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Field Support Group Update

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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

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

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

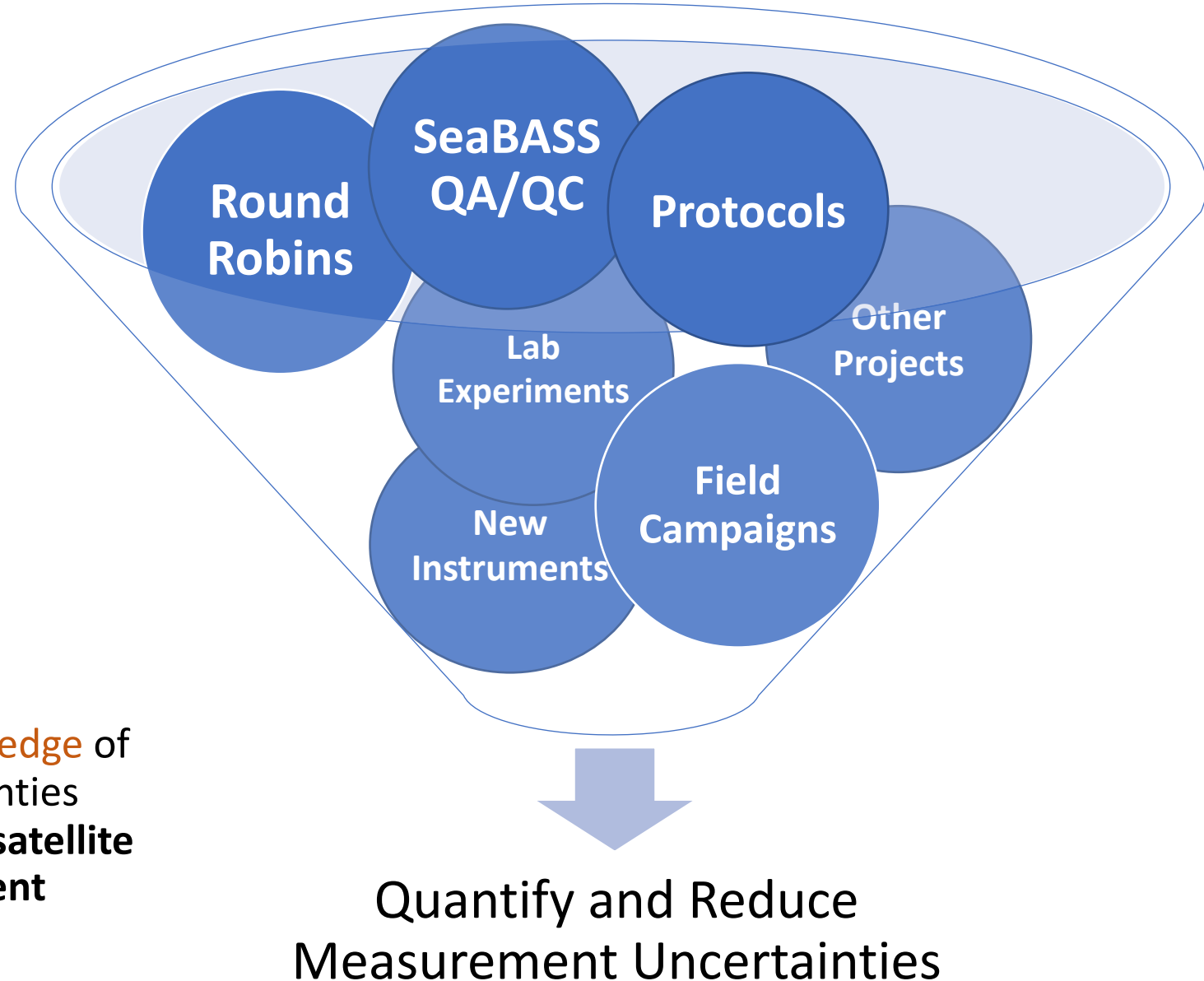
Field & Lab activities in support of NASA

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

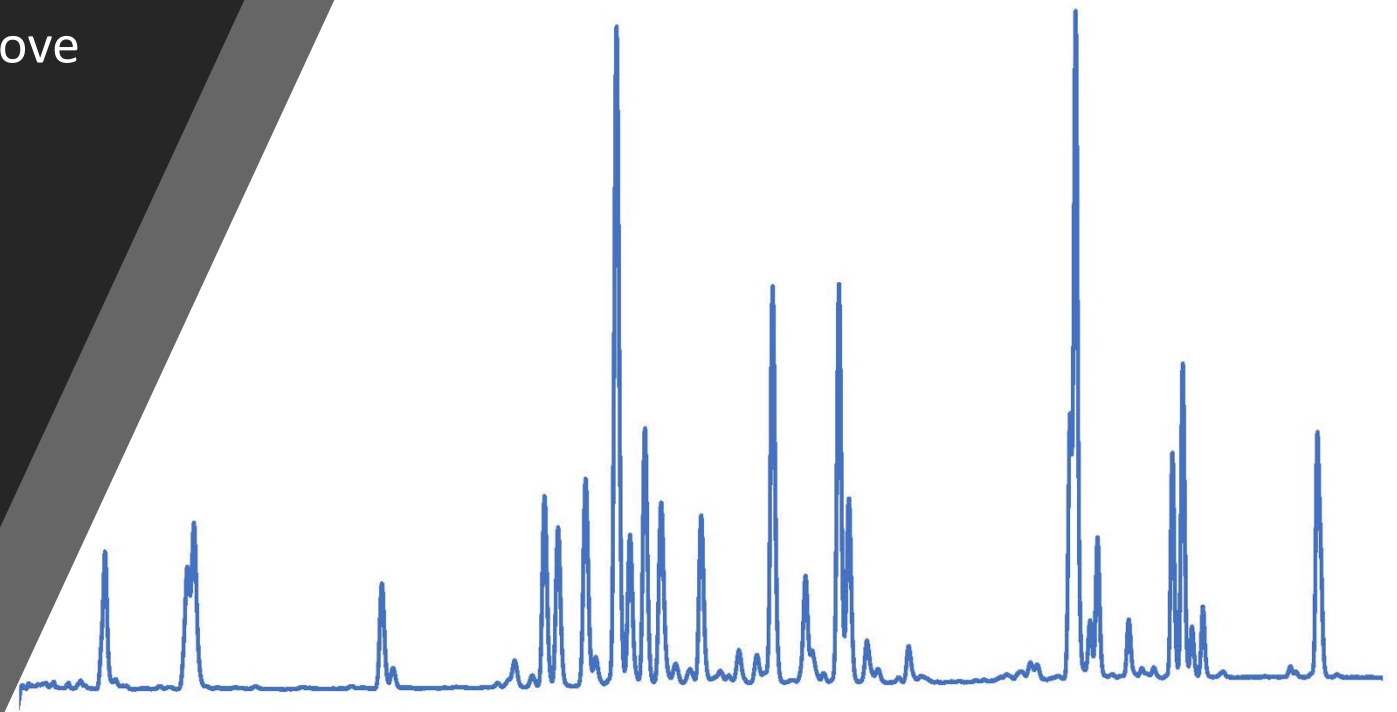
- Reported ~2700 HPLC pigment samples
- On-going efforts to maintain and improve data quality and analytical efficiency
- Methods development for phycobilin pigments

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

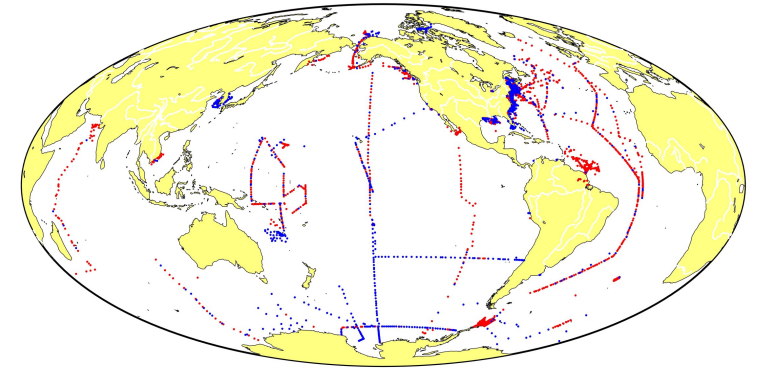
Crystal S. Thomas^{*a,b}, Joaquín E. Chaves^{a,b}, and Antonio Mannino^b

^aScience Systems & Applications, Inc. 10210 Greenbelt Road, Lanham, MD 20706

^bNASA, Goddard Space Flight Center, Greenbelt, MD 20771

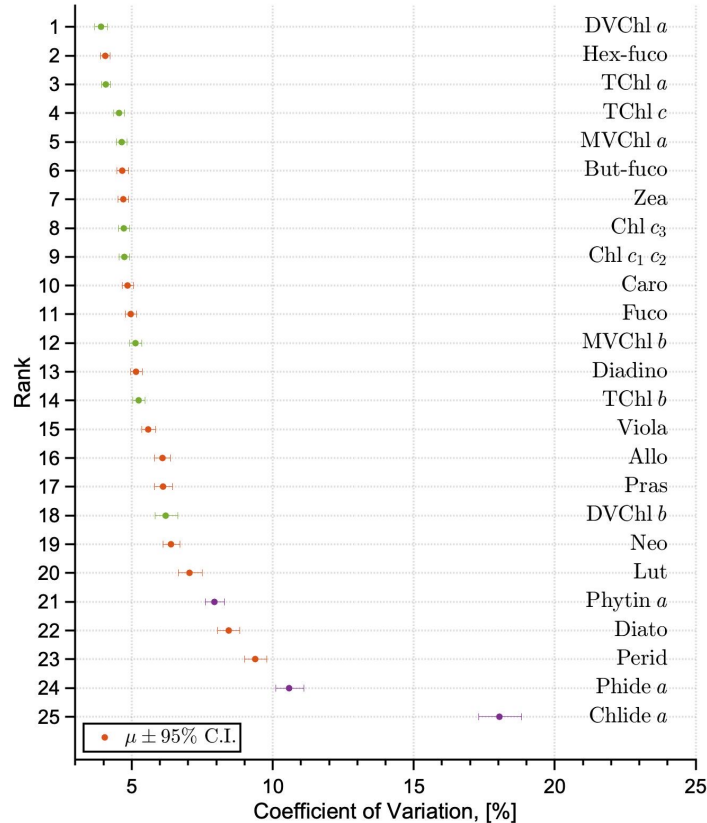
Draft version: May 2, 2022

N datasets=114; n = 12594; n replicates=4873



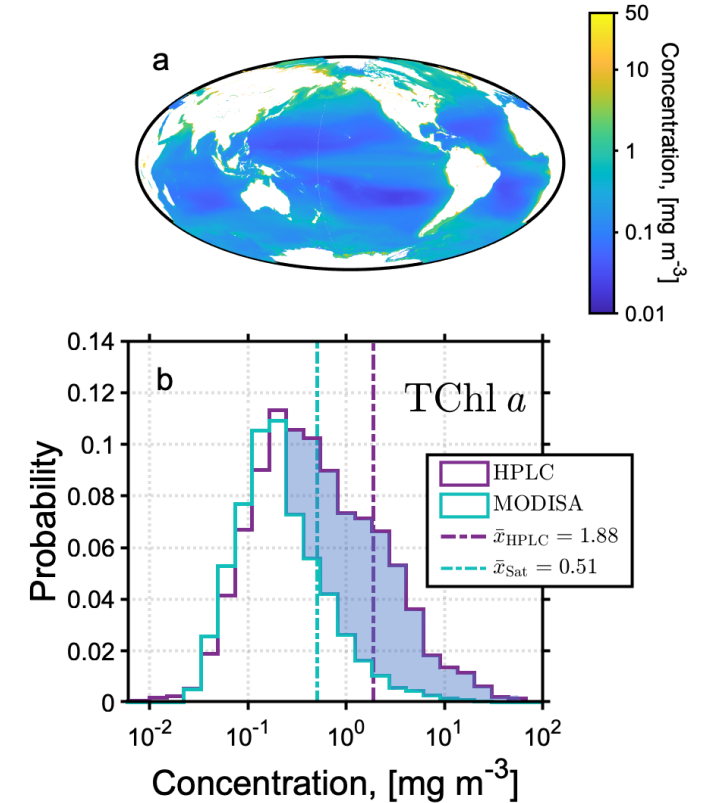
● Observations with replicates ● Observations without replicates

Pigments ranked by analytical precision



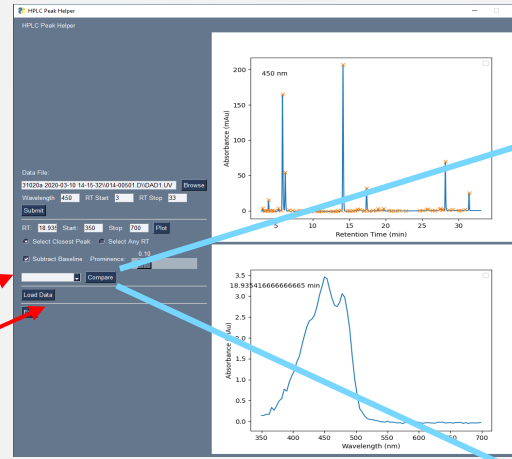
- Manuscript in preparation that gleans information from thousands of replicate filter sets from all major ocean basins
- Investigates the impacts of filtration volume, water basin, pigment concentration, etc. on replicate filter precision
- **Main conclusions**
 - Concentration is not a major driver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

Satellite v. HPLC Chl *a* concentration

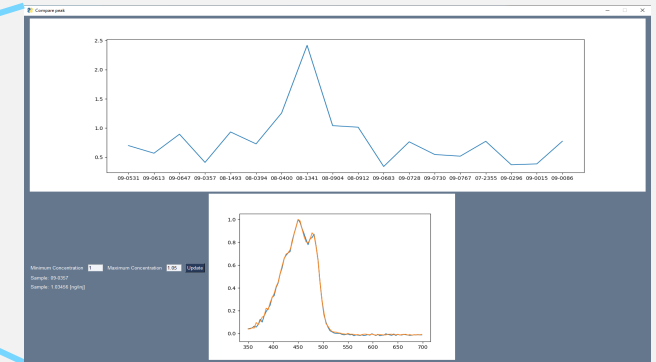


Pigment ID through Machine Learning

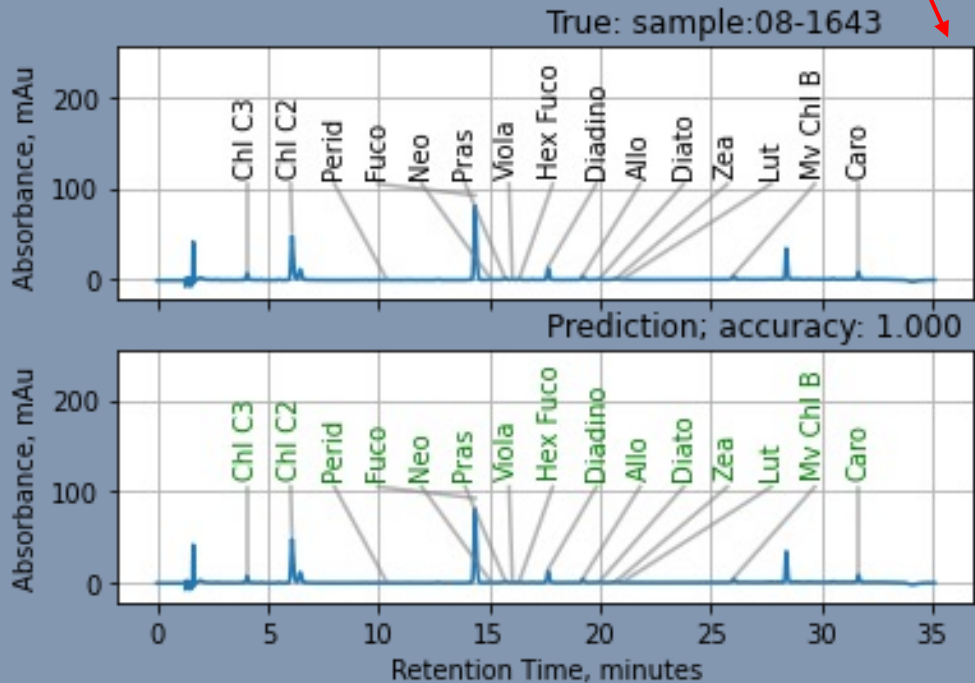
- A Graphical User Interface was developed this summer for an HPLC analyst to use for peak validation.
- We used existing expert-labeled phytoplankton pigment chromatogram peaks to train a convolutional neural network (CNN).
- Harnesses the entire body of HPLC analysis conducted at GSFC to aid decision-making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



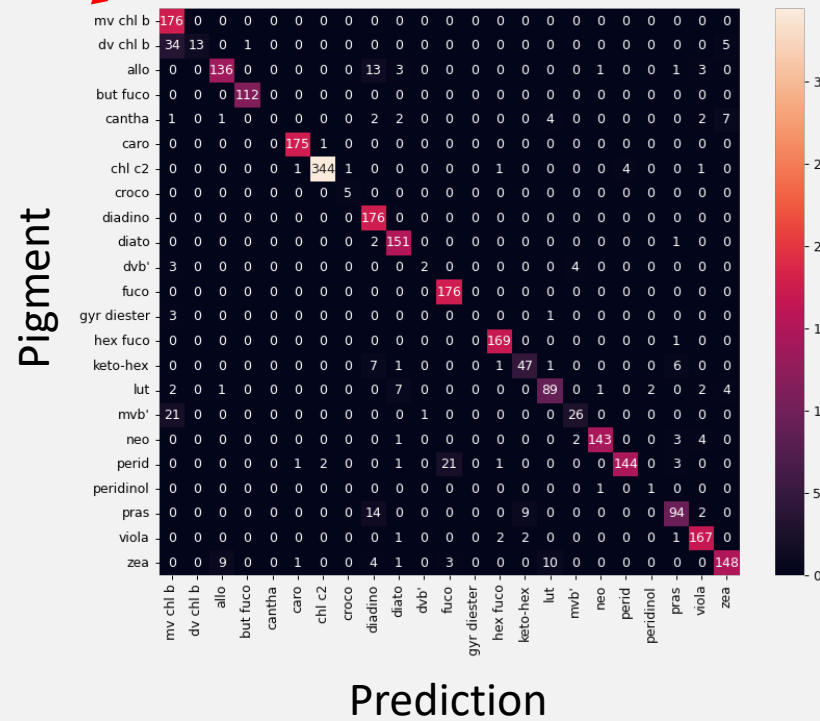
HPLC analyst GUI tool



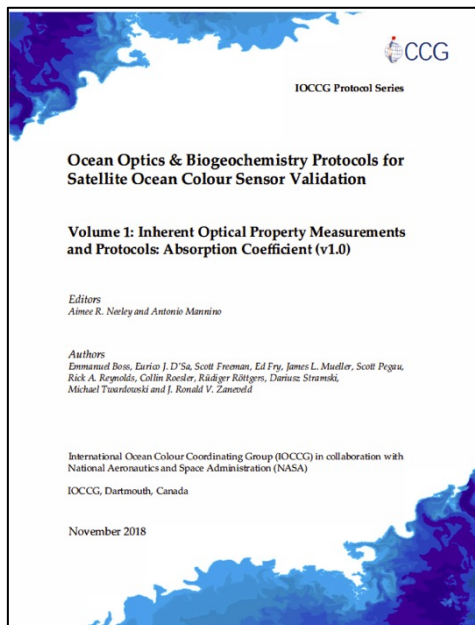
Validation set peak ID predictions



Validation sample Prediction

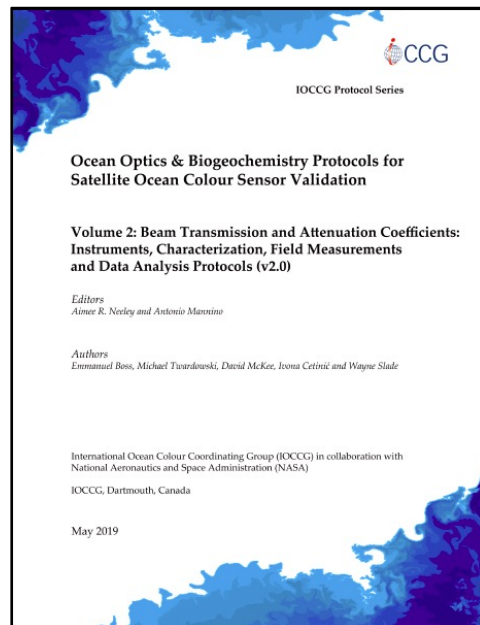


“Confusion Matrix” showing ML model predictions on validation set



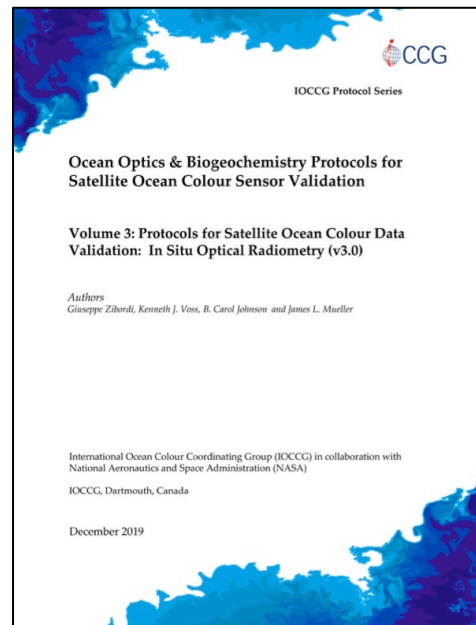
Vol. 1.0
Absorption
(particles)

Nov. 2018



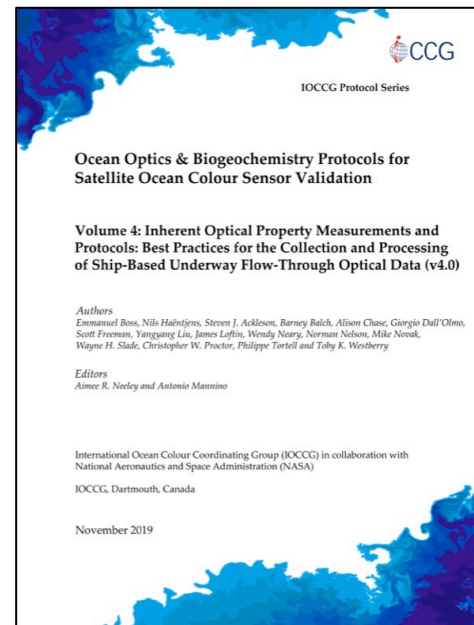
Vol. 2.0
Beam
Attenuation

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

Status of Protocols – Primary Productivity



CCG
IOCCG Protocol Series

Ocean Optics & Biogeochemistry Protocols for Satellite Ocean Colour Sensor Validation

Volume 7: Aquatic Primary Productivity Field Protocols for Satellite Validation and Model Synthesis

Authors:
Balch, W.M., Carranza, M., Cetinic, I., Chaves, J.E., Duhamel, S., Fassbender, A., Fernandez-Carrera, A., Ferrón, S., García-Martín, E., Goes, J., Gomes, H., Gundersen, K., Halsey, K., Hirawake, T., Isada, T., Juranek, L., Kulk, G., Langdon, C., Letelier, R., López-Sandoval, D., Mannino, A., Marra, J., Neale, P., Nicholson, D., Silsbe, G., Stanley, R.H., Vandermeulen, R.A.

Editors:
Ryan A. Vandermeulen and Joaquín E. Chaves

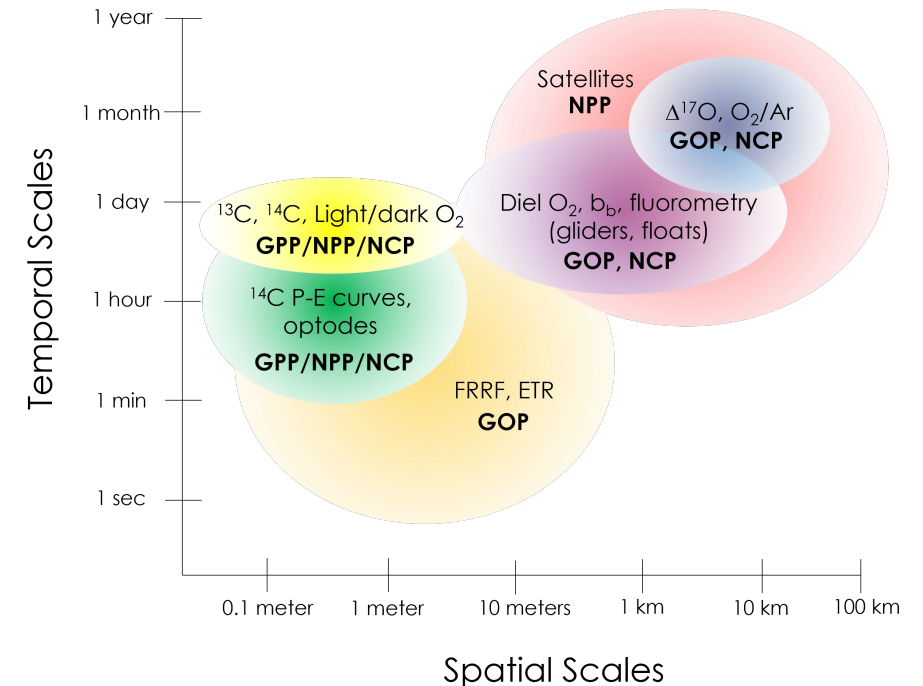
International Ocean Colour Coordinating Group (IOCCG) in collaboration with National Aeronautics and Space Administration (NASA)

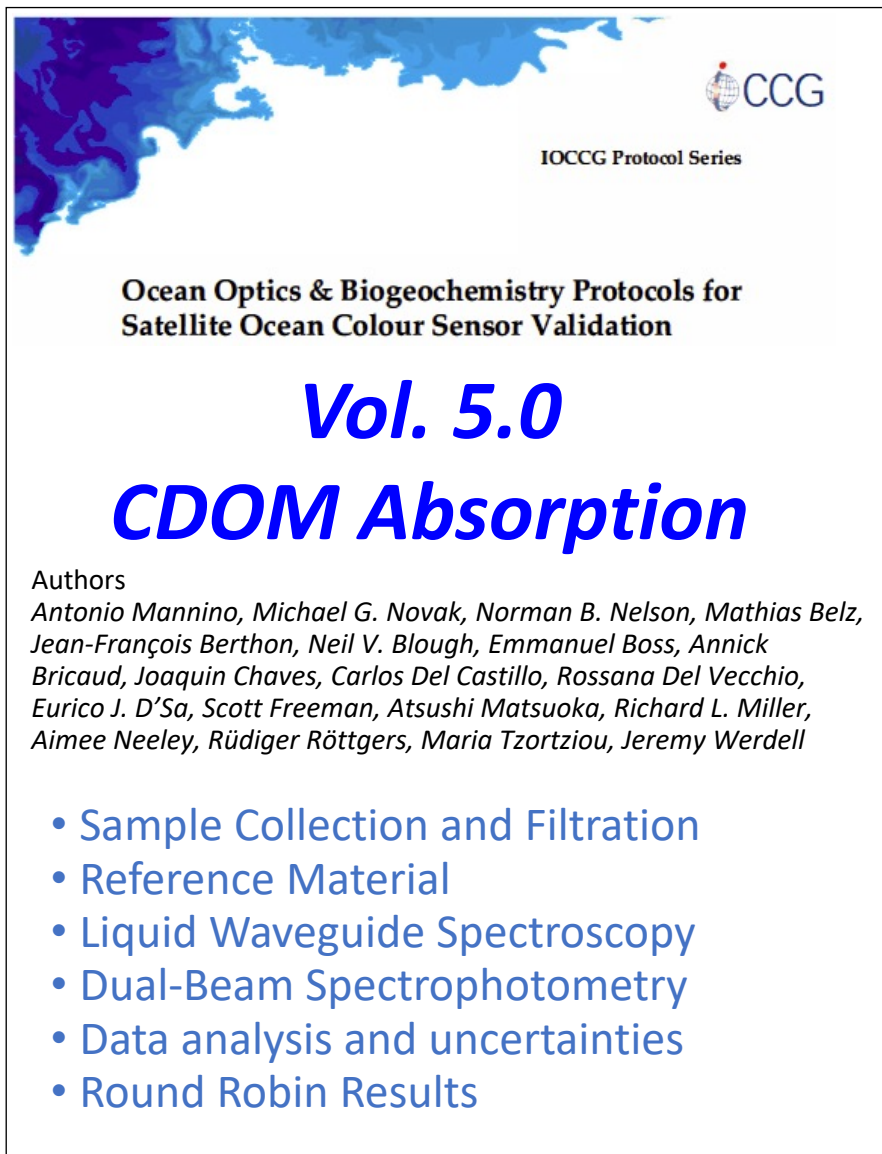
IOCCG, Dartmouth, Canada
September 2022

<http://dx.doi.org/10.25607/OBP-1835>

The image shows the front cover of a book. At the top left is a satellite image of a coastline. The title and volume information are centered. The authors and editors' names are listed below. At the bottom, there is a URL and the publisher information.

- 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)





IOCCG Protocol Series

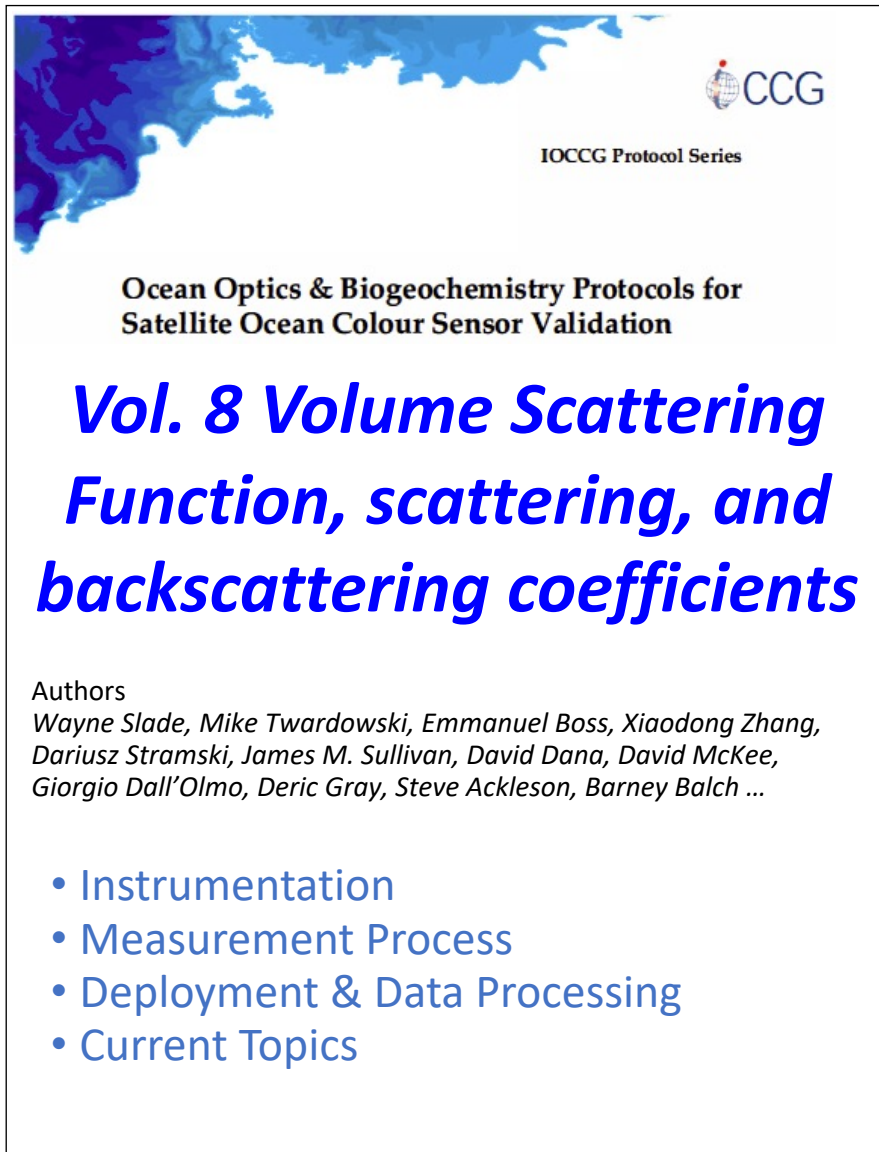
Ocean Optics & Biogeochemistry Protocols for
Satellite Ocean Colour Sensor Validation

Vol. 5.0
CDOM Absorption

Authors
*Antonio Mannino, Michael G. Novak, Norman B. Nelson, Mathias Belz,
Jean-François Berthon, Neil V. Blough, Emmanuel Boss, Annick
Bricaud, Joaquin Chaves, Carlos Del Castillo, Rossana Del Vecchio,
Eurico J. D'Sa, Scott Freeman, Atsushi Matsuoka, Richard L. Miller,
Aimee Neeley, Rüdiger Röttgers, Maria Tzortziou, Jeremy Werdell*

- Sample Collection and Filtration
- Reference Material
- Liquid Waveguide Spectroscopy
- Dual-Beam Spectrophotometry
- Data analysis and uncertainties
- Round Robin Results

- 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



CCG
IOCCG Protocol Series

Ocean Optics & Biogeochemistry Protocols for
Satellite Ocean Colour Sensor Validation

***Vol. 8 Volume Scattering
Function, scattering, and
backscattering coefficients***

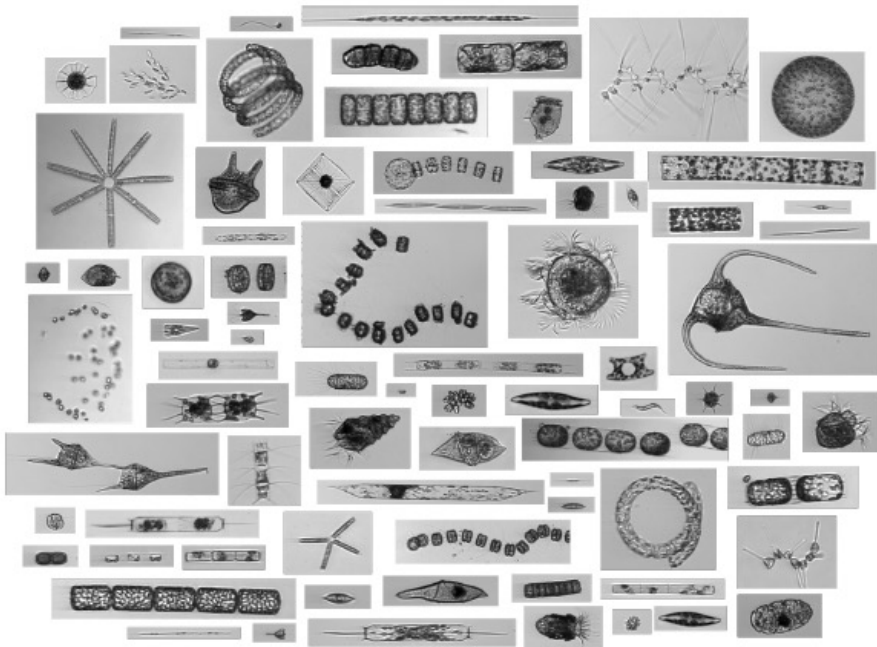
Authors
*Wayne Slade, Mike Twardowski, Emmanuel Boss, Xiaodong Zhang,
Dariusz Stramski, James M. Sullivan, David Dana, David McKee,
Giorgio Dall’Olmo, Deric Gray, Steve Ackleson, Barney Balch ...*

- Instrumentation
- Measurement Process
- Deployment & Data Processing
- Current Topics

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

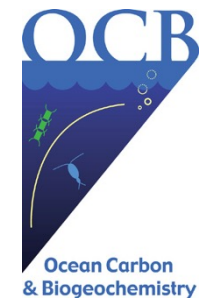
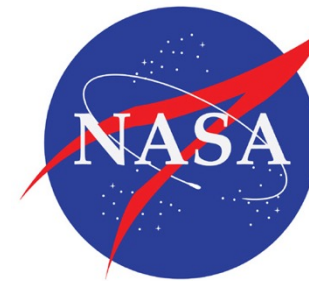
Reporting Data from Particle Images

Standards and practices for reporting plankton and other particle observations from images Technical Manual



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>



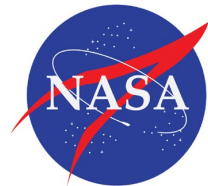
Reporting Data from Flow Cytometry

Standards and practices for reporting flow cytometry data

Technical Manual

Authors: Aimee Neeley, Inia Soto Ramos, Chris Proctor, Jason Graff, Michael Lomas, and Nicole Poulton

- Standardized data table
- Flexible reporting of both taxonomic and morphological information
- Implements Darwin Core and SeaDataCloud vocabulary
- Discussion of supporting documentation is included



- 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

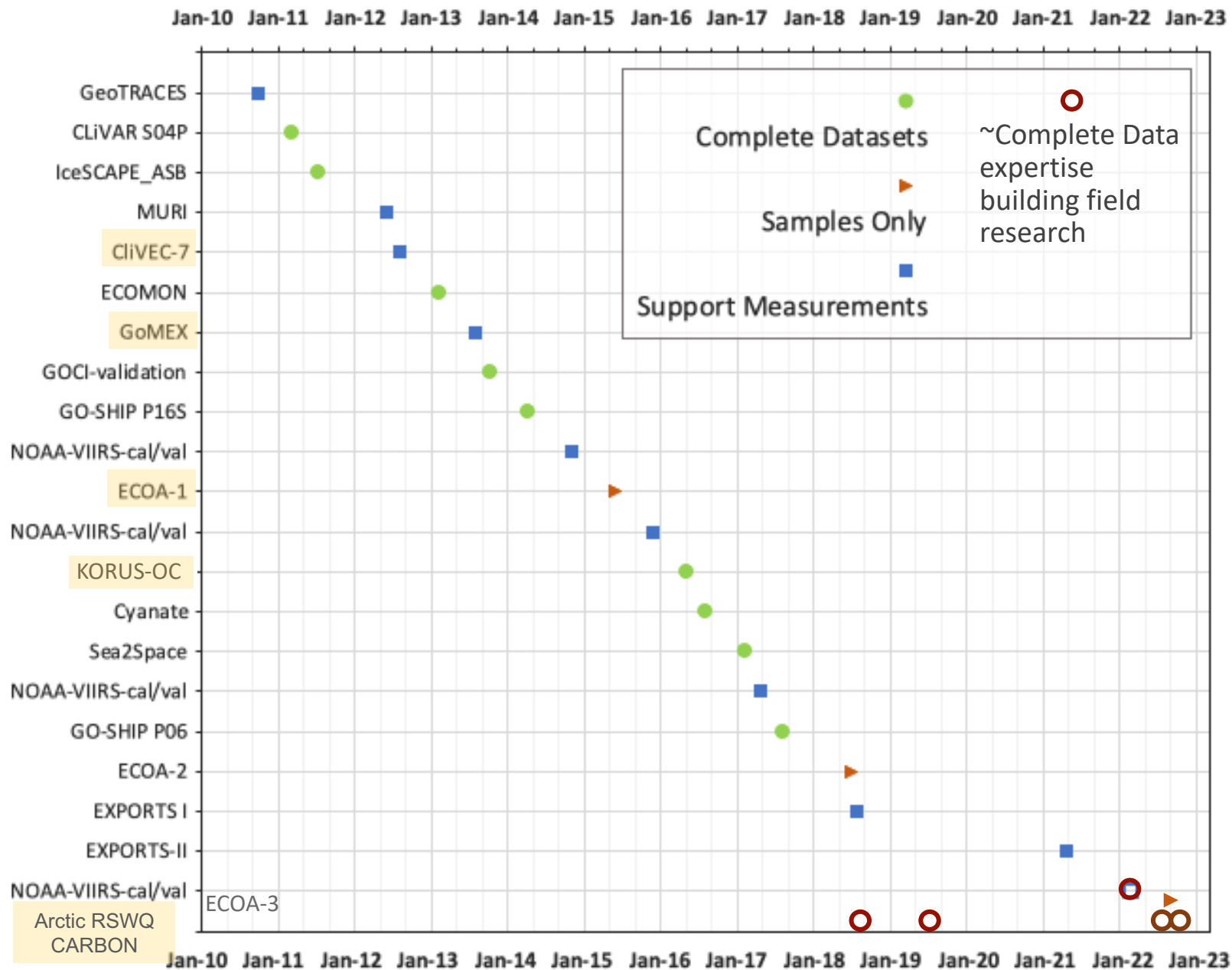
- Hyper-bb (b_{bp})
- SC-6 (b_{bp})
- PSICAM & QFT-ICAM (a)
- SBA (R_{rs})
- Sorting flow cytometry
- ML particle ID

SBIR Pipeline

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

- 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

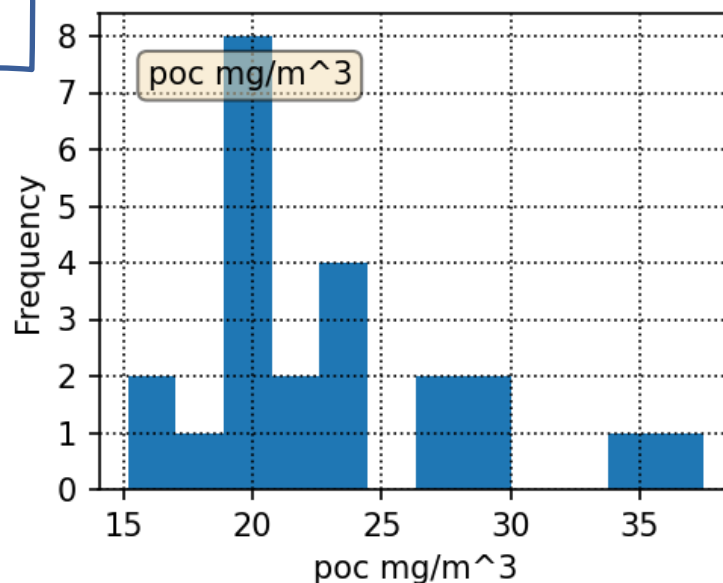
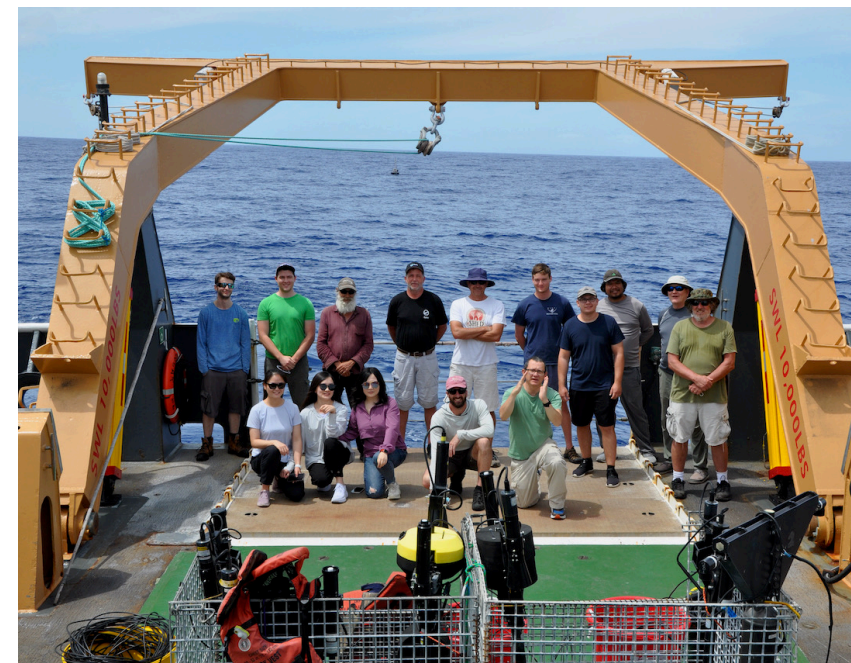
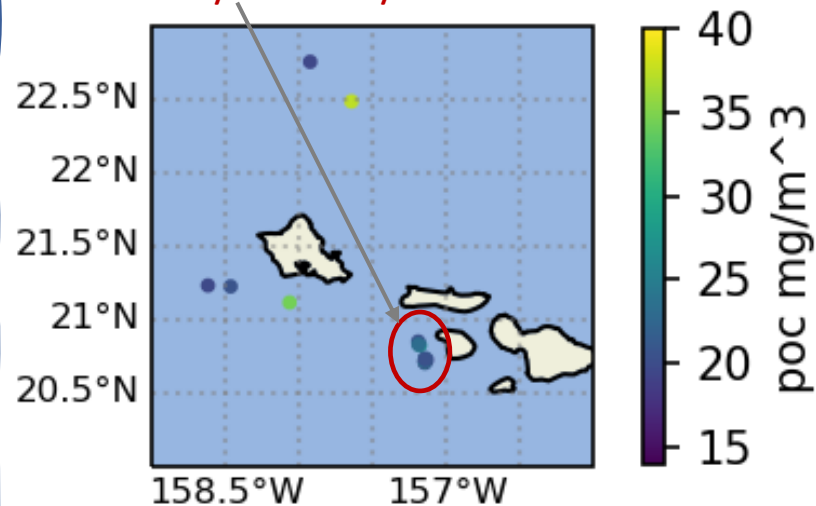
March 8-19, 2022. Hawai'i.

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

MOBY/Refresh/MarONet



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:

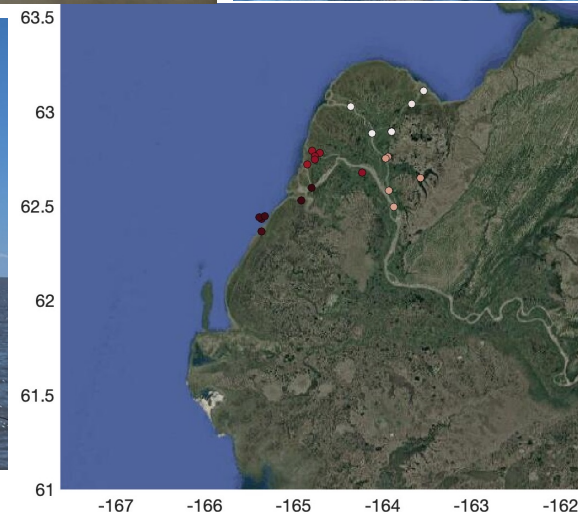
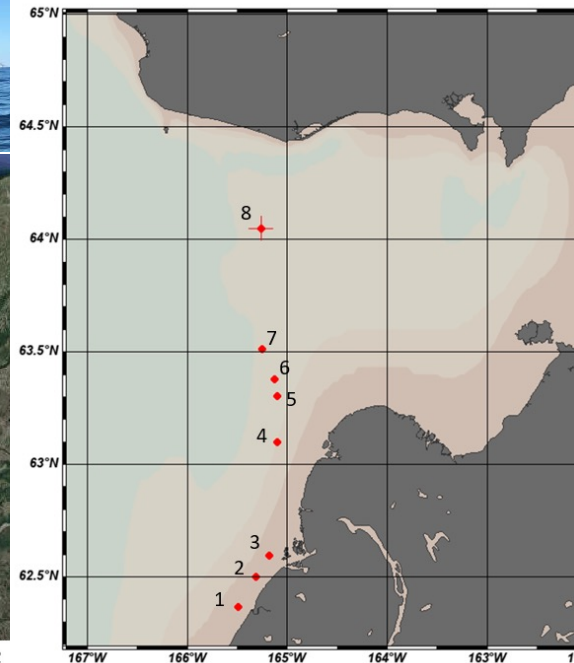
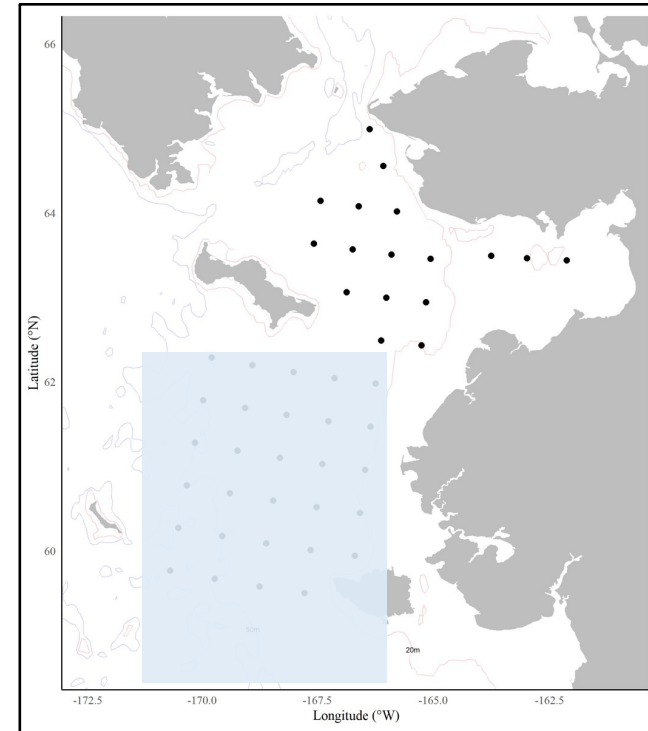
Tzortziou, Clark, Hernes, Mannino & Spencer

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

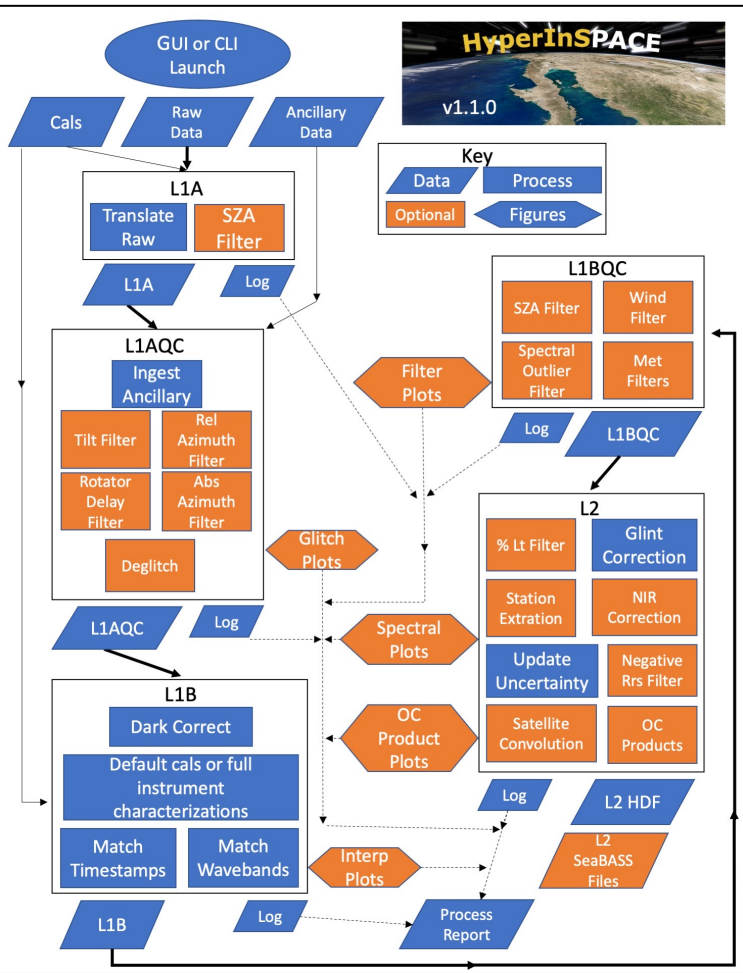
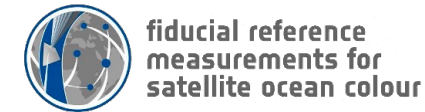


Automated, underway, above-water radiometry submitted to SeaBASS

- ✓ KORUS-OC (2016)
- ✓ EXPORTS-NP (2018)
- ✓ Archimedes/Superyacht (2018, collaboration with R. Brewin, )
- ✓ 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

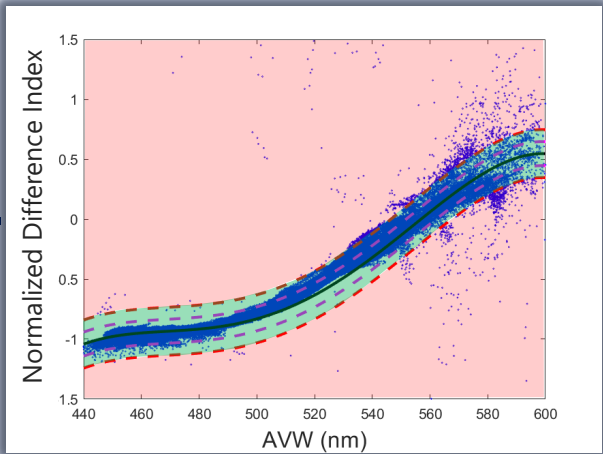
<https://github.com/nasa/HyperInSPACE>

New OC product

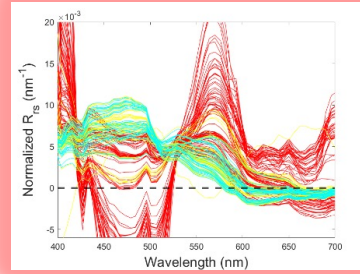
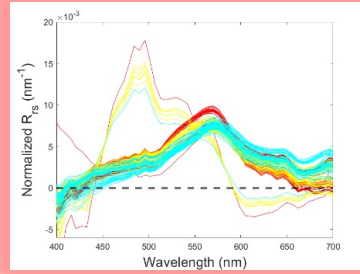
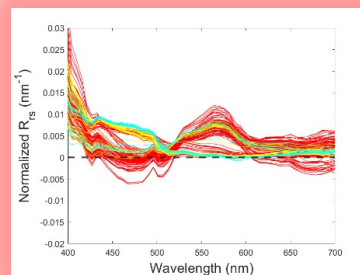
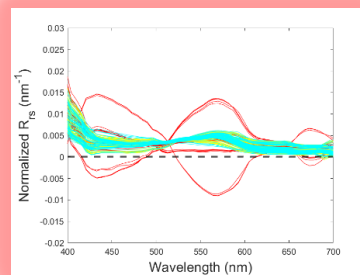
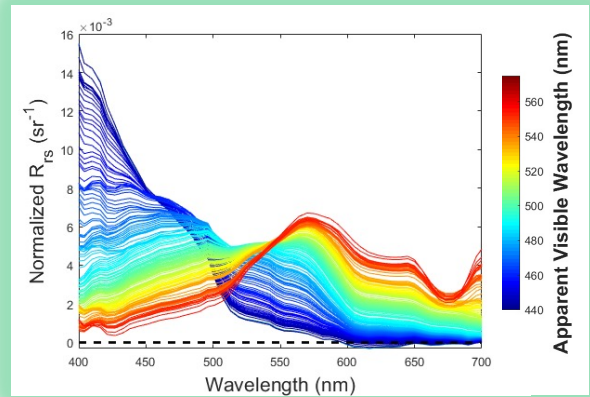
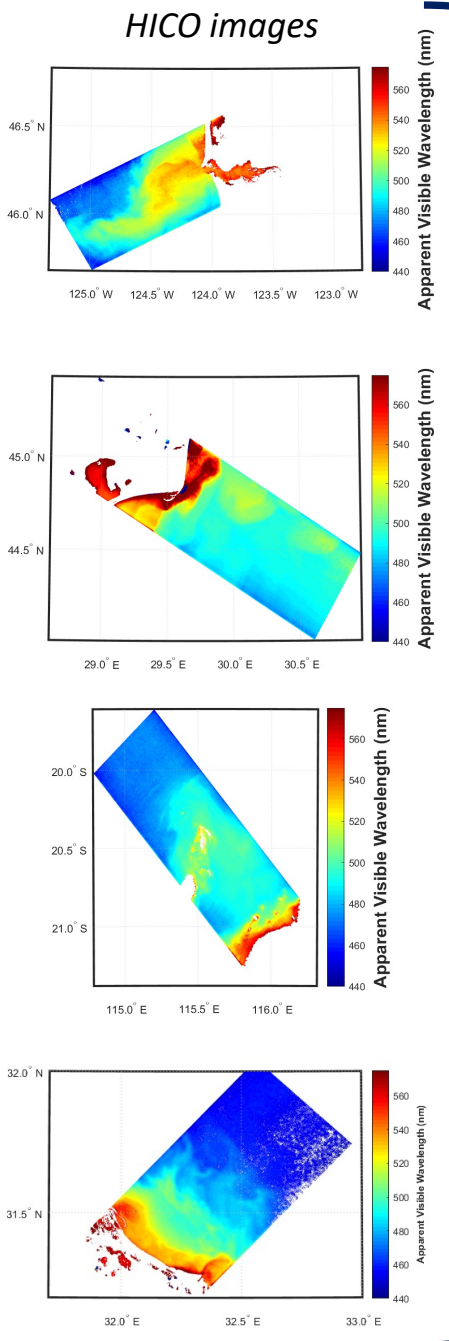
QWIP – Quality
Water Index
Polynomial

Accept
 $-0.2 < QWIP < 0.2$

Reject
 $-0.2 > QWIP > 0.2$



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.





Thank You

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