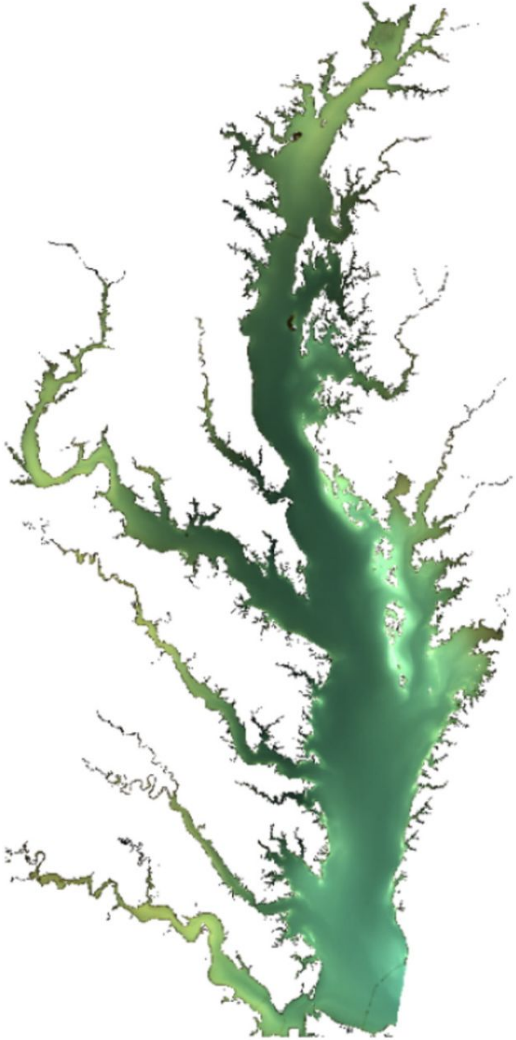

Optical water typing in optically complex waters: a case study of Chesapeake Bay

Anna E. Windle[1*], Sairah Y. Malkin[1], Raleigh R. Hood[1], Greg M. Silsbe[1]

[1]University of Maryland Center for Environmental Science, Horn Point Laboratory, Cambridge, MD
Present address: Ocean Ecology Laboratory, NASA Goddard Space Flight Center, Greenbelt, MD / Science Systems and Applications, Inc., Lanham, MD

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Optical water typing in optically complex waters: A case study of Chesapeake Bay

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University of Maryland Center for Environmental Science, Horn Point Laboratory, Cambridge, MD 21613, USA

Why and how do we monitor water quality?

Why?

- Understanding ecosystem health
- Detecting environmental change
- Evaluate effectiveness of management actions

How?

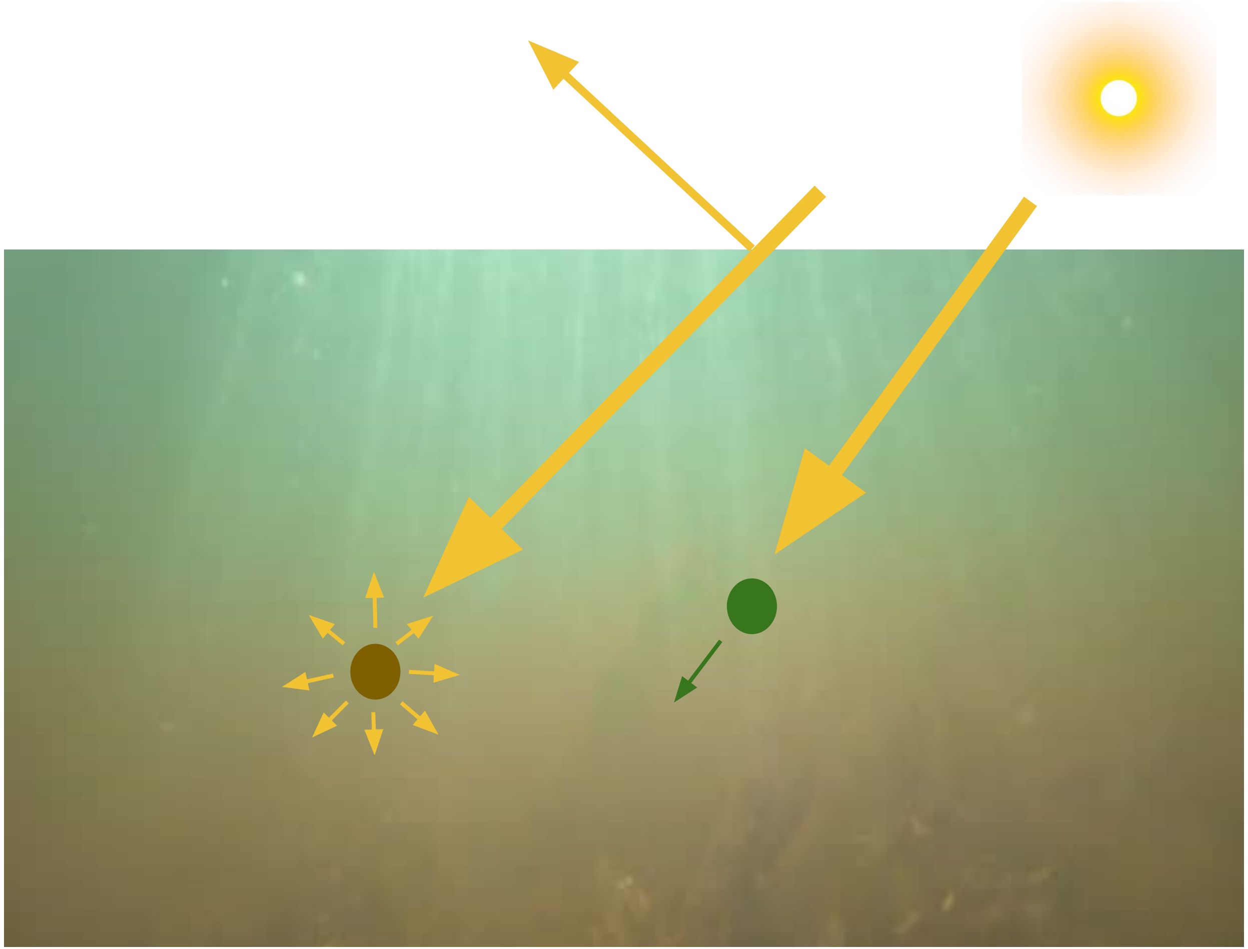
- Collecting discrete water column measurements
- Numerical modelling
- **Satellite remote sensing**

Light in water

Two important processes determine fate of light in water:

1) **Absorption**: light is taken up by molecules or water matter

2) **Scattering**: light is redirected with no loss



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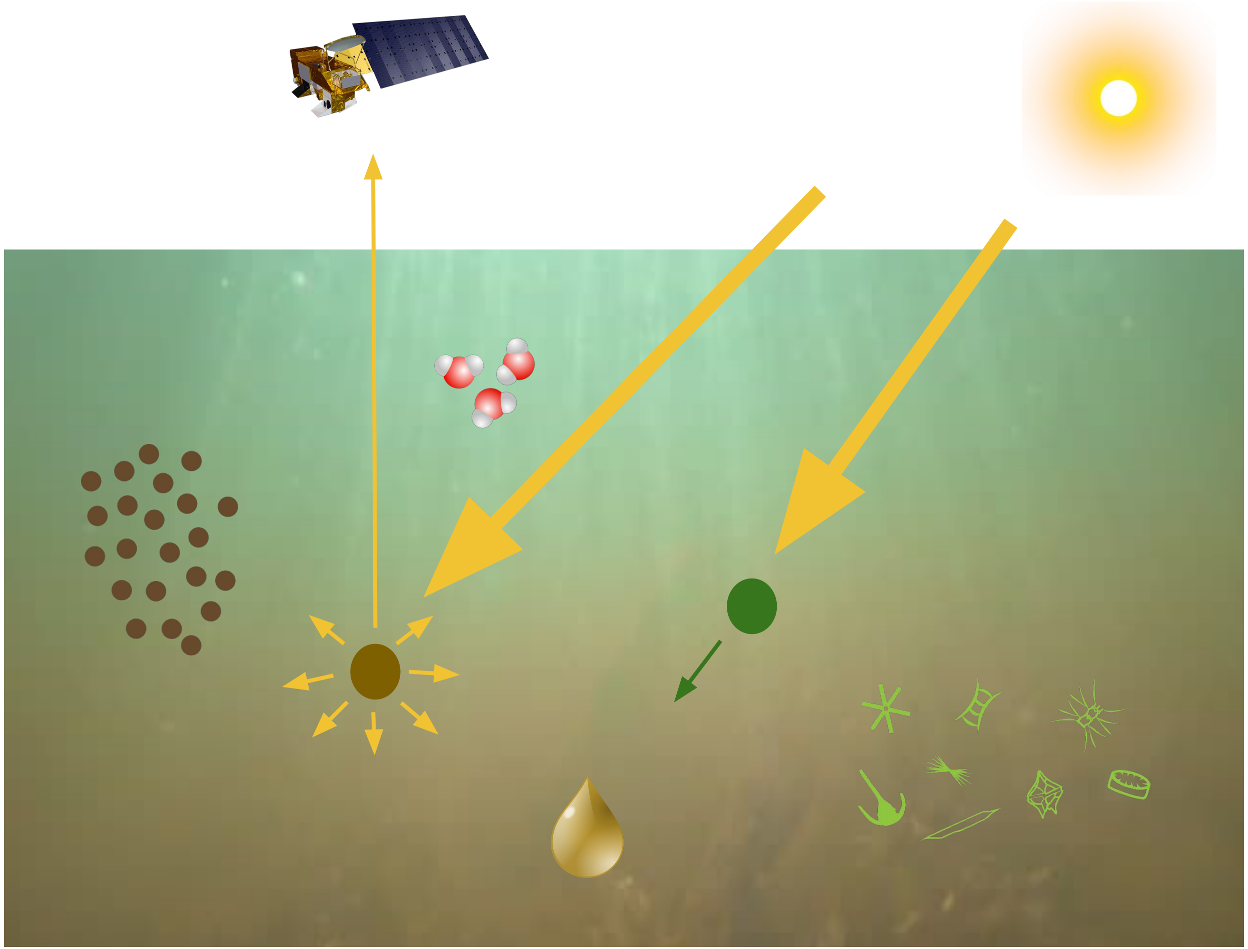
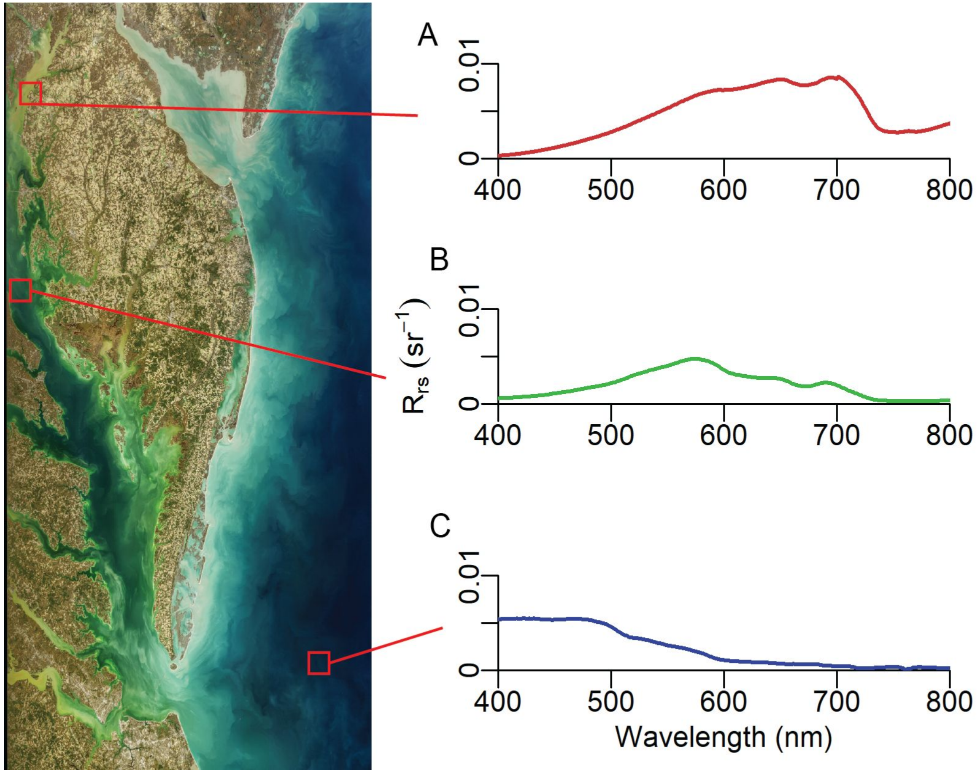


Satellite remote sensing

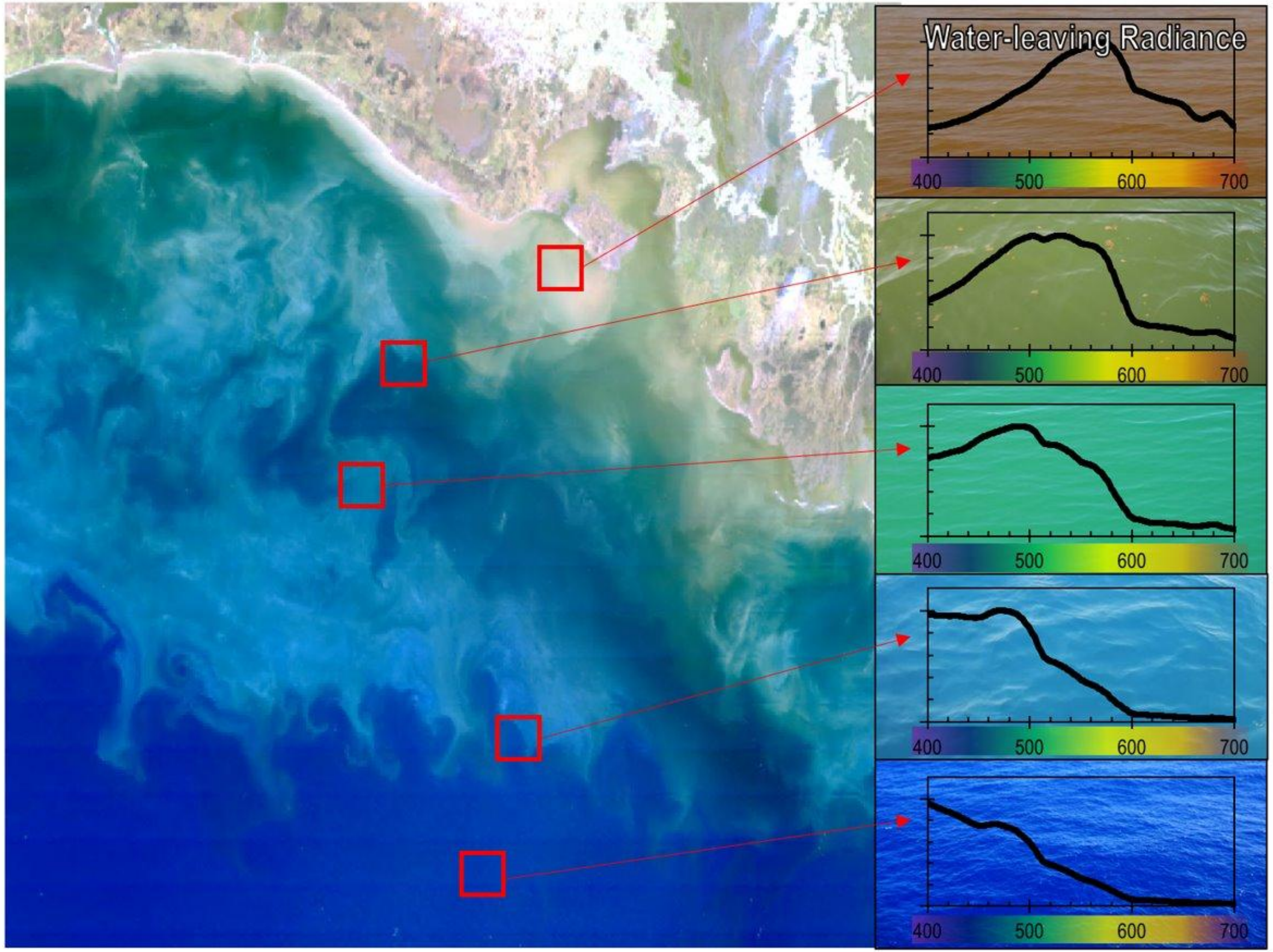
- Remote sensing reflectance (R_{rs}) used to infer underlying water quality concentrations

- $$R_{rs} \approx \frac{\text{backscattering } (b_b)}{\text{absorption (a)}}$$

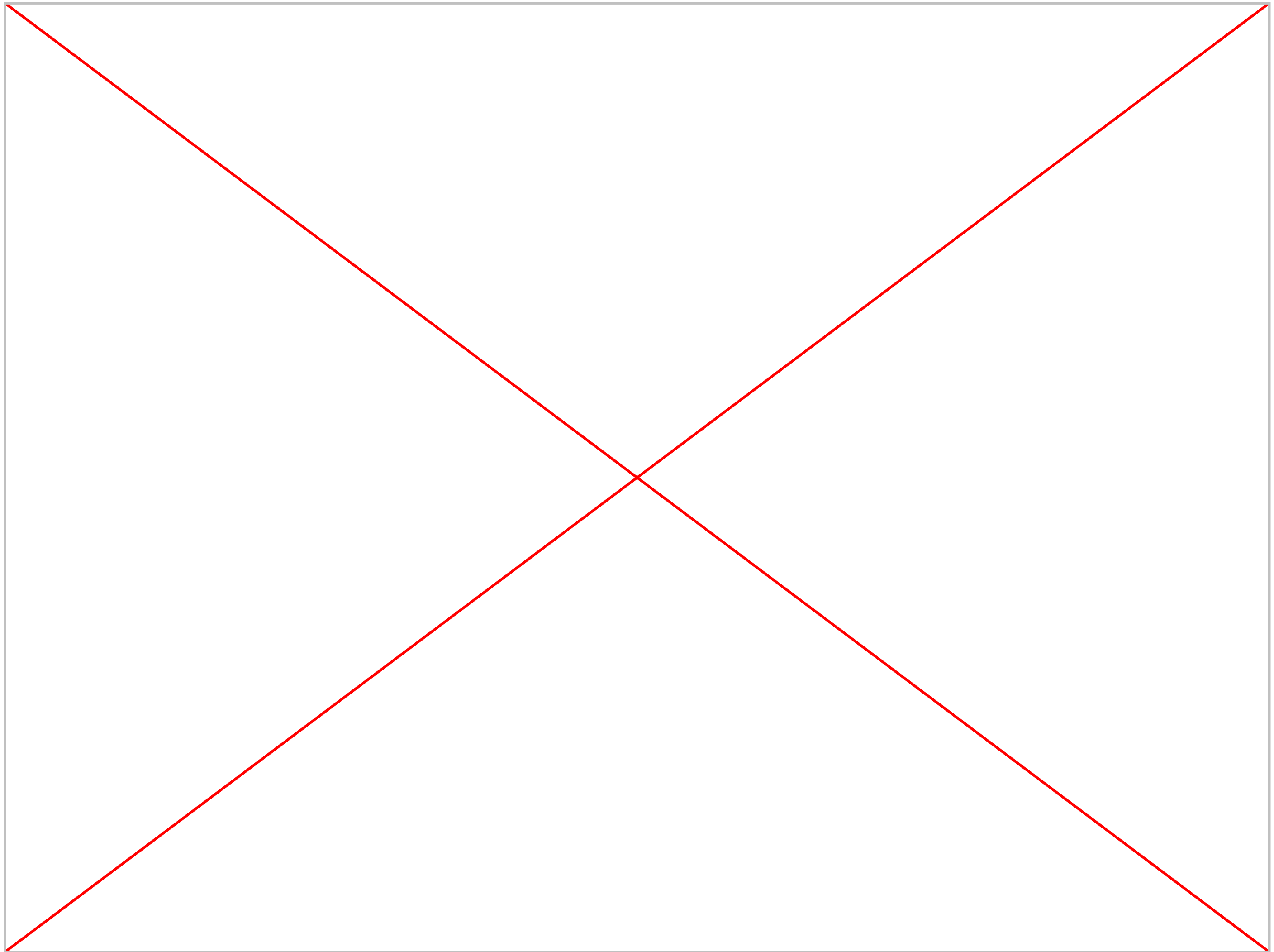
- Amount of absorption and backscattering (e.g., inherent optical properties, IOPs) determines color of water



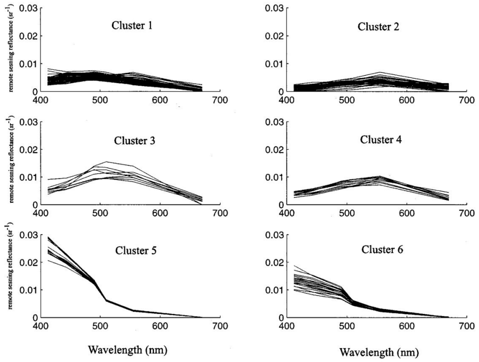
In situ R_{rs} spectra collected in A) turbid Upper Bay, B) productive Mid Bay, and C) open ocean



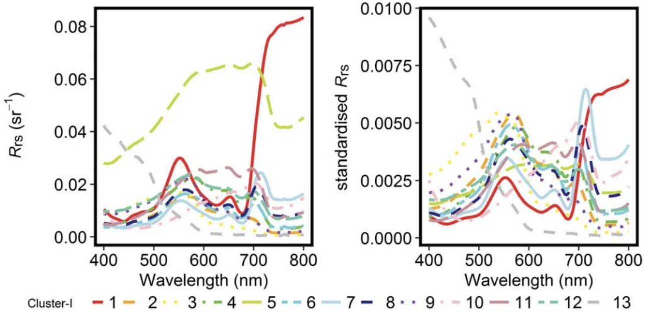
Credit: NASA



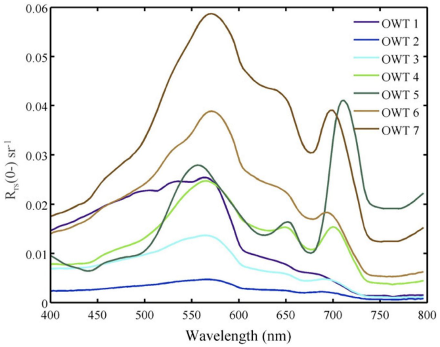
Optical water typing: Classifying water based on their IOPs as perceived through water color (e.g., R_{rs} spectra)



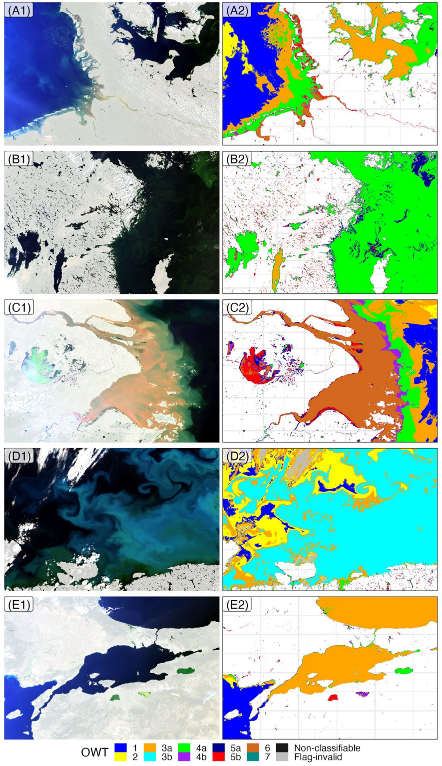
Moore et al., 2001



Spyrakos et al., 2018



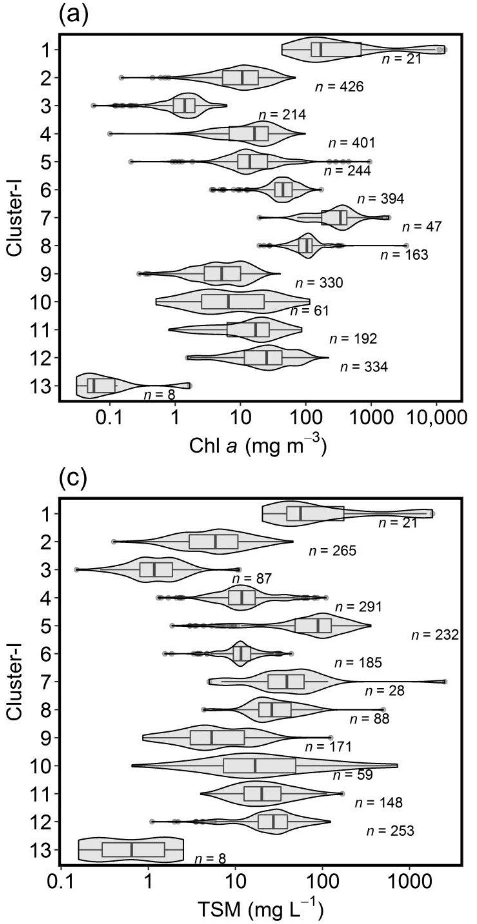
Moore et al., 2014



Bi & Hieronymi, 2024

Pairing results to coincident discrete data

- Most studies have paired OWTs exclusively with optically active discrete water quality variables that directly influence R_{rs}
- Covariance of other water quality variables that neither influence R_{rs} or whose influence is indirect (e.g., nutrients) has received less attention



Spyrakos et al., 2018

Study site: Chesapeake Bay

- Optically complex estuary
- History of eutrophication → Ches Bay Program water quality monitoring
- (Bi)-monthly discrete water quality measurements (> 130 fixed stations)

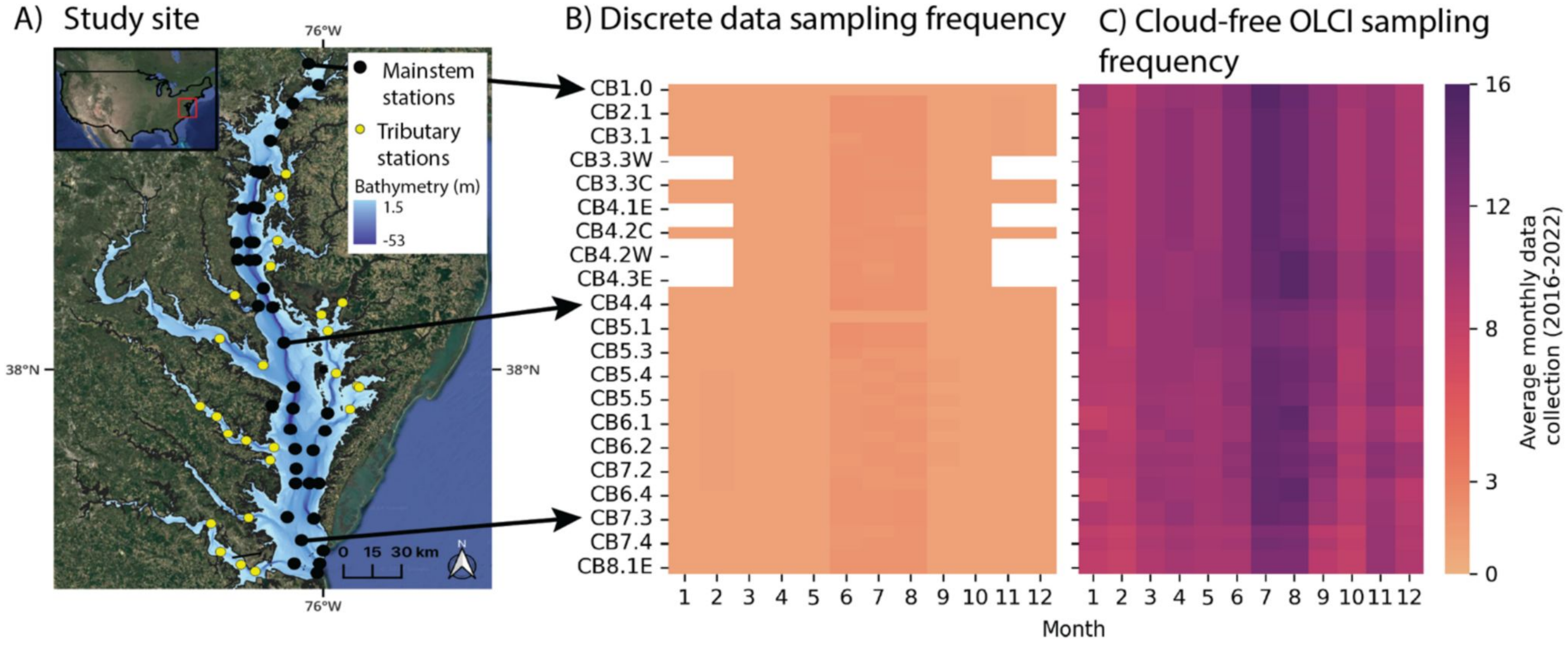
📸: Aqua MODIS

Satellite data

- Ocean Land Color Instrument (OLCI) onboard Sentinel-3A-B satellites
- 300 m spatial resolution
- 12 spectral bands from 400 - 753 nm
- Atmospherically corrected by Case 2 Regional Coast Color (C2RCC) algorithm
  - Windle et al., 2022
- Used data from 2016-2022
  - 2,038 scenes, 64,424,531 pixels

https://oceancolor.gsfc.nasa.gov/about/missions/s3a/

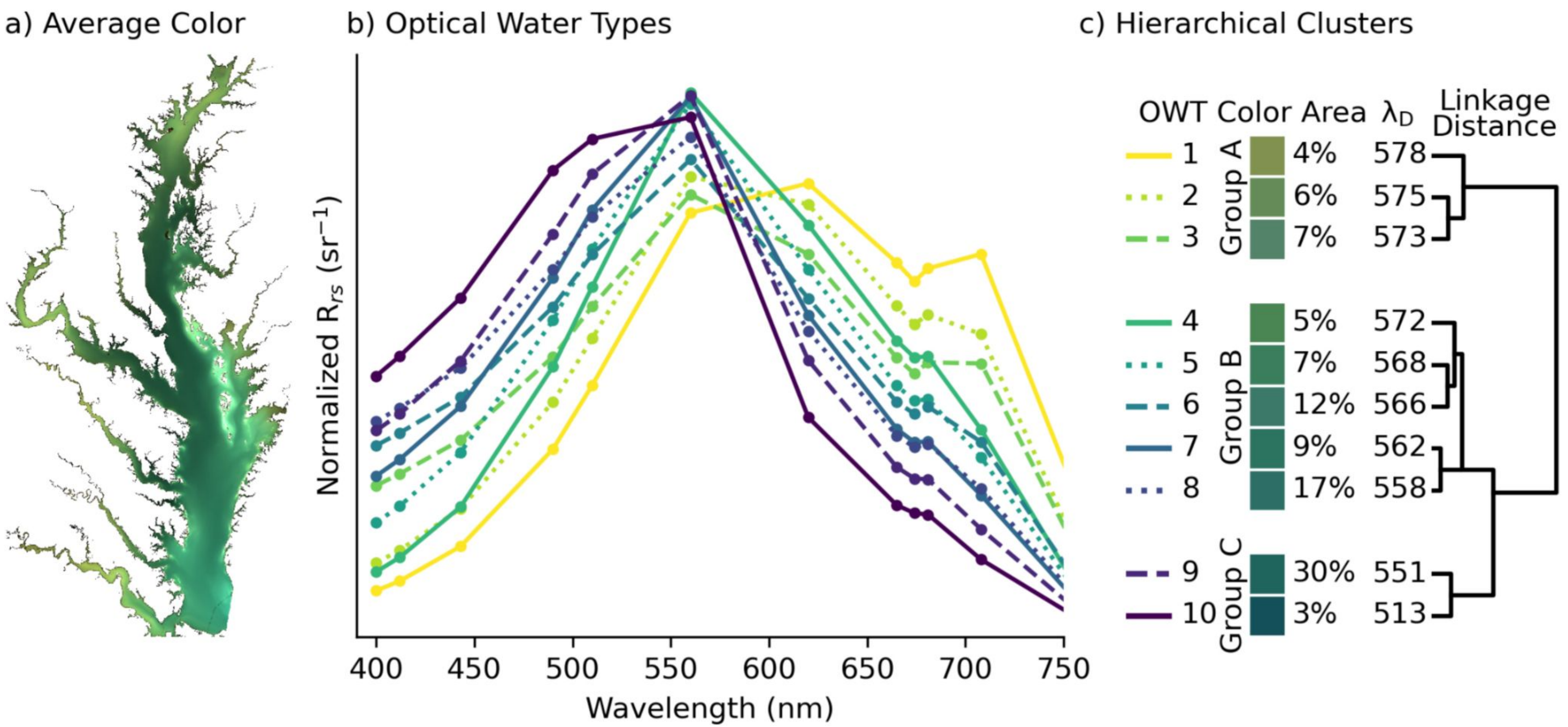
Study site


A) Study site
76°W
Mainstem stations
Tributary stations
Bathymetry (m)
1.5
-53
38°N
38°N
0 15 30 km
N
76°W
B) Discrete data sampling frequency
CB1.0
CB2.1
CB3.1
CB3.3W
CB3.3C
CB4.1E
CB4.2C
CB4.2W
CB4.3E
CB4.4
CB5.1
CB5.3
CB5.4
CB5.5
CB6.1
CB6.2
CB7.2
CB6.4
CB7.3
CB7.4
CB8.1E
1 2 3 4 5 6 7 8 9 10 11 12
C) Cloud-free OLCI sampling frequency
1 2 3 4 5 6 7 8 9 10 11 12
Month
16
12
8
3
0
Average monthly data collection (2016-2022)

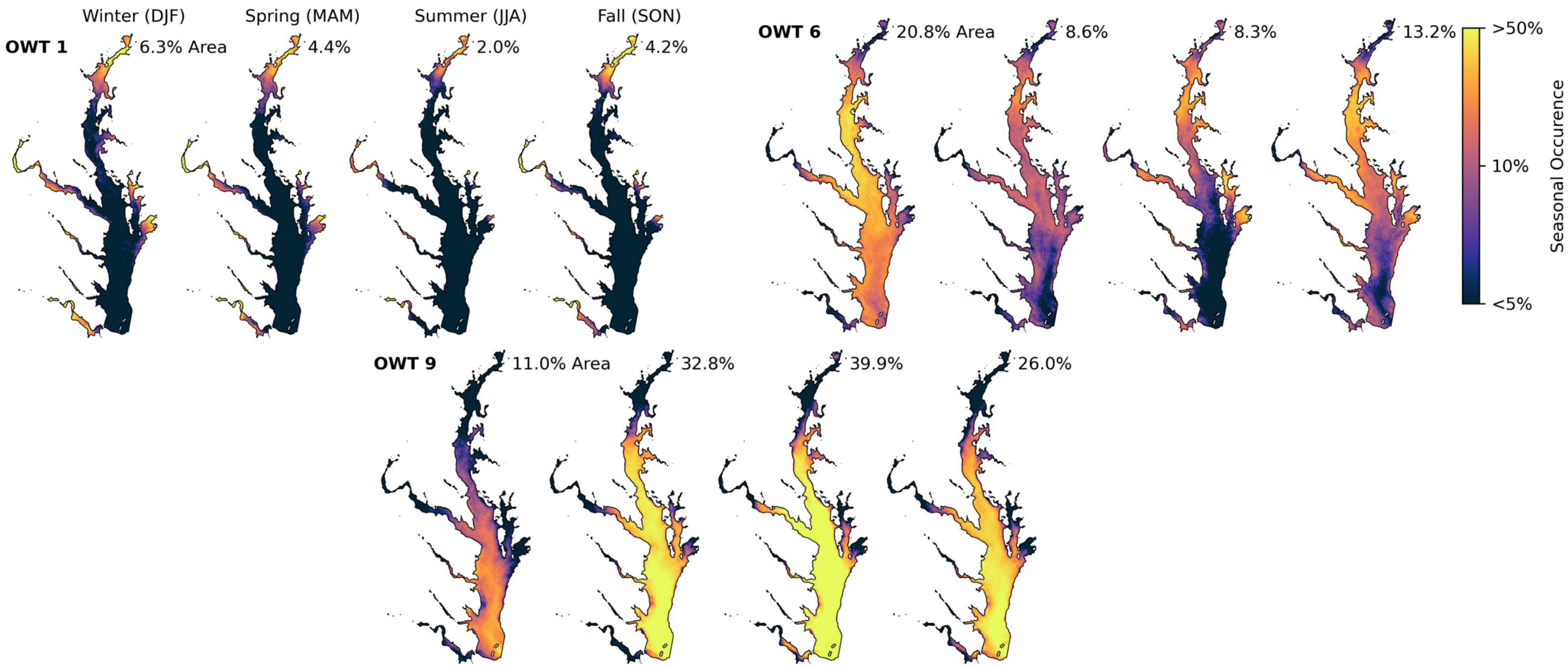
K-means and hierarchical clustering analysis

- Normalized R_{rs} (trapezoidal integration across λ)
- sklearn.cluster.KMeans algorithm from Python package *scikit-learn*
- Optimal number of clusters was determined by computing the Gap statistic (Tibshirani et al., 2001): 10 clusters
- For each pixel, R_{rs} spectra were assigned to the nearest OWT (sum of the absolute squared distance at each waveband)
- A hierarchical clustering analysis (scipy.cluster.hierarchy.linkage algorithm from Python package *SciPy*) of the OWT spectra was computed to ascertain and represent spectral (dis)similarities as a dendrogram.
- Discrete water quality data co-located in time and space with corresponding satellite pixels → 1,151 coincident matchups

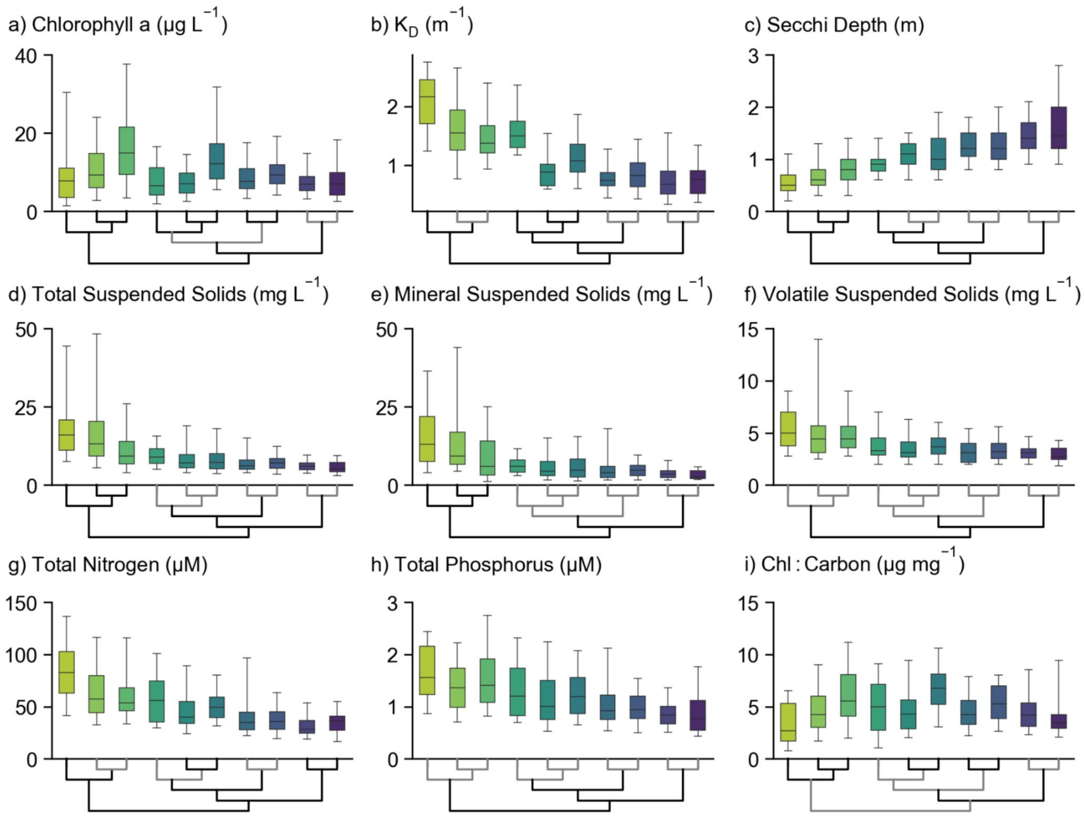
OWT classification

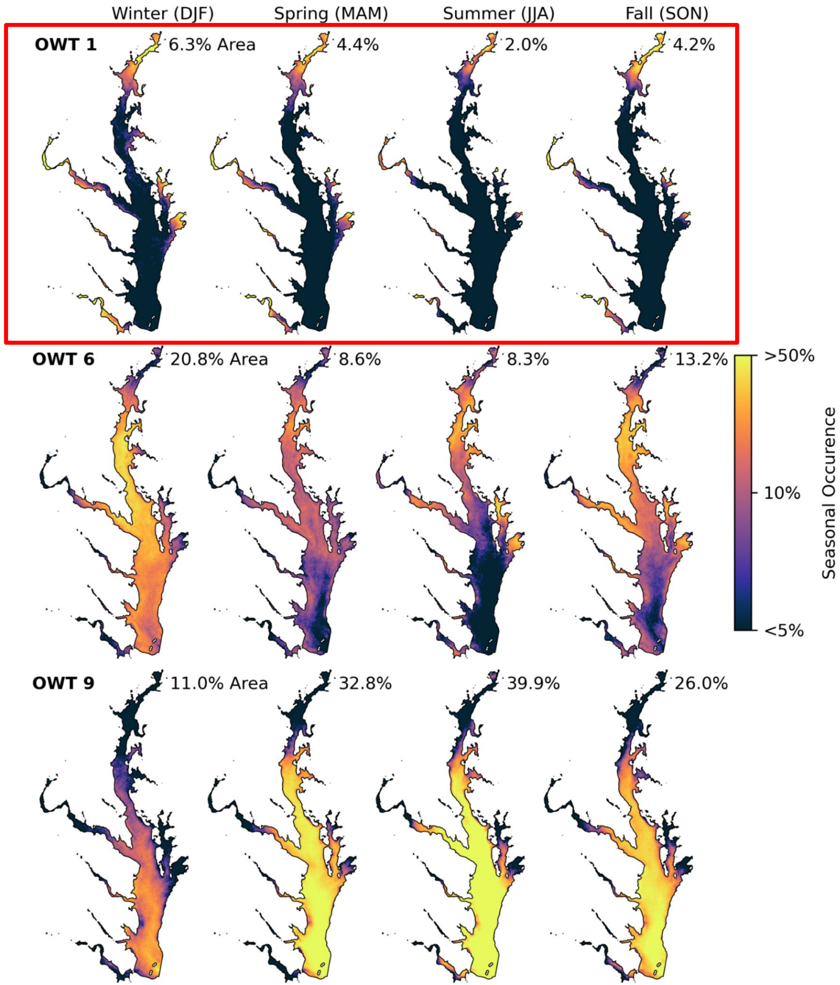


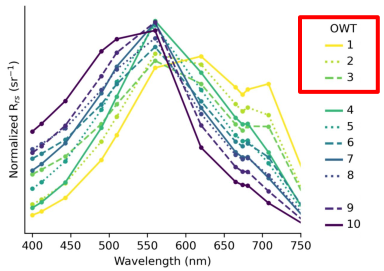
Spatial and seasonal occurrence of OWTs

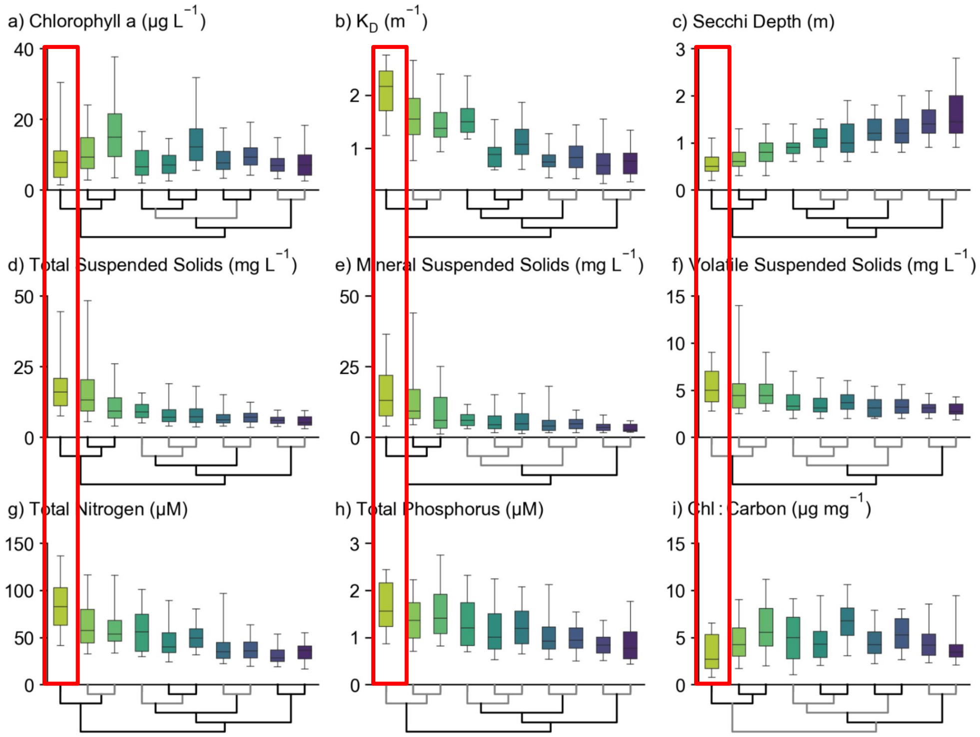


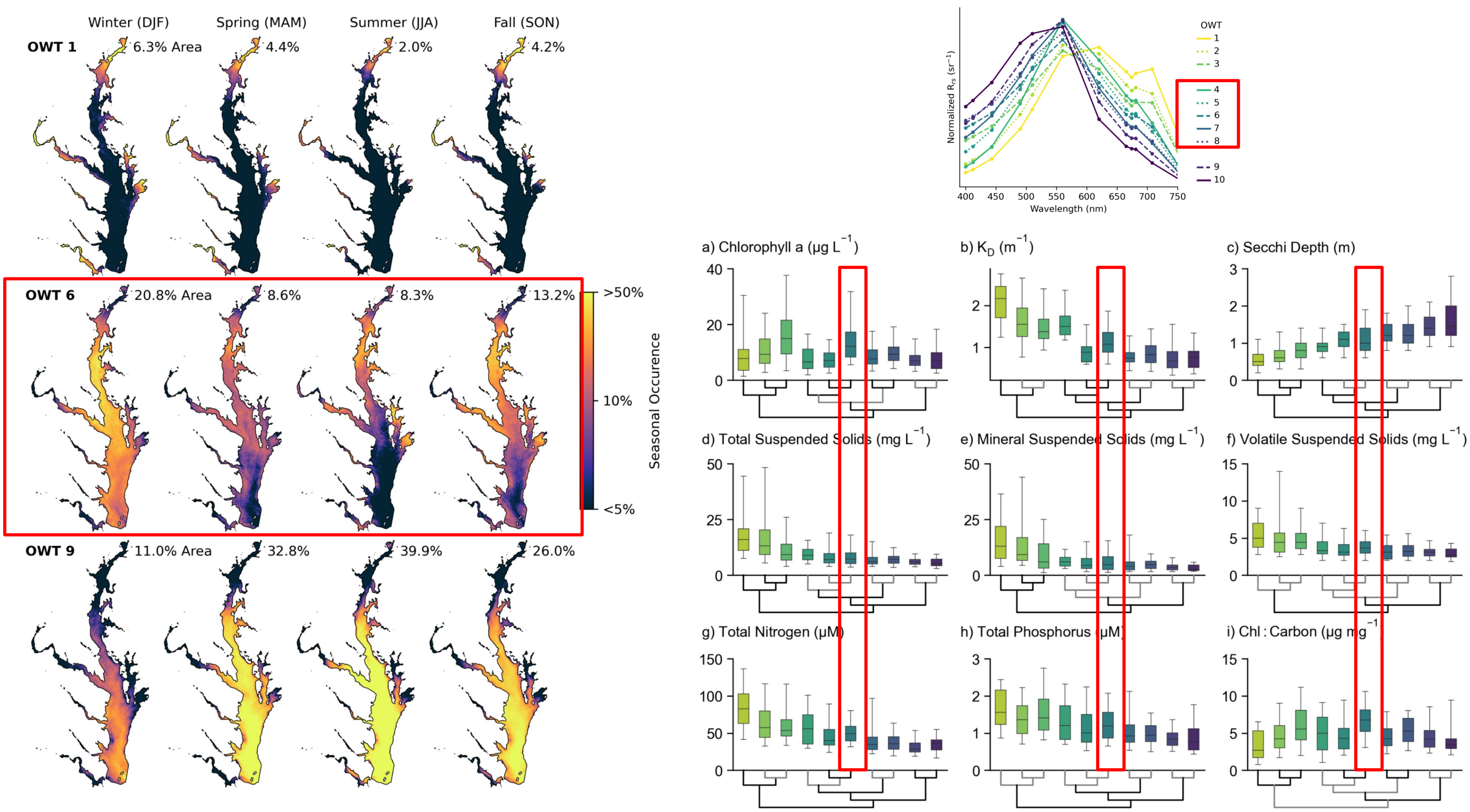
Discrete water quality data within OWTs




Winter (DJF)
Spring (MAM)
Summer (JJA)
Fall (SON)
OWT 1
6.3% Area
4.4%
2.0%
4.2%
OWT 6
20.8% Area
8.6%
8.3%
13.2%
OWT 9
11.0% Area
32.8%
39.9%
26.0%
>50%
10%
<5%
Seasonal Occurence


Normalized R$_{rs}$ (sr^{-1})
Wavelength (nm)
400
450
500
550
600
650
700
750
OWT
1
2
3
4
5
6
7
8
9
10


a) Chlorophyll a (µg L^{-1})
b) K$_D$ (m^{-1})
c) Secchi Depth (m)
d) Total Suspended Solids (mg L^{-1})
e) Mineral Suspended Solids (mg L^{-1})
f) Volatile Suspended Solids (mg L^{-1})
g) Total Nitrogen (µM)
h) Total Phosphorus (µM)
i) Chl : Carbon (µg mg^{-1})



Winter (DJF)
Spring (MAM)
Summer (JJA)
Fall (SON)
OWT 1
6.3% Area
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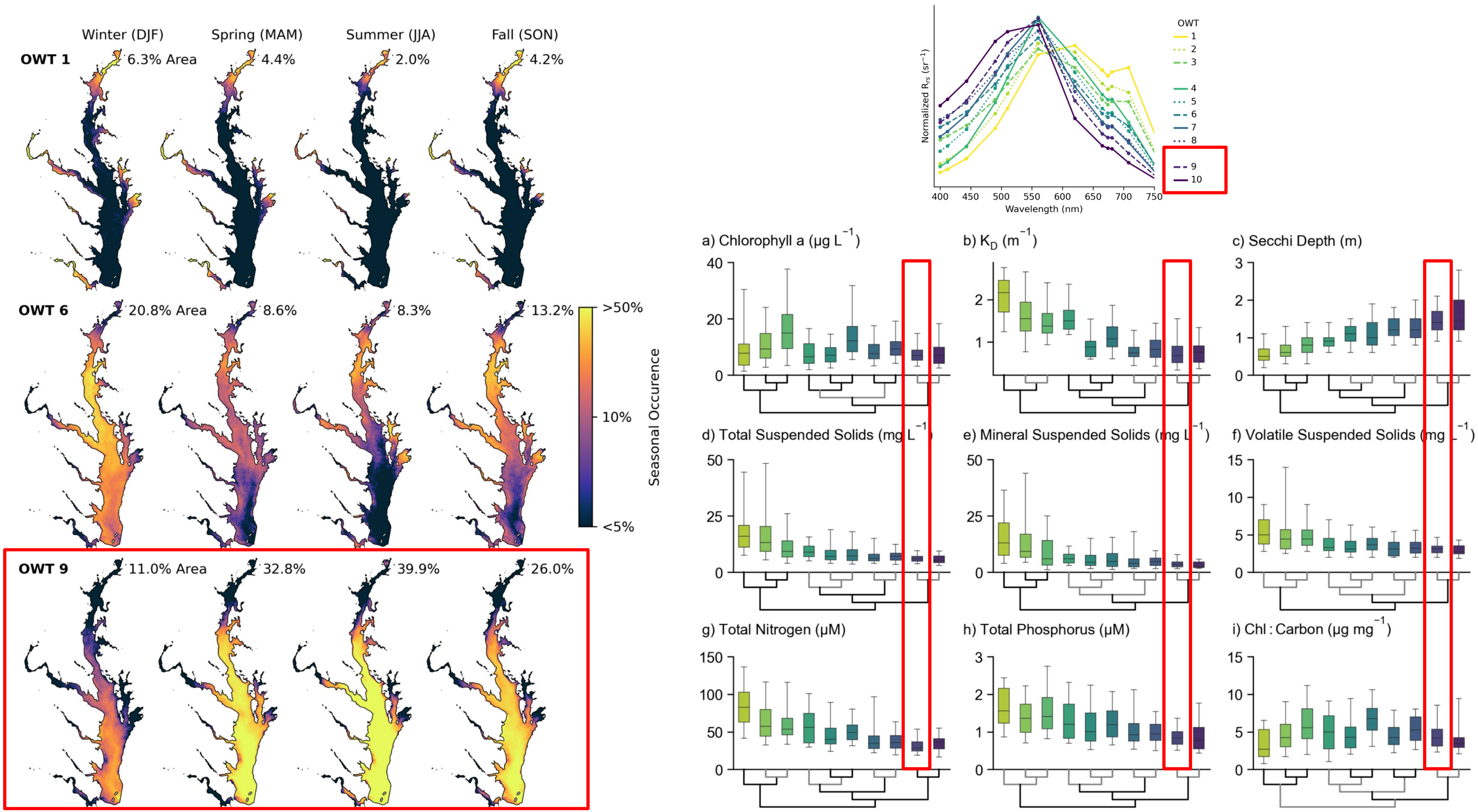
2.0%
4.2%
OWT 6
20.8% Area
8.6%
8.3%
13.2%
OWT 9
11.0% Area
32.8%
39.9%
26.0%
>50%
10%
<5%
Seasonal Occurence
Normalized Rrs (sr−1)
Wavelength (nm)
OWT
a) Chlorophyll a (μg L−1)
b) KD (m−1)
c) Secchi Depth (m)
d) Total Suspended Solids (mg L−1)
e) Mineral Suspended Solids (mg L−1)
f) Volatile Suspended Solids (mg L−1)
g) Total Nitrogen (μM)
h) Total Phosphorus (μM)
i) Chl : Carbon (μg mg−1)



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OWT 9
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32.8%
39.9%
26.0%
>50%
10%
<5%
Seasonal Occurence
Normalized R_rs (sr^-1)
Wavelength (nm)
OWT
1
2
3
4
5
6
7
8
9
10
a) Chlorophyll a (μg L^-1)
b) K_D (m^-1)
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g) Total Nitrogen (μM)
h) Total Phosphorus (μM)
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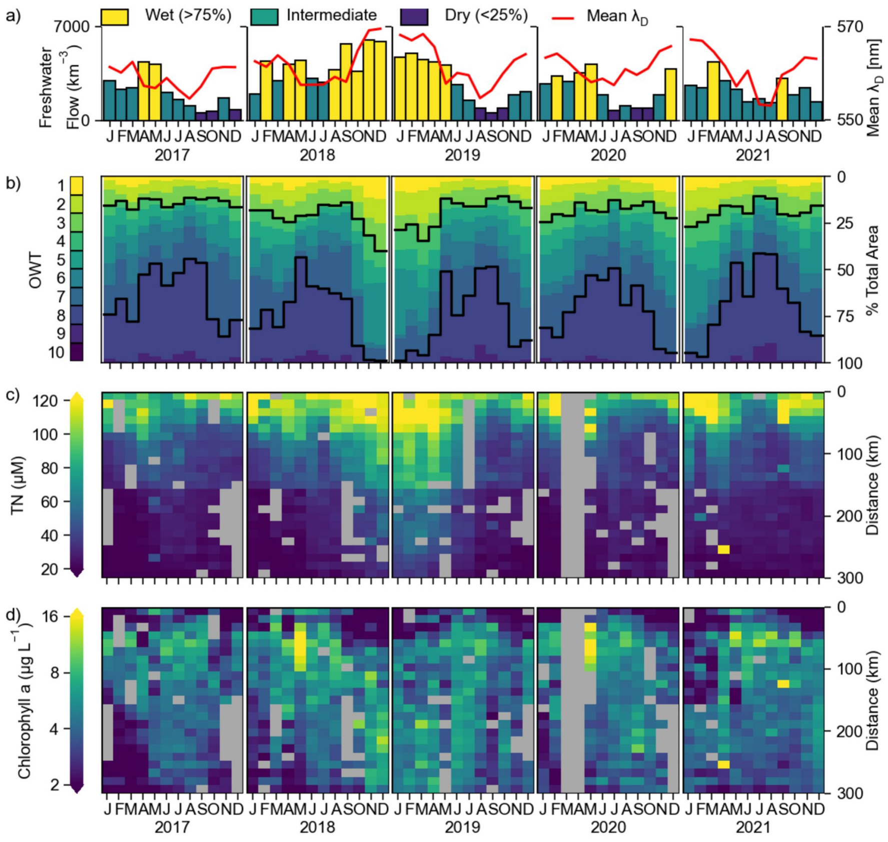
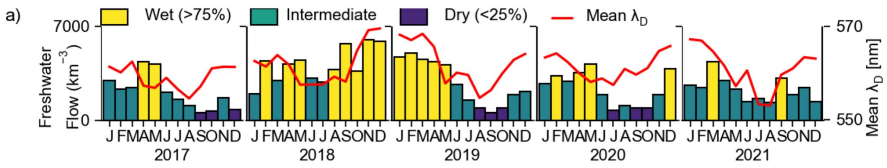
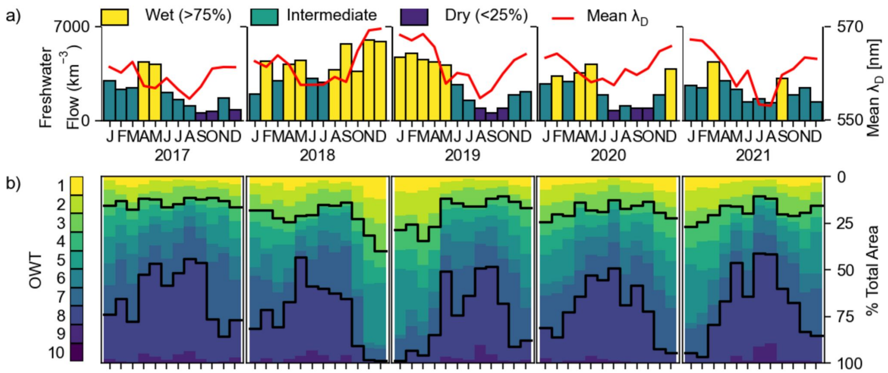
Seasonal and interannual variability



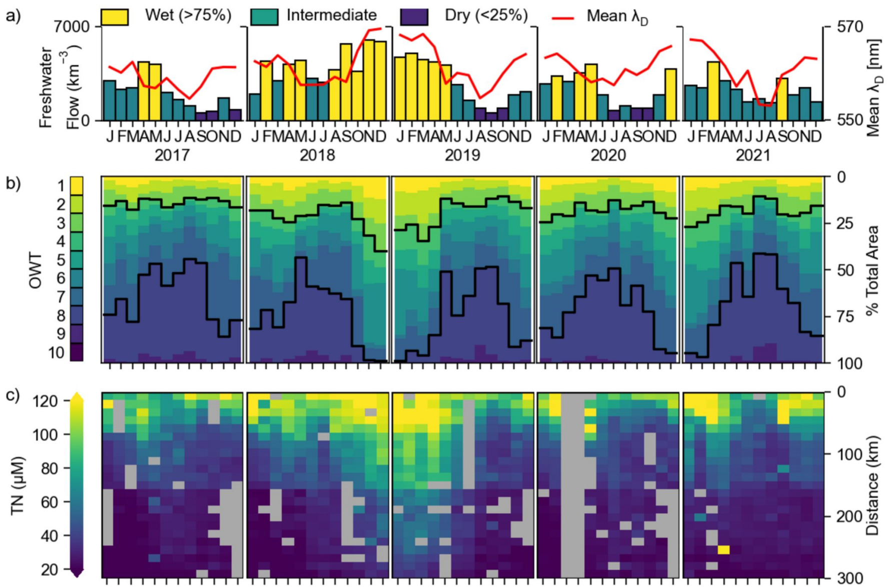
Seasonal and interannual variability



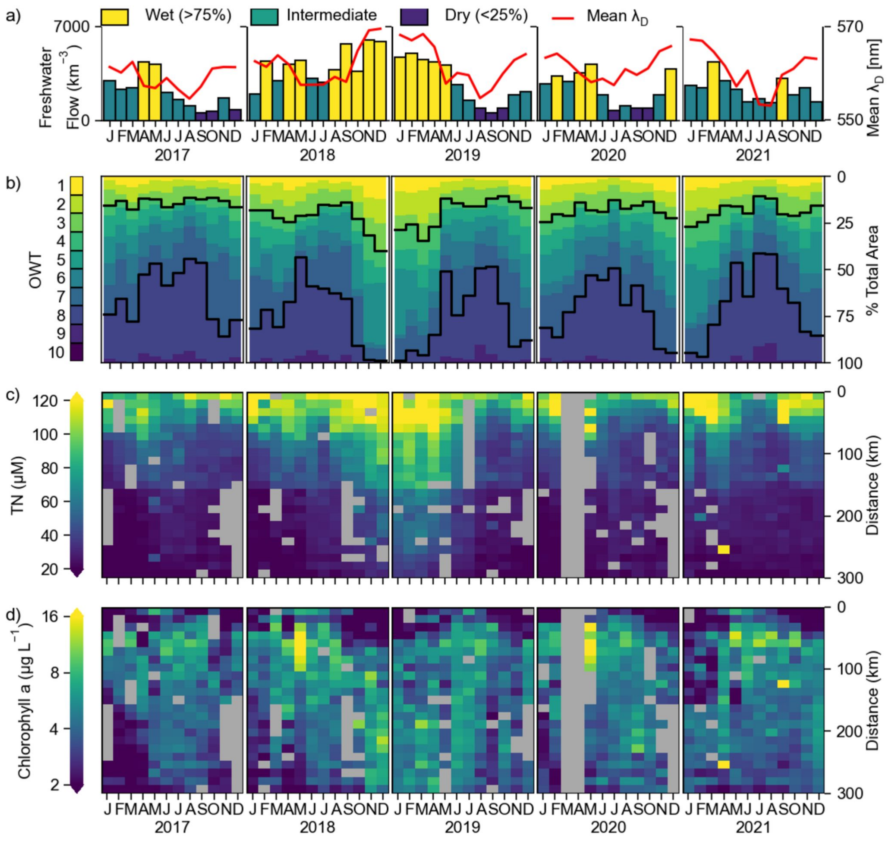
Seasonal and interannual variability



Seasonal and interannual variability



Seasonal and interannual variability



Is covariation between water color and nutrient loading stronger than Chl *a*?

Elevated discrete TN corresponding to OWT occurrence and freshwater flow

Correspondence with discrete Chl *a* is less clear

Interesting findings

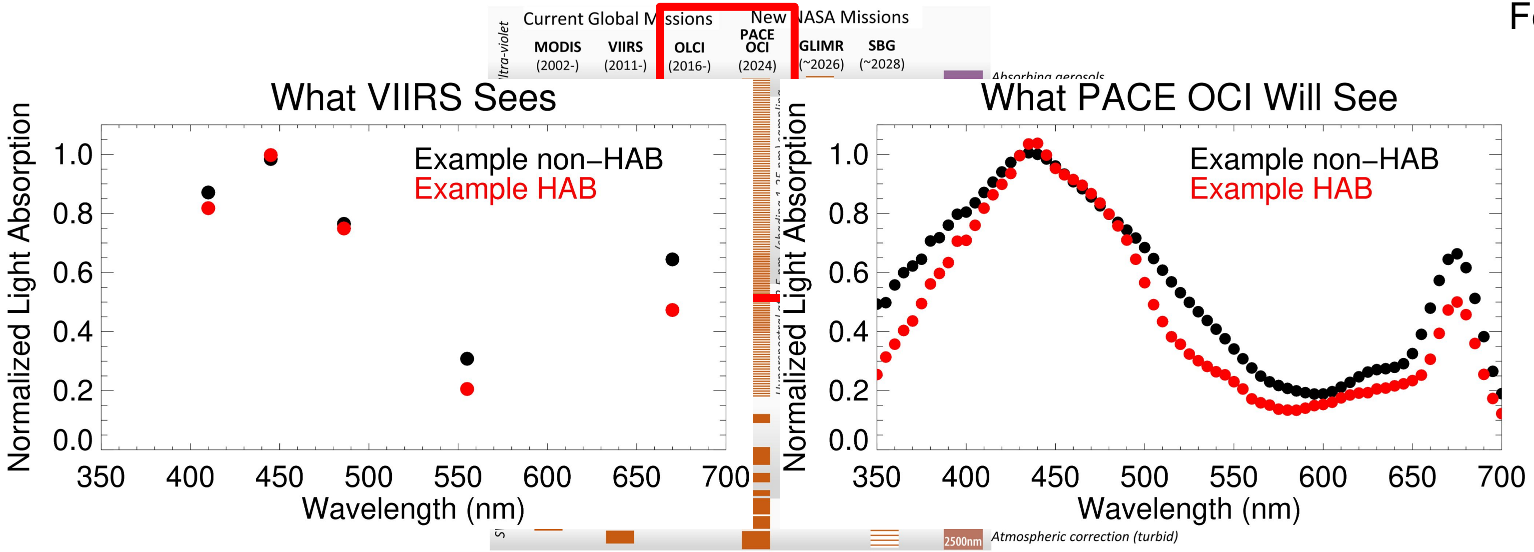
“When synchronously comparing all water quality parameters grouped by corresponding OWTs, ***TN concentrations emerged as having more statistically significant differences than known optically important parameters (e.g., Chl a),*** *demonstrating that this approach may have the potential to improve our understanding of nutrient loading variability at the scale of a large, optically complex estuary.”*

*“**Chl a**, commonly used as both a proxy for light absorption and an indicator of primary production,* ***exhibited lower than expected separability among OWTs****, suggesting that phytoplankton physiological status, particularly their degree of light or nutrient limitation, substantially influences the optical properties of this eutrophic system.”*

Keeping PACE: Hyperspectral OWTs

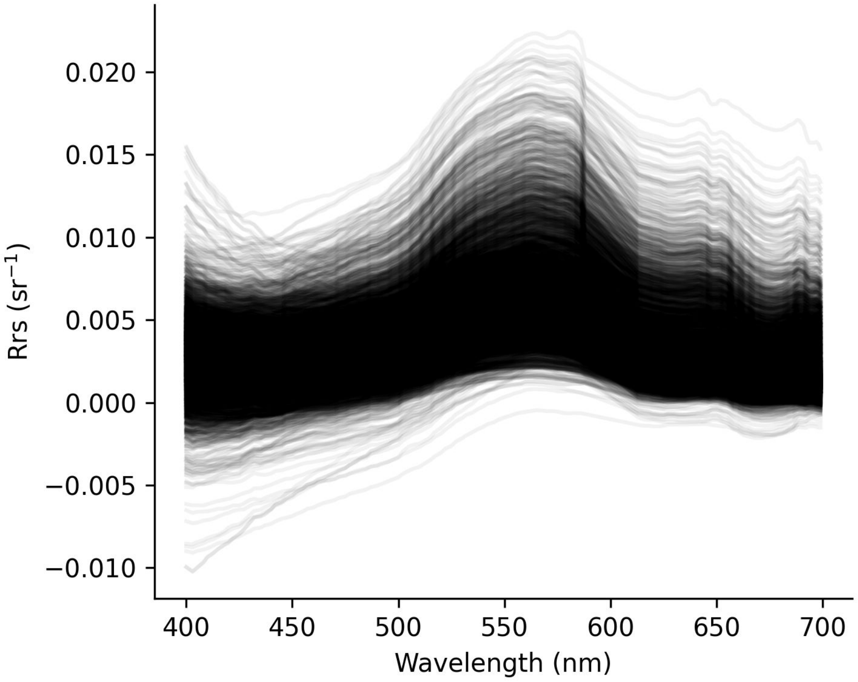
Can hyperspectral OWTs tell us *more* about the underlying inherent optical properties or water constituents?

PACE launched Feb 2024



Dierssen et al., 2023

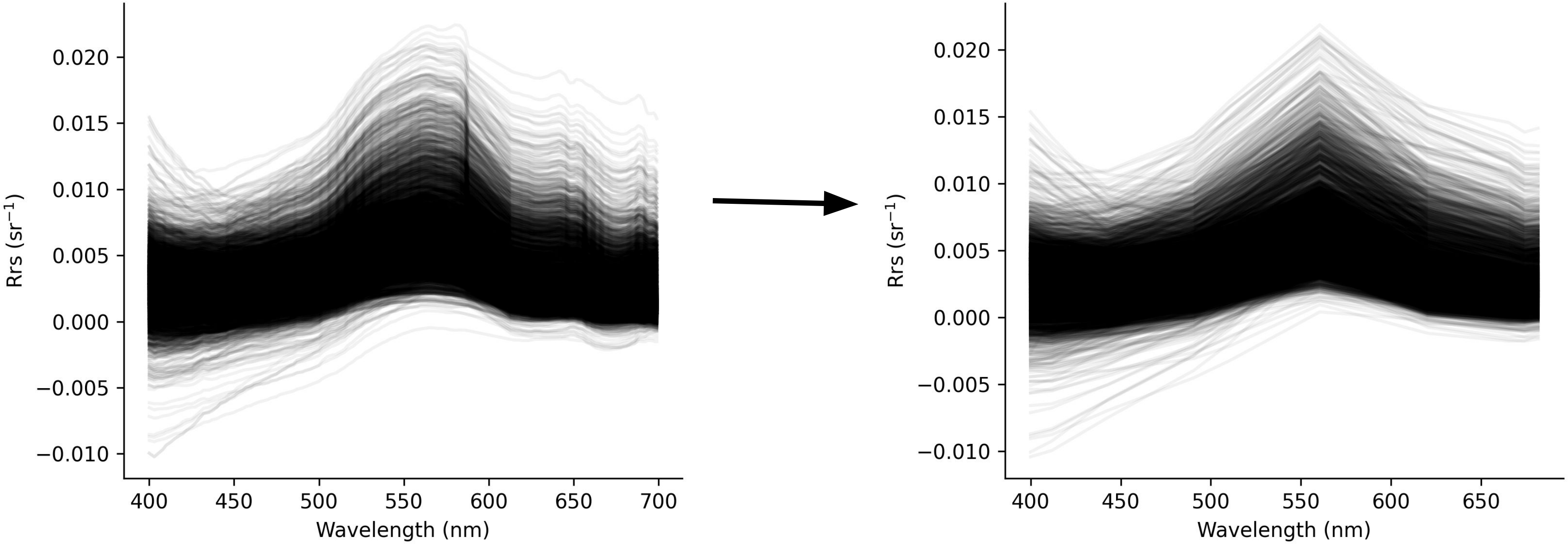
PACE OCI R_{rs} (v3.1) in Chesapeake Bay (July 2025)



R_{rs} spectra from random 5000 pixels

45 scenes (30 days) -> 35,211 pixels x 136 wavelengths

Deconvolved PACE OCI R_{rs} to 10 OLCI wavelengths



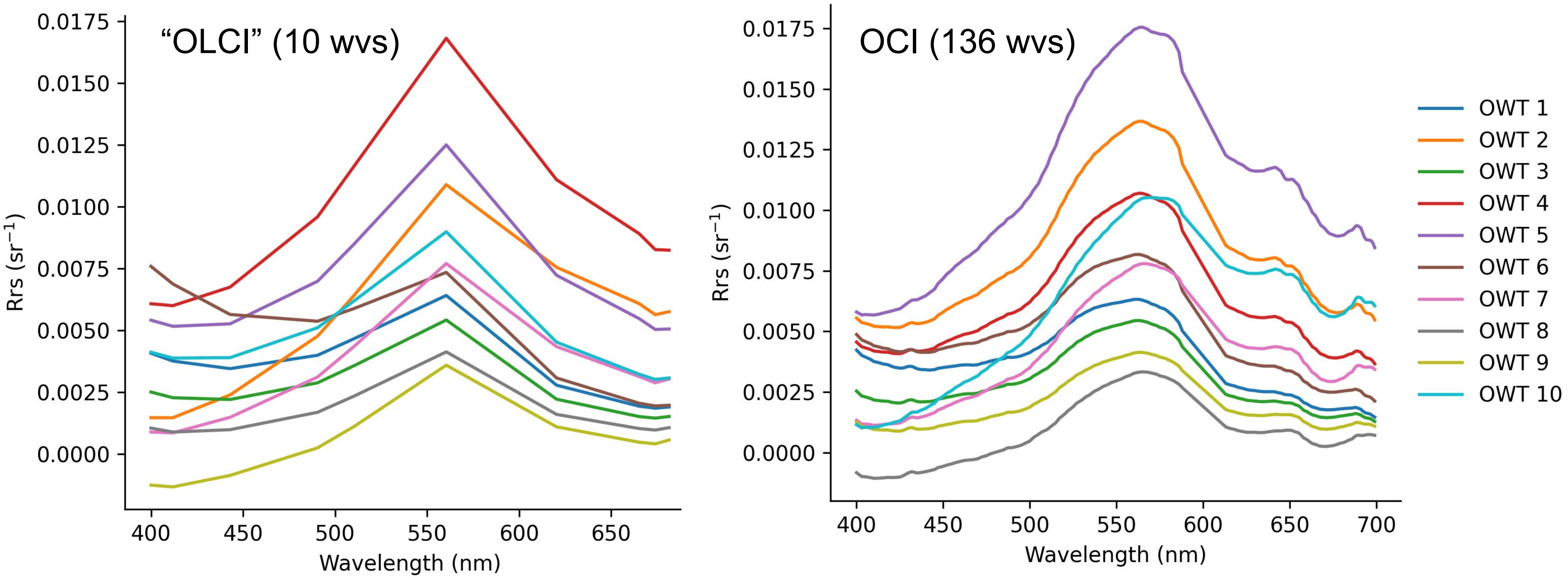
Using OLCI-S3A SRFs found here:
https://oceancolor.gsfc.nasa.gov/resources/docs/rsr_tables/

Gap statistic to find optimum number of clusters (100 iterations)

- PACE OCI R_{rs}: median = **10**, s.d. = 2.90

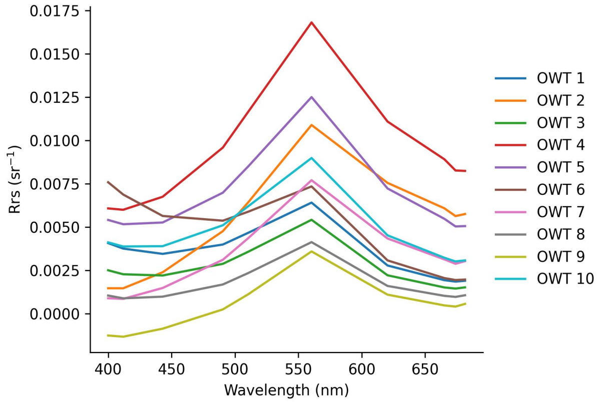
- OLCI R_{rs}: median = **10**, s.d. = 3.03

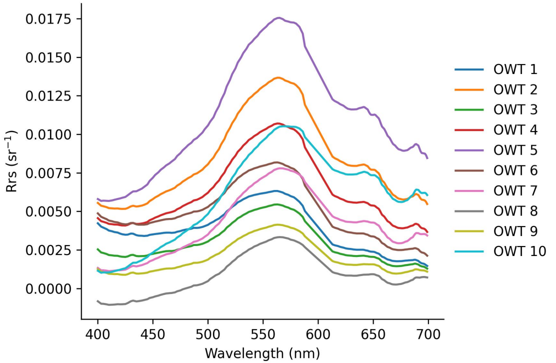
OWTs in Chesapeake Bay (k-means clustering)

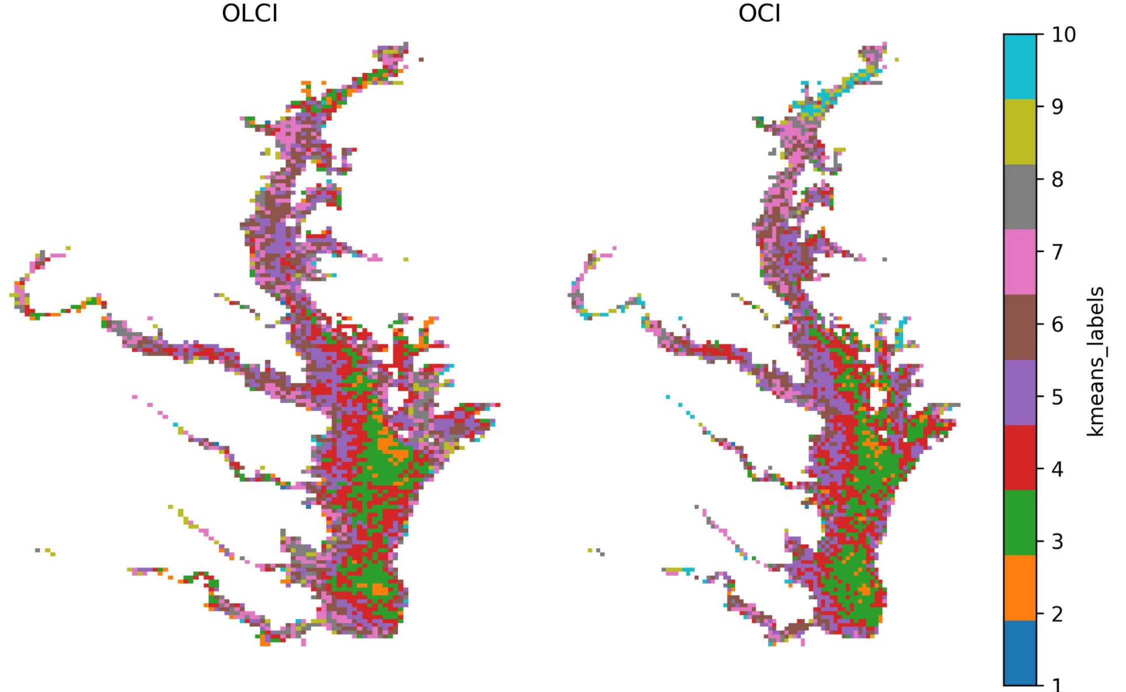


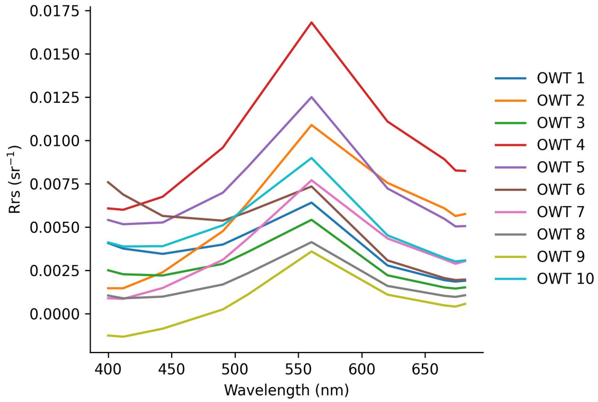
Why different colors? Different feature spaces → different cluster assignment. K-means isn’t aware that these are “the same pixels” — it clusters solely based on distances in whatever space you give it. Even small spectral shape changes from convolution/downsampling can cause points to jump cluster boundaries. Future work will include applying a label-reordering algorithm so that cluster numbers post-hoc are based on spectral similarity.

Median OWT July 2025

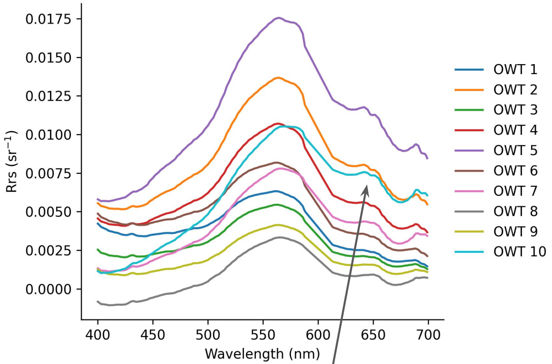


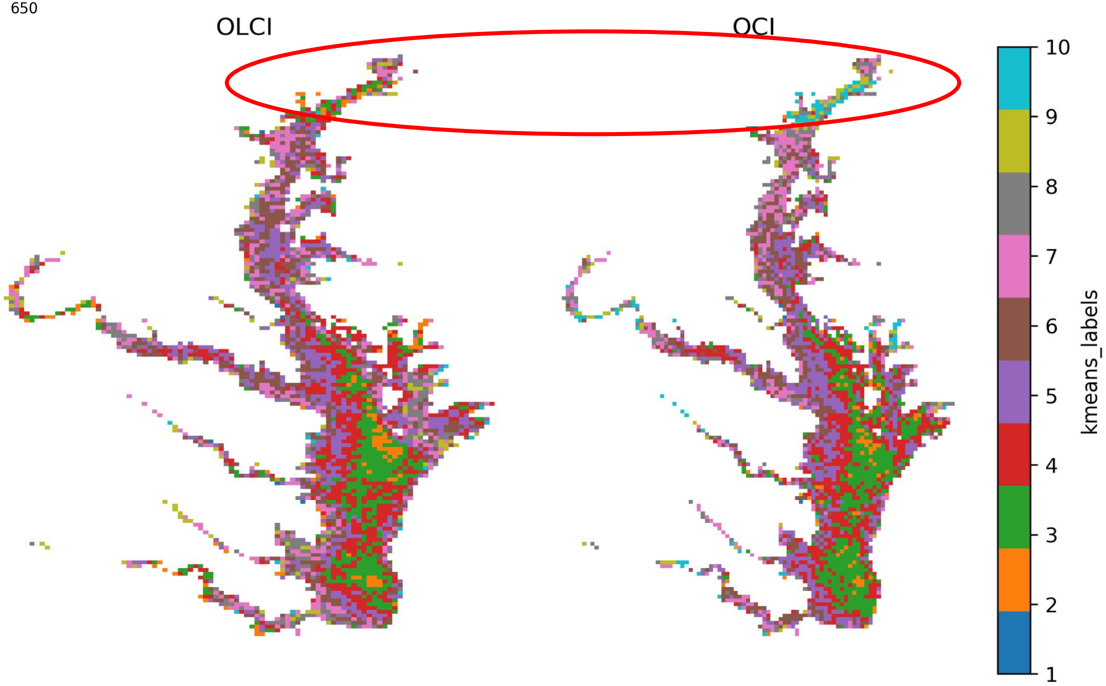






Median OWT July 2025



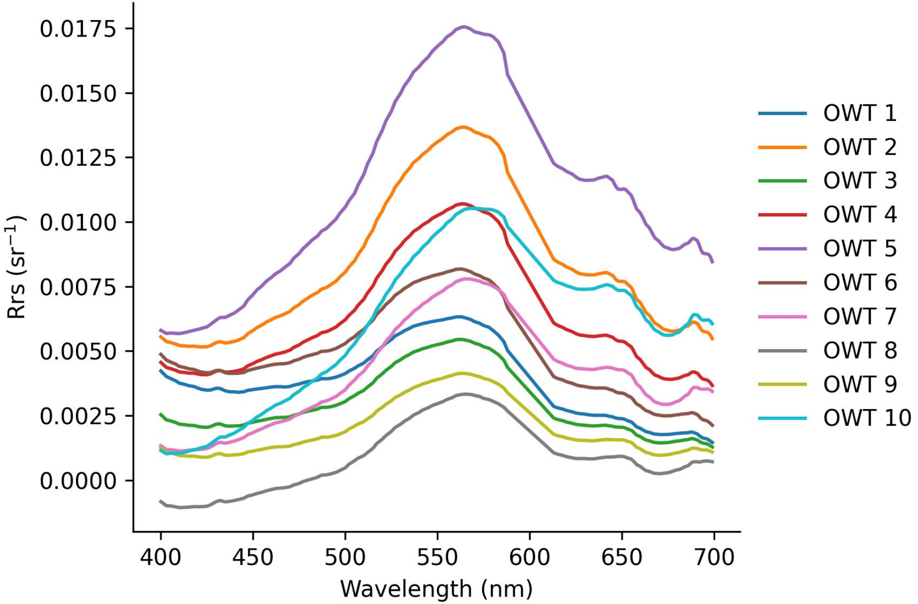


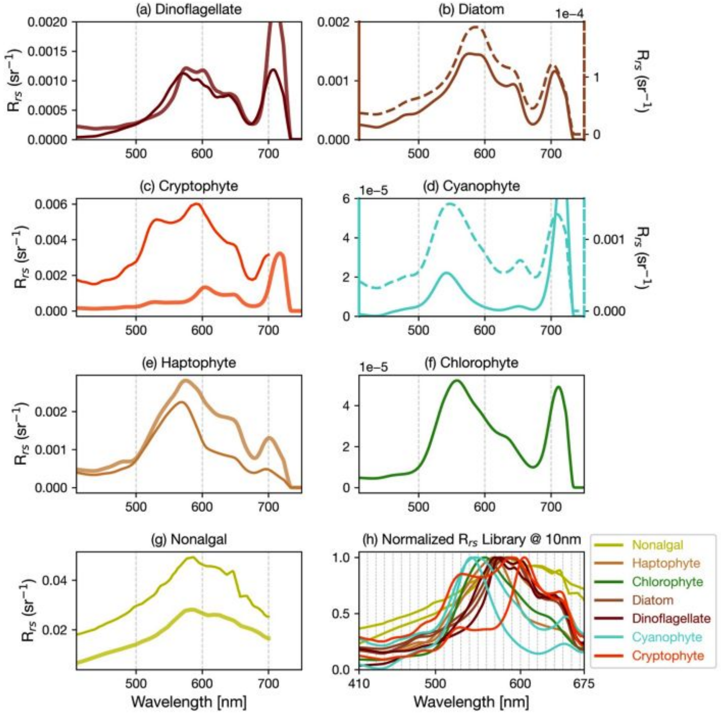
Wiggles in the longer wvs could tell us more? Diagnostic of certain taxa?

Peak in 680–700 nm can indicate fluorescence

Other pigments (like phycoerythrin in cyano) can create subtle features in the red (≈600–650 nm)

Are any OWTs similar to phytoplankton Rrs spectra?





Could an OWT be used to identify a (H)AB?

McKibben et al., 2024

Management implications

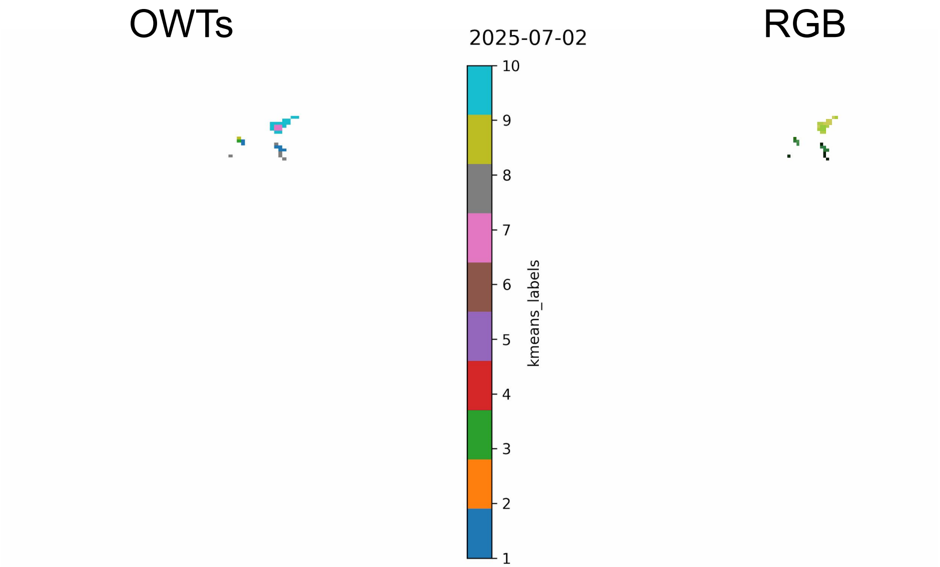
- Timing and location of OWTs can be used to inform discrete water quality monitoring
  - Targeted discrete sampling in winter or nearshore waters

- Assist with assessing water quality standards
  - Track the location and timing of increased sediment loading or areas not meeting water clarity criteria

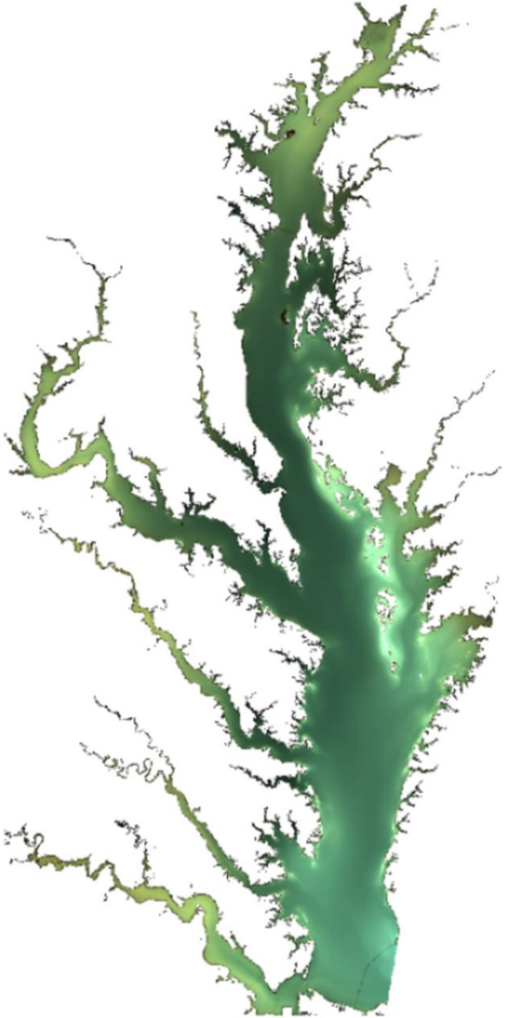
Future work

- Extend time period: re-do analysis for whole PACE mission life (Apr 2024 - now)
- Compare to coincident discrete Chesapeake Bay Program water quality data to see if/how underlying data are grouped differently compared to OLCI
- Evaluate bio-optical algorithms within each OWT. Would a blended algorithm approach improve results?
- Search for *in situ* phytoplankton taxa data in Chesapeake Bay that could be compared to hyperspectral R_{rs} to help develop/evaluate coastal phytoplankton community composition algorithms?

A combination of optically active constituents comprise the R_{rs} signal in optically complex estuarine waters. Measuring an individual metric, such as remotely sensed Chl a concentration, may not provide a comprehensive understanding of the aquatic system.



Can satellite-based OWT classifications be incorporated into numerical models to better predict water quality dynamics and quantify progress of Bay-wide restoration goal?



Questions?

anna.windledipaola@nasa.gov