Field Support Group Update

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- Introduction
- Accomplishments
  - Pigment Analysis Activities
  - *in situ* Protocol updates
  - Field campaign efforts
  - HyperInSPACE & QWIP

Field Support Group Update

Antonio Mannino
NASA Goddard Space Flight Center

Core members:
Joaquin Chaves, Scott Freeman, Chris Kenemer, Chelsea Lopez, Aimee Neeley, Harrison Smith, and Crystal Thomas

Other contributors to FSG activities:
Dirk Aurin and Ryan Vandermeulen

NASA OCRT Meeting – 7 September 2022

Our Staff

Core Members

Joaquin Chaves

Scott Freeman

Chris Kenemer

Chelsea Lopez

Aimee Neeley

Harrison Smith

Crystal Thomas

Other contributing staff

Dirk Aurin

Ryan Vandermeulen

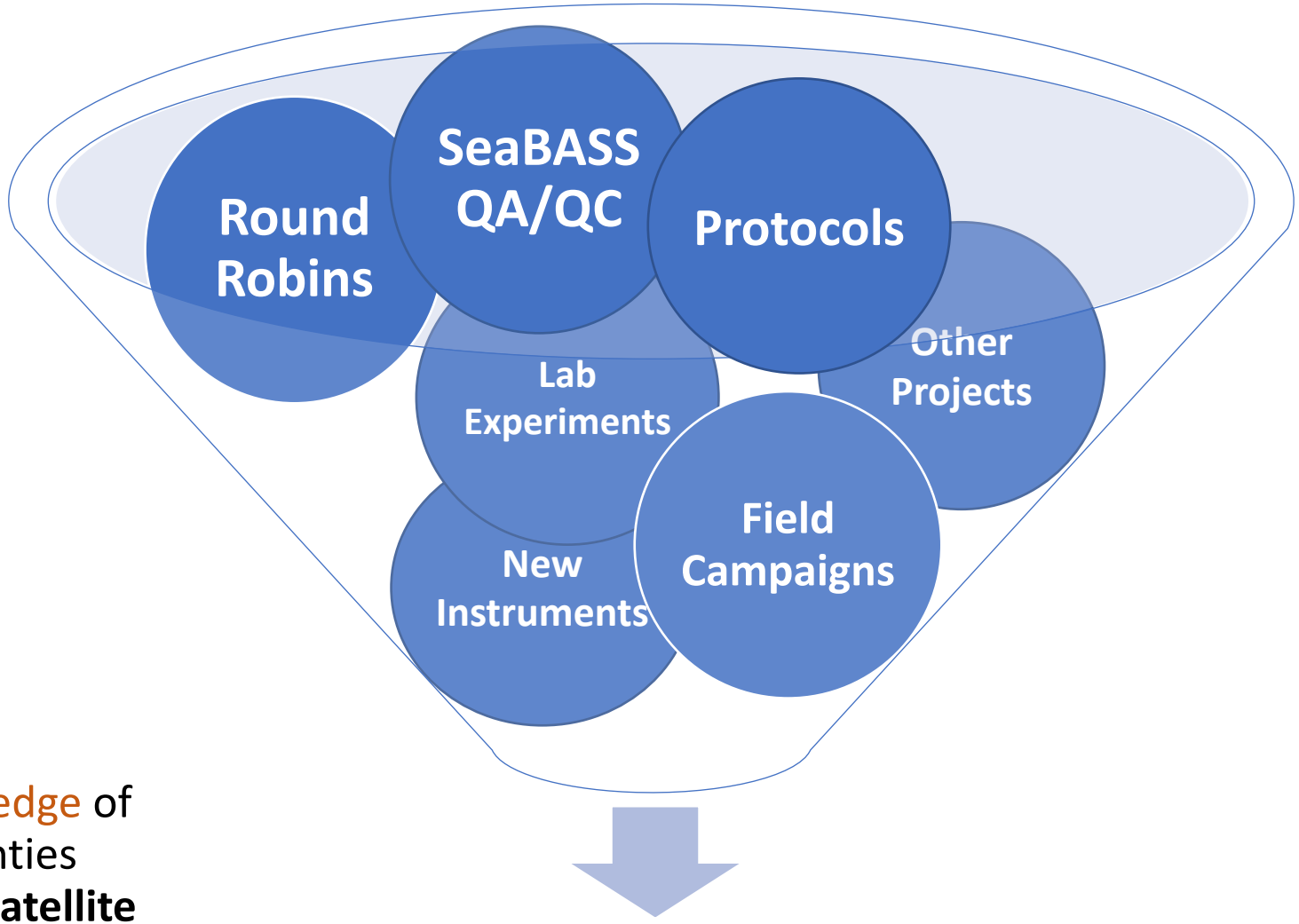
Field & Lab activities in support of NASA

our Mission Statement:

Engage in activities to ensure the quality of NASA's optical and biogeochemical field datasets used in the development of Ocean Color (OC) satellite algorithms and in the validation of OC satellite data products (and models).

THIS IS CRITICAL TO PACE'S SUCCESS

Everything we do feeds into improving knowledge of and reduction of *field measurement* uncertainties and thus through interdependence **improve satellite data products and knowledge of their inherent uncertainties**.



Phytoplankton pigment analysis lab

Dedicated quality-assured lab necessary for validation and maintenance of chl-*a* climate data record and production of suite of HPLC-amenable phytoplankton pigments

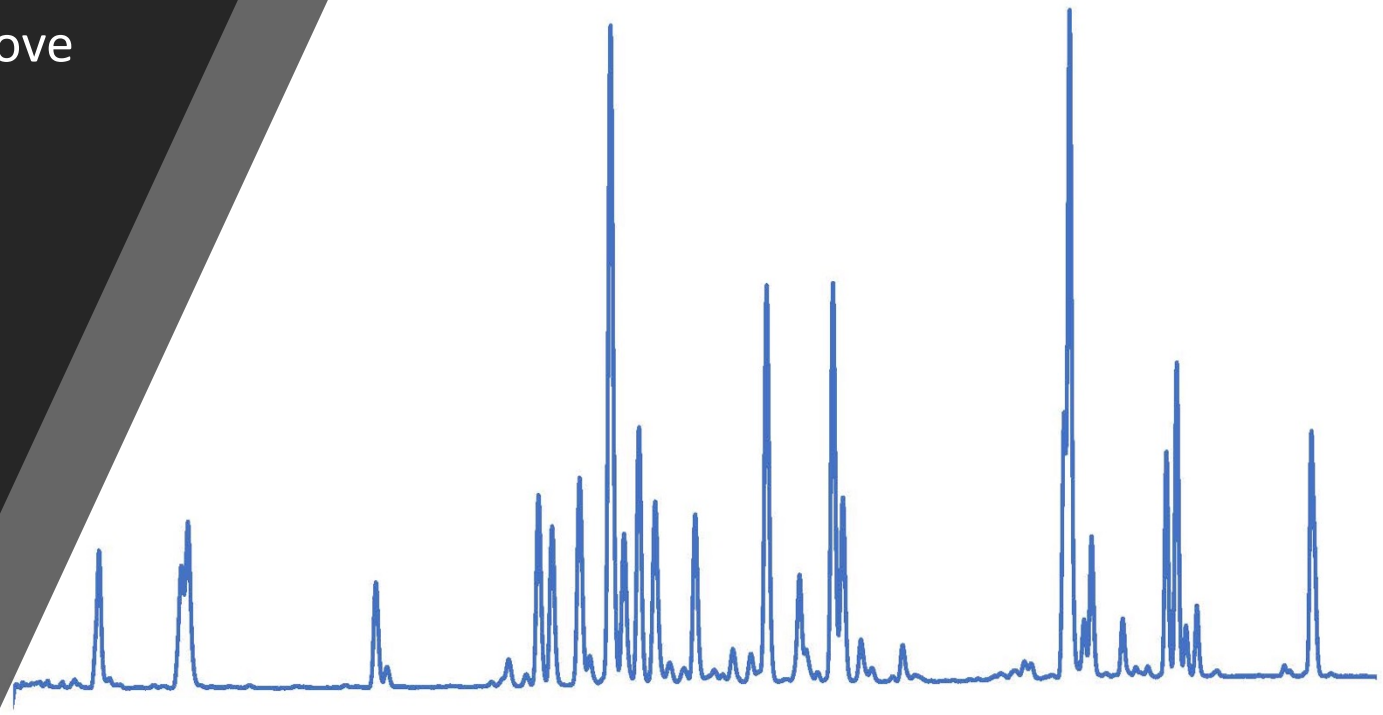
Past Year Accomplishments

- Reported ~2700 HPLC pigment samples
- On-going efforts to maintain and improve data quality and analytical efficiency
- Methods development for phycobilin pigments

Future Work

- Methods development/assessment for uHPLC and uHPLC-LC-MS
- Method selection for phycobilin pigments

Chromatogram of pigments from
High-Performance Liquid Chromatography (HPLC)



Technical lead contact: crystal.s.thomas@nasa.gov

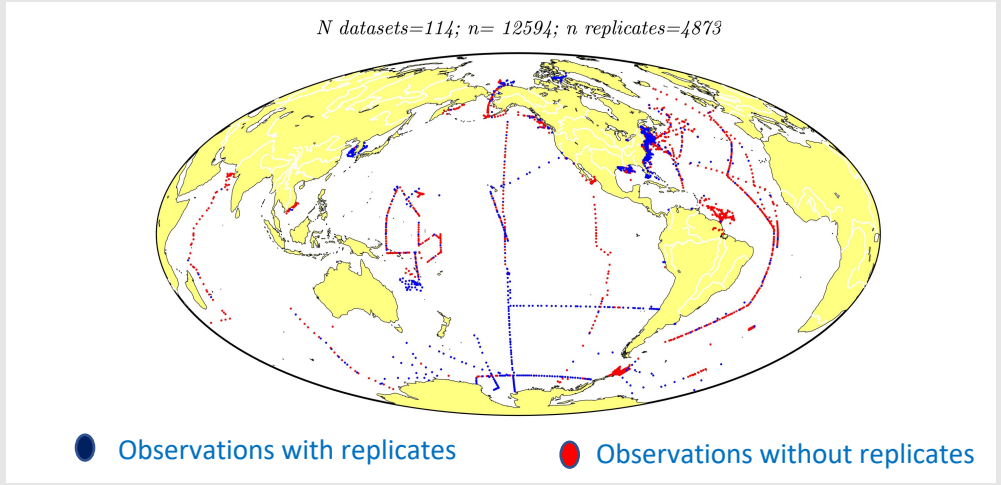
Sources of Uncertainty in HPLC Pigment Measurements

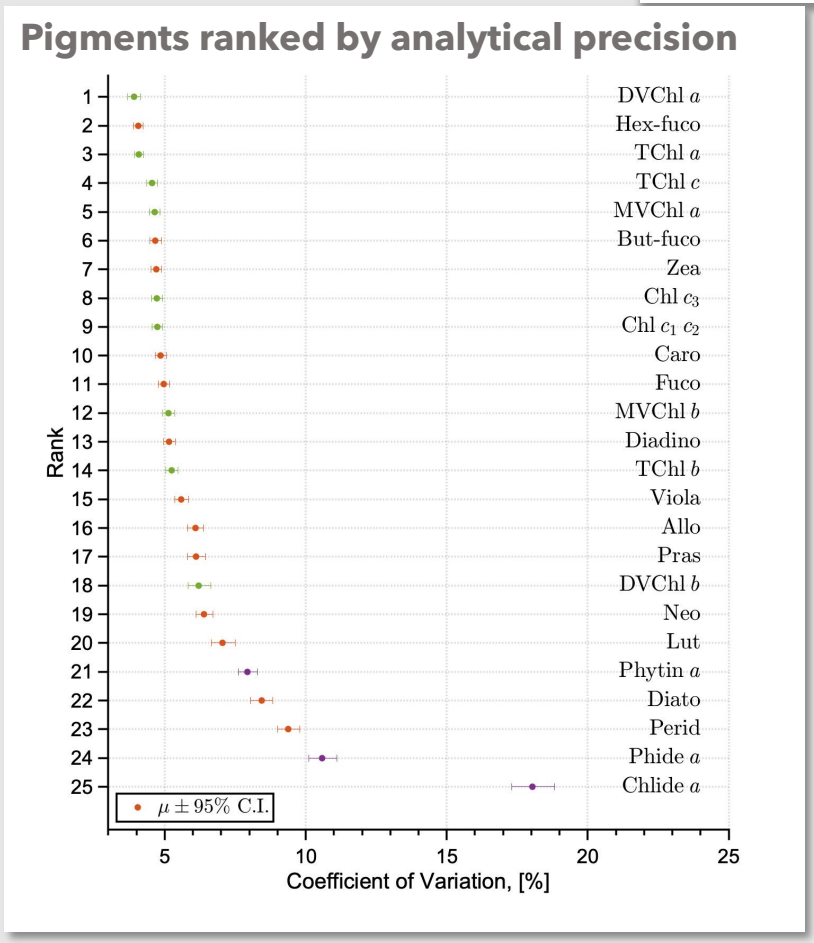
GLOBAL VARIABILITY OF PHYTOPLANKTON PHOTOSYNTHETIC PIGMENTS MEASURED BY HIGH PERFORMANCE LIQUID CHROMATOGRAPHY (HPLC): A PRECISION ASSESSMENT OF THE DATASET ANALYZED BY NASA

Crystal S. Thomas[*a,b], Joaquín E. Chaves[a,b], and Antonio Mannino[b]

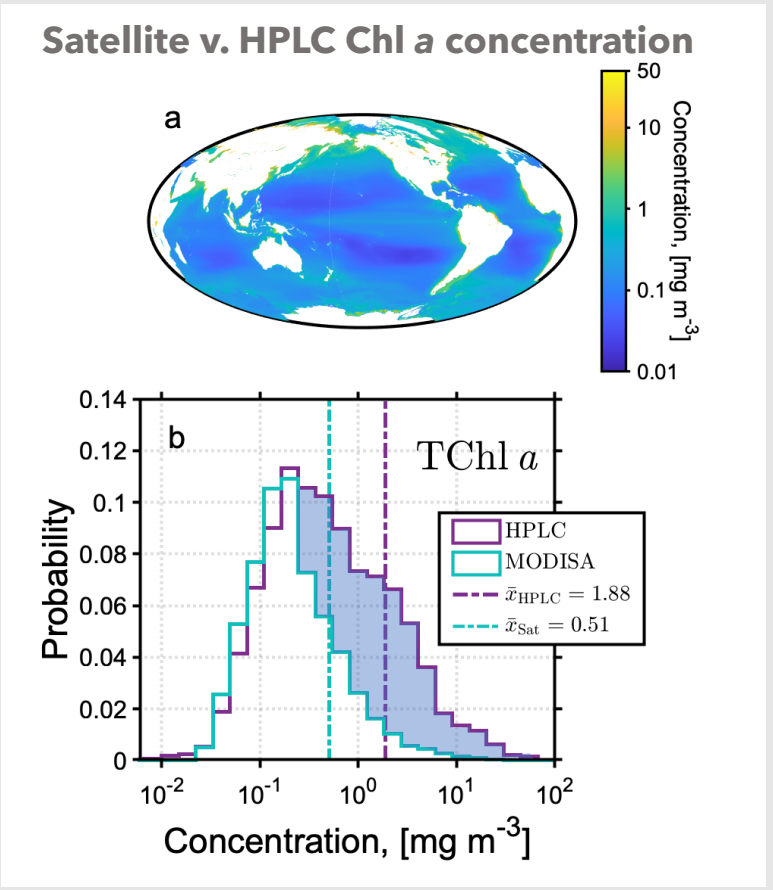
[a]*Science Systems & Applications, Inc. 10210 Greenbelt Road, Lanham, MD 20706*
[b]*NASA, Goddard Space Flight Center, Greenbelt, MD 20771*

Draft version: May 2, 2022



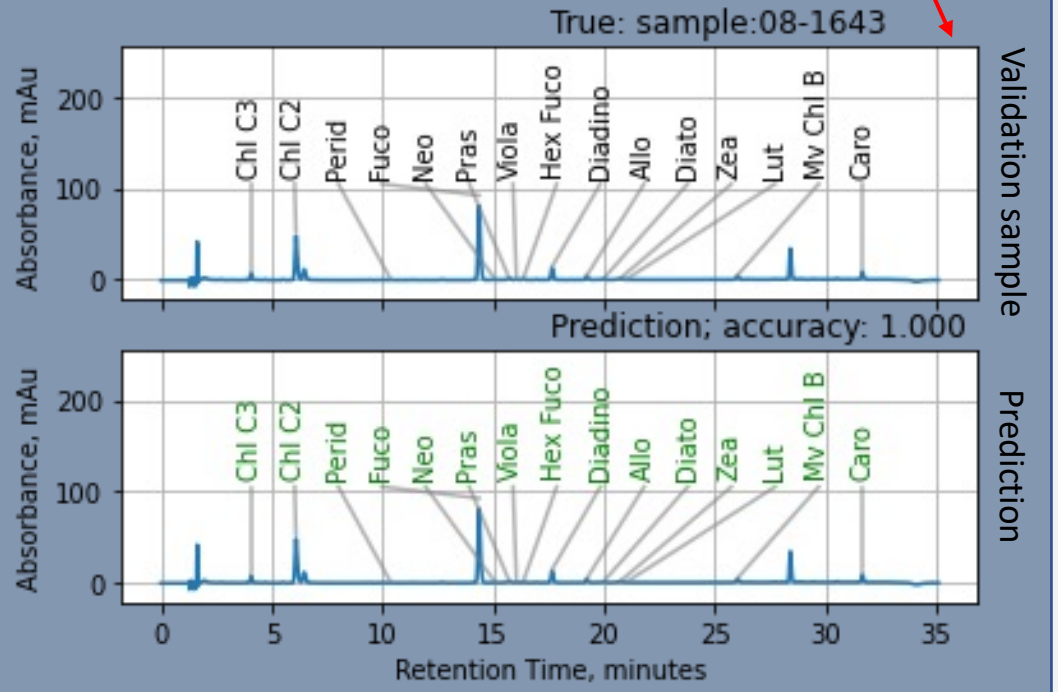


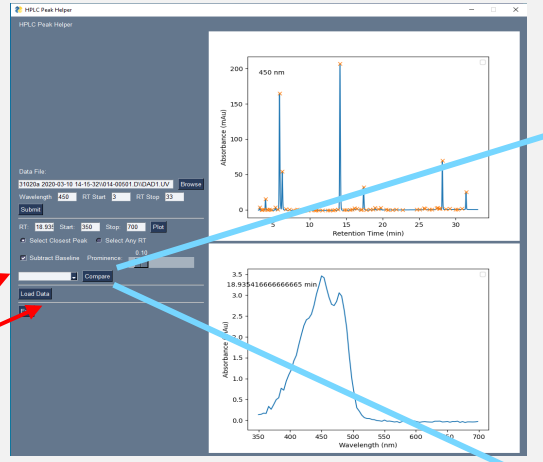
- Manuscript in preparation that gleans information from thousands of replicate filter sets from all major ocean basins
- Investigates the impacts of filtration volume, water basin, pigment concentration, etc. on replicate filter precision
- **Main conclusions**
  - Concentration is not a major driver of precision
  - Most pigments have poorer precision in coastal waters
  - Most variability appears to be random, not systematic or driven by the above variables



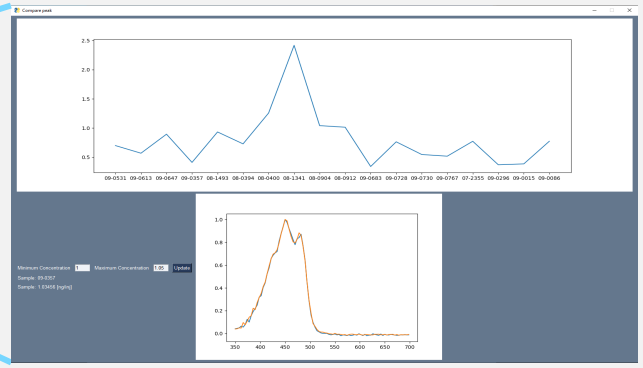
Pigment ID through Machine Learning

- A Graphical User Interface was developed this summer for an HPLC analyst to use for peak validation.
- We used existing expert-labeled phytoplankton pigment chromatogram peaks to train a convolutional neural network (CNN).
- Harnesses the entire body of HPLC analysis conducted at GSFC to aid decision-making in addition to standard spectral matching.

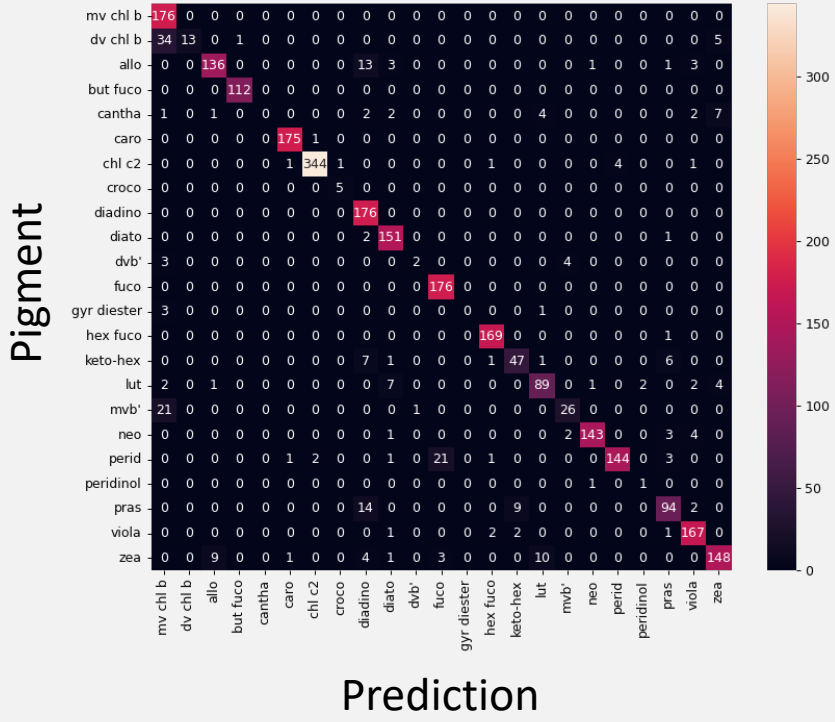




HPLC analyst GUI tool

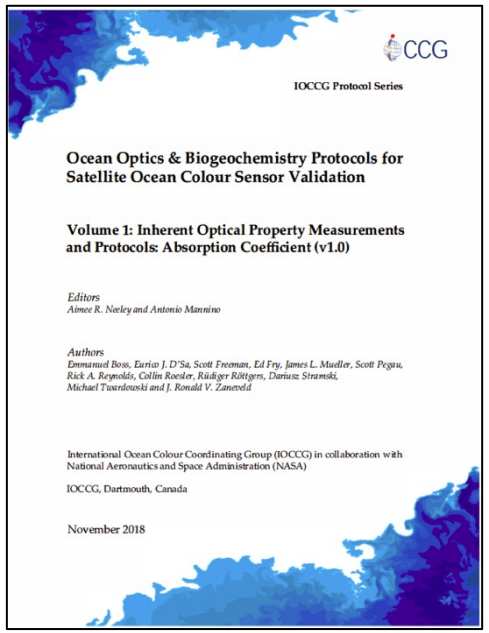


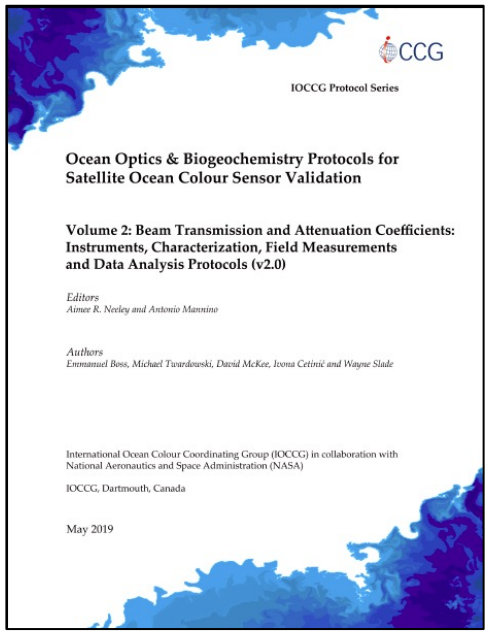
Validation set peak ID predictions

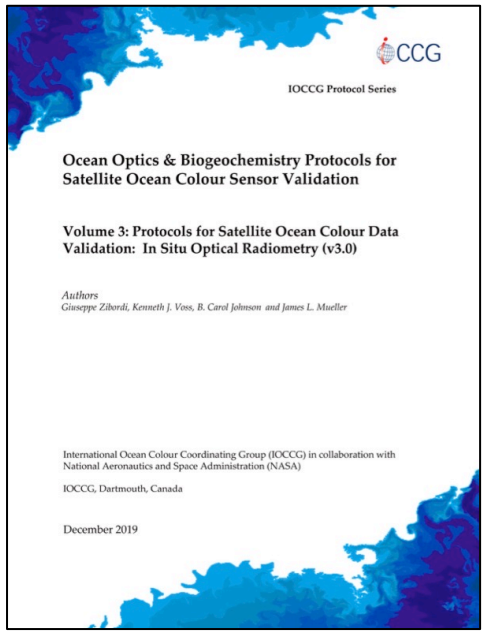


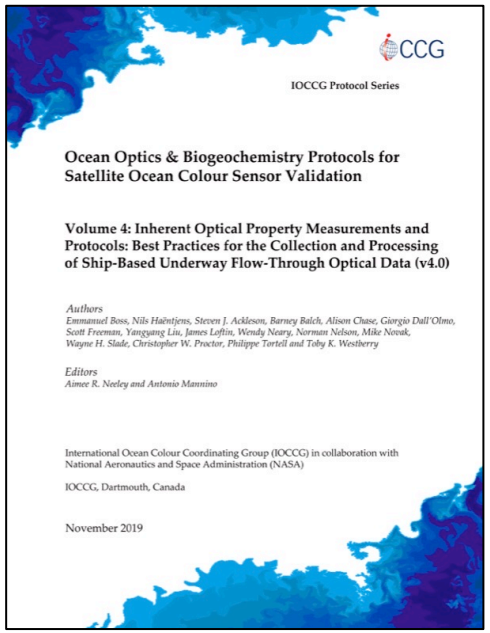
"Confusion Matrix" showing ML model predictions on validation set

Status of Field Measurement Protocols - Published









Vol. 1.0 Absorption (particles)

Nov. 2018

Vol. 2.0 Beam Attenuation

April 2019

Vol. 3.0 Radiometry for Validation

Dec. 2019

Vol. 4.0 Inline Flow-Through IOPs

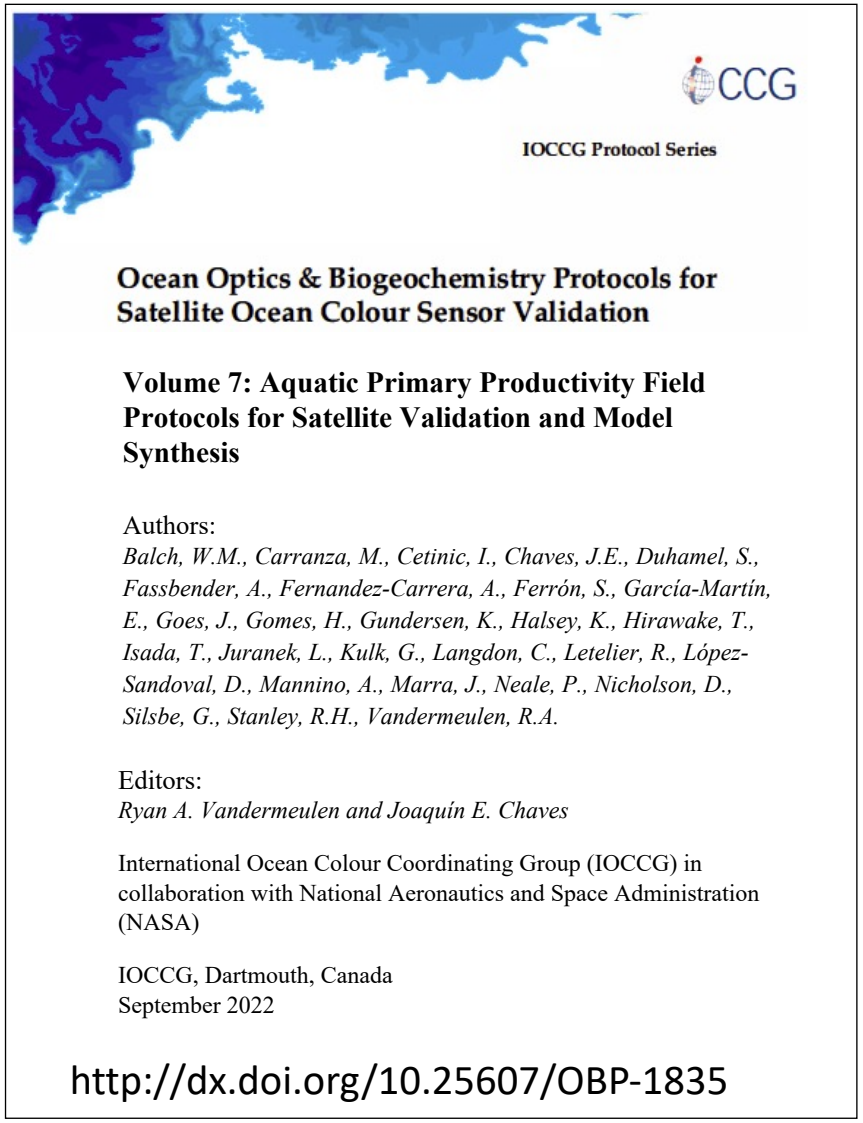
Nov. 2019

Vol. 6.0 Particulate Organic Carbon

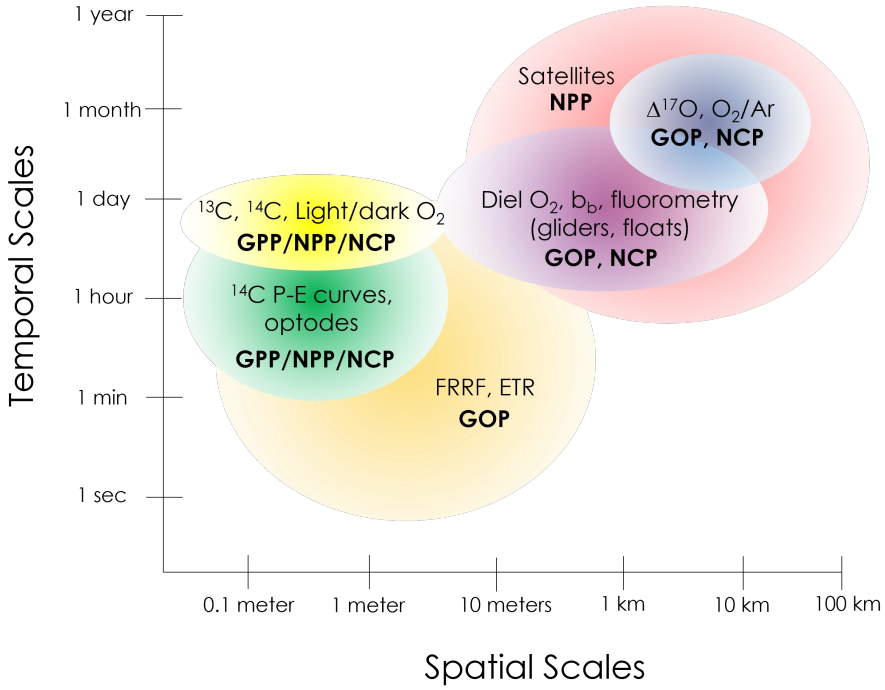
August 2021

https://ioccg.org/what-we-do/ioccg-publications/ocean-optics-protocols-satellite-ocean-colour-sensor-validation/

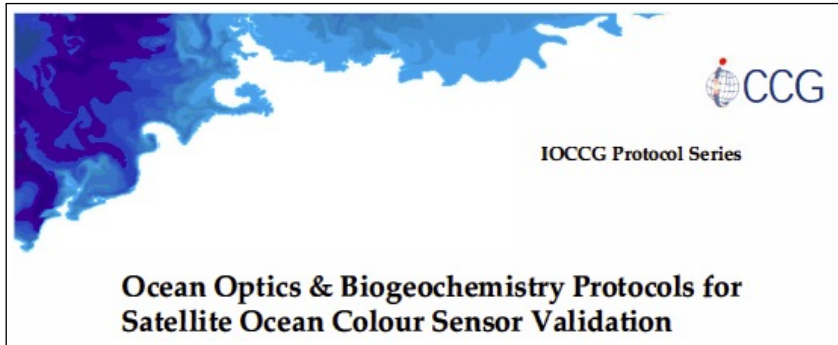
Status of Protocols – Primary Productivity



- Protocol published **September 2022**
- 27 authors + 7 AEPRs, representing 28 institutions from 9 countries
- "One-stop-shop" for measurements of aquatic primary productivity (9 distinct methods covered in detail)

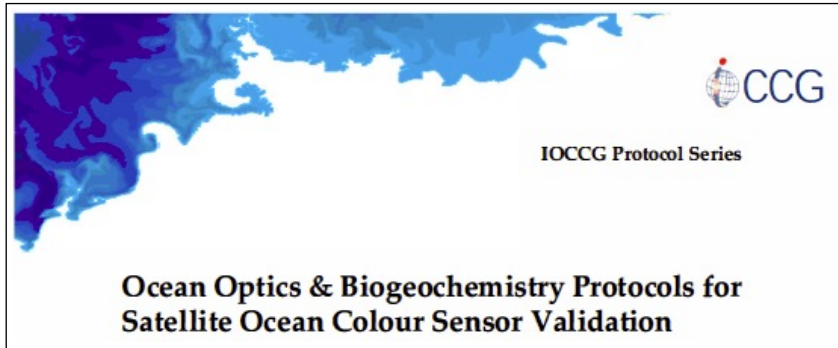


Status of Protocols – CDOM Absorption



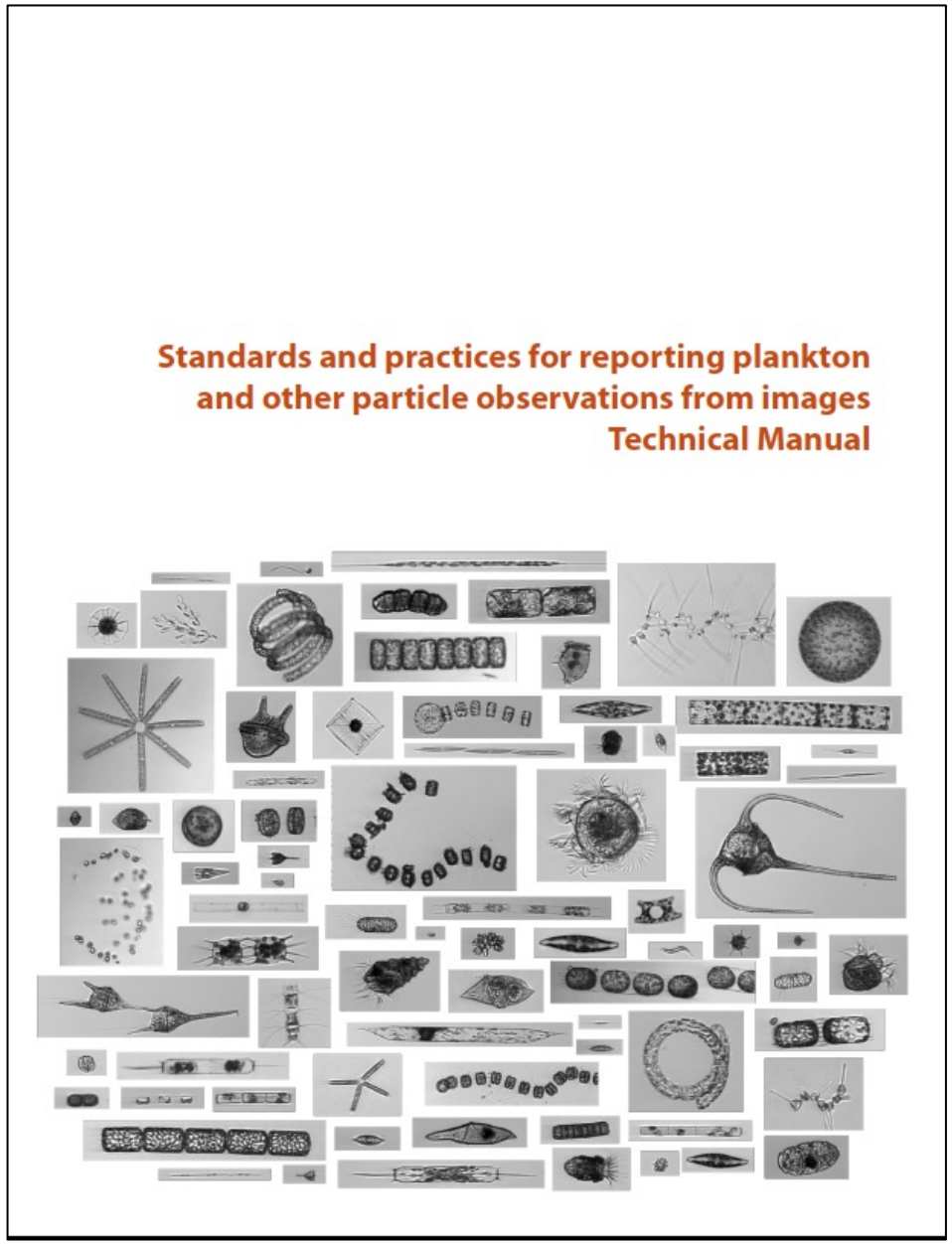
- Protocol has undergone review by AEPRs & Community
- Currently being revised per those comments
  - Updated CDOM reference material to SRFA-III
  - Merging of LWCC UV-Vis and spectrophotometer UV
- Back to AEPRs *circa* Nov 2022
- Final version in 2023

Status of Protocols – Scattering Properties



- Draft protocol in preparation
- Post protocol for community & AEPR review by end of 2022

Reporting Data from Particle Images

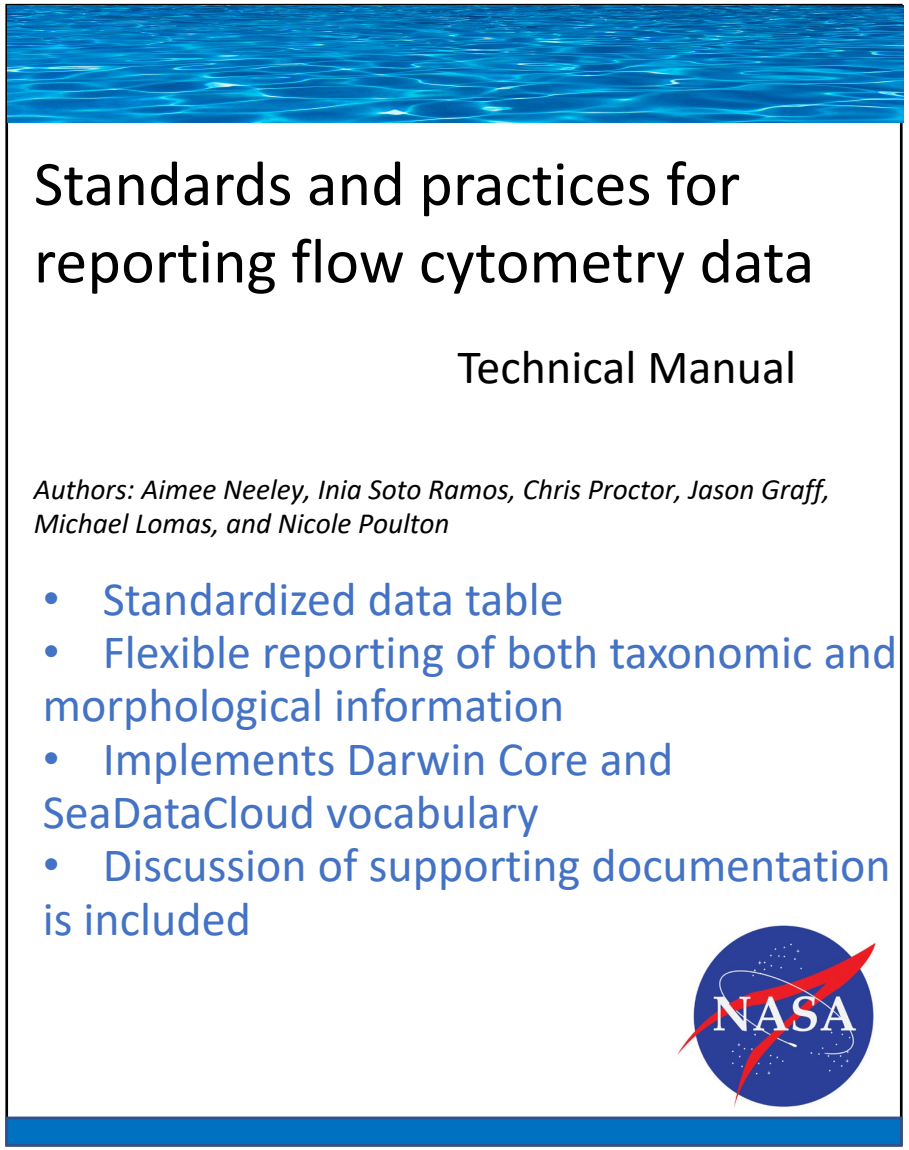


Published August 2021

Neeley, Aimee, Beaulieu, Stace E., Proctor, Chris, Cetinić, Ivona, Futrelle, Joe, Soto Ramos, Inia, Sosik, Heidi M., Devred, Emmanuel, Karp-Boss, Lee, Picheral, Marc, Poulton, Nicole, Roesler, Collin S., Shepherd, Adam, "Standards and practices for reporting plankton and other particle observations from images", 2021-07-26, DOI:10.1575/1912/27377, https://hdl.handle.net/1912/27377

NSF NASA OCB Ocean Carbon & Biogeochemistry

Reporting Data from Flow Cytometry



- Draft protocol in final preparation
- Final version: Fall 2022
- Provides standards for reporting taxonomic and morphology data collected by flow cytometry

Preparing for PACE Validation

PACE Ocean Products	IOCCG/other Field Protocols
R_{rs} (350 to 720nm every 5nm @ 2.5nm steps) and spectral k_d	Vol. 3 & 9
Spectral absorption coefficients (a_t, a_p, a_{ph}, a_{cdm}, a_g)	Vols. 1, 4 & 5
Spectral backscatter coefficients (350 to 700 nm)	Vols. 4 & 8
Chlorophyll-*a*	NASA TM
Phytoplankton pigments (HPLC & Phycobilins)	NASA TM & planning
Phytoplankton community composition	planning
Daily and instantaneous PAR	Vol. 3; NASA TM
Fluorescence line height	~Vol. 3
Net primary production (NPP)	Vol. 7
Particulate organic carbon	Vol. 6
Particulate inorganic carbon	planning
Phytoplankton carbon	planning
Dissolved organic carbon	Draft
Suspended particulate matter	planning
Particle size distribution	planning

Evaluating instruments and approaches

- Hyper-bb (b_{bp})
- SC-6 (b_{bp})
- PSICAM & QFT-ICAM (a)
- SBA (R_{rs})
- Sorting flow cytometry
- ML particle ID

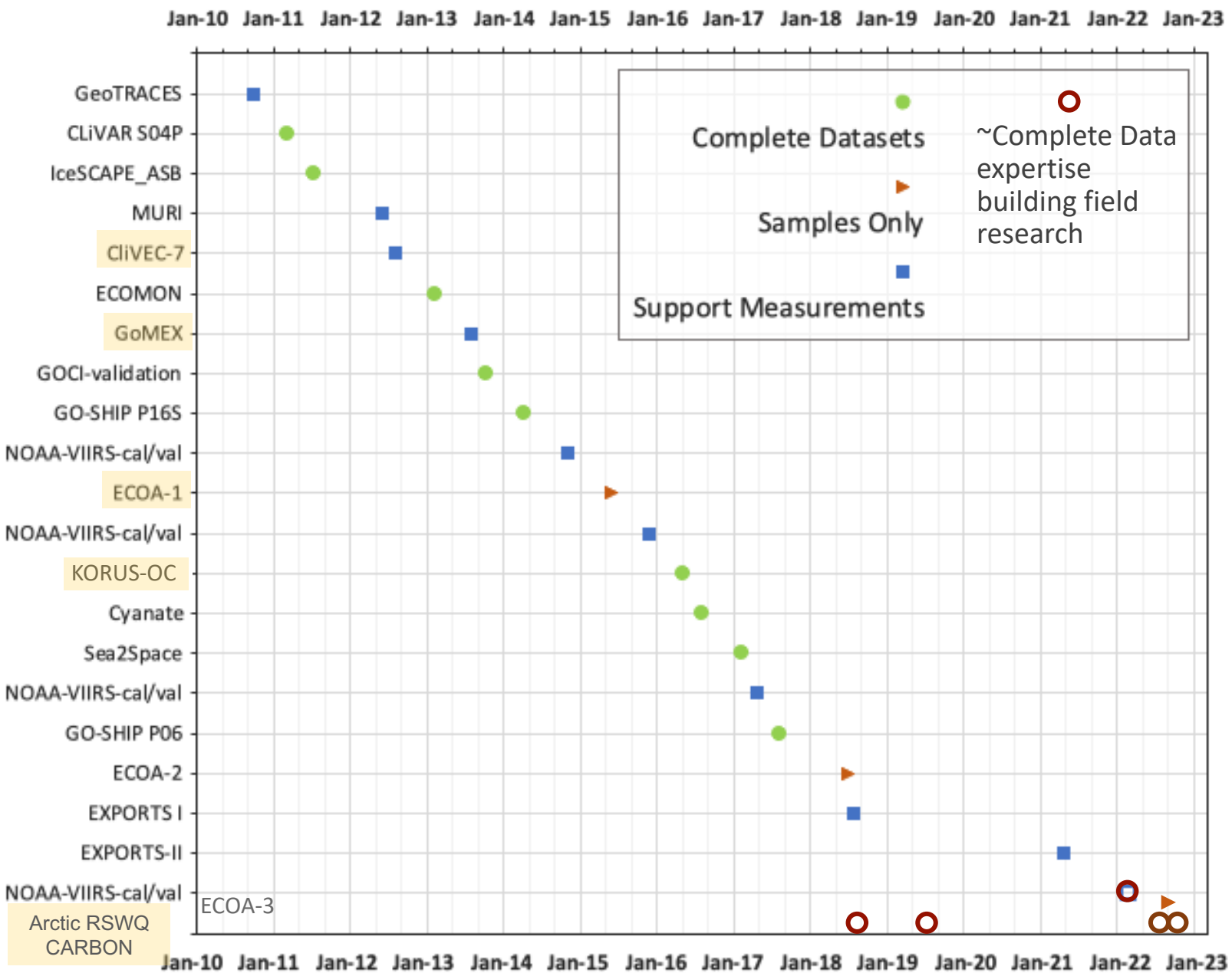
SBIR Pipeline

- OKSI AquaFloat (R_{rs})
- Sequoia “a-sphere” (a)
- Resonon airborne (R_{rs})

Planned Field Protocol Activities

- Future Field Protocols - in planning stage
  - Phytoplankton community composition & biovolume – kicking off soon
  - Phytoplankton Carbon – kicking off soon
  - HPLC Pigments update – in-house activity underway
  - Suspended Particulate Matter – in house activity
  - Dissolved Organic Carbon - draft in development
  - Phycobilin Pigments – in-house activity underway
  - Particulate Inorganic Carbon – kicking off in 2023
- Other recommended protocol topics
  - Optical and Biogeochemical Properties in Very Turbid Waters
  - Fluorescence properties
  - Review ship-based atmospheric aerosol and trace gas measurement protocols
- Updates to current IOCCG protocols as required

Field Campaign Participation and Support



Support from other funding

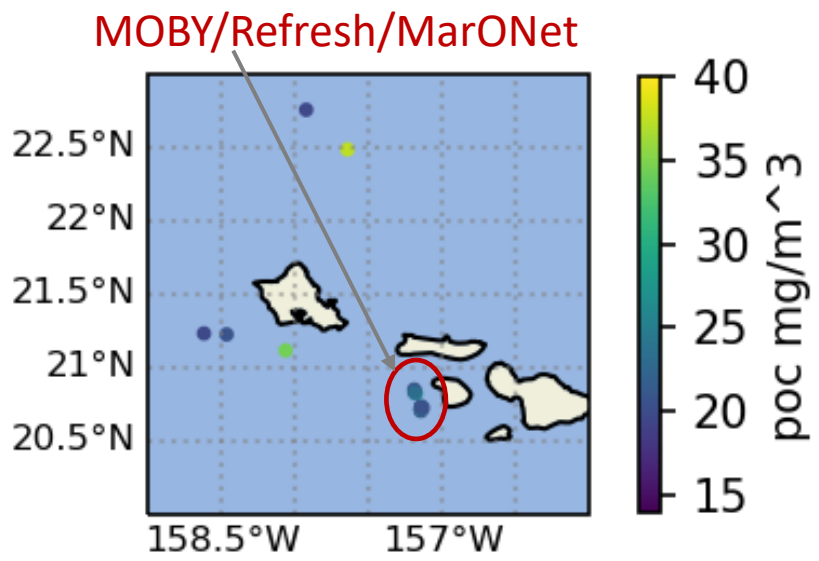
NOAA, NASA VIIRS 2022 Validation Campaign

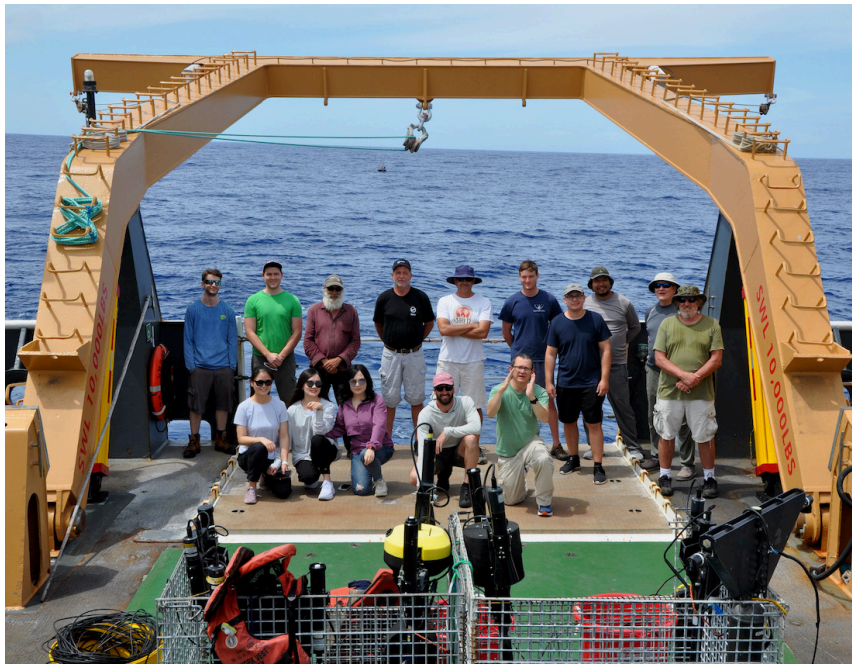
March 8-19, 2022. Hawai'i.

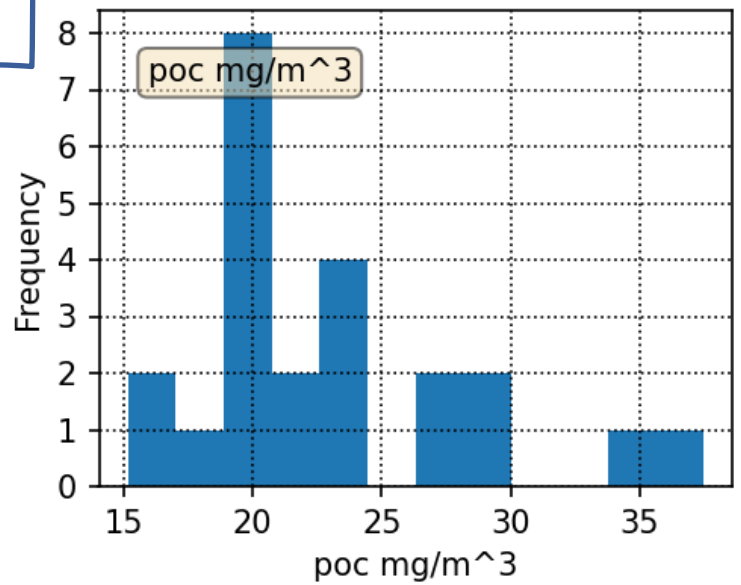
Measurements

- Radiometry intercomparison
- Above- and in-water R_{rs}
- Profiling IOPs; Hyper-bb
- HPLC pigments
- Particle and CDOM* absorption
- POC*, DOC*, PIC, SPM

* submitted to SeaBASS







Yukon River Delta/Plume/Norton Sound/northern Bering Sea

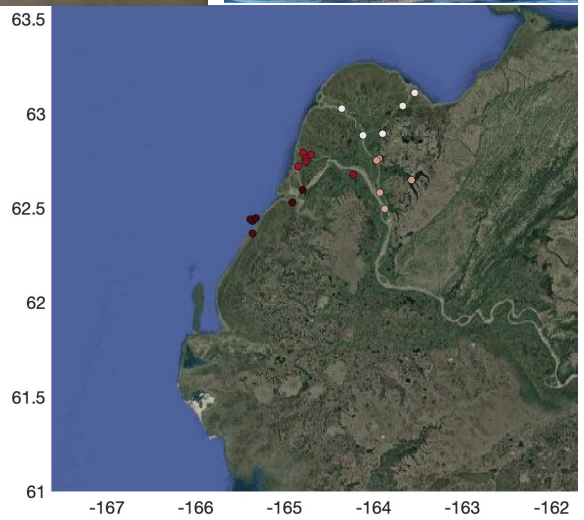
August 3-10, Aug 31-Sept 7, Sept. 9-20, 2022. Alaska

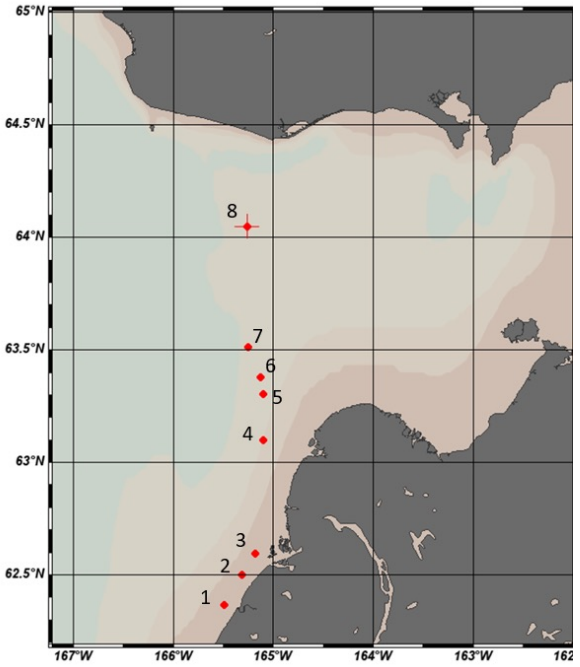
ROSES CCS Multi-investigator project:
Tzortziou, Clark, Hernes, Mannino & Spencer
Collaborators: ADF&G, NOAA, Alakanuk Tribal IGAP

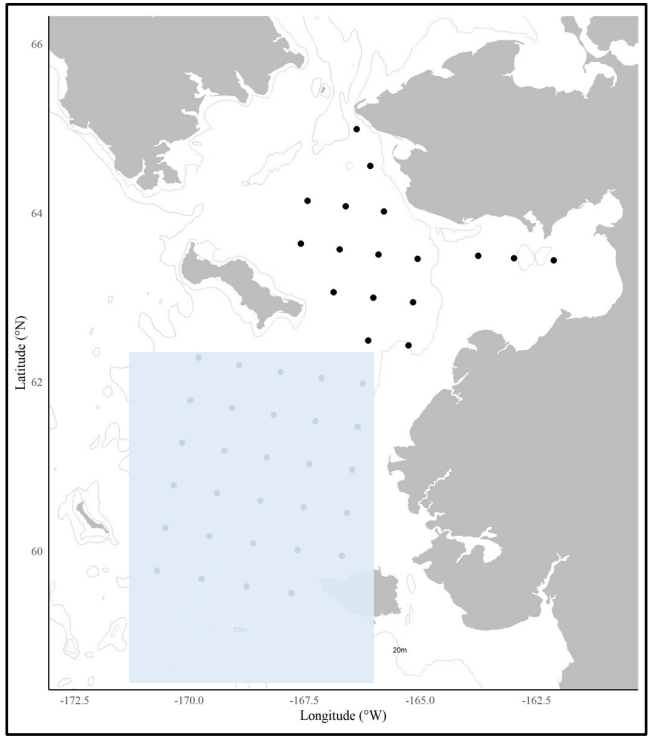
https://www.arcticriverscarbon.org/blog

Measurements

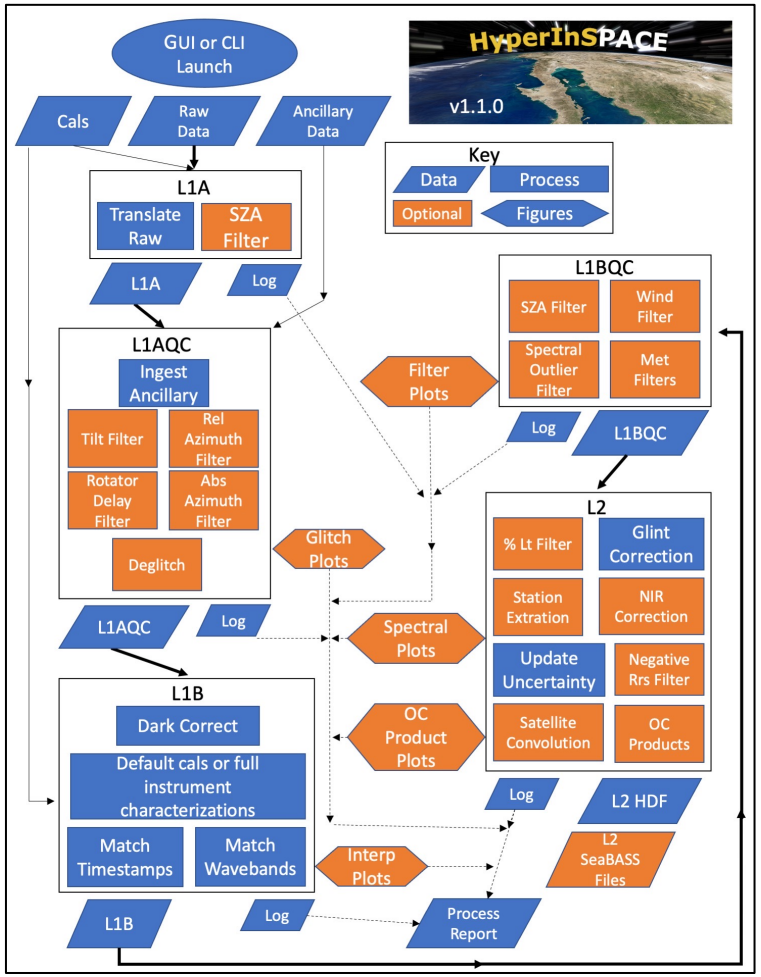
- SBA R_{rs}
- Profiling IOPs (SC-6), LISST, pH
- Particle and CDOM absorption
- POC, DOC, PIC, DIC, TA, SPM
- HPLC Pigments







HyperInSPACE Community Processor



Automated, underway, above-water radiometry submitted to SeaBASS

- ✓ KORUS-OC (2016)
- ✓ EXPORTS-NP (2018)
- ✓ Archimedes/Superyacht (2018, collaboration with R. Brewin, University of Exeter)
- ✓ NOAA VIIRS_2019_Gunter (2019)
- ✓ EXPORTS-NA (2021)

…and more in process

Collaboration with FRM4SOC2

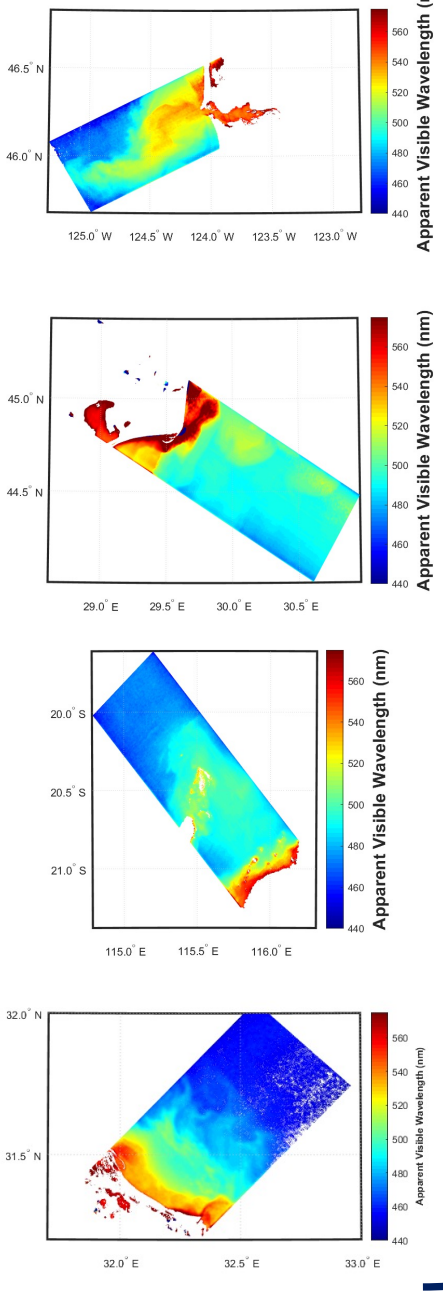
- ➢ Add TriOS-RAMSES radiometry
- ➢ Incorporate instrument characterization per IOCCG 2019 Protocols
- ➢ Complete uncertainty budget propagation
- ✓ FICE22 Field Intercomparison Campaign
  - July 2022 @ AAOT, Italy; 8 international organizations
  - Compare legacy processing to HyperInSPACE, In-water, AERONET-OC

Open-source Python on NASA GitHub

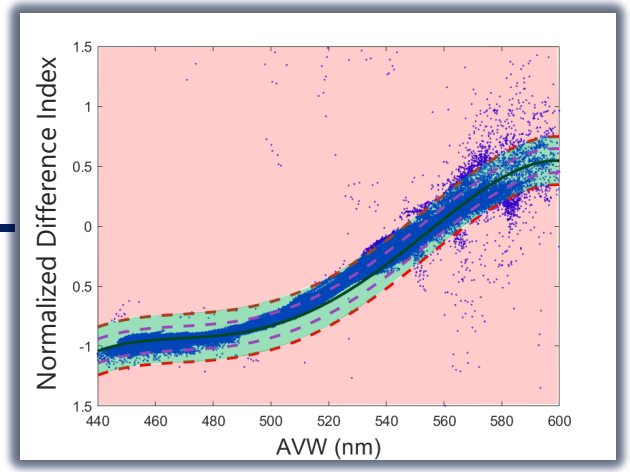
https://github.com/nasa/HyperInSPACE

New OC product

HICO images

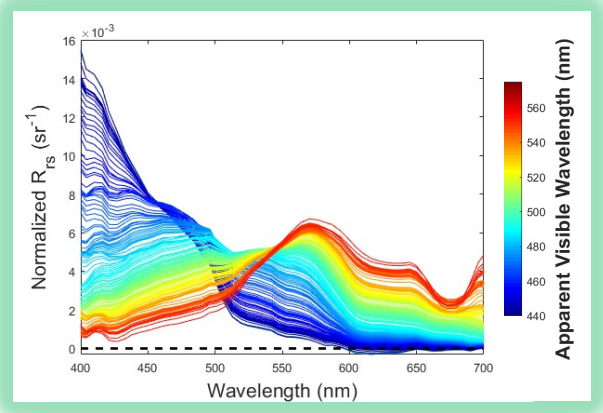


QWIP – Quality Water Index Polynomial



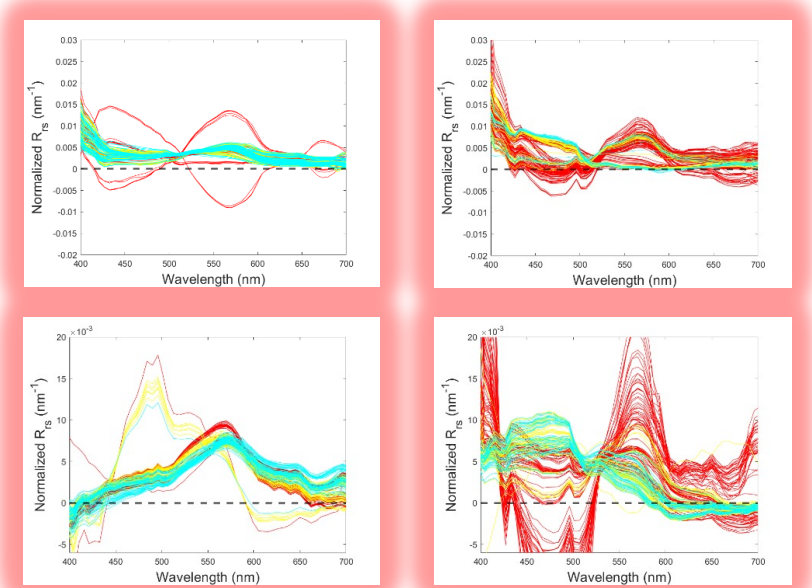
Accept

-0.2 < QWIP < 0.2



-0.2 > QWIP > 0.2

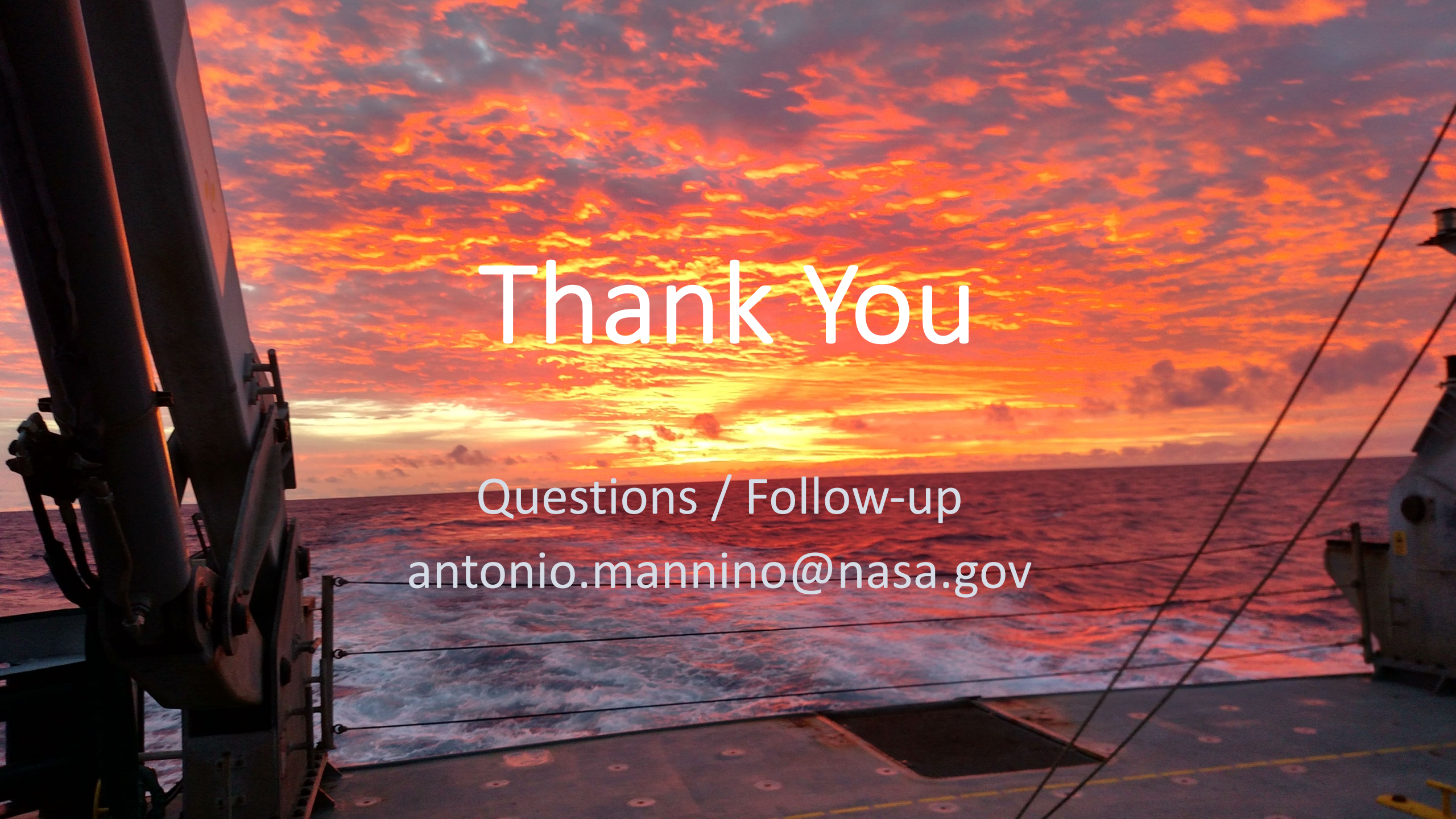
Reject



*Based on the Apparent Visible Wavelength, the QWIP score provides an automated, quick and efficient means of assessing the relative quality of hyperspectral **satellite** and **in situ** data.*

Deviation score 0.2 – 0.25 | 0.25 – 0.35 | > 0.35

Dierssen, Vandermeulen, et al., 2022


Thank You
Questions / Follow-up
antonio.mannino@nasa.gov