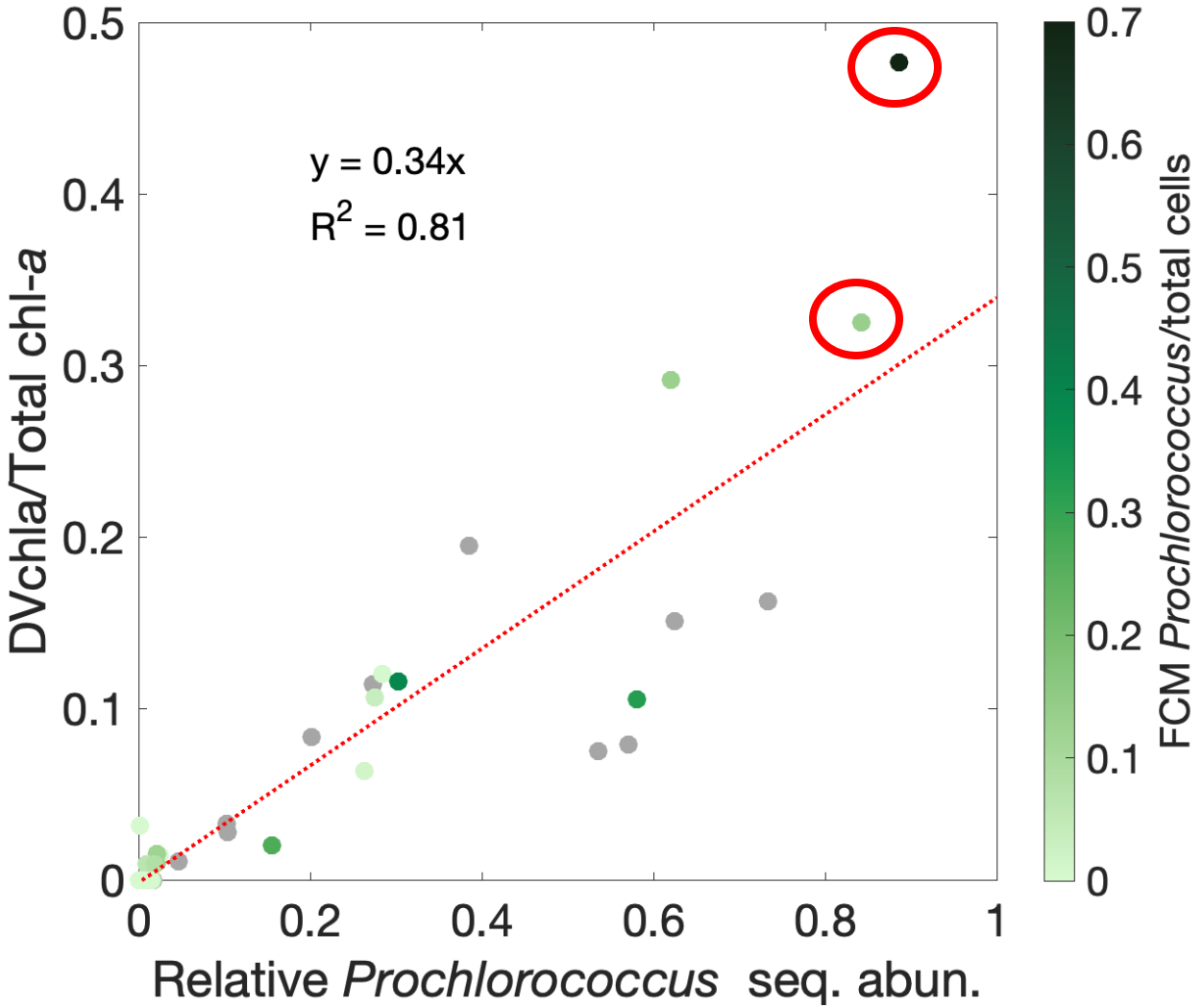
Methods with higher taxonomic resolution correct community assignment

Kramer et al., 2024 *Limnology & Oceanography: Methods*

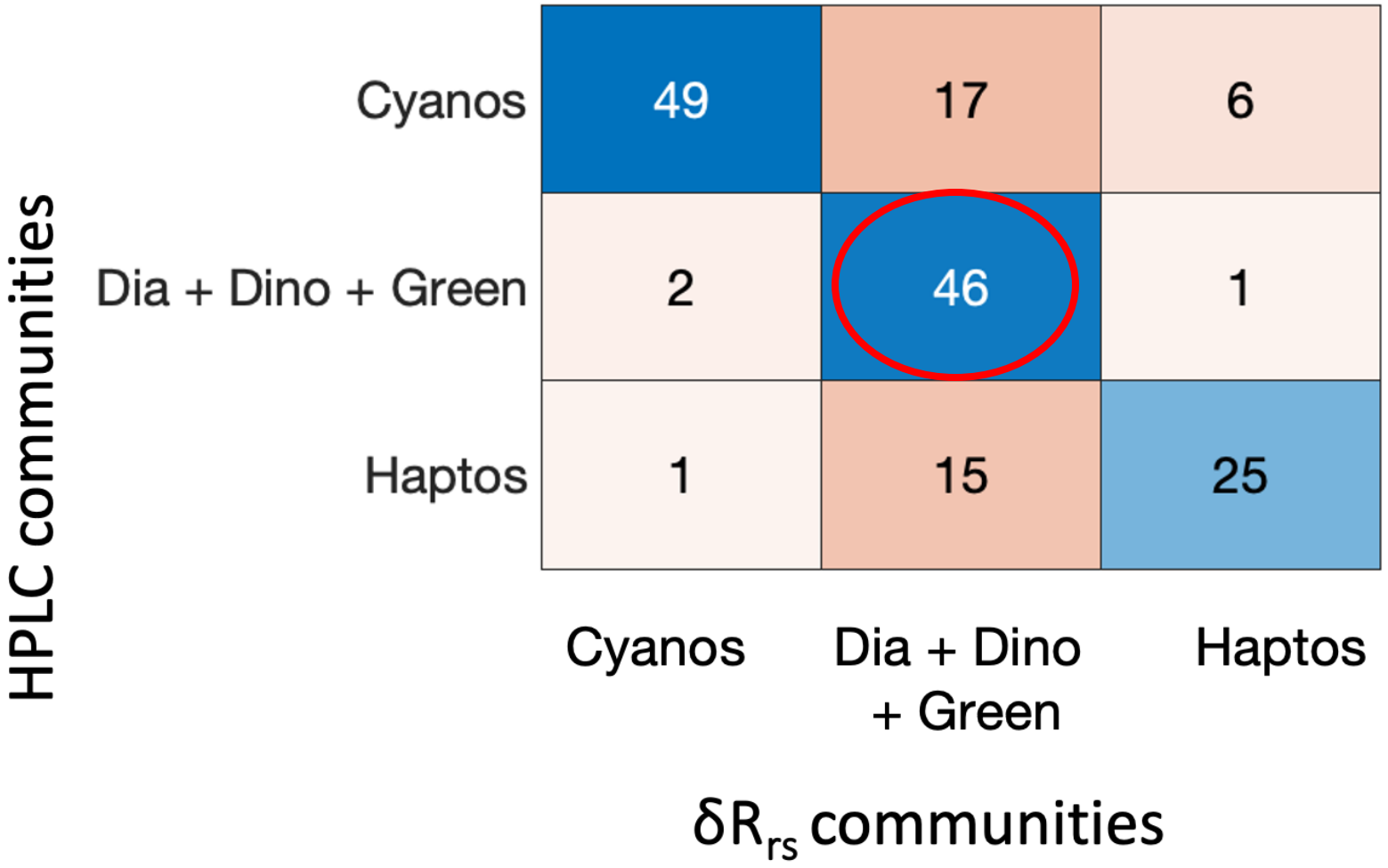
δR_{rs} community:
diatoms + dinos + greens
HPLC community: cyanos

16S rRNA + FCM: *Prochlorococcus*





Can we use other methods to investigate “confused” samples?



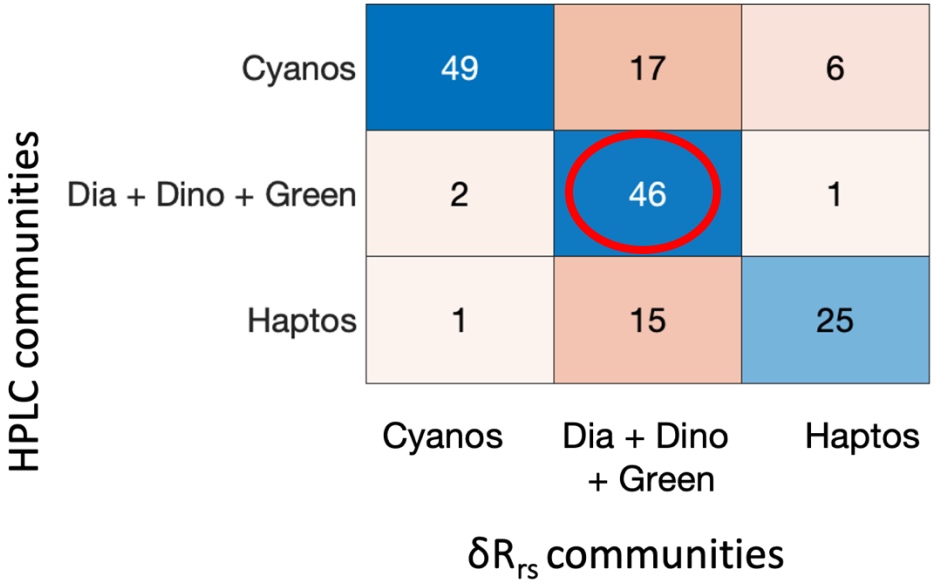
Kramer et al., 2024 *Optics Express*

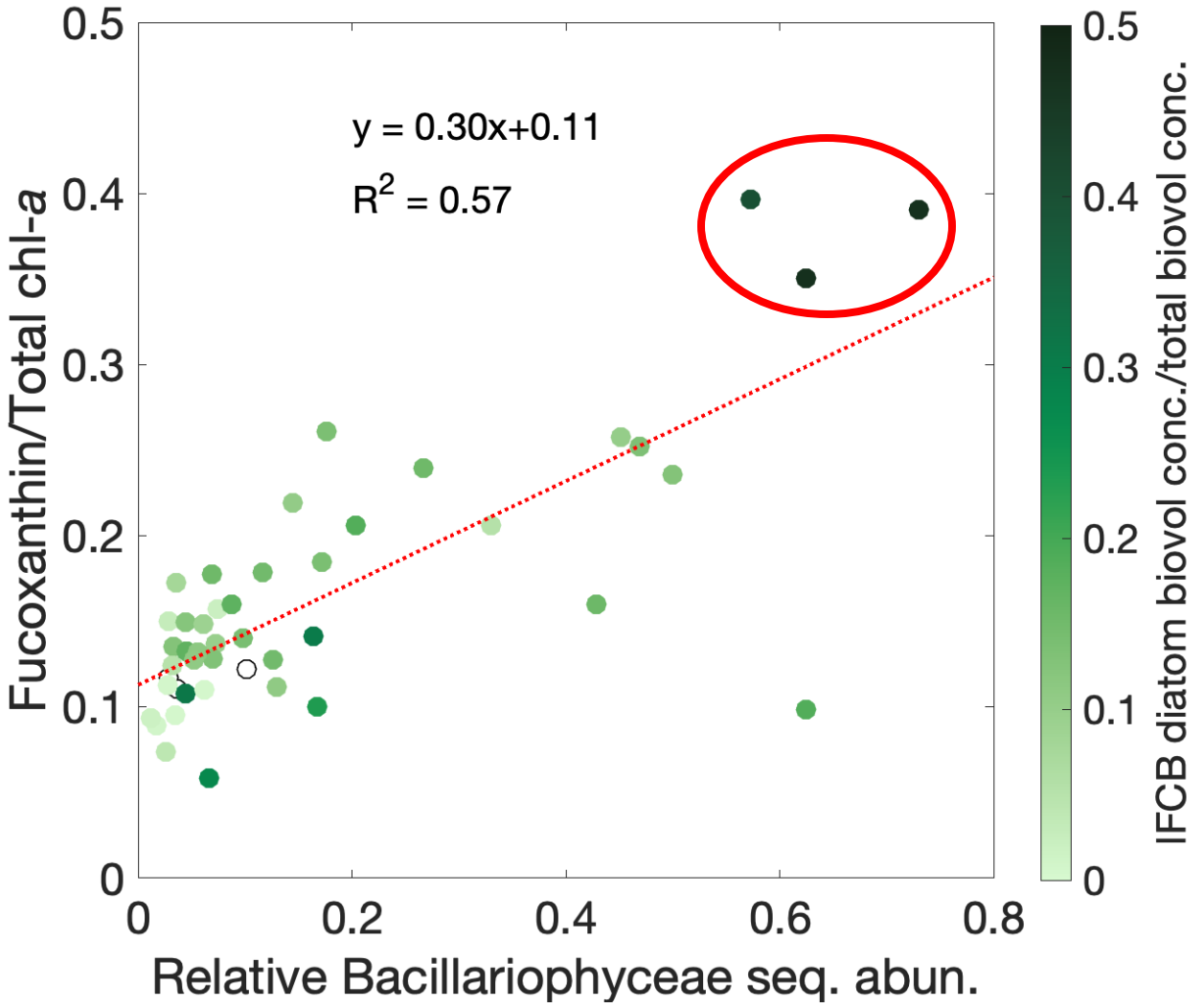
Methods with higher taxonomic resolution confirm community assignment

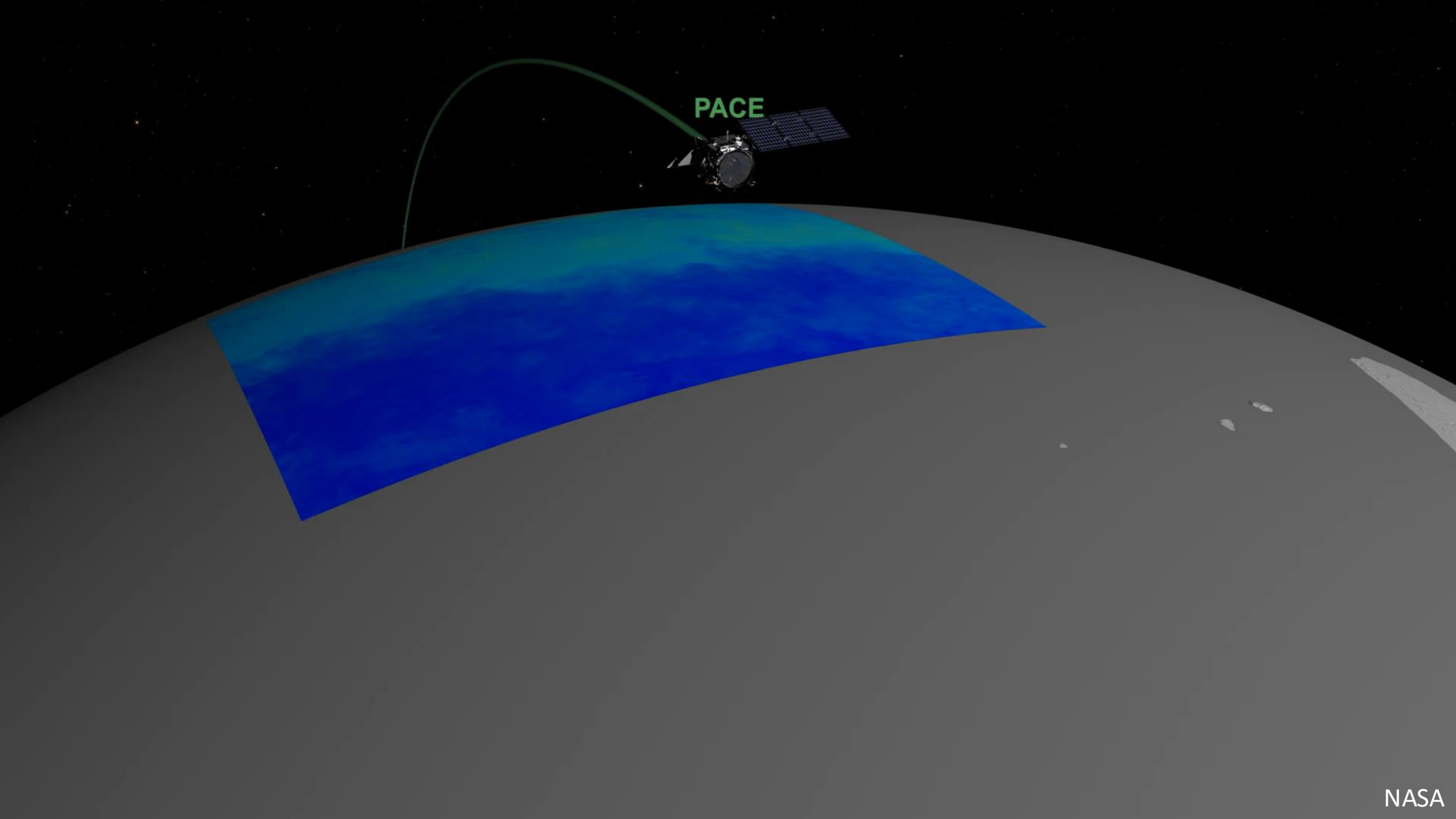
Kramer et al., 2024 *Limnology & Oceanography: Methods*

HPLC + δR_{rs} communities: diatoms + dinos + green algae

18S rRNA + IFCB: diatoms

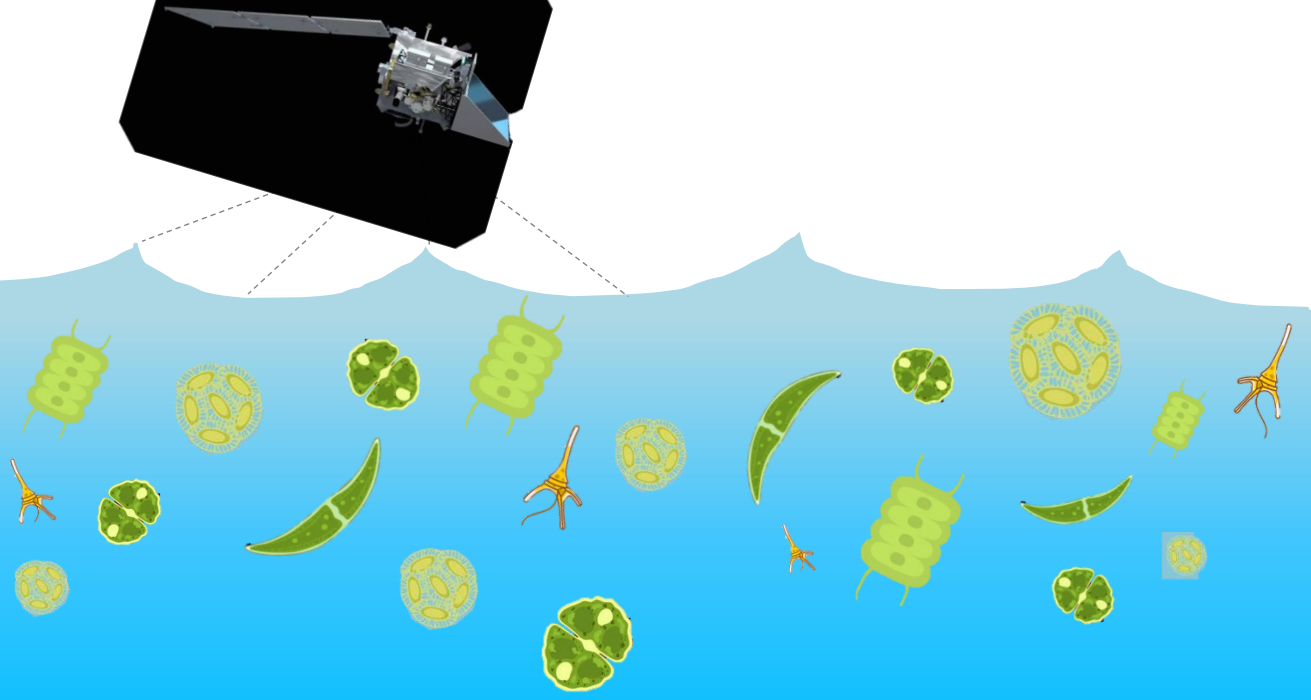






NASA

Next steps



1) SDP model is currently being implemented for PACE to model phytoplankton pigments

2) $\delta R_{rs}(\lambda)$ spectra will be available as a product from SDP and PACE: compare variability in space and time, compare communities from PVST HPLC.

Thanks and acknowledgements

Coauthors on work shown here: Dave Siegel, Jason Graff, Stéphane Maritorena, Jeremy Werdell, Ivona Cetinić, Dylan Catlett, Colleen Durkin, Erin Jones, Nicola Paul, Meg Estapa, Tatiana Rynearson, Alyson Santoro, Sebastian Sudek.

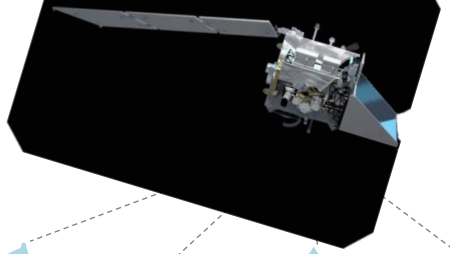
All researchers, technicians, captains, and crew who contributed to data collection, preparation, analysis, and submission (particular thanks to Ali Chase, Emmanuel Boss, Nils Haëntjens, Brian VerWey, Pat Kelly, Sean O'Neill, Melissa Omand, Ken Buesseler, and Elaine Steinberg).

The EXPORTS, NAAMES, and PACE science teams; the Carbon Flux Ecology lab at MBARI; BU Department of Earth & Environment.

Funding sources for work shown here: National Defense Science and Engineering Graduate Fellowship, NASA Ocean Biology and Biogeochemistry, Simons Foundation Postdoctoral Fellowship in Marine Microbial Ecology, David and Lucile Packard Foundation.

Questions?

sjkramer@bu.edu



Phytoplankton pigments can be successfully modeled from short spectral scale variability in hyperspectral $R_{rs}(\lambda)$.

Communities from $\delta R_{rs}(\lambda)$ and from HPLC identify the same 3 pigment-based phytoplankton groups with good (74%) agreement across paired global samples.

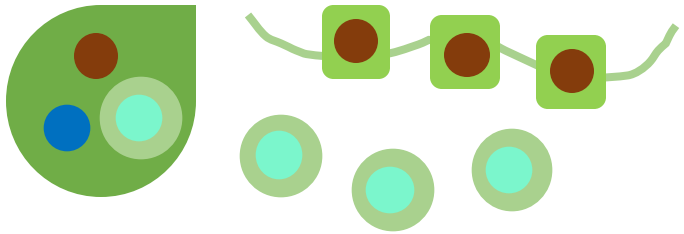
Aquatic Cathartic documentary

Migrations magazine

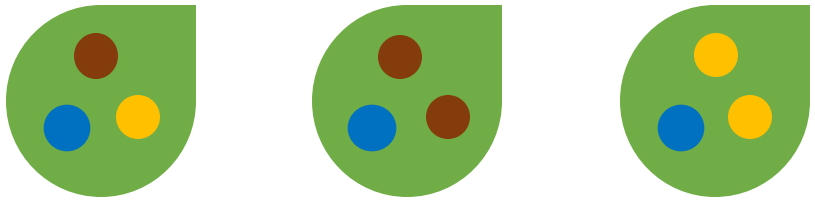
EXTRA SLIDES

Four major challenges for pigment-based PCC

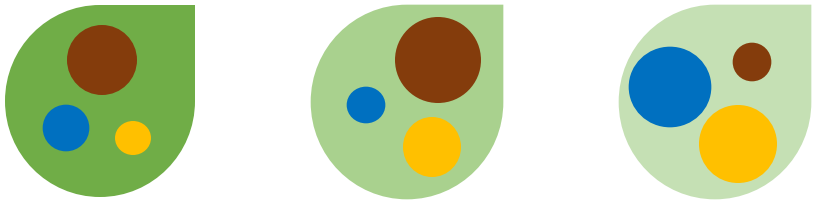
1. Many phytoplankton groups share pigments, either due to evolution or mixotrophy.



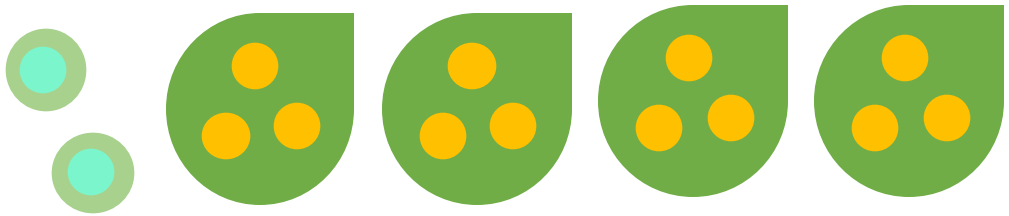
2. Within the same broad phytoplankton group, there can be variations in pigment composition.



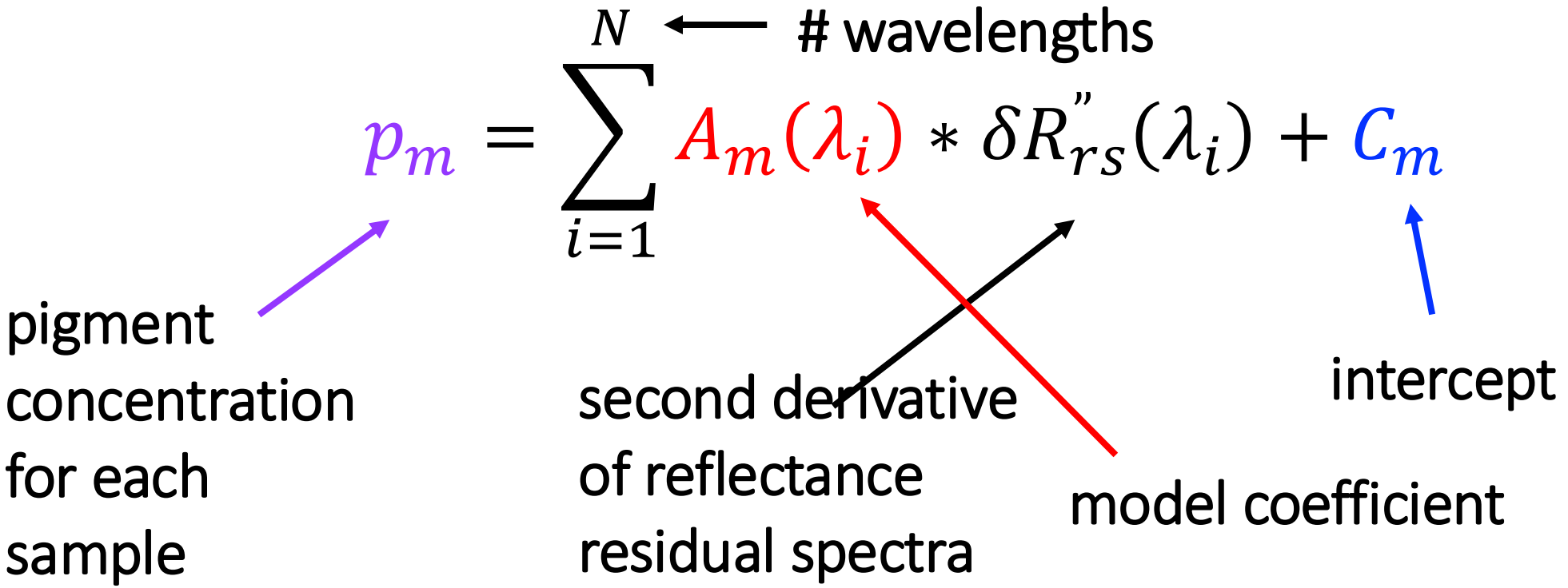
3. Pigment concentration and composition can be affected by the environment (light, nutrients).



4. Correlations between pigments and other methods may happen due to co-occurrence in nature.



Principal components regression model:



Repeat for all pigments. 100-fold cross validation used to test model. Use 75% of dataset for model training, 25% for testing.