Retrieval of phytoplankton pigments and functional types from underway spectrophotometry in the Fram Strait, Arctic Ocean

1. What are phytoplankton pigments and why important?
2. What is the link between phytoplankton pigments and functional types?
3. Why and how to retrieve?
4. What is underway spectrophotometry?
5. What is the current phytoplankton research state in the Fram strait?

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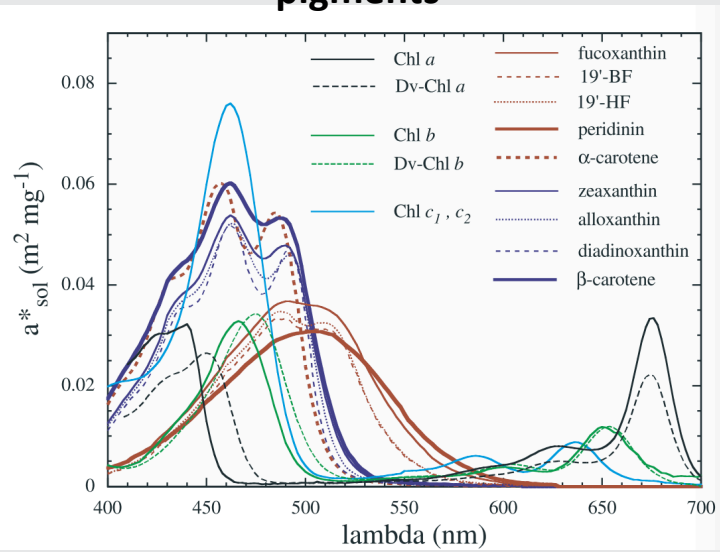
Phytoplankton pigments

- ✓ Help Snacking on SUNLIGHT — photosynthesis
- ✓ Protect against SUN BURNT — photoprotection

Source: Ocean Optics Web Book

Light absorption spectra of various pigments

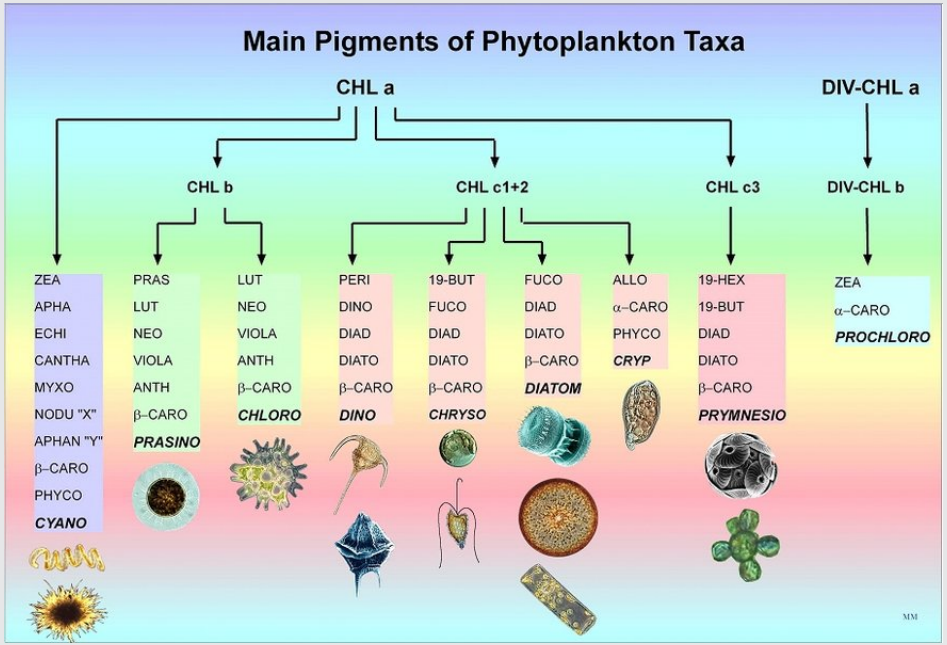


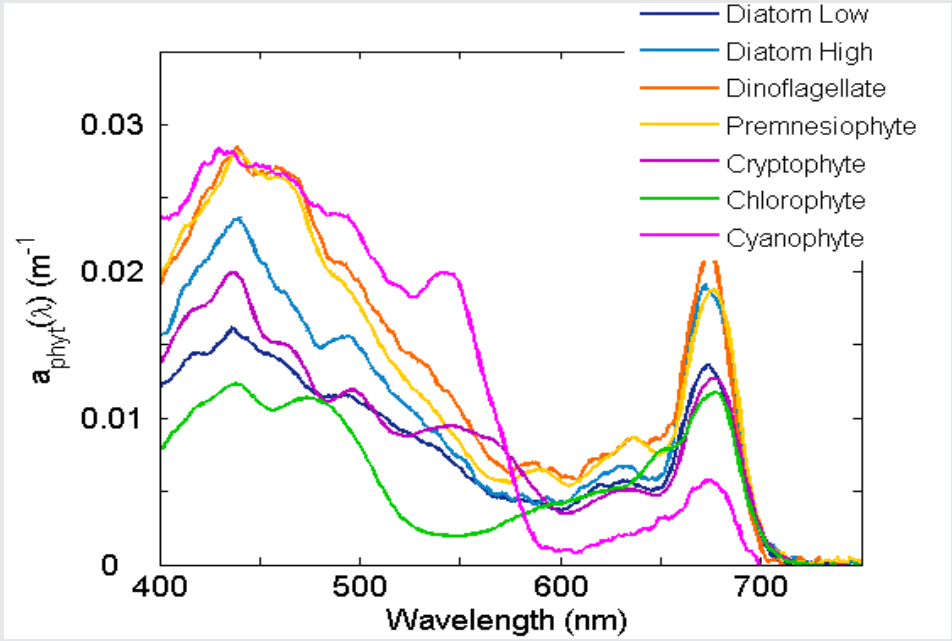
Source: Bricaud et al., 2004

Phytoplankton pigments and functional types

Each group of phytoplankton owns its specific pigment composition.

Different phytoplankton groups have distinct absorption due to different pigment composition



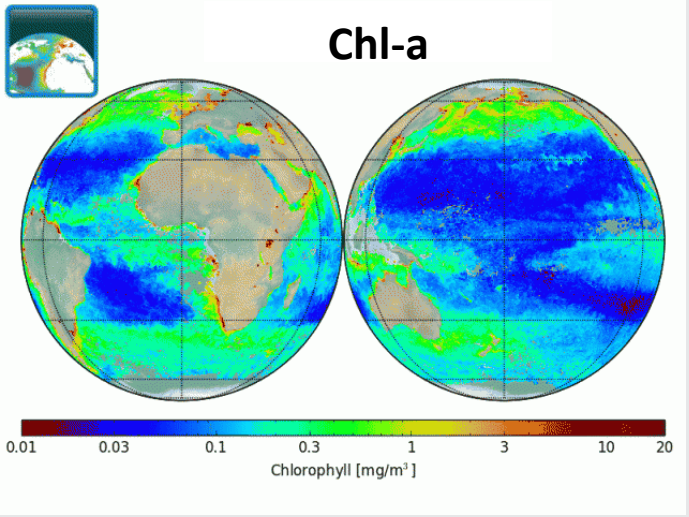


Sources: https://www.geomar.de/en/research/fb2/fb2-bi/infrastructure/hplc-analyses/ (left) and Ocean Optics Web Book (right)

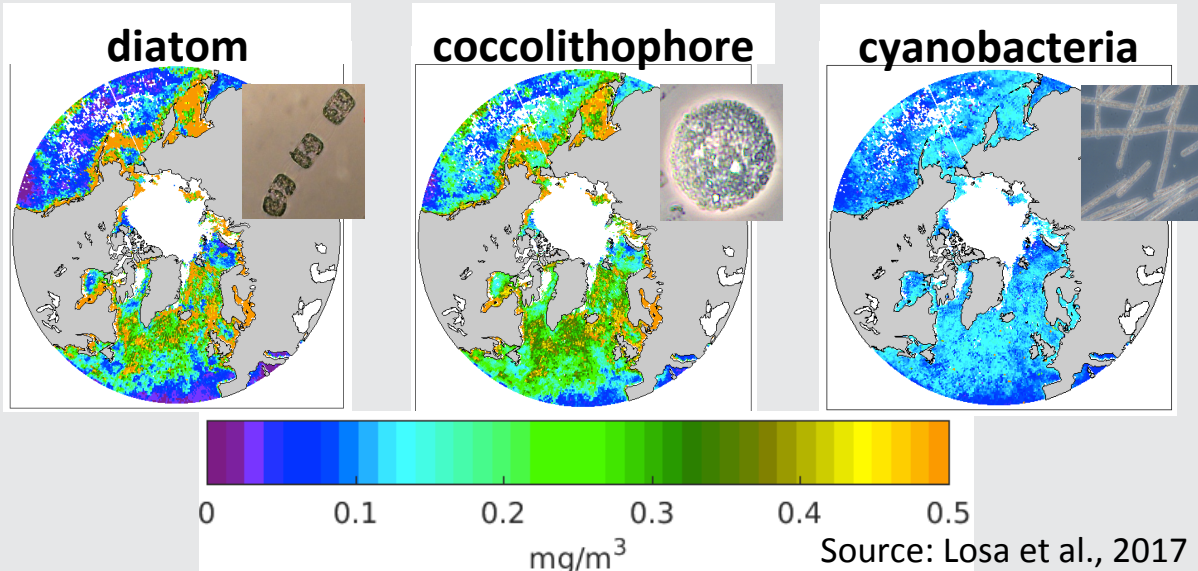
Phytoplankton pigments in remote sensing applications

develop, validate or refine bio-optical algorithms

- ✓ Phytoplannkton biomass
- ✓ Functional types:
  - cell size (micro-, nano- and pico-)
  - biogeochemical functions (e.g. calcication, silicication, DMS production, nitrogen fixation)



Source: ESA Ocean Color CCI



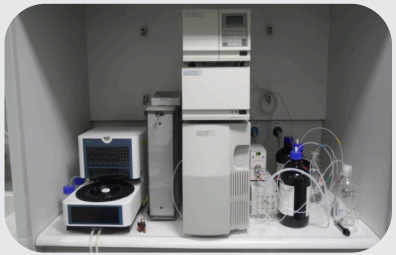
Source: Losa et al., 2017

Quantify phytoplankton pigments

1. Measure them using High Performance Liquid Chromatography (HPLC)


Discrete water sampling


---> Filtration


---> HPLC

2. Retrieve them from optical measurements (e.g. absorption, reflectance)

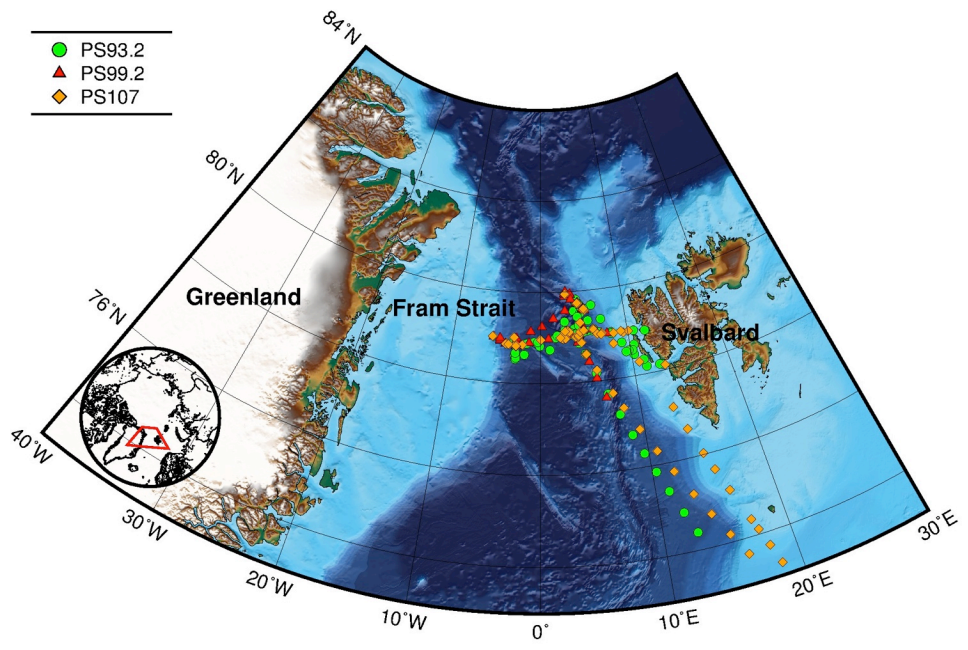
- ✓ **Spectral decomposition:**
  phytoplankton absorption = absorption of (pigment 1 + pigment 2 + …)
- ✓ **Spectral reconstruction:**
  absorption of (pigment 1 + pigment 2 + …) = phytoplankton absorption
- ✓ …

Esp. from *in situ* Optical sensors!

This study

3…

Fram Strait

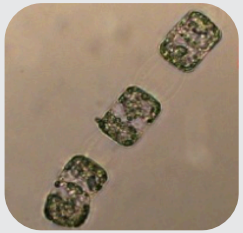


- ✓ Mass (75%), heat (90%) exchanges
- ✓ Sea ice mass export (10%)

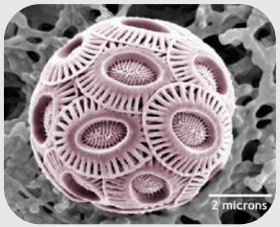
- ○ Climate change
- ○ Light & nutrient conditions change
- ○ **phytoplankton community change**

Satellite data: poor spatial-temporal resolution; lack of assessment of the applicability of global bio-optical algorithms

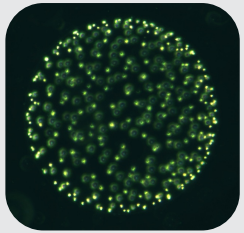
***In situ* data**: insufficient HPLC data, even less optical measurements



diatom

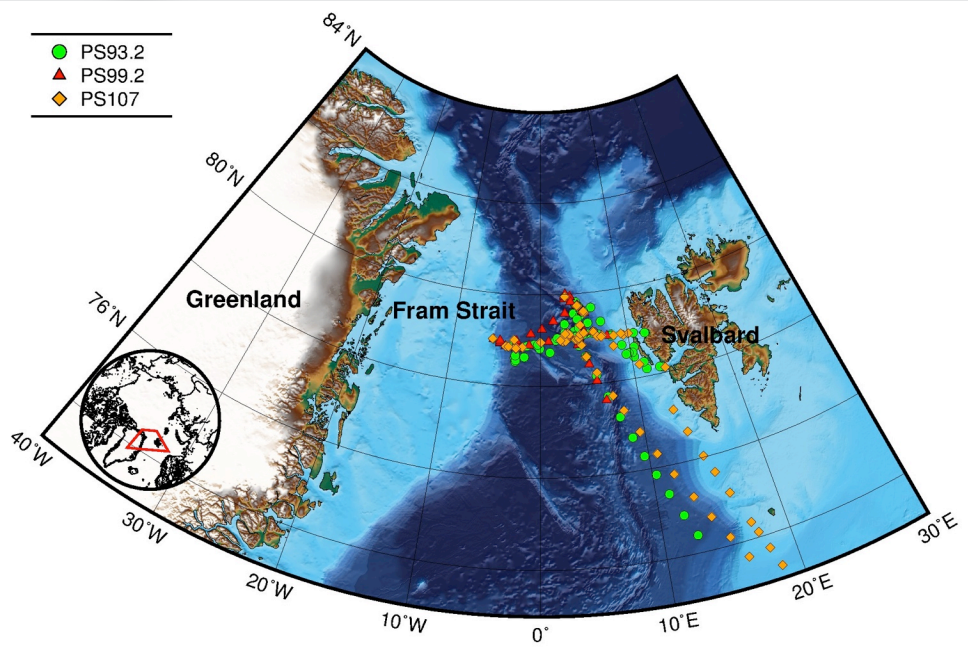


coccolithophore



phaeocystis

Data set



Expedition: icebreaker *R/V Polarstern*

- PS93.2 (Jul - Aug 2015)
- PS99.2 (Jun - Jul 2016)
- PS107 (Jul - Aug 2017)

✓ HPLC pigments (18 types) from 299 discrete samples

✓ Collocated particle absorption a_p from underway spectrophotometry

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Objectives

01 Evaluate the applicability of 2 pigment retrieval algorithms to the Fram Strait: Gaussian decompostion (Chase et al., 2013) and Singular Value Decomposition+Non-Negative Least squares (SVD-NNLS) (Moisan et al., 2011).

02 Retrieve pigments from continuous *in situ* particulate absorption data measured by underway spectrophotometry.

03 Obtain the time series of phytoplankton functional types during cruise periods via diagnostic pigment analysis.

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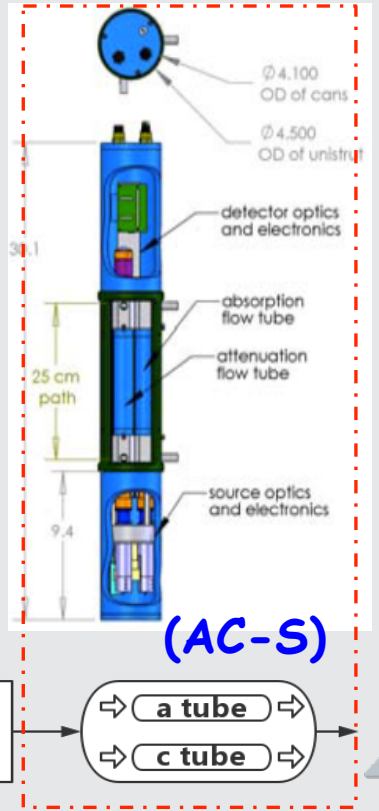
Underway spectrophotometry

AC-S spectrophotometer



- Hyperspectral: 400-735 nm, > 80 wavelengths outputs
- spectral resolution: 10 nm
- Sampling frequency: 4 Hz

Final output: particle absorption a_p

Diagram of the underway AC-S flow-through system

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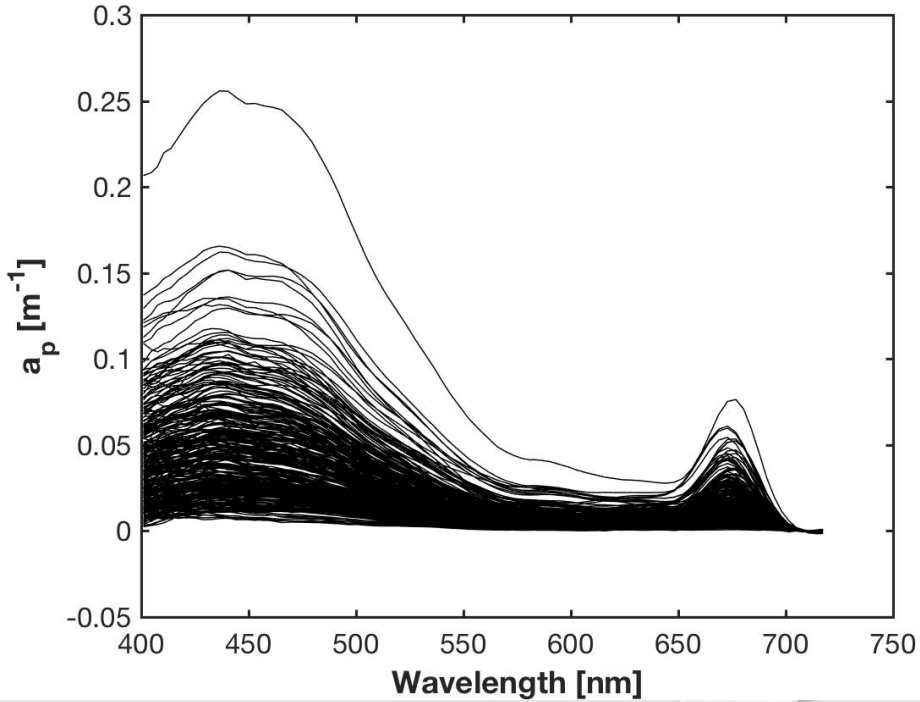

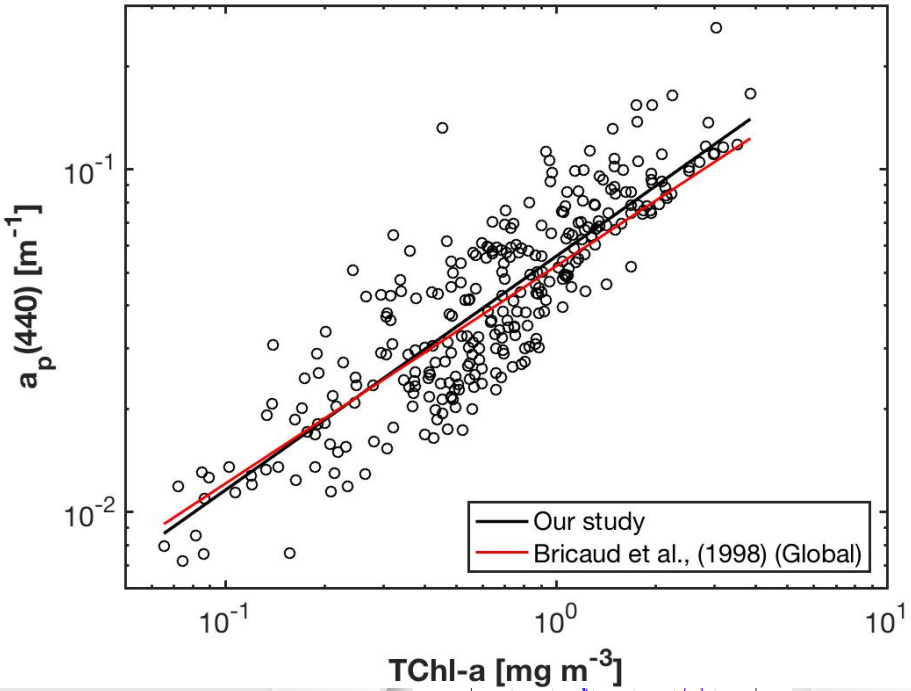

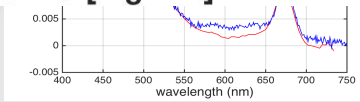

1-min interval bin

4 measurements per sec.

a_p calculation

Linear interpolation

Validated with filter-pad data

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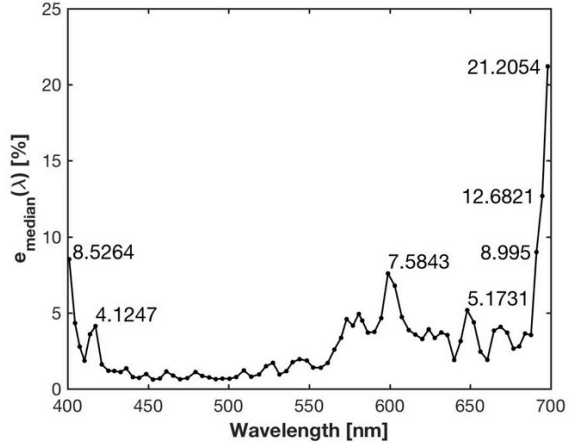
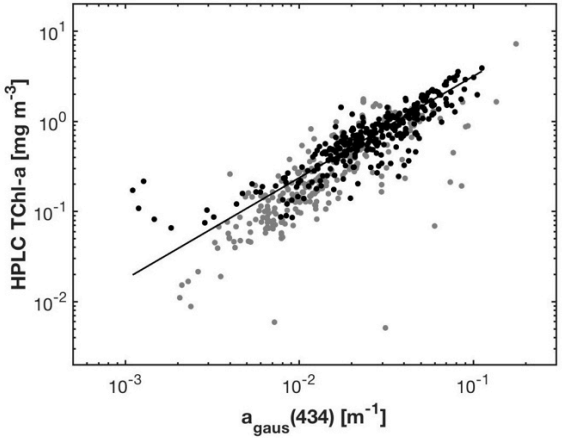
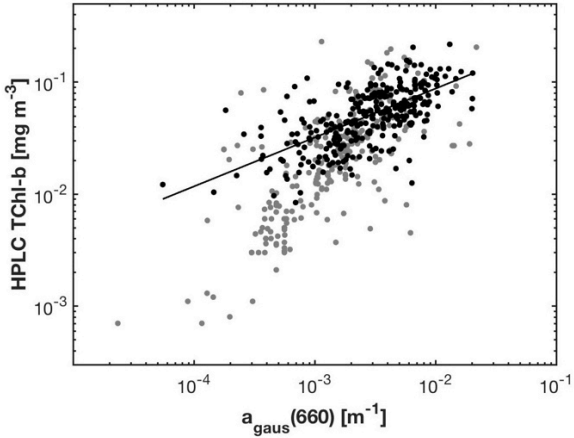
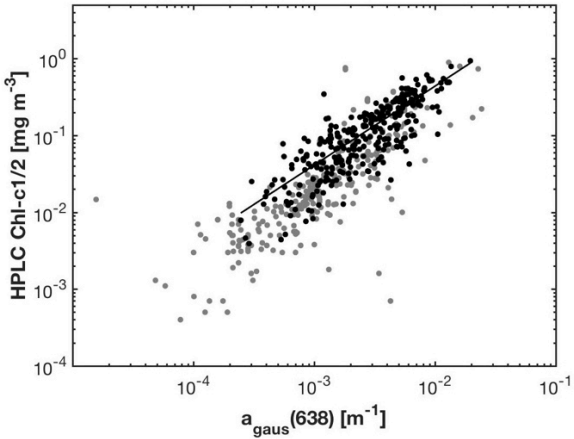
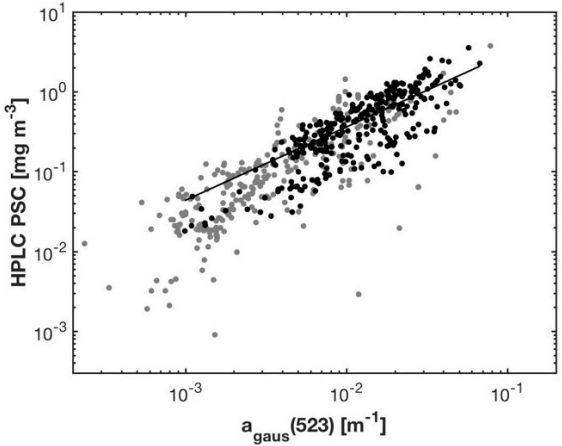
Guassian decomposition (Spectral decomposition)

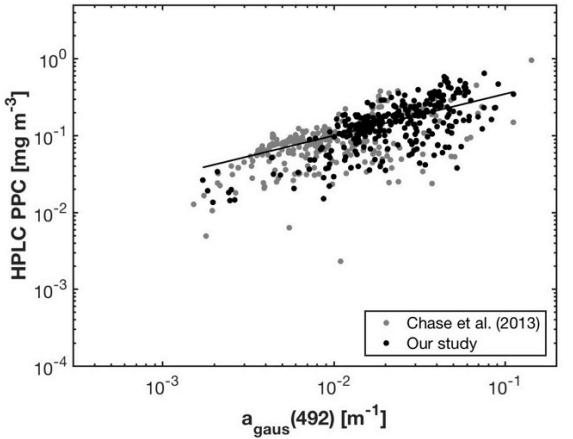






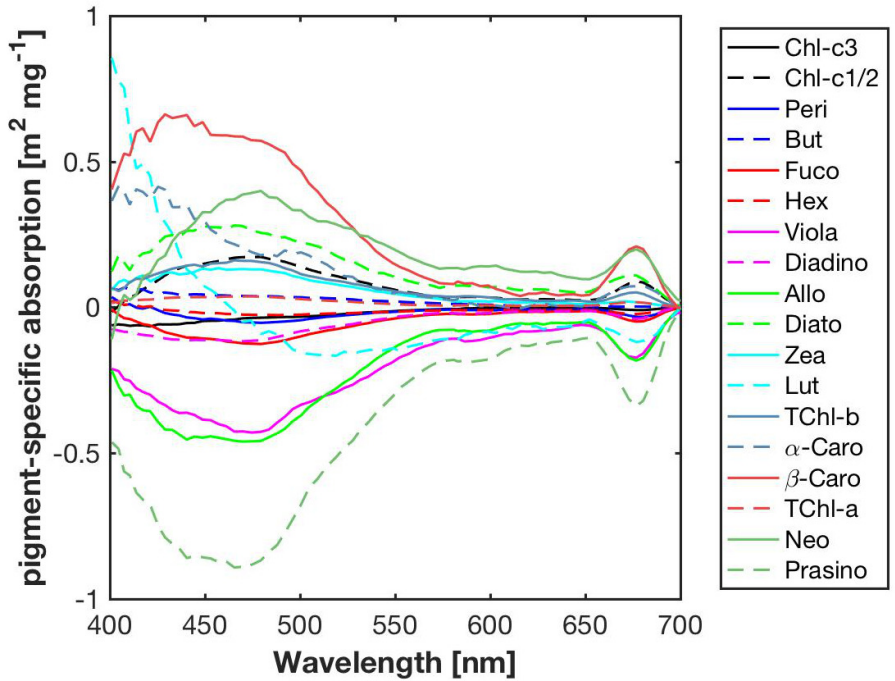


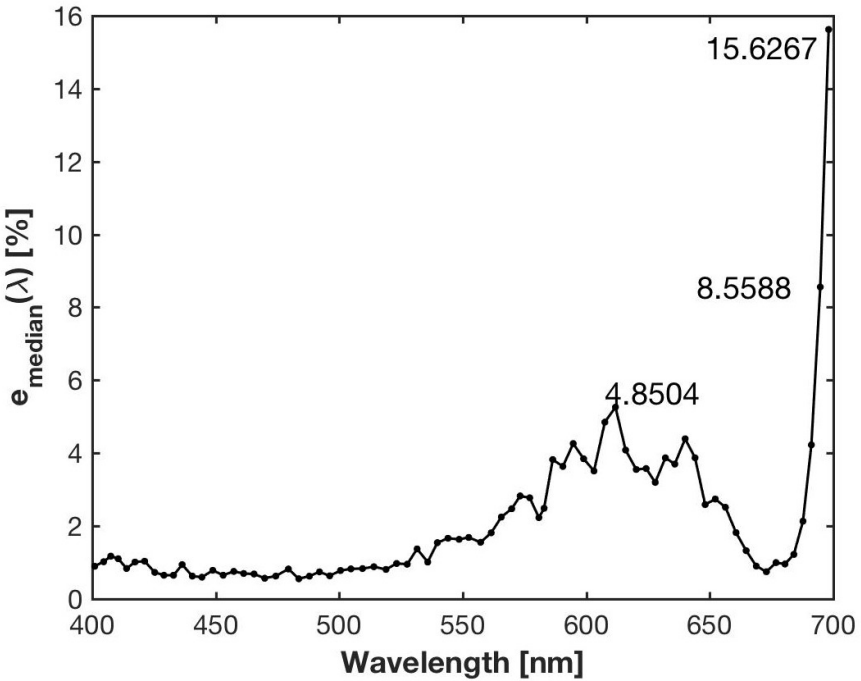




SVD - NNLS（Spectral reconstruction）

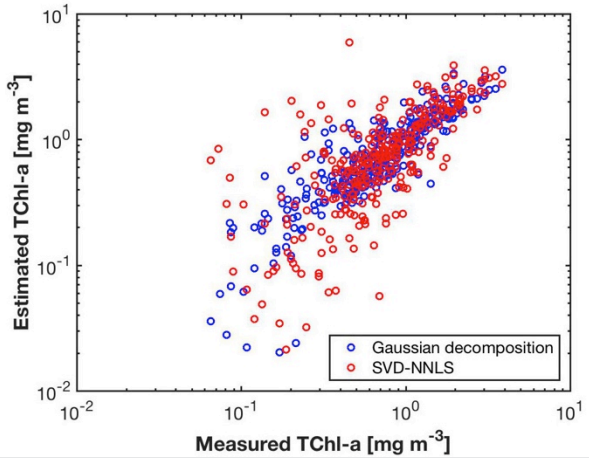
$$a'_{ph}(\lambda) = \sum_{i=1}^{m} c_i a_i^*(\lambda),$$



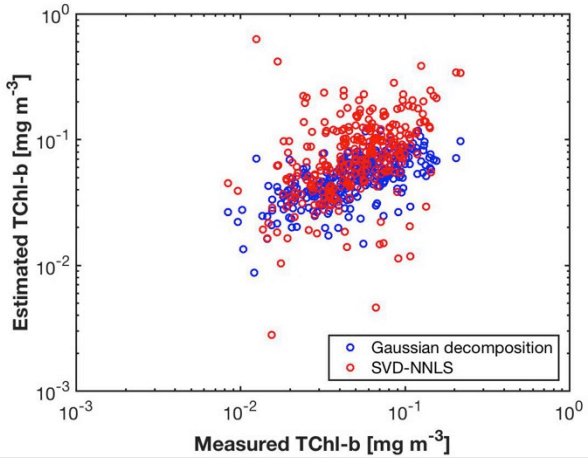


Comparison of the 2 methods

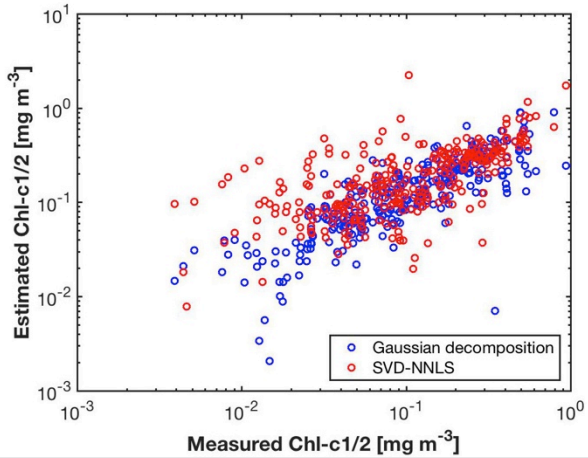
TChl-a



TChl-b



Chl-c1/2



Training accuracy

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Comparison of the 2 methods

pigments	abbreviation	Gaussian decomposition				SVD-NNLS			
		R^2	RMSE	MAE	RPD (%)	R^2	RMSE	MAE	RPD (%)
alloxanthin	Allo	-	-	-	-	0.20	0.408	0.294	114.6
chlorophyll-c1/2	Chl-c1/2	0.69	0.264	0.207	40.0	0.51	0.416	0.308	157.0
chlorophyll-c3	Chl-c3	-	-	-	-	0.35	0.648	0.500	484.6
α-carotene	α-Caro	-	-	-	-	0.16	0.528	0.425	217.6
β-carotene	β-Caro	-	-	-	-	0.26	0.306	0.229	60.8
diadinoxanthin	Diadino	-	-	-	-	0.26	0.464	0.330	171.5
diatoxanthin	Diato	-	-	-	-	0.28	0.401	0.321	48.9
fucoxanthin	Fuco	-	-	-	-	0.52	0.326	0.243	53.8
19′-hexanoyloxyfucoxanthin	Hex	-	-	-	-	0.47	0.485	0.344	227.1
19′-butanoyloxyfucoxanthin	But	-	-	-	-	0.16	0.739	0.585	589.8
neoxanthin	Neo	-	-	-	-	0.43	0.568	0.480	123.3
lutein	Lut	-	-	-	-	0.10	0.461	0.354	47.6
peridinin	Peri	-	-	-	-	0.32	0.500	0.395	181.5
prasinoxanthin	Prasino	-	-	-	-	0.75	0.344	0.316	60.6
violaxanthin	Viola	-	-	-	-	0.14	0.413	0.307	89.4
zeaxanthin	Zea	-	-	-	-	0.18	0.354	0.279	74.1
total chlorophyll-a	TChl-a	0.78	0.182	0.131	12.2	0.55	0.316	0.215	39.6
total chlorophyll-b	TChl-b	0.40	0.200	0.158	15.4	0.14	0.403	0.286	100.2
photosynthetic carotenoids	PSC	0.60	0.246	0.211	49.8	-	-	-	-
photoprotective carotenoids	PPC	0.39	0.278	0.188	34.3	-	-	-	-

Blue: Gaussian decomposition

Red: SVD-NNLS

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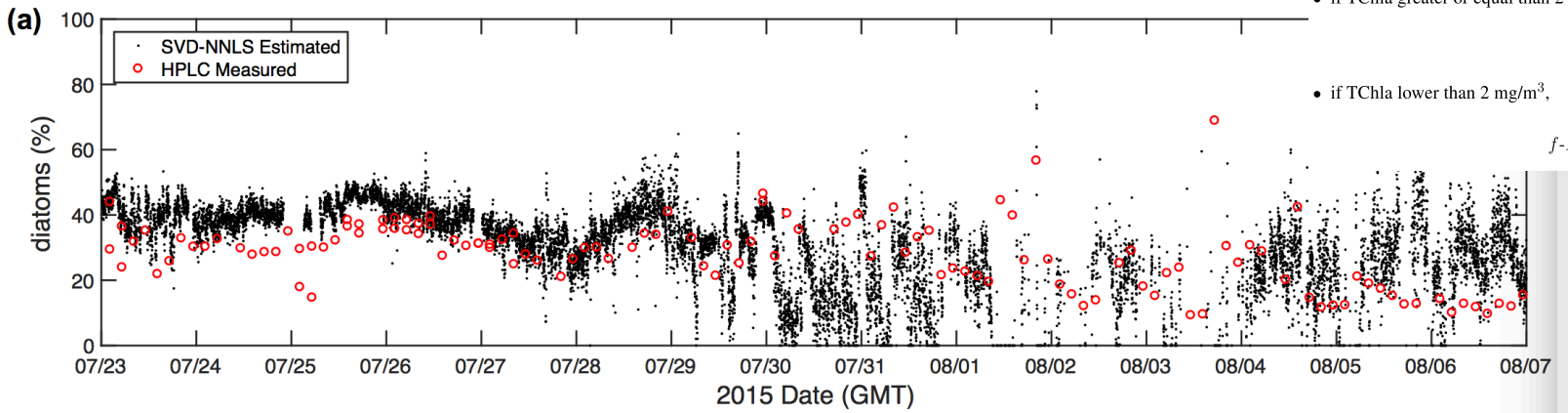
10-fold cross validation

Phytoplankton functional types time series

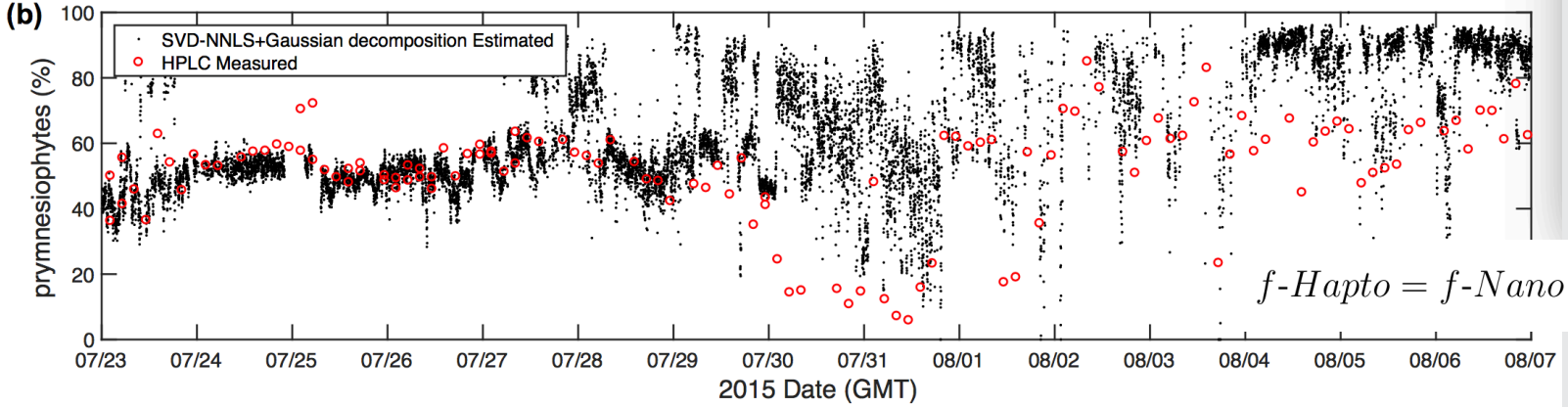


- if TChla greater or equal than 2 mg/m^3,

$$f\text{-}Diatoms = \frac{1.27 \cdot fuco}{TChla_w}$$

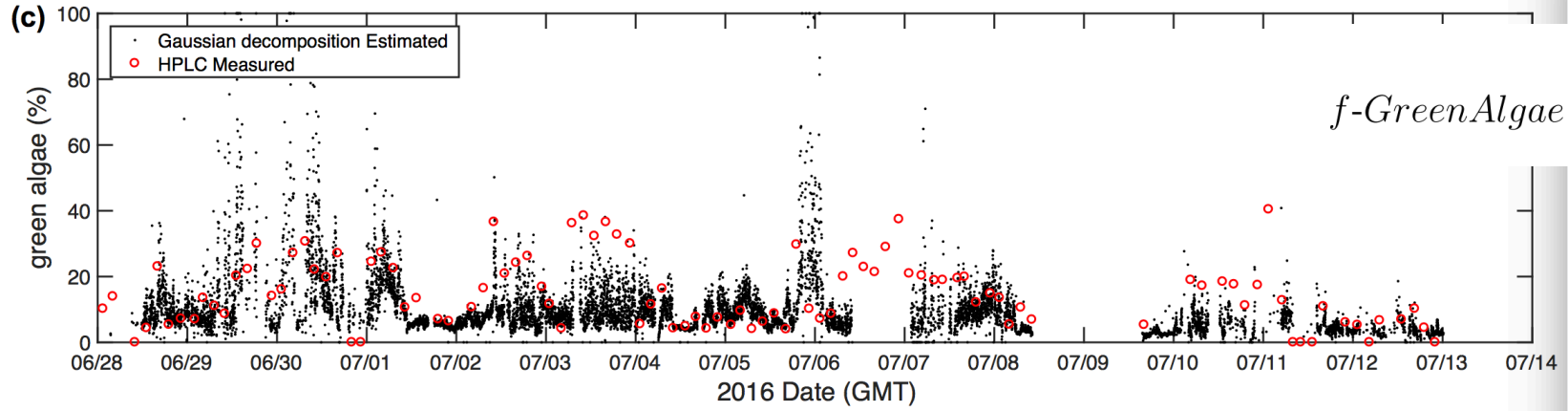
- if TChla lower than 2 mg/m^3,

$$f\text{-}Diatoms = \frac{1.27 \cdot (fuco - fuco_{Nano})}{TChla_w}$$

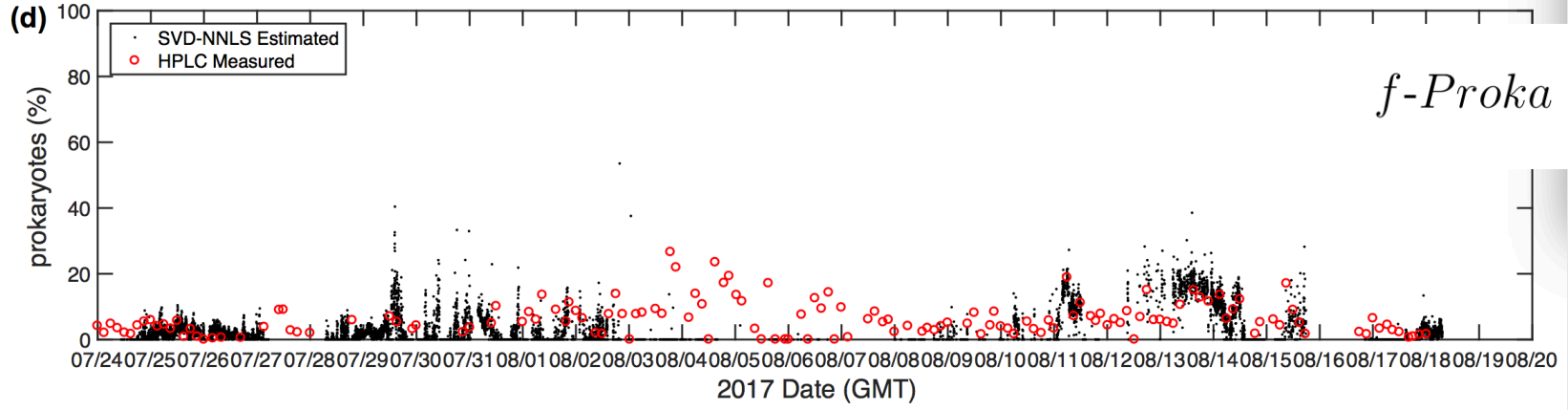


$$f\text{-}Hapto = f\text{-}Nano - f\text{-}GreenAlgae$$

Phytoplankton functional types time series



$$f\text{-}GreenAlgae = \frac{1.30 \cdot TChlb}{TChla_w}$$



$$f\text{-}Proka = \frac{2.36 \cdot zea}{TChla_w}$$

Conclusions

01

Evaluate the applicability of 2 pigment inversion algorithms to the Fram Strait: Gaussian decompostion (Chase et al., 2013) and Singular Value Decomposition+Non-Negative Least squares (SVD-NNLS) (Moisan et al., 2011).

- ✓ both methods tend to overestimate specific pigment concentration.
- ✓ the combination of the methods still provide robust estimates for many of the tested 18 phytoplankton pigments and two pigment groups (PSC and PPC) .

- The Gaussian decomposition: TChl-a, TChl- b, Chl-c1/2, PSC and PPC.
- The SVD-NNLS: TChl-a, Fuco, Diato, b-Caro, Prasino, TChl-b, Zea, Viola and Lut.

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Conclusions

02 **Retrieve pigments from continuous *in situ* particulate absorption data measured by underway spectrophotometry.**

03 **Obtain the time series of phytoplankton functional types during cruise periods via diagnostic pigment analysis.**

- ✓ diatoms, prymnesiophytes, green algae and prokaryotes were determined by combining the results from the two retrieval methods.
- ✓ We obtained high resolution phytoplankton pigment data and relative biomass of key phytoplankton groups in the Fram Strait.

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Outlook

Further discern the factors governing the retrieval uncertainties e.g. package effect.

A

B

coupling of phytoplankton composition and distribution to physical and biogeochemical properties.

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