Sentinel-3 OLCI L2 report for baseline collection OL_L2M_003

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Table of Contents

Table of Figures

Table of Tables

1 EXECUTIVE SUMMARY – OLCI BASELINE COLLECTION OC_L2M.003

Major updates have been introduced to Sentinel-3 OLCI Level-2 Ocean Colour processing. These updates constitute OLCI Collection-3 products (OL_L2M.003) and are based on L2 processor IPF-OL-2 version 07. IPF-OL-2 v.07 was installed in EUMETSAT operational processing on 16 February 2021 and is used for the full mission reprocessing of OLCI-A and OLCI-B L2 products in the first half of 2021.

The goal of Collection-3 is to achieve accuracy and consistency across OLCI-A and -B Ocean Colour products and to introduce several algorithm improvements. Among the main updates

- System Vicarious Calibration gains are updated in OLCI-A and OLCI-B,
- revised Bright Pixel Correction (BPC) and new Chlorophyll Index algorithm are introduced in the open water processing chain,
- new Neural Network v.2 is introduced in the complex water processing chain,
- new and updated flags are available, together with a new flag recommendation for users.

The updates implemented in Collection OL_L2M.003 follow EUMETSAT's Marine Roadmap and recommendations from the Sentinel-3 OLCI/SYN Quality Working Group and Sentinel-3 Validation Team, Ocean Colour.

Collection OL_L2M.003 demonstrates

- high consistency between OLCI-A and OLCI-B Ocean Colour products
- oligotrophic algal pigment concentration within mission requirements
- improved coastal retrievals
- reduced «salt and pepper» noise

New Ocean Colour System Vicarious Calibration gains ensure traceable and harmonised SVC strategy for OLCI-A and -B. OC-SVC produces an excellent agreement between the two missions, which opens new capabilities to use both OLCIs together and merging their data.

New OC-SVC gains have a significant impact on OLCI-A blue bands, where a more accurate spectral shape is now retrieved, and on OLCI-B, where they provide notable reduction of biases in radiometry.

The updated Bright Pixel Correction eliminates frequent failures of the previous BPC. It reduces salt-and-pepper noise in products and improves coverage of coastal retrievals.

The new Chlorophyll Index algorithm introduced for application in low-chlorophyll oligotrophic waters reduces biases in open ocean chlorophyll retrievals. Algal pigment concentration product for open water now meets Sentinel-3 Mission Requirements.

Cloud flagging improvements eliminate many cloud omissions and the need to apply other flags to compensate for cloud flagging failure. The list of user recommended flags is updated.

NNv2 provides an important improvement in the three bio-optical products, particularly in TSM_NN and CHL_NN following S3VT-OC validations.

OLCI Collection OL_L2M.003 has achieved much progress, but there is room for improvement. Sentinel-3 Mission Requirements are partially met for water reflectance products, significant uncertainties are still present in more complex waters, and there is residual noise in products. To address these issues, the following evolutions of OLCI Level-2 Ocean Colour processing will focus on the standard/baseline atmospheric correction and other detailed algorithm improvements.

Members of CMEMS OC-TAC, S3VT-OC and OLCI/SYN QWG as well as NOAA/MOBY, AERONET-OC, NASA/OC, AMT, BC and Cefas teams who provided data to make this OLCI L2 release and its validation possible are gratefully acknowledged.

2 INTRODUCTION

This document describes Sentinel-3 OLCI Level-2 processor updates and product validation for the baseline collection OL_L2M.003.

Baseline collection OL_L2M.003 is produced using OLCI L2 processor IPF-OL-2 version 07 applied on Level-1B products. IPF-OL-2 version 07 was installed in EUMETSAT operational processing on 16 February 2021 and was used for the full mission reprocessing of OLCI-A and OLCI-B L2 products in the first half of 2021.

The updates implemented in Collection OL_L2M.003 follow EUMETSAT's Marine Roadmap and numerous recommendations from the Sentinel-3 OLCI/SYN Quality Working Group and Sentinel-3 Validation Team, Ocean Colour.

Details of Collection OL_L2M.003 subversions and corresponding IPF-OL-2 deployment timeline are described in Appendix A.

OLCI is an imaging spectrometer on board of Sentinel-3 satellites belonging to the European Union's Earth Observation data and information services of the Copernicus Programme (https://www.copernicus.eu/en). The first of the Sentinel-3 satellites, S3A, was launched in February 2016 and the second, S3B, in April 2018. Current OLCI product time series span the period from 26 April 2016 for OLCI-A, and from 15 May 2018 for OLCI-B.

2.1 Scope

The goal of this document is to provide to all users of OLCI Level-2 Marine products the status of the updated Ocean Colour baseline collection OL_L2M.003.

This document provides the required detail in complement to the 'Sentinel-3 Product Notice – OLCI Level-2' for OL_L2M.003 (RD-1) and to other information available on EUMETSAT Ocean Colour Services web pages (https://www.eumetsat.int/ocean-colour-services, RD-2), in particular 'Sentinel-3 OLCI Marine User Handbook' (RD-3).

Collection OL_L2M.003 only relates to OLCI Level-2 Marine processing, i.e. Ocean Colour processing. Collection OL_L2M.003 is implemented using the existing OLCI Level-1B products from Baseline 002.

The validations presented here are mostly based on EUMETSAT's own analyses. EUMETSAT has been cooperating closely with many international groups from the OC-TAC CMEMS, Sentinel-3 Validation Team (RD-4), and the OLCI/SYN Quality Working Group. Selected results from a few teams are presented here and further references are included.

2.2 Applicable Documents

	Document Title	Reference
AD-1	Sentinel-3: Mission Requirements Document, M.R Drinkwater and H. Rebhan (MRD)	EOP-SMO/1151/MD-md, Feb 2007, *http://esamultimedia.esa.int/docs/GMES/GMES_Sentinel3_MRD_V2.0_update.pdf*
AD-2	Sentinel-3 Mission Requirements Traceability Document, C. Donlon	EOP-SM/2184/CD-cd, Feb 2011, *http://download.esa.int/docs/EarthObservation/GMES_Sentinel-3_MRTD_Iss-1_Rev-0-issued-signed.pdf*
AD-3	Sentinel-3 Calibration and Validation Plan	*S3-PL-ESA-SY-0265, Issue 2.0, 2014, website.*

2.3 Reference Documents

	Document Title	**Reference**
RD-1	Sentinel-3 Product Notice – OLCI Level-2' for OC_L2M.003	*https://www.eumetsat.int/media/47783*
RD-2	EUMETSAT Ocean Colour Services	*https://www.eumetsat.int/ocean-colour-services*
RD-3	Sentinel-3 OLCI Marine User Handbook	*EUM/OPS-SEN3/MAN/17/907205 at https://www.eumetsat.int/ocean-colour-services*
RD-4	Sentinel-3 Scientific Validation Team Implementation Plan	*https://earth.esa.int/eogateway/news/announcement-of-opportunity-for-sentinel-3-validation-team*
RD-5	OLCI Processing Baselines	*https://www.eumetsat.int/olci-processing-baselines*
RD-6	Mission Requirements for Future Ocean-Colour Sensors. McClain, C.R. and Meister, G. (eds.), Reports of the International Ocean-Colour Coordinating Group, No. 13, IOCCG, Dartmouth, Canada.	*IOCCG, Report 13, 2012, https://ioccg.org/wp-content/uploads/2015/10/ioccg-report-13.pdf*
RD-7	Sensor-independent approach to the vicarious calibration of satellite ocean colour radiometry. B.A. Franz, S.W. Bailey, P.J. Werdell, and C.R. McClain.	*Applied Optics, 46: 5068–5082, 2007*
RD-8	MOBY. Provides vicarious calibration of ocean colour satellites.	*https://www.mlml.calstate.edu/moby/; https://coastwatch.noaa.gov/cw/field-observations/MOBY.1.html*
RD-9	Ocean Colour System Vicarious Calibration tool. EUMETSAT study: SOLVO and Brockmann Consult.	*EUM/CO/19/4600002359/EJK, https://www.eumetsat.int/ocean-colour-system-vicarious-calibration-tool*
RD-10	Ocean Colour System Vicarious Calibration tool. C. Mazeran and A. Ruescas.	*https://www.eumetsat.int/media/47502*
RD-11	S3 Product Notice – OLCI L1	*S3.PN-OLCI-L1.07; EUM/OPS-SEN3/DOC/19/1128998; 2020, https://www.eumetsat.int/media/44035*
RD-12	S3 OLCI Tandem Phase results	*https://s3tandem.eu/*
RD-13	Validation of the SLSTR & OLCI Sentinel-3 calibration/radiometry using natural targets, C. Desjardins, X. Lenot, L. Landier, S. Marcq, A. Meygret, C. Miquel, N. Guilleminot, I. Soleihlhavoup	*CNES, S3VT#6 meeting website available to the S3VT team https://s3vt2020.vcd-eventsforce.com/*
RD-14	Case II.S Bright Pixel Atmospheric Correction. J. Aiken, G. Moore, S. Lavender, C. Mazeran, J.-P. Huot	*MERIS ATBD 2.6, 2017, https://www.eumetsat.int/media/41514*
RD-15	Ocean Colour Bright Pixel Correction. EUMETSAT/Copernicus study: SOLVO, HYGEOS, Helmholtz-Zentrum Geesthacht	*EUM/C0/18/4600002103/EJK, https://www.eumetsat.int/OC-BPC*
RD-16	Ocean Colour Bright Pixel Correction. C. Mazeran, F. Steinmetz, and M. Hieronymi	*https://www.eumetsat.int/OC-BPC*

RD-17	Examining the consistency of products derived from various ocean color sensors in open ocean (Case 1) waters in the perspective of a multi-sensor approach. A. Morel, Y. Huot, B. Gentili, P.J. Werdell, S.B. Hooker, and B.A. Franz	*Remote Sensing of Environment, 111, 69-88, 2007.*
RD-18	Ocean Colour Products in Case 1 waters, OLCI Level-2 Algorithm Theoretical Basis. D. Antoine	*S3-L2-SD-03-C10-LOV-ATBD, 2010, https://www.eumetsat.int/media/38635*
RD-19	Sentinel-3 OLCI Chlorophyll Index switch for low-chlorophyll waters. I. Cazzaniga and E. Kwiatkowska	*OLCI L2 ATBD, EUM/RSP/DOC/18/1028360, 2020, https://www.eumetsat.int/media/47752*
RD-20	Chlorophyll algorithms for oligotrophic oceans: A novel approach based on three-band reflectance difference. C. Hu, Z. Lee, and B.A. Franz	*J. Geophys. Res., 117, C01011, doi: 10.1029/2011JC007395, 2012.*
RD-21	VIIRS-derived chlorophyll-a using the ocean color index method. M. Wang and S. Son	*Remote Sensing of Environment 182: 141–149, 2016.*
RD-22	SeaBASS, Bio-optical Archive and Storage System, NASA Ocean Biology Processing Group	*https://seabass.gsfc.nasa.gov/*
RD-23	Effective reflectance of oceanic whitecaps. P. Koepke.	*Appl. Opt., 23, 1816– 1824, 1984.*
RD-24	Spectral reflectance of sea foam in the visible and near infrared: In situ measurements and remote sensing implications. R. Frouin, M. Schwindling, and P. Y. Deschamps.	*J. Geophys. Res., 101, 14,361–14,371, 1996.*
RD-25	Observations of oceanic whitecaps in the north polar waters of the Atlantic. M. Stramska and T. Petelski.	*J. Geophys. Res., 108C3, 3086. doi: 10.1029/2002JC001321, 2003.*
RD-26	OLCI Level 2 White Caps Correction. OLCI Level-2 Algorithm Theoretical Basis Document. S. Lavender.	*S3-L2-SD-03-C06-ARG-ATBD, 2010, https://www.eumetsat.int/media/38640*
RD-27	Ocean Colour Turbid Water. OLCI Level 2 Algorithm Theoretical Basis Document. Roland Doerffer	*S3-L2-SD-03-C11-GKSS-ATBD, 2010, https://www.eumetsat.int/media/38636*
RD-28	Uncertainty estimation of case2 water IOP products of OLCI using artificial neural networks. Roland Doerffer	*2019, https://www.eumetsat.int/media/43613*
RD-29	SNAP Sentinel Toolbox. Brockmann Consult, SkyWatch and C-S	*https://step.esa.int/main/download/snap-download/*
RD-30	Cloud Masking for Ocean Color Data Processing in the Coastal Regions. M. Wang and W. Shi	*IEEE Trans. Geosc. Remote Sens., VOL. 44, NO. 11, 2006*
RD-31	CMEMS, Ocean Colour Thematic Centre	*https://marine.copernicus.eu/about/producers/oc-tac*
RD-32	Sentinel-3 Validation Team Call	*S3VT announcement and documentation website*
RD-33	Sentinel-3 Validation Team annual meeting #6, presentations	*meeting website available to the S3VT team https://s3vt2020.vcd-eventsforce.com/*

RD-34	Copernicus Ocean Colour Fiducial Reference In Situ Database (OC-DB)	*https://ocdb.eumetsat.int*
RD-35	Sentinel-3 OLCI Spectral Response Function Data	*https://sentinel.esa.int/web/sentinel/technical-guides/sentinel-3-olci/olci-instrument/spectral-response-function-data*
RD-36	Aerosol Robotic Network (AERONET) – Ocean Color	*https://aeronet.gsfc.nasa.gov/new_web/ocean_color.html*
RD-37	Advances in the Ocean Color component of the Aerosol Robotic Network (AERONET-OC). G. Zibordi, B.N. Holben, M. Talone, D. D'Alimonte, I. Slutsker, D.M. Giles and M.G. Sorokin.	*Journal of Atmospheric and Oceanic Technology (in press), https://doi.org/10.1175/JTECH-D-20-0085.1, 2020.*
RD-38	Atlantic Meridional Transect (AMT) programme	*https://www.amt-uk.org/*
RD-39	Ocean Color Web, NASA Ocean Biology Processing Group	*https://oceancolor.gsfc.nasa.gov/*
RD-40	Recommendations for Sentinel-3 OLCI Ocean Colour product validations in comparison with in situ measurements – Matchup Protocols	*EUM/SEN3/DOC/19/1092968, https://www.eumetsat.int/media/44087*
RD-41	Diffuse reflectance of oceanic waters. III. Implication of bidirectionality for the remote-sensing problem. A. Morel and B. Gentili	*Applied Optics Vol. 35, Issue 24, pp. 4850-4862, 1996.*

2.4 Terminology

Acronyms and Abbreviations

Acronym/Abbr.	Explanation
AAC	Alternative Atmospheric Correction
ACS	WET Labs ACS hyperspectral spectrophotometer
AMT	Atlantic Meridional Transect
BAC	Baseline Atmospheric Correction
BC	Brockmann Consult, GmbH, in Germany
BPC	Bright Pixel Correction
cal/val	calibration and validation
CDOM	Coloured Dissolved Organic Matter
Cefas	Centre for Environment, Fisheries and Aquaculture Science in the UK
CI	Chlorophyll Index
CMEMS	Copernicus Marine Environment Monitoring Service (marine.copernicus.eu)
FR	Full Resolution, i.e. OLCI 300m spatial resolution product
HPLC	High Performance Liquid Chromatography
IOP	Inherent Optical Properties
IPF	Instrument Processing Facility
L1	Level-1
L2, L2M	Level-2, Level-2 Marine
MOBY	Marine Optical Buoy
NASA	National Aeronautics and Space Administration in the USA
NIR	Near infra-red bands or a wavelength range
NN	Neural Network
NOAA	National Oceanic and Atmospheric Administration in the USA
OC	Ocean Colour
OC-TAC	Ocean Colour Thematic Assembly Centre of CMEMS
OLCI and OL	Ocean and Land Colour Instrument
PB	Processing Baseline
PDU	Product Dissemination Unit, i.e. OLCI file directory
PML	Plymouth Marine Laboratory in the UK
RR	Reduced Resolution, i.e. OLCI 1.2km spatial resolution product
QWG	Quality Working Group
S3	Sentinel-3
S3VT	Sentinel-3 Validation Team
SLSTR	Sea and Land Surface Temperature Radiometer
SPG	South Pacific Gyre
SVC	System Vicarious Calibration
SYN	Synergy products (referring to Land products from OLCI and SLSTR synergy)
TSM	Total Suspended Matter
VIS	Visible bands or a wavelength range

Definitions

Definition/Term	Explanation
OL_L2M.003.xx	Baseline Collection 003, the definition of Collection 003 can be found in: - PDU name e.g. S3A_OL_2_WFR____20190702T142513_20190702T142813_20201109T084348_0179_046_267_2700_MAR_F_NT_**003**.SEN3 - inside the xfdumanifest.xml file: <sentinel3:baselineCollection>**003**</sentinel3:baselineCollection> Collection 003 subversions .xxx are described in Appendix A.
IPF-OL-2 version 07.yy	IPF-OL-2 processor version 07.yy, the definition of processor version 07.yy can be found in: - inside the xfdumanifest.xml file: e.g. <sentinel-safe:software name="IPF-OL-2" version="**07.00**"/> - in global attributes in NetCDF data files :source = "IPF-OL-2 **07.00**" IPF-OL-2 processor subversions .yy are described in Appendix A.
Rrs	Remote sensing reflectance [sr-1]

2.5 Document Structure

The follow-on sections of this document include:

- Section 3 describes the algorithm changes introduced in Collection OL_L2M.003,
- Section 4 describes the methods used for validation of products presented in the next sections,
- Section 5 presents results of the Collection OL_L2M.003 validations,
- Section 6 focuses on inter-comparison results between Collection OL_L2M.003 and the previous processor,
- Section 7 summarizes Collection OL_L2M.003 status and its performance towards meeting Sentinel-3 Mission Requirements,
- Section 8 acknowledges teams and institutions contributing to Collection OL_L2M.003 and its validation.

3 ALGORITHM EVOLUTIONS IN PROCESSING BASELINE COLLECTION OL_L2M.003

Sentinel-3 OLCI L2 Marine processor baseline collection OL_L2M.003 defines OLCI Level-2 Marine processing at EUMETSAT, i.e. Ocean Colour processing, which was deployed in operational production on 16 February 2021 (Near Real Time and Non Time Critical chains) and was used in OLCI-A/B full mission reprocessing in the first half of 2021 (see Appendix A).

Collection OL_L2M.003 constitutes the first major change in OLCI L2 Marine processing since November 2017.

'Sentinel-3 OLCI Marine User Handbook' describes the background behind OLCI products and Ocean Colour Level-2 processing (RD-3).

The main Ocean Colour evolutions introduced in OL_L2M.003 include the following:

- New L2 System Vicarious Calibration gains for OLCI-A and OLCI-B
- In the Baseline Atmospheric Correction processing chain (clear waters):
  - Updated Bright Pixel Correction
  - CHL_OC4ME: new chlorophyll index (CI) algorithm for oligotrophic waters
  - Introduction of spectrally-resolved whitecap correction
- In the Alternative Atmospheric Correction processing chain (complex waters, NN products)
  - Introduction of new Neural Network v.2
  - TSM_NN: maximum value of Total Suspended Matter changed from 100 to 400 g/m^3
- Flag updates
  - New flags: COASTLINE, TURBID_ATMOSPHERE
  - OC4ME_FAIL maximum chlorophyll value changed from 30 to 100 mg/m^3
  - New additional test for CLOUD_AMBIGUOUS
  - Updated definition of ADJAC, ANNOT_DROUT

With collection OL_L2M.003, the user recommendation is updated for a list of flags to be applied to mask bad and questionable pixels in the products from the Baseline Atmospheric Correction (clear waters BAC) processing chain. The new list of OLCI L2 recommended flags is defined in section 3.4.4.

Figure 1 displays a schematic of OLCI L2 Marine processing chain and highlights in red the parts of the processing which were updated with collection OL_L2M.003.

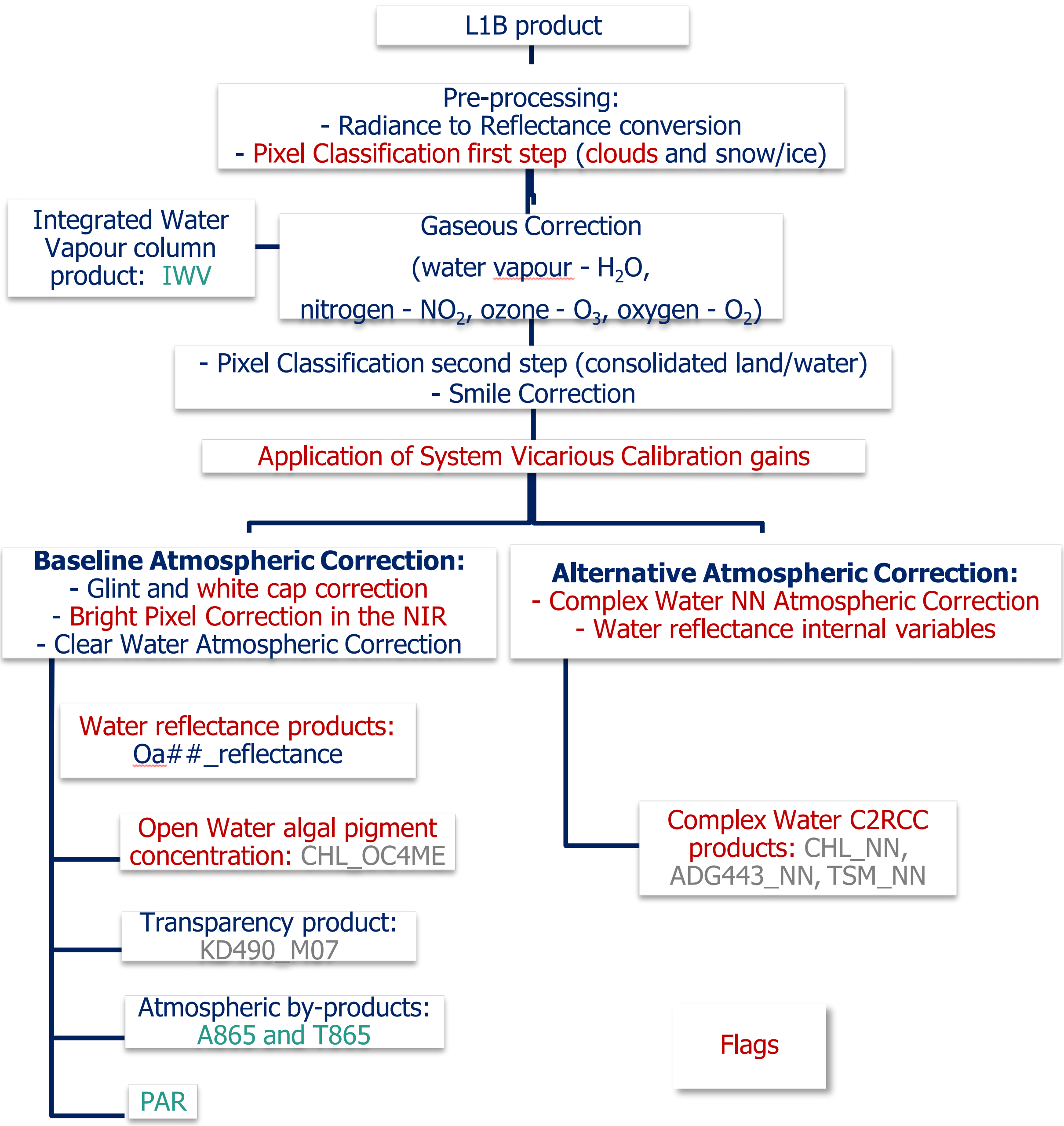


Figure 1: Schematic of OLCI L2 Marine processing chain. The processor updates introduced with OL_L2M.003 are highlighted in red.

OLCI-A and OLCI-B Marine L2 processing is identical, except for the System Vicarious Calibration (SVC) gains which are unique to the sensor.

The complete history of OLCI processing updates can be found on EUMETSAT webpages dedicated to Ocean Colour Services (https://www.eumetsat.int/ocean-colour-services, RD-2) in the table of Product Notices, as well as the associated graphic (https://www.eumetsat.int/olci-processing-baselines, RD-5). The last update of OLCI Level-2

Marine processing occurred in November 2017, when processing baseline v.2.23 was introduced for OLCI-A and used in operational processing as well as in OLCI-A full mission reprocessing at the time. There were no L2 updates related to OLCI-B launch in 2018 and public release, except that OLCI-B SVC gains were set to 1 because no reliable SVC could be performed at that time.

The website shows numerous processing baseline updates from 2018 onwards (RD-2, RD-5). These updates are associated with ongoing OLCI calibration and characterization monitoring and Level-1B processing adjustments in radiometric evolution, dark signal and geolocation modelling in order to ensure the consistency and continuity of OLCI L1B time series. Collection OL_L2M.003 is implemented using these existing OLCI L1B operational products and previously reprocessed L1B product time series, where available. OLCI L1B products belong to baseline collection 002.

The subsections below shortly describe the main Ocean Colour evolutions introduced in Collection OC_L2M.003.

3.1 New L2 System Vicarious Calibration gains for OLCI-A and OLCI-B

The goal of this new System Vicarious Calibration is to implement traceable and harmonised SVC gains for OLCI-A and OLCI-B and to ensure high quality and uniform Ocean Colour retrievals from both missions.

The SVC gains, described below, are applied in L2 processing to Collection OL_L2M.003 data.

System Vicarious Calibration of Ocean Colour sensors is required, along with the sensor calibration, to meet stringent accuracy requirements of water-leaving radiance products and all downstream water bio-optical products (IOCCG, 2012: RD-6). OLCI SVC has been a major recommendation from S3 OLCI/SYN QWG and S3VT-OC.

SVC gains were derived independently for OLCI-A and OLCI-B. The standard Ocean Colour SVC methodology was used, as documented in Franz *et al.* (2007) (RD-7), including South Pacific Gyre coverage for NIR-band SVC gains and MOBY hyperspectral measurements for the VIS-band SVC gains (RD-8). The methodology was used to derive the SVC gains for OLCI Baseline Atmospheric Correction processing chain (clear waters). Nevertheless, the same SVC gains are currently also applied in the Alternative Atmospheric Correction processing chain (complex waters, NN products) because the NN SVC strategy requires more development, yet SVC gains improve the NN products.

For the SVC gain retrieval, a generic SVC tool was implemented. The SVC process, protocol, the tool as well as the SVC gains and validation results are described in detail on EUMETSAT webpage (https://www.eumetsat.int/ocean-colour-system-vicarious-calibration-tool, RD-9) and in the linked document (RD-10).

OLCI-A SVC gains are given in Table 1. Only bands used in OC processing are listed. The missing bands associated with atmospheric gas absorption do not have SVC gains derived and their gains are set to 1.

VIS bands	*400*	*412.5*	*442.5*	*490*	*510*	*560*	*620*	*665*	*673.75*	*681.25*
S3A new	0.97546	0.97406	0.97492	0.9689	0.97184	0.97571	0.98001	0.97834	0.9786	0.97908

NIR bands	*708.75*	*753.75*	*778.75*	*865*	*885*	*1020*
S3A new	0.98013	0.98552	0.98772	0.986	0.98657	0.91316

Table 1: OLCI-A SVC gains for Collection OL_L2M.003

OLCI-B SVC gains are given in Table 2.

VIS bands	*400*	*412.5*	*442.5*	*490*	*510*	*560*	*620*	*665*	*673.75*	*681.25*
S3B	0.99458	0.9901	0.99221	0.9862	0.98898	0.99114	0.99769	0.99684	0.99716	0.99802

NIR bands	*708.75*	*753.75*	*778.75*	*865*	*885*	*1020*
S3B	0.99782	1.00163	1.00259	1	1.00089	0.94064

Table 2: OLCI-B SVC gains for Collection OL_L2M.003

For OLCI-A, the standard assumption on the 865 nm gain to be 1 (RD-7) was modified because of the known over-estimation of top-of-the-atmosphere radiance by OLCI-A (RD-11). Instead of the gain equal to 1, an average difference between OLCI-A and OLCI-B in this band of 1.4% was taken, coming from the analysis of S3A and S3B tandem data (RD-12).

Figure 2 shows the spectral distribution of SVC gains for OLCI-A and OLCI-B. The bands associated with atmospheric gas absorption, in the range of 761 – 768 nm and 900 – 940 nm, have SVC gains set to 1. About 2% difference between the OLCI-A and -B gains reflects well the results of OLCI L1 radiometry validations and tandem phase data (RD-13).

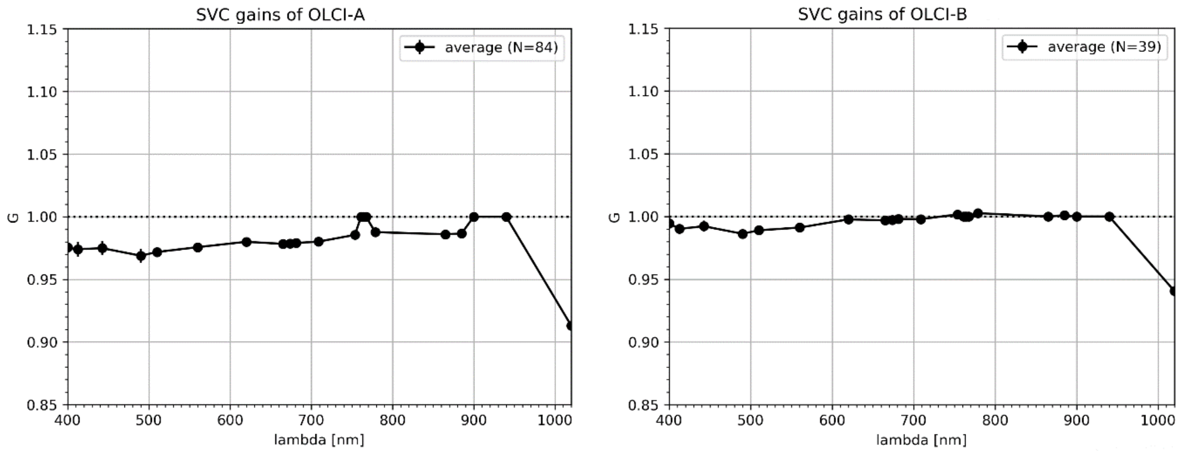


Figure 2: Distribution on SVC gains retrieved for OLCI-A and OLCI-B in Collection OL_L2M.003

OLCI-A SVC gains for the previous processing versions were derived for the processing baseline v.2.23 and used in OLCI-A operational processing from 29 November 2017 as well as in its mission reprocessing 26 April 2016 – 29 November 2017. For these gains, the process of VIS-band SVC retrieval used a provisional strategy of a mix of in situ (MOBY and BOUSSOLE) as well as satellite climatology (GlobCOLOUR) datasets.

OLCI-B did not have SVC gains retrieved before this Collection OL_L2M.003. Earlier OLCI-B SVC attempts failed due to insufficient number of matchups with the SVC in situ source, MOBY, and OLCI-B SVC gains were set to 1.

3.2 Updates in the Baseline Atmospheric Correction processing chain

3.2.1 Updated Bright Pixel Correction

The goal of this Bright Pixel Correction update is to improve OLCI retrievals in complex waters and to reduce noise in OLCI products.

The BPC's objective is approximation and removal of the water signal in the NIR bands in order to enable the subsequent Baseline Atmospheric Correction. The subsequent BAC models the atmosphere, and aerosols in particular, by assuming there is no water-leaving radiance in the NIR via the so-called 'black ocean pixel assumption'. Therefore, BPC is a critical step preceding the BAC to remove any residual NIR water reflectances which particularly occur in complex waters, coastal and inland environments with a sediment load. S3 OLCI/SYN QWG and S3VT-OC recommended major improvements in OLCI BPC.

In OLCI processing, the application of BPC is global for all water types, in order to ensure the continuity of the correction and the spatial consistency of Ocean Colour products.

In the OLCI L2M processing, BPC is implemented as an iterative algorithm using a coupled water and atmosphere model in the NIR (RD-14). The Collection OL_L2M.003 implements the following updates to this algorithm:

- 6 bands in the NIR are used by the coupled model, weighted by per-pixel uncertainties: 709, 753, 779, 865, 885 and 1020 nm,
- numerical inversion is revised,
- first guess is revised.

In particular, including band 1020 nm has helped to improve retrieval of NIR water reflectance in the most turbid cases, not achieved to date.

BPC used in the previous OLCI processing versions frequently failed, raising the flag BPAC_FAIL. Consequently, the correction was not applied for the failed pixels and contributed to visible salt-and-pepper noise in L2 BAC products. Additionally, the quality of near coast and complex water retrievals was relatively poor.

The Collection OL_L2M.003 implements a fully updated BPC processing. The algorithm and its validation results are described in detail on EUMETSAT webpage (https://www.eumetsat.int/OC-BPC, RD-15) and in the linked document (RD-16).

3.2.2 CHL_OC4ME: new chlorophyll index (CI) algorithm for oligotrophic waters

The goal of this OLCI algorithm update is to remove the systematic underestimation of low chlorophyll concentrations by the OC4Me Algal Pixel Concentration product, for chlorophyll lower than 0.2 mg/m^3 obtained via the BAC processing chain.

The OC4Me is a maximum-band-ratio semi-analytical chlorophyll algorithm developed by Morel et al. (2007) (RD-17) which defines the BAC Algal Pigment Concentration product. The algorithm uses maximum-band-ratios of irradiance reflectance $R=E_u(0^-)/E_d(0^-)$ [dimensionless] for blue-to-green bands ($R^{443}{}_{560}$; $R^{490}{}_{560}$; $R^{510}{}_{560}$), where $E_u(0^-)$ and $E_d(0^-)$ are the upward and downward irradiance beneath the surface (at null depth, symbol 0^-) corrected for the bi-directional effects (via the "f /Q correction") (RD-18). OC4Me is different to many other band-ratio algorithms which use maximum-band-ratios of Remote sensing reflectance (Rrs, [sr^{-1}]).

To complement the OC4Me algorithm, a chlorophyll index (CI) approach was developed for Collection OL_L2M.003 for application specifically in low-chlorophyll oligotrophic waters (RD-19). The CI implementation is in response to S3 OLCI/SYN QWG and S3VT-OC recommendations. The CI methodology follows Hu et al. (2012) (RD-20), and the switching between CI and OC4Me (i.e. low and higher chlorophyll concentrations) follows Wang and Son (2016) (RD-21).

The CI algorithm equation was parametrised for OLCI bands at 442.5, 560, and 665 nm, which are different from the original SeaWiFS bands used in the paper by Hu et al. (2012) (RD-20). The parametrization applied in situ HPLC measurements of chlorophyll concentrations in the range below 0.16 mg/m^3 and simultaneous in situ Rrs measurements in the three OLCI bands, from NASA's SeaBASS database (RD-22). The switching between CI and OC4Me algorithms, based on Wang and Son (2016) (RD-21) Rrs ratio approach, 442.5/560 nm, uses the thresholds and the algorithm mixing span adapted to OLCI bands and to the chlorophyll range from the CI parametrization.

Collection OL_L2M.003 keeps the historical name of OC4Me Algal Pigment Concentration product but implements CI and OC4Me algorithms. The details of OLCI CI algorithm implementation and its validation results are described in EUMETSAT document (RD-19).

The original OC4Me algorithm used in the previous OLCI processing versions systematically underestimated the low range of chlorophyll concentrations, as documented by S3 OLCI/SYN QWG and S3VT-OC (RD-23).

3.2.3 Introduction of spectrally-resolved whitecap correction

The goal of this update is to revise OLCI whitecap correction.

The whitecap correction is a combination of the whitecap reflectance and the whitecap coverage, i.e. the fraction of the water surface that is covered by whitecaps. The whitecap reflectance is composed of the effective whitecap irradiance reflectance (Koepke, 1984; RD-23) and the normalized reflectance factor that varies with wavelength (Frouin et al., 1996; RD-24). The whitecap coverage increases significantly with an increase in wind speed (or wind friction velocity) (Stramska and Petelski, 2003; RD-25).

The new OLCI whitecap correction in Collection OL_L2M.003 applies the following formulations:

- effective whitecap irradiance reflectance of 0.22 taken from Koepke (1984) (RD-23)
- normalized whitecap reflectance factor taken from Fougnie (2020)
- whitecap coverage for undeveloped seas from Stramska and Petelski (2003), Figure 8 (RD-25)

and is implemented for wind speeds $6.33 \leq v \leq 12$ m/s.

The normalized whitecap reflectance factors, a_{wc}, from Fougnie (2020) is given for OLCI bands in Table 3 and plotted in Figure 3.

VIS bands	*400*	*412.5*	*442.5*	*490*	*510*	*560*	*620*	*665*	*673.75*	*681.25*
$\mathbf{a_{wc}}$	1.0000	1.0000	1.0000	1.0006	1.0001	0.9947	0.9593	0.9428	0.9376	0.9283

NIR bands	*708.75*	*753.75*	*761.25*	*762.375*	*767.5*	*778.75*	*865*	*885*	*900*	*940*	*1020*
a_{wc}	0.8788	0.7191	0.7260	0.7272	0.7327	0.7453	0.6416	0.6110	0.5887	0.5059	0.4855

Table 3: Normalized whitecap reflectance factor from Fougnie (2020) model applied in Collection OL_L2M.003

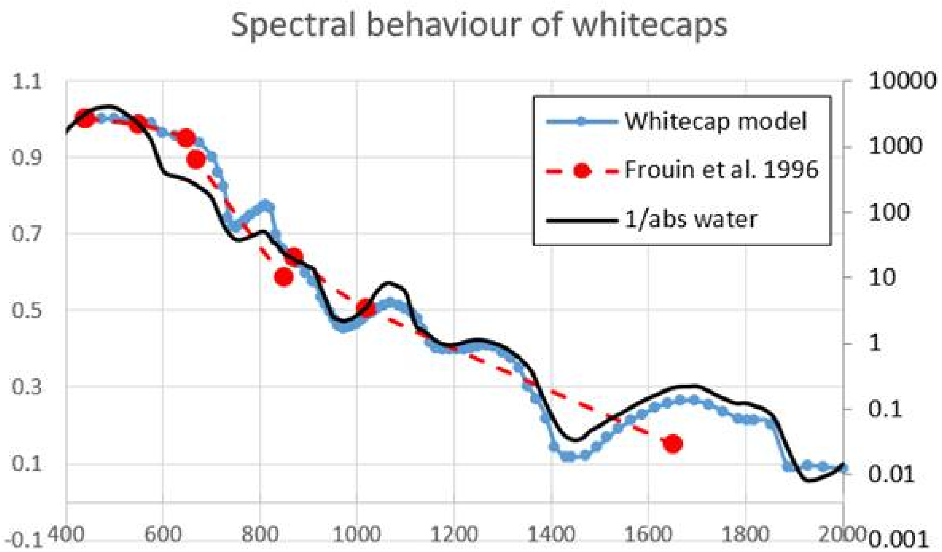


Figure 3: Normalized whitecap reflectance factor from Fougnie (2020) model in comparison with Frouin et al., 1996, measurements (RD-24)

Below wind speeds of 6.33 m/s the whitecap effect over a pixel is considered negligible and above 12 m/s the pixel is considered to be too contaminated for an accurate retrieval and the WHITECAPS flag is turned ON. The WHITECAPS flag belongs to the list of user recommended flags, available in Table 3.

The original whitecap correction used in the previous OLCI processing versions was different in its implementation of all three whitecap formulations (RD-26). The differences were in the effective whitecap irradiance reflectance, the normalized whitecap reflectance factor was spectrally constant, and the whitecap coverage was from Stramska and Petelski (2003), Figure 4 (RD-25), for wind speeds $4.93 \leq v \leq 12$ m/s.

3.3 Updates in the Alternative Atmospheric Correction processing chain

3.3.1 New Neural Network v.2 (NNv2)

The goal of the new NNv2 implementation is to reduce noise in NN OLCI products and to achieve more accurate product value in open ocean waters.

There are two NNs used in the AAC processing chain: a NN performing the atmospheric correction and retrieving water reflectances, and a NN retrieving water Inherent Optical Properties (RD-27, RD-28). The three OLCI NN operational products (i.e. CHL_NN, ADG443_NN, and TSM_NN) are derived from IOPs outputted by the second NN.

The new NNv2 includes improvements in both NNs, which are the following:

- New water bio-optical model, including new exponent for detritus spectrum

- Extended training range and co-variance ranges, including better coverage of high backscatter water such as river estuaries and lakes
- Updated forward modelling: combining Hydrolight and CC atmosphere model
- Increased number of training samples and more robust training to reduce noise in data

The extended training range used by NNv2 applies the following limits on IOPs at 442.5 nm:

a_{pig} = 0.001 – 6.0 (absorption by phytoplankton pigments)

$a_{detritus}$ = 0.001 – 22.0 (absorption by humic and fulvic acid)

a_g = 0.001 – 22.0 (absorption by Gelbstoff)

a_{tot} = 0.003 - 50.0 (total absorption, $a_{tot} = a_{detritus} + a_g + a_{pig}$)

$b_{b,p}$ = 0.001 – 250.0 (backscattering by suspended matter)

$b_{b,white}$ = 0.001 – 250.0 (backscattering by white particles such as coccolithophore and bubbles)

$b_{b,total}$ = 0.0021 – 500.0 (total backscattering, $b_{b,total} = b_{b,p} + b_{b,white}$)

NNv2 output IOPs (i.e. a_{pig}, a_g, $a_{detritus}$, $b_{b,p}$, and $b_{b,white}$) are converted in follow-on processing to mass concentrations for Total Suspended Matter (TSM) and Algal Pigment Concentration products.

With NNv2 in Collection OL_L2M.003, there are two updates in the NN TSM product:

- new conversion is used for the TSM: TSM_NN [g/m^3] = 1.06*($b_{b,total}$)^0.942
- TSM_NN output is scaled between 0.01 and 400 g/m^3 (in OL_L2M.003.01, see Appendix A)

NNv2 in Collection OL_L2M.003 does not include any updates in the NN Algal Pigment Concentration product:

- conversion for CHL_NN [mg/m^3] = 21*(a_{pig})^1.04
- CHL_NN output is scaled between 0.01 and 100 mg/m^3

NNv2 has been tested by the Ocean Colour community in SNAP processing through Case-2 Regional CoastColour (C2RCC) (RD-29). NNv2 was recommended for application in the OLCI operational processing by the S3VT and the OLCI/SYN QWG. The original NNv1 used in the previous OLCI processing versions showed significant overestimation of TSM and poor Algal Pigment Concentration retrievals in low chlorophyll waters.

Users are cautioned that there may be small differences between OLCI operational NN products and outputs from the SNAP C2RCC processing. The pre-processing steps applied before the AAC can explain most of those differences (e.g. different OLCI pixel classification, application of the gaseous correction at different steps). The application of the OC-SVC gains may have the biggest impact, as the gains are not automatically included in the SNAP C2RCC processing.

3.3.2 TSM_NN: maximum value of Total Suspended Matter changed from 100 to 400 g/m^3

The range of Total Suspended Matter concentration was updated to be 0.01 to 400 g/m^3 in Collection subversion OL_L2M.003.01 (see Appendix A).

The previous TSM scaling, implemented up to Collection OL_L2M.003.00, limited the maximum concentration to 100 g/m^3, which is too restrictive in most turbid waters, such as the estuary of Rio de la Plata.

The IOP NNv2 training applied $b_{b,total}$ values up to 500.0 that rounds up to TSM of about 400 g/m^3. The only new change in the TSM_NN product is therefore the scaling factor which now allows maximum output of TSM up to 400 g/m^3.

3.4 Flag updates

Users are strongly cautioned to apply the flag definitions from the products, if implementing own OLCI L2M product readers. There are new flags included in the OLCI Collection OL_L2M.003 and the flag order has changed. Having flag bits hard coded in a product reader may cause bad flags to be retrieved and applied. To avoid the hard-coding, use bit-to-flag mapping specified in the *flag_meanings* and *flag_masks* attributes in the WQSF netCDF file contained in every OLCI PDU. This warning does not apply to OLCI tools like SNAP, which are implemented to correctly read the flag bit definition from the products.

3.4.1 New flags: COASTLINE, TURBID_ATMOSPHERE

There are two new flags implemented in OLCI Collection OL_L2M.003:

- COASTLINE
- TURBID_ATMOSPHERE

The COASTLINE flag is a direct copy into L2 flag output of the L1 product COASTLINE flag.

The TURBID_ATMOSPHERE flag is composed of two conditions:

- pixel's diffuse path transmittance in band 865 nm obtained from the NN AAC is lower than a threshold (0.955), or
- pixel is saturated or excessively bright in band 442.5 nm.

3.4.2 OC4ME_FAIL maximum chlorophyll value changed from 30 to 100 mg/m^3

This OL_L2M.003 change regards higher values of chlorophyll concentrations retrieved by OLCI through the BAC processing chain. The goal of the change is to allow user access to the full range of the OC4Me Algal Pigment Concentration product to enable its validation and to support coastal studies.

The update reduces the number of pixels marked with the OC4ME_FAIL flag. In the previous processor, OC4ME_FAIL was set for all CHL_OC4ME values higher than a 30 mg/m^3 threshold. With OL_L2M.003, OC4ME_FAIL is changed to be set at the threshold of CHL_OC4ME values equal or higher than 100 mg/m^3.

The OC4ME_FAIL flag is defined based on the chlorophyll threshold and also based on tests that identify unavailable or bad chlorophyll retrievals, e.g. because of negative reflectance values and parameters not being within the scope of the applicability of the OC4Me algorithm.

The OC4Me chlorophyll algorithm has been specifically developed for open oceanic waters (RD-17). The algorithm has an asymptotic behaviour as the curve of the blue-to-green ratio flattens when chlorophyll concentrations become large, already above ~10 mg/m^3. For the higher chlorophyll, small uncertainties in the ratio translate to larger uncertainties in the chlorophyll. Nevertheless, OC4Me retrieves chlorophyll values up to 100 mg/m^3 in concentration.

With this update, OC4ME_FAIL does not limit the higher range of OC4Me chlorophyll retrieval, thus retrievals beyond 30 mg/m^3 are not flagged, unless for other OC4Me issues. As OC4ME_FAIL is a standard flag recommended for use with BAC Algal Pigment Concentration, product values up to 99.99 mg/m^3 are now available to users.

Users are cautioned that higher OC4ME chlorophyll concentration, above ~10 mg/m^3, may have higher uncertainties. Users are also encouraged to support validations of these higher chlorophyll concentrations.

3.4.3 New additional test for CLOUD_AMBIGUOUS

The goal for updating the CLOUD_AMBIGUOUS flag is to improve OLCI L2 processor skill in masking cloudy pixels over water, particularly cloud edges. The goal is also to eliminate the need of using ANNOT flags to substitute for incomplete cloud flagging by standard cloud flags.

OLCI L2 products include three standard cloud flags: CLOUD, CLOUD_AMBIGUOUS, and CLOUD_MARGIN. The CLOUD flag masks the pixels classified with high confidence as cloudy, the L2 processing is not continued for these pixels. CLOUD_AMBIGUOUS flags pixels suspected of cloud contamination, the follow-on L2 processing is performed for these pixels. The CLOUD_MARGIN flag is set for areas around the pixels flagged as CLOUD or CLOUD_AMBIGUOUS to further eliminate any potential cloud contamination or straylight, within 2 pixel radius for Reduced Resolution products and 4 pixel radius for Full Resolution products. The cloud algorithm is based on a cloud classification NN and on a series of additional tests, including spectral thresholds.

A new cloud test is introduced which is a part of the spectral tests performed to set the CLOUD_AMBIGUOUS flag. The test is based on the Wang and Shi (2006) algorithm (RD-30), where clouds are differentiated from bright water in the NIR and small particle aerosols by taking an advantage that clouds are spectrally flat. The method allocates thresholds to Rayleigh corrected reflectance and reflectance ratio in the NIR: $\rho_{RC}(869) \geq \text{threshold}_1$ and $\varepsilon_{RC}(748,869) \leq \text{threshold}_2$, where

- $\rho_{RC}(\lambda) = \rho_{TOA}(\lambda) - \rho_{R}(\lambda)$
- $\varepsilon_{RC}(\lambda_i,\lambda_j) = \rho_{RC}(\lambda_i) / \rho_{RC}(\lambda_j)$

The algorithm developed by Wang and Shi (2006) for MODIS spectral bands is recalibrated for OLCI bands with the following thresholds: $\rho_{RC}(865) \geq 0.08$ and $\varepsilon_{RC}(753,865) \leq 1.04$.

The cloud flagging used in the previous OLCI processing versions significantly missed cloud contamination over water. Therefore, additional flags had to be recommended to users in order to ensure the proper cloud masking. Those additional flags were the ANNOT flags, such as ANNOT_ABSO_D, ANNOT_MIXR1, ANNOT_DROUT, and ANNOT_TAU06. Especially the ANNOT_DROUT flag enabled good screening of cloud edges over water. Nevertheless, the ANNOT flags were not designed for cloud masking and were additionally flagging coastal areas of high importance to user applications. The elimination of ANNOT flags from the list of user recommended flags has been a consistent recommendation from S3VT and OLCI/SYN QWG. Wang and Shi (2006) cloud test now enables improved flagging of the clouds and allows removal of the ANNOT flags from the list of recommended flags.

An example of cloud flagging is displayed in Figure 4. The preceding processor version on the left of Figure 4 shows yellow and light green pixels around clouds which are not masked by cloud flagging. At the same time, Collection OL_L2M.003 on the right of Figure 4 does not leave behind the questionable pixel retrievals and masks those cloud pixels.

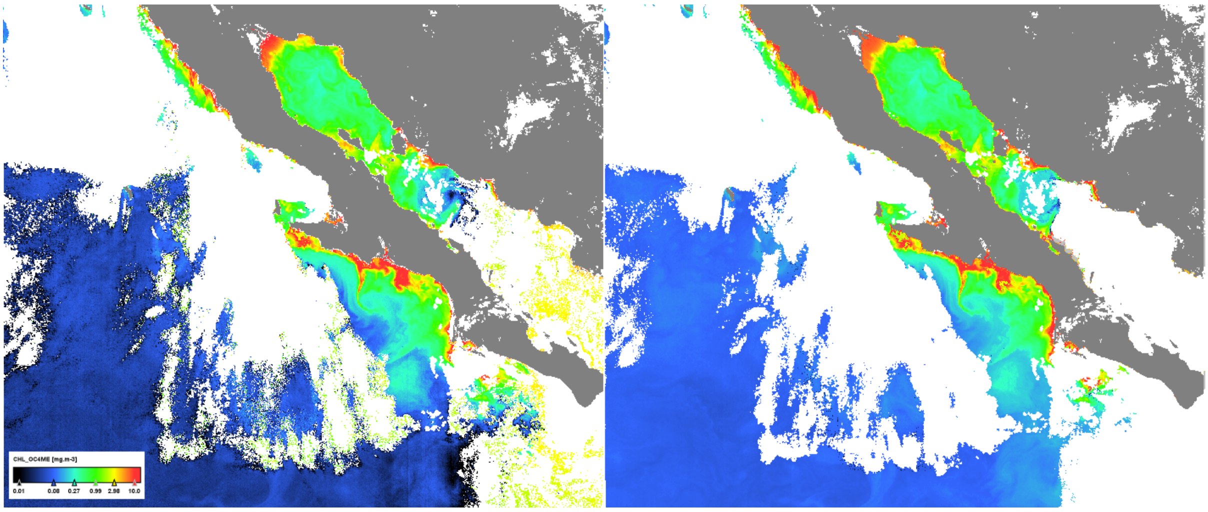


Figure 4: OLCI-A scene processed using the preceding processor version on the left and the processor Collection OL_L2M.003 on the right. The scene: S3A_OL_2_WRR____20190702T172158_20190702T180621. In both cases, all cloud flagged pixels are shown in white, i.e. identified as CLOUD, CLOUD_AMBIGUOUS, and CLOUD_MARGIN.

3.4.4 Updated definition of ADJAC, ANNOT_DROUT

The definition of the ADJAC and ANNOT_DROUT flags is updated with this Collection OC_L2M.003 to allow a better representation of surface conditions defined by these flags.

3.4.4.1 ADJAC flag update

The ADJAC flag is in OLCI to indicate pixel adjacency to bright targets. This flag existed but was not used in the previous processor versions. Collection OC_L2M.003 applies ADJAC for flagging of specific cases along bright coastlines.

The Wang and Shi (2006) cloud test (RD-30) contributing to CLOUD_AMBIGUOUS flagging, described in section 3.4.2, allows significant improvement in OLCI cloud screening over water. However, this test occasionally becomes also positive along coastlines. OLCI water processing goes closely up to a coastline where the specific condition of NIR band brightness and cloud-like NIR band ratio is sometimes met, even with no clouds present. The Ocean Colour retrievals for these pixels are unreliable and should be flagged. Consequently, the unused ADJAC flag was selected to indicate these coastline pixels.

The procedure uses a radius to search the area around the pixels which pass the Wang and Shi (2006) cloud test. If the area is adjacent to a coastline, along either open or inland waters, and it does not contain any high confidence CLOUD flagging, the CLOUD_AMBIGUOUS flag is replaced with ADJAC for these pixels. The search radius of 1 pixel in RR and FR products is used in Collection subversion OL_L2M.003.00. The radius is extended to 2 pixels in FR products with subversion OL_L2M.003.01 (see Appendix A).

The procedure above eliminates most of cloud misclassification. Yet, there may be cases where Wang and Shi (2006) identified NIR cloud conditions are positive but they extend further away from the coastline with no clouds present. In these rarer cases the pixels will be assigned the CLOUD_AMBIGUOUS flag and CLOUD_MARGIN will further expand the cloud flagging.

Users are cautioned against using the pixels identified by the Wang and Shi (2006) test in Ocean Colour analyses. Therefore, the ADJAC flag is added to the list of recommended flags for OLCI Collection OL_L2M.003.

3.4.4.2 ANNOT_DROUT flag update

The goal of ANNOT_DROUT is to detect anomalously bright waters, for example with coccolithophore algae. The ANNOT_DROUT flag is set for pixels for which the residual reflectance in band 510 nm is higher than a threshold after the Baseline Atmospheric Correction and the subtraction of water reflectance at 510 nm from a climatology.

Nevertheless, the ANNOT_DROUT flag systematically comes-on in a variety of other circumstances where the residual reflectance in band 510 nm is beyond the threshold. For example, this occurs in most complex waters as well as in water pixels contaminated by clouds.

To limit one of these additional ANNOT_DROUT activation cases, the flag definition is updated to exclude its activation over 'case-2' waters. The 'case-2' water pixels are determined by their particulate backscatter retrieved by the Bright Pixel Correction.

3.4.5 User recommended flags for application with OLCI Collection OL_L2M.003

Table 3 contains the definition of user recommended flag combinations for masking of cloudy and unreliable pixels in OLCI Level-2 Ocean Colour products from Collection OL_L2M.003. This list of recommended flags is applied in the following OLCI product validations in this report.

Users are advised to apply the flag recommendations from Table 3. Implementing the recommendations is central to the traceability of OLCI L2 product status across applications and the validation process. This flag recommendation is particularly important for large scale analyses and automated processes. It is understood that advanced users would want to experiment with application of flags that suit their particular local region or application. However, it is advised that, at the same time, the results based on the recommended flags are also reported.

Product names	Products	Common flags	Processing chain flags	Product flags
Water reflectance – BAC Open Waters	Oa**_reflectance → Oa**_reflectance	**Ocean Colour Products** (WATER *or* INLAND_WATER) *and not* (CLOUD CLOUD_AMBIGUOUS CLOUD_MARGIN INVALID COSMETIC SATURATED SUSPECT HISOLZEN HIGHGLINT SNOW_ICE)	**Baseline Atmospheric Correction Open Water Products** *not* (AC_FAIL WHITECAPS ADJAC RWNEG_O2 RWNEG_O3 RWNEG_O4 RWNEG_O5 RWNEG_O6 RWNEG_O7 RWNEG_O8)	*none*
Algal pigment concentration – BAC Open Waters	chl_oc4me → CHL_OC4ME			*not* OC4ME_ FAIL
Diffuse attenuation coefficient – BAC Open Waters	trsp → KD490_M07			*not* KDM_FAIL
Photosynthetically Active Radiation – BAC Open Waters	par → PAR			*not* PAR_ FAIL
Aerosol Optical Thickness and Ångström exponent – BAC Open Waters	w_aer → T865, A865			*none*
Algal pigment concentration – AAC Complex Waters	chl_nn → CHL_NN		**Alternative Atmospheric Correction Complex Water Products** *no specific flags to be applied*	*not* OCNN_FAIL
Total suspended matter concentration – AAC Complex Waters	tsm_nn → TSM_NN			*not* OCNN_FAIL
Coloured Detrital and Dissolved Material absorption – AAC Complex Waters	iop_nn → ADG443_NN			*not* OCNN_FAIL
Integrated Water Vapour Column	iwv → IWV	**Atmospheric Products**	**Water Vapour** *not* MEGLINT	*not* WV_FAIL

Table 3: Recommended OLCI Level 2 flag combinations for masking of cloudy and unreliable pixels for Collection OL_L2M.003.

4 VALIDATION METHODOLOGY

The validation methodology for Collection OL_L2M.003 products follows the cal/val tasks defined for OLCI L2 Ocean Colour products in the 'Sentinel-3 Calibration and Validation Plan' (AD-3). The main methods encompass

- validations with in situ measurements (OLCI-L2WLR-CV-300),
- validations with Level-3 products (OLCI-L2WLR-CV-400), and
- processing quality verifications (OLCI-L2WLR-CV-500).

Collection OL_L2M.003 algorithm verifications and product validations were supported by OC-TAC CMEMS (RD-31), S3VT-OC (RD-32) and S3 OLCI/SYN QWG. EUMETSAT provided hundreds of thousands of reprocessed L2 products to the teams, covering regions of interest and with in situ measurements available to the teams, and received crucial feedback and validation results.

Validation results presented in this OL_L2M.003 report are based on EUMETSAT's own activities and a limited set of results from external teams. This is because, at this stage, the external teams still await result publication in journal papers. When these papers are published, the current report will be updated with corresponding references. Collection OL_L2M.003 findings from S3VT-OC are available to the S3VT members on the website of the S3VT virtual meeting, which took place on 15-17 December 2020 (RD-33).

4.1 Validation data sets

4.1.1 OLCI products

OLCI L1B products from Baseline Collection 002 available in the EUMETSAT CODA, CODAREP, and Data Centre (see Appendix A) were reprocessed to Level 2 in the EUMETSAT Climate Data Record environment using IPF-OL-2 version 07, producing Collection OL_L2M.003 products. The reprocessed L2 data sets include:

- FR products matching in situ locations and times as specified below,
- RR products over the first 4 days of each month for the period 06/2018-07/2020. Daily global binned Level-3 products at 9.2 km resolution were derived for validation purposes (not distributed).

OLCI L2 pixels are filtered according to the list of recommended flags defined in section 3.4.4.

4.1.2 In situ reference data sets

The in situ validation strategy and matchup datasets are available to all users in the Copernicus Fiducial Reference In Situ Ocean Colour Database OC-DB (https://ocdb.eumetsat.int/, RD-34). OC-DB serves as a data repository for all EUMETSAT's in situ validation activities.

4.1.2.1 MOBY radiometric measurements

MOBY optical measurements include:

- Hyperspectral normalized water-leaving radiance resampled to the OLCI bands

MOBY data are used for System Vicarious Calibration of OLCI VIS bands. While the highest quality MOBY matchups are selected for SVC, as described in section 3.1, the full extended set of matchups is used for SVC verification and presented in section 5.2.1. The verification does not constitute OLCI product validation but is reviewed here to confirm the quality of the SVC process.

The MOBY measurements cover the period 2016-04-01 – 2020-06-30. They are convolved with OLCI mean spectral response functions (RD-35) and shifted to OLCI's nominal band wavelengths.

See RD-8 for details, documentation and data access.

4.1.2.2 AERONET-OC radiometric measurements

AERONET-OC optical measurements include:

- Multispectral normalized water-leaving radiance

EUMETSAT's OLCI in situ validations heavily rely on AERONET-OC as the only source of operational fiducial reference measurements for validation, which are openly and easily available to all users.

The AERONET-OC measurements cover the period 2016-04-01 – 2020-04-30.

One should know that the AERONET-OC sites are in coastal waters, typically characterised by complex optical properties.

See RD-36 and RD-37 for details, documentation and data access.

4.1.2.3 SeaBASS chlorophyll-a concentration measurements

SeaBASS chlorophyll measurements include:

- HPLC chlorophyll-a concentrations

Chlorophyll in situ measurements for OLCI validations are acquired from NASA SeaBASS bio-optical archive and storage system.

The SeaBASS measurements cover the period 2016-04-01 – 2020-04-30.

See RD-22 for details, documentation and data access.

4.1.2.4 Atlantic Meridian Transect (AMT) cruise bio-optical measurements

The AMT bio-optical measurements include:

- Chlorophyll concentrations obtained from WET Labs ACS underway hyperspectral spectrophotometers, calibrated against HPLC values
- Normalized remote sensing reflectance obtained from underway hyperspectral spectroradiometers

AMT field campaigns are managed by Plymouth Marine Laboratory (PML) in the UK. In situ data cover AMT cruises AMT26, 27 and 28 in 2016, 2017 and 2018, respectively. AMT in situ reference data sets included in this report were prepared, processed by the PML team and original PML results are included.

See RD-38 for details and documentation.

4.1.2.5 Cefas smart buoy turbidity measurements

Centre for Environment, Fisheries and Aquaculture Science (Cefas) in the UK operates autonomous moored smart buoys, which measure, among others

- In situ water turbidity at 1 m depth

Brockmann Consult, GmbH, uses the buoy measurements to perform validations of OLCI Total Suspended Matter product.

4.1.3 Satellite reference data sets

MODIS-Aqua daily global binned Level-3 products at 9.2 km resolution include processing version R2018.1:

- Rrs_xxx: Normalized remote sensing reflectance at wavelengths 412, 443, 488, 555, and 667 nm.
- Chlor_a: Chlorophyll-a concentration

MODIS-Aqua datasets for OLCI validations are acquired from NASA's Ocean Color Web.
See RD-39 for details, documentation and data access.

4.2 Validation Tests

Following the S3 OLCI cal/val plan (AD-3), OLCI validation tests include validations with in situ measurements (OLCI-L2WLR-CV-300), mission inter-comparisons with Level-3 products (OLCI-L2WLR-CV-400), and processing quality verifications via visual inspections and further analyses (OLCI-L2WLR-CV-500).

4.2.1 Ocean colour validation with in situ measurements

Collection OL_L2M.003 validations with situ measurements address the tasks OLCI-L2WLR-CV-300 from the S3 cal/val plan (AD-3). The validated products include

- Water reflectance products at bands where in situ data are available
- Algal pigment concentration products, open water CHL_OC4ME and complex water CHL_NN

The validations consist of scatter plots of in situ vs. OLCI data with respective statistics, after stringent matchup criteria are applied to both datasets.

The OLCI matchup criteria are defined in EUMETSAT's document 'Recommendations for Sentinel-3 OLCI Ocean Colour product validations in comparison with in situ measurements – Matchup Protocols' (RD-40).

The specific matchup parameters (such as a window size) and corrections (such as BRDF or band-shift) used in the validations of OLCI Collection OL_L2M.003 presented in this report are summarised in Table 4. They describe the parameters and corrections performed for validations with AERONET-OC, HPLC, as well as OL_L2M.003 verification with MOBY.

In situ validations reported for the previous processing version PB2.43/1.15 also follow the specific description in Table 4, except that a different flag list is used. For Open Water products this old flag list is as follows: CLOUD, CLOUD_AMBIGUOUS, CLOUD_MARGIN, INVALID, COSMETIC, SATURATED, SUSPECT, HISOLZEN, HIGHGLINT, SNOW_ICE, AC_FAIL, WHITECAPS, RWNEG_O2, RWNEG_O3, RWNEG_O4, RWNEG_O5, RWNEG_O6, RWNEG_O7, RWNEG_O8. This flag list does not include the four ANNOT flags: ANNOT_ABSO_D, ANNOT_MIXR1, ANNOT_DROUT, ANNOT_TAU06, which are among the previous user recommended flags as they remove residual cloudy pixels.

Parameter/Correction	What is stated in RD-40	What was done in this report for: OLCI vs. AERONET-OC, OLCI vs. MOBY, OLCI vs. HPLC
In situ – OLCI maximum time difference	1 hour (standard) Exceptionally: <1 hour (if very dynamic waters) 3 hours to enlarge dataset	3 hours
Spatial window	Centered on the measurement point/platform position. 25 (5x5) window Exceptionally: Non-homogeneous site: 3x3 Extremely non-homogeneous site: 1x1	Centered on the measurement point/platform position. 25 (5x5) window
Zenith angles	SZA < 70 (solar) OZA < 60 (viewing)	Same as in RD-40
Flags: Standard products	Same as specified in Table 3.	Same as specified in Table 3.
Flags: NN products	Same as specified in Table 3.	Same as specified in Table 3
Minimum number of valid pixels	50%+1 Exceptionally: 100%	50%+1 (13/25)
Outlier detection	Distance to the mean (μ) should be less than 1.5 times the standard deviation (σ): $|\text{pixel value}- \mu| < 1.5\sigma$	Same as in RD-40
High CV criterion	If CV[560 nm] > 0.2, the whole match-up should be discarded.	Same as in RD-40

Reported value and absolute error **(Satellite)**	**Reported value**: Median (after outlier extraction). **Absolute error**: Standard deviation (after outlier extraction).	Same as in RD-40
Band-shifting correction	Always apply if Δλ>1 nm **Exceptions** In the **red**, always apply if Δλ>2 nm [Follow guidelines by Zibordi et al. 2006 or Melin and Sclep 2015]	Applied
BRDF Correction	Always apply	Applied
Maximum measurement depth	Depth of **measurement** should be no more than 2 to 5 m.	Applied
Measurement aggregation	Independent casts over the same OLCI scene should be aggregated within each defined ROI	Same as in RD-40
Non-spectral statistics: **Rrs, band-by-band**	• MAD • MAPD • MD • MPD • Same statistics as before but median-based (MdAD, MdAPD, MdD, MdPD) • Slope, Intercept and linear regression performance statistics	Same as in RD-40 Presentation of statistics on the plots: Mean_Stats / Median_Stats Linear regression was performed using an Orthogonal Distance Regressor (ODR)
Non-spectral statistics:	Same but additionally computed over the logarithmic values	Also shown on the OLCI vs. HPLC plots.

Other products (ADG443, CHL, TSM, etc)	(LMAD, LMD and same but median-based).	
Spectral statistics [only Rrs]	*May* additionally present Spectral Angle Mapper (SAM), and Chi-square vectorial statistics	Not shown in this document

Table 4: Listing of specific matchup parameters and corrections used in Collection OL_L2M.003 in situ validations (columns 3 and 4), versus general validation recommendations described in the OLCI Matchup Protocol (RD-40) (column 2).

4.2.2 Ocean colour validation with Level-3 products

Collection OL_L2M.003 validations with L3 products address the tasks OLCI-L2WLR-CV-400 from the S3 cal/val plan (AD-30). The validated products include

- Normalized water reflectance at all OC bands
- Algal pigment concentration from the clear water BAC processing, i.e. CHL_OC4ME

OLCI-A and OLCI-B are compared with each other during the S3-A-B tandem phase (June-October 2018, RD-12) and, afterwards, in routine operation and until July 2020. OLCI-A and -B products are also inter-compared with third party reference mission, which is MODIS-Aqua described in section 4.1.3.

The comparisons are performed using Level 3 global daily products, and rely on the standardized bin coverage of the globe with matching bins having identical ground location across the missions.

OLCI RR L2 products, processed with Collection OL_L2M.003 algorithms, are assembled to Level 3 internally for validation purposes, using the 9.2 km sampling grid and the binning algorithm consistent with the MODIS 9.2 km L3 binned products.

Only those L2 pixels are binned to L3, which pass the flag screening criteria. The flags used in L3 binning of Collection OL_L2M.003 are defined in Table 3. The results in section 6 also include inter-comparisons with the previous processing version PB2.43/1.15. For PB2.43/1.15, the old flag list is applied: CLOUD, CLOUD_AMBIGUOUS, CLOUD_MARGIN, INVALID, COSMETIC, SATURATED, SUSPECT, HISOLZEN, HIGHGLINT, SNOW_ICE, AC_FAIL, WHITECAPS, ANNOT_ABSO_D, ANNOT_MIXR1, ANNOT_DROUT, ANNOT_TAU06, RWNEG_O2, RWNEG_O3, RWNEG_O4, RWNEG_O5, RWNEG_O6, RWNEG_O7, RWNEG_O8.

Because the performance of the L2 processing algorithms depends, among other factors, on the type of water observed, the analyses are stratified between

- Oligotrophic waters (Chl <= 0.1 mg/m^3)
- Mesotrophic waters (0.1 < Chl <= 1 mg/m^3)
- Eutrophic waters (Chl > 1 mg/m^3)

The comparisons consist of time series over the first 4 days of each calendar month for
- the mean of the product for each of the missions compared,
- the relative percentage (RPC) difference (e.g. (OLCI-B-OLCI-A)/OLCI-A).

4.2.3 Ocean colour processing quality verifications

The verifications of Ocean Colour processing quality for the Collection OL_L2M.003 primarily include verifications of consistency of OLCI retrievals and of quality of cloud and other flagging. They addressed the tasks OLCI-L2WLR-CV-500 from the S3 cal/val plan (AD-3). These verifications rely on L2 diagnostic scenes and L3 maps and their visual inspections.

5 PRODUCT VALIDATION RESULTS FOR BASELINE COLLECTION OL_L2M.003

Section 5 describes product validations performed at EUMETSAT and at a few external partners for Sentinel-3 OLCI L2 Marine processor Collection OL_L2M.003. The validations are reported for standard products of Water reflectance and Algal pigment concentrations. Readers are pointed to further validation results from S3VT for these and the other standard products, which are available to S3VT members from the S3VT#6 meeting (RD-33).

The presented validations apply the methodology, data sets, protocols and user recommended flags described in section 4.

5.1 High level overview of OLCI-A and -B Ocean Colour products

Figure 5 and Figure 6 below are an illustration of the very good alignment of OLCI-A and -B. These images show Collection OL_L2M.003 CHL_OC4ME algal pigment concentration product binned to Level-3 and mapped for the first four days of January 2020. To ease the comparison, only the coverage available from both sensors is displayed.

Figure 7 shows Collection OL_L2M.003 algal pigment concentrations for the west coast of France. Retrievals are available all along the west coast, including Gironde, Loire, Vilaine and Seine estuaries. There is a good retrieval in the bay of Mont-Saint-Michel relatively close to the coast considering some of the biggest tides in Europe occurring in this bay and large sediment and water bottom exposure.

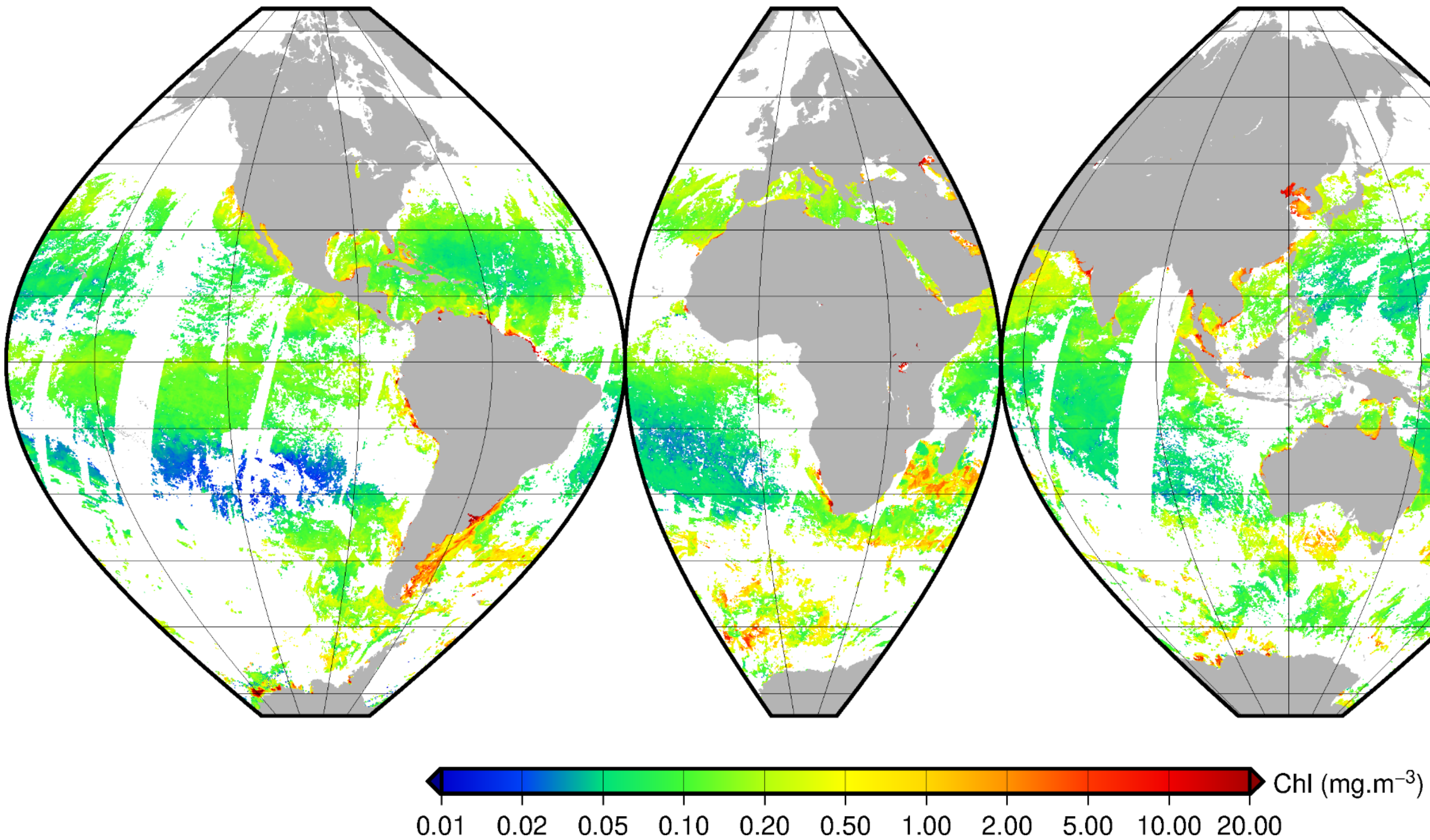


Figure 5: OLCI-A OC4ME chlorophyll concentration synthesis for the first four days of January 2020

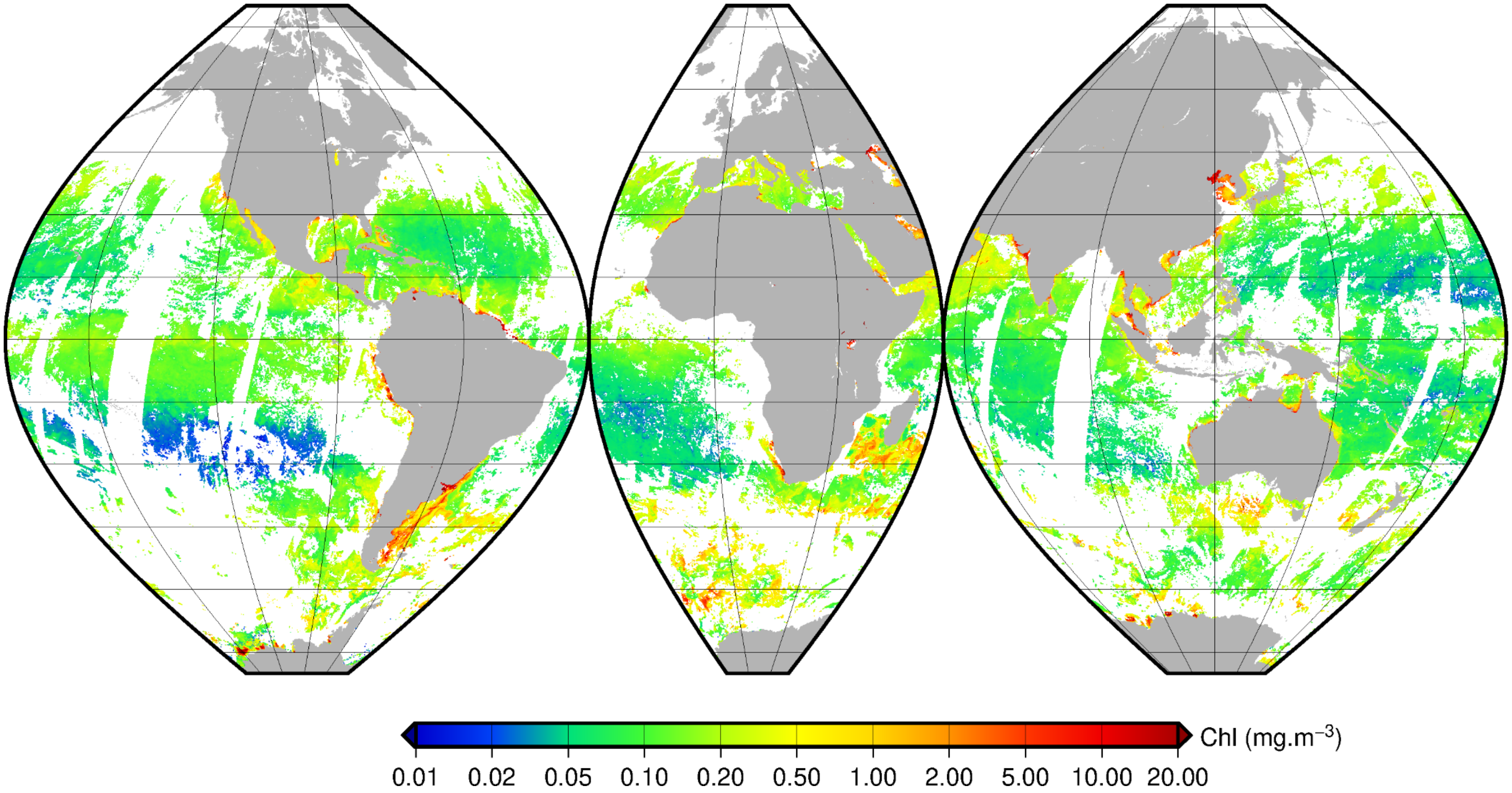


Figure 6: OLCI-B OC4ME chlorophyll concentration synthesis for the first four days of January 2020

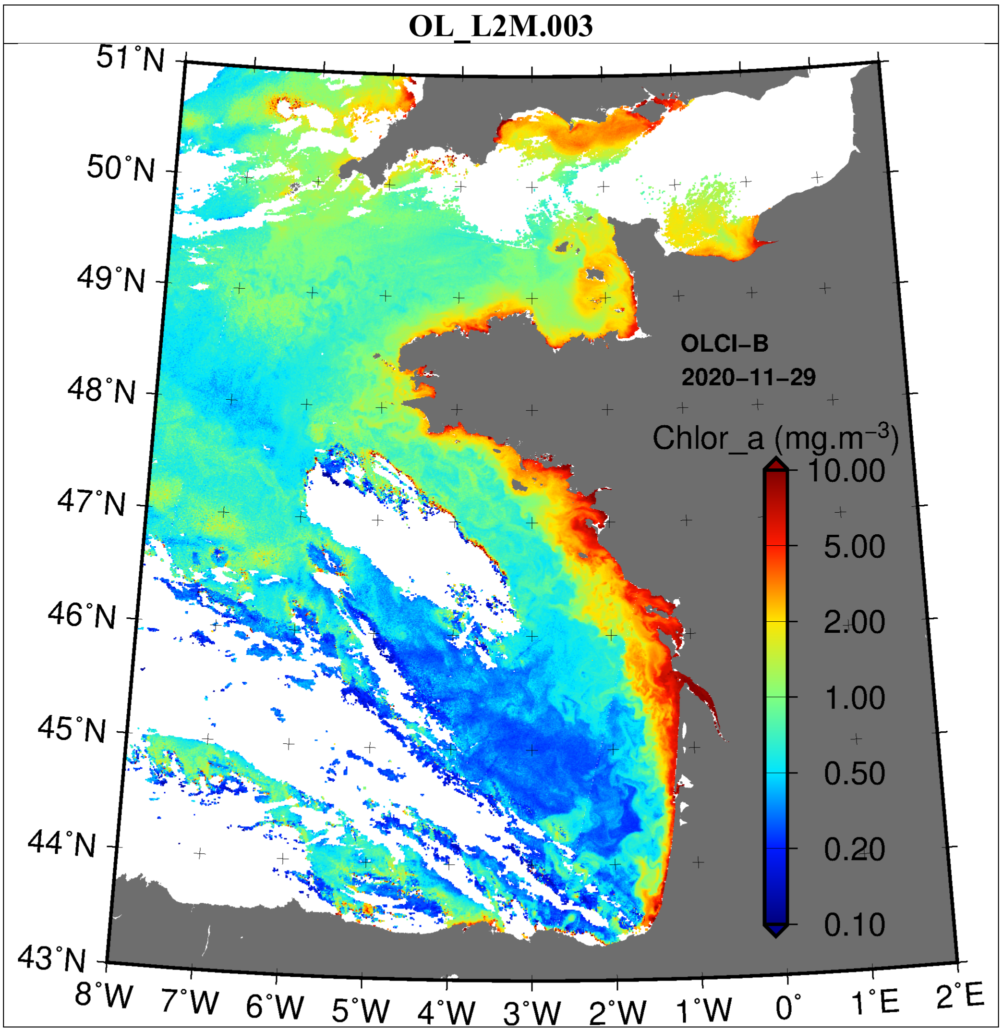


Figure 7: OC4ME Algal pigment concentrations with OL_L2M.003 for French west coast on 29 November 2020

5.2 Validations of SVC gains

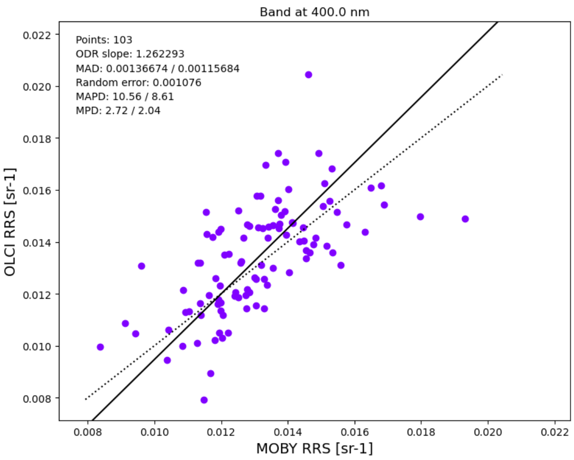
Verifications of new OLCI-A and -B SVC gains are performed with MOBY in situ radiometry measurements. Verifications and validations of the SVC gains are also accomplished with water reflectance time series and inter-comparisons with MODIS-A data over the oligotrophic South Pacific Gyre.

5.2.1 Verification with MOBY in situ radiometric measurements

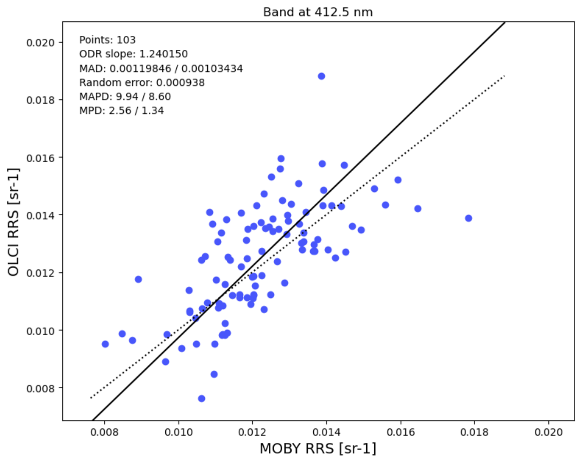
The goal of OLCI matchups with MOBY in situ measurements is to sanity check the System Vicarious Calibration process, as described in section 3.1, and to confirm the accuracy of the SVC gains. The results presented below are not OLCI validation but the SVC verification. MOBY measurements used in these verifications are significantly extended in comparison with the MOBY subset screened for the SVC gain retrieval.

The applied datasets and methodology are described in sections 4.1.1, 4.1.2.1, 4.2.1.

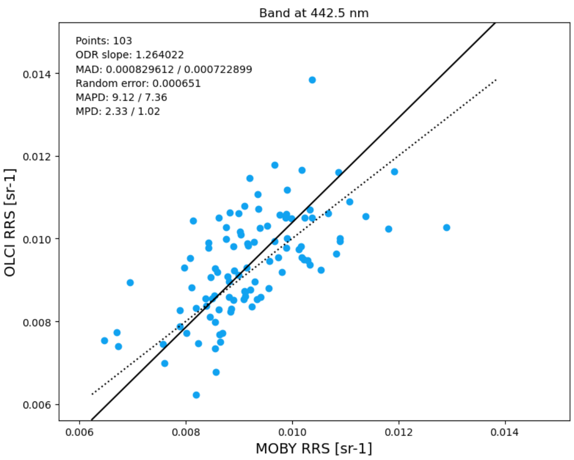
5.2.1.1 OLCI-A matchups



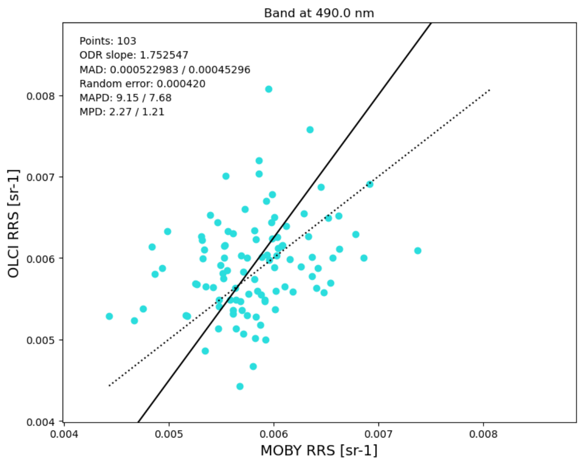
(a)



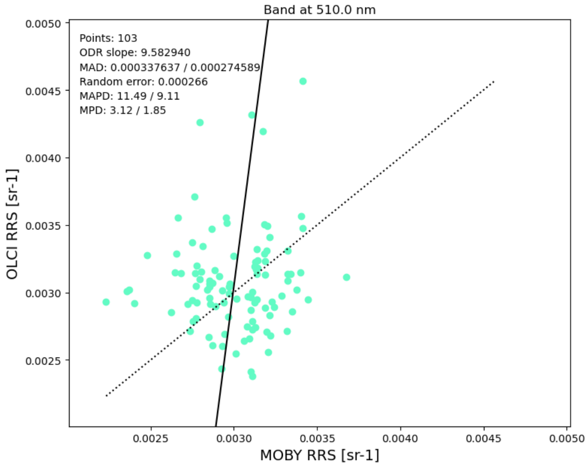
(b)



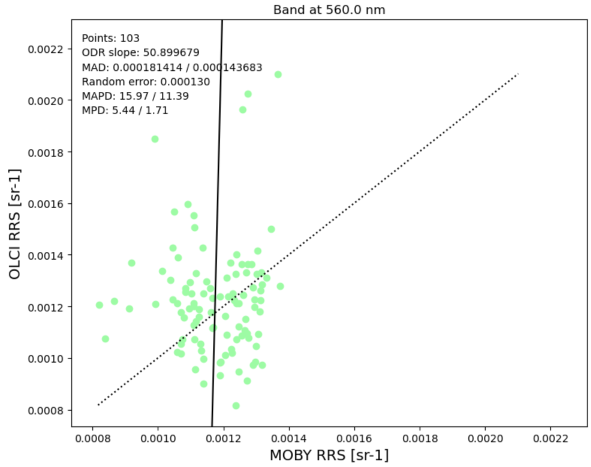
(c)



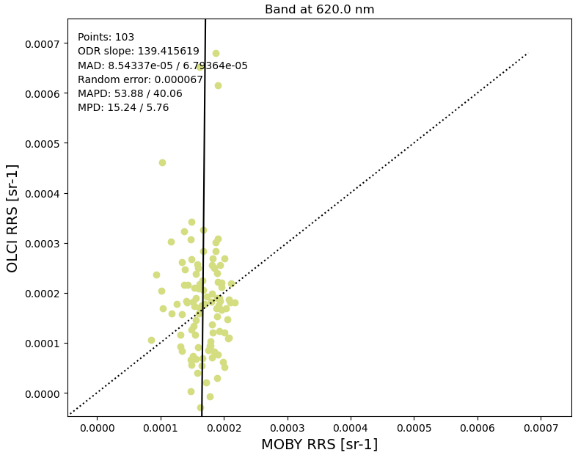
(d)


Band at 510.0 nm
Points: 103
ODR slope: 9.582940
MAD: 0.000337637 / 0.000274589
Random error: 0.000266
MAPD: 11.49 / 9.11
MPD: 3.12 / 1.85
OLCI RRS [sr-1]
MOBY RRS [sr-1]

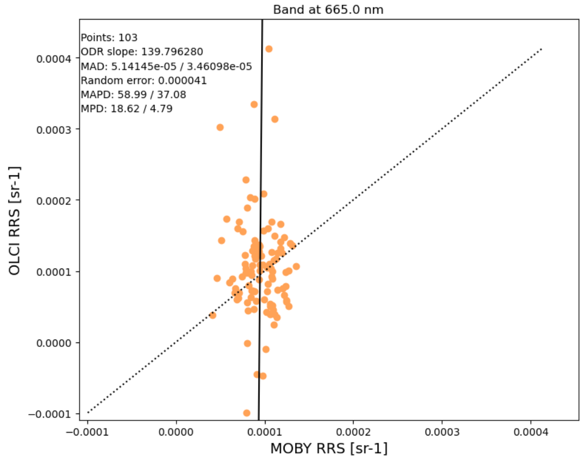
(e)


Band at 560.0 nm
Points: 103
ODR slope: 50.899679
MAD: 0.000181414 / 0.000143683
Random error: 0.000130
MAPD: 15.97 / 11.39
MPD: 5.44 / 1.71
OLCI RRS [sr-1]
MOBY RRS [sr-1]

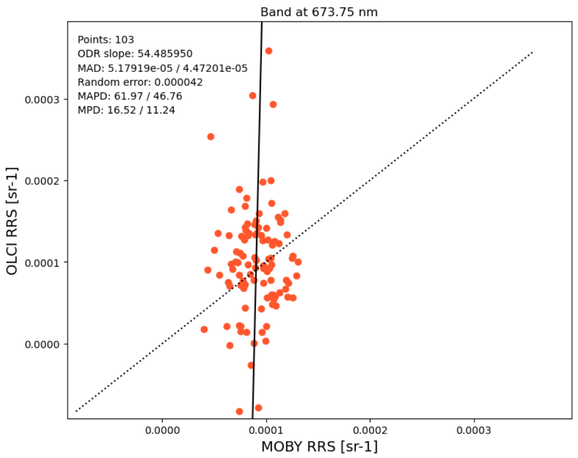
(f)


Band at 620.0 nm
Points: 103
ODR slope: 139.415619
MAD: 8.54337e-05 / 6.79364e-05
Random error: 0.000067
MAPD: 53.88 / 40.06
MPD: 15.24 / 5.76
OLCI RRS [sr-1]
MOBY RRS [sr-1]

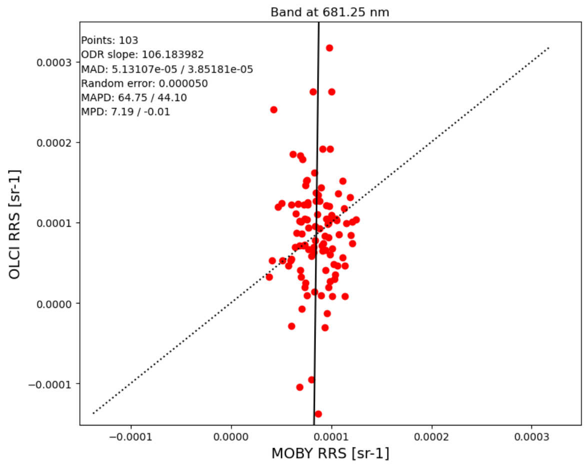
(g)


Band at 665.0 nm
Points: 103
ODR slope: 139.796280
MAD: 5.14145e-05 / 3.46098e-05
Random error: 0.000041
MAPD: 58.99 / 37.08
MPD: 18.62 / 4.79
OLCI RRS [sr-1]
MOBY RRS [sr-1]

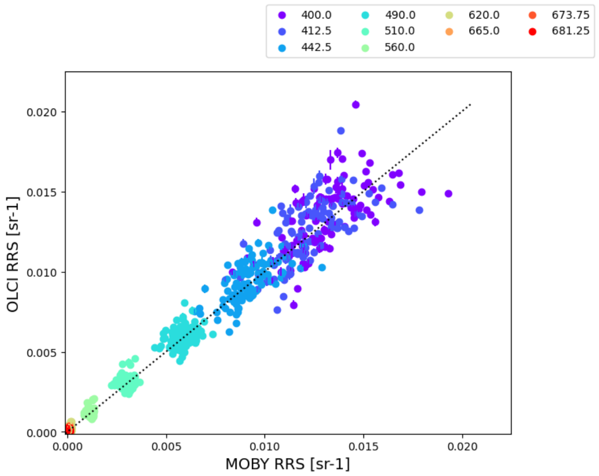
(h)


Band at 673.75 nm
Points: 103
ODR slope: 54.485950
MAD: 5.17919e-05 / 4.47201e-05
Random error: 0.000042
MAPD: 61.97 / 46.76
MPD: 16.52 / 11.24
OLCI RRS [sr-1]
MOBY RRS [sr-1]

(i)


Band at 681.25 nm
Points: 103
ODR slope: 106.183982
MAD: 5.13107e-05 / 3.85181e-05
Random error: 0.000050
MAPD: 64.75 / 44.10
MPD: 7.19 / -0.01
OLCI RRS [sr-1]
MOBY RRS [sr-1]

(j)



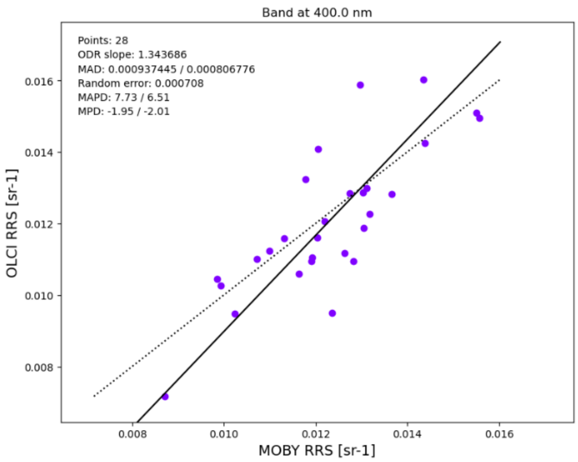
(k)

Figure 8: OLCI-A verification with MOBY Rrs at all VIS wavelengths, including Raman correction

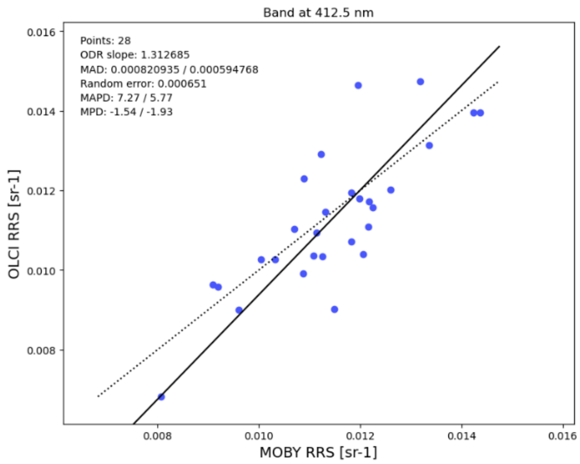
Wavelength	***400***	***412.5***	***442.5***	***490***	***510***	***560***	***620***	***665***
Median %D	2.04	1.34	1.02	1.21	1.85	1.71	5.76	4.79
Wavelength	***673.75***	***681.25***	***708.75***	***753.75***	***778.75***	***865***	***885***	***1020***
Median %D	11.24	-0.01	-	-	-	-	-	-

Table 5: Median percentage difference between MOBY and OLCI-A Rrs in the wavelength range of MOBY hyperspectral data

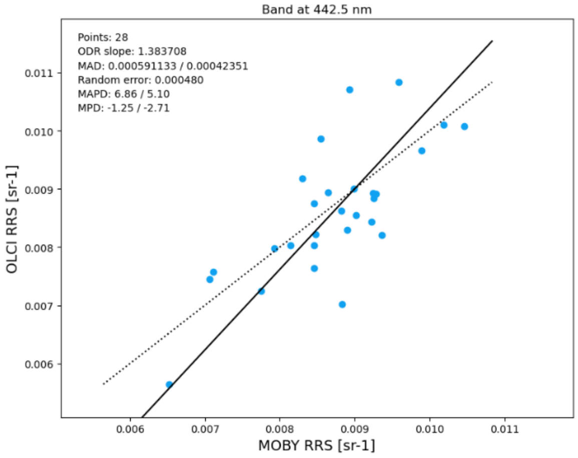
5.2.1.2 OLCI-B matchups

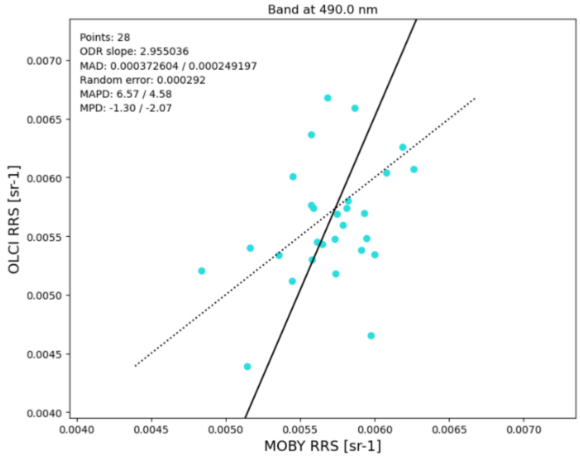


(a)

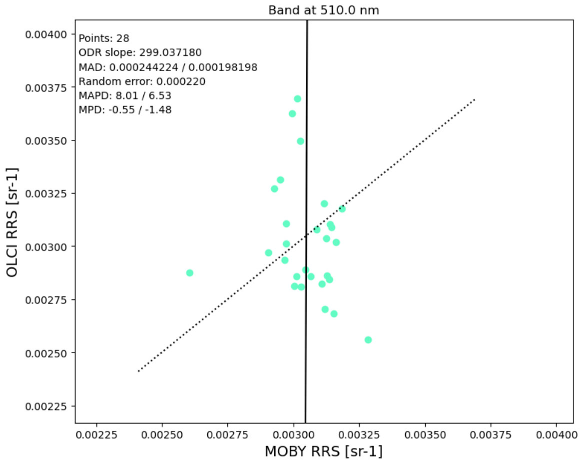


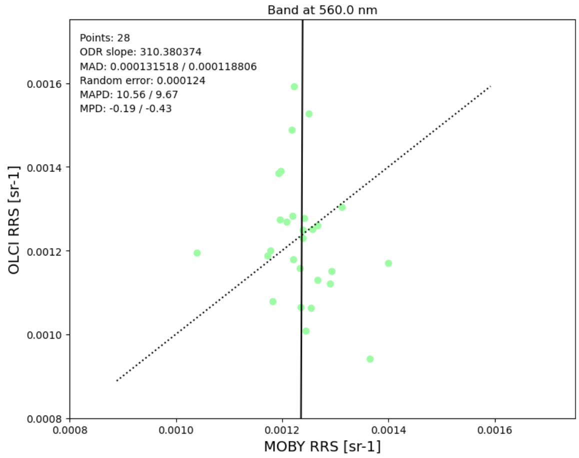
(b)


Band at 442.5 nm
Points: 28
ODR slope: 1.383708
MAD: 0.000591133 / 0.00042351
Random error: 0.000480
MAPD: 6.86 / 5.10
MPD: -1.25 / -2.71
OLCI RRS [sr-1]
MOBY RRS [sr-1]

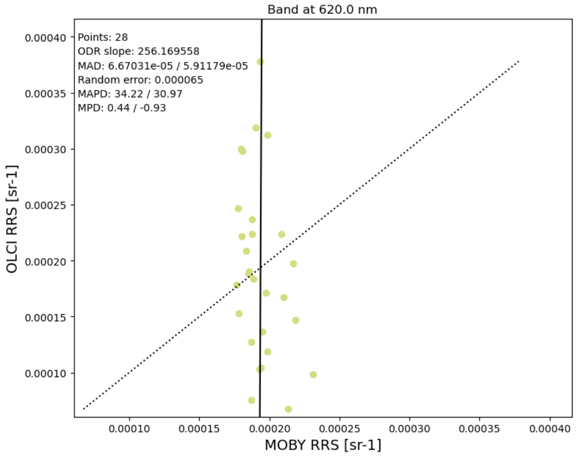

Band at 490.0 nm
Points: 28
ODR slope: 2.955036
MAD: 0.000372604 / 0.000249197
Random error: 0.000292
MAPD: 6.57 / 4.58
MPD: -1.30 / -2.07
OLCI RRS [sr-1]
MOBY RRS [sr-1]

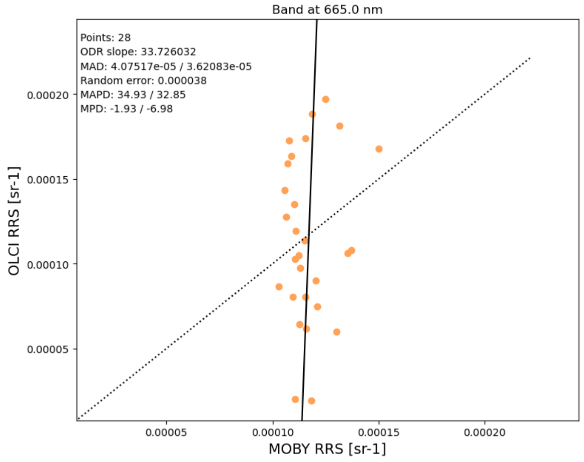
(c) (d)


Band at 510.0 nm
Points: 28
ODR slope: 299.037180
MAD: 0.000244224 / 0.000198198
Random error: 0.000220
MAPD: 8.01 / 6.53
MPD: -0.55 / -1.48
OLCI RRS [sr-1]
MOBY RRS [sr-1]

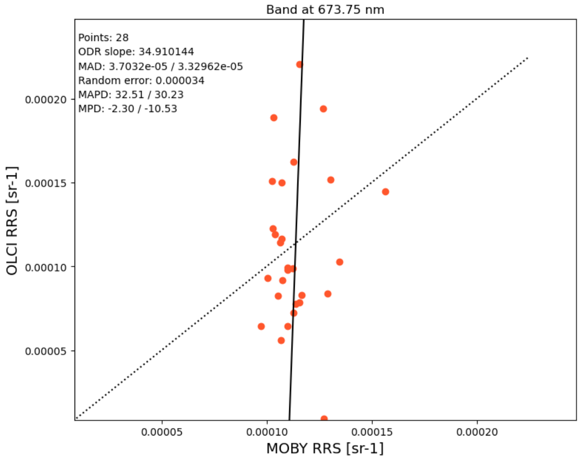

Band at 560.0 nm
Points: 28
ODR slope: 310.380374
MAD: 0.000131518 / 0.000118806
Random error: 0.000124
MAPD: 10.56 / 9.67
MPD: -0.19 / -0.43
OLCI RRS [sr-1]
MOBY RRS [sr-1]

(e) (f)

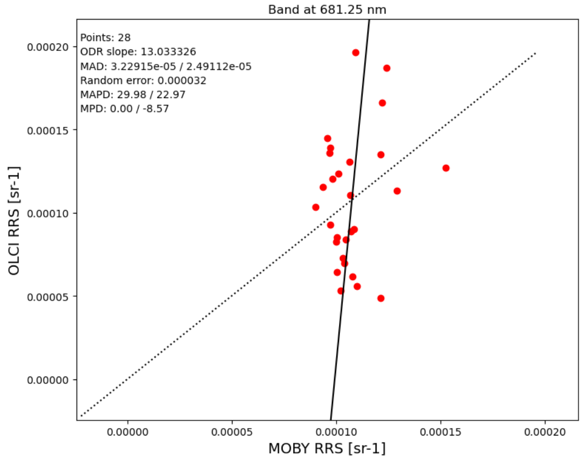

Band at 620.0 nm
Points: 28
ODR slope: 256.169558
MAD: 6.67031e-05 / 5.91179e-05
Random error: 0.000065
MAPD: 34.22 / 30.97
MPD: 0.44 / -0.93
OLCI RRS [sr-1]
MOBY RRS [sr-1]


Band at 665.0 nm
Points: 28
ODR slope: 33.726032
MAD: 4.07517e-05 / 3.62083e-05
Random error: 0.000038
MAPD: 34.93 / 32.85
MPD: -1.93 / -6.98
OLCI RRS [sr-1]
MOBY RRS [sr-1]

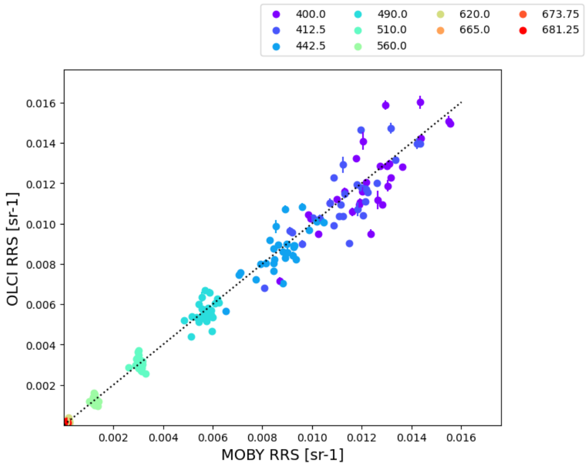
(g) (h)



(i)



(j)



(k)

Figure 9: OLCI-B verification with MOBY Rrs at all VIS wavelengths, including Raman correction

Wavelength	*400*	*412.5*	*442.5*	*490*	*510*	*560*	*620*	*665*
Median %D	-2.01	-1.93	-2.71	-2.07	-1.48	-0.43	-0.93	-6.98
Wavelength	*673.75*	*681.25*	*708.75*	*753.75*	*778.75*	*865*	*885*	*1020*
Median %D	-10.53	-8.57	-	-	-	-	-	-

Table 6: Median percentage difference between MOBY in situ and OLCI-B Rrs in the wavelength range of MOBY hyperspectral data

5.2.2 Verification and validation with mission time series over the South Pacific Gyre

The goal of OLCI-A and -B inter-comparisons in the South Pacific Gyre is to verify the consistency and long-term stability of OLCI measurements in the stable oligotrophic gyre and to validate their accuracy against MODIS-Aqua.

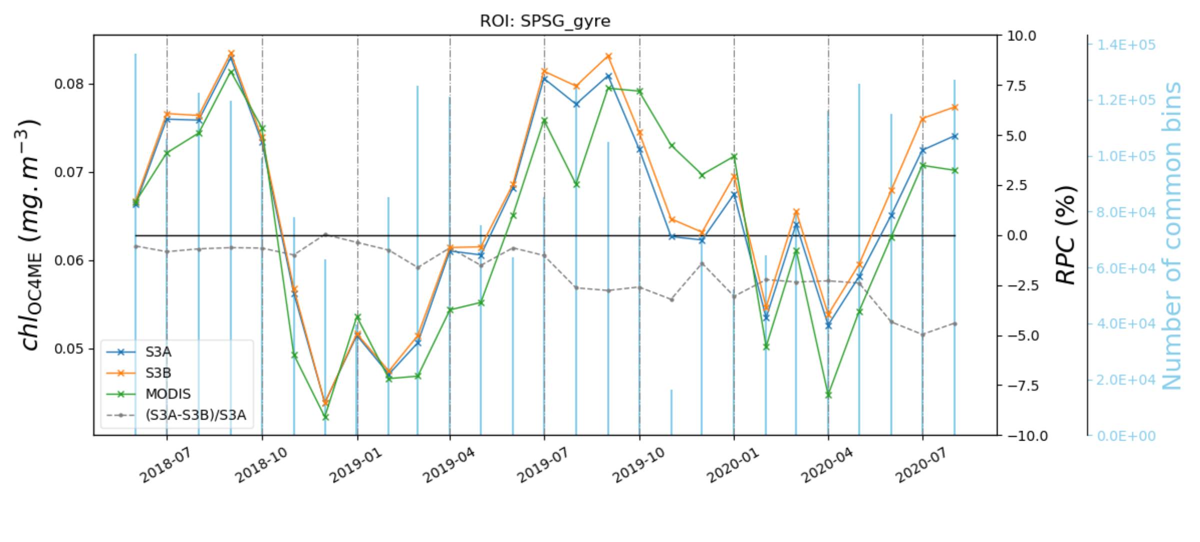
The analysis is performed with L3 time series covering four first days of each month with common bins in the SPG area between OLCI-A and OLCI-B, as well as between OLCI-A, -B, and MODIS, when corresponding MODIS bands are available. Within those common bins, the mean of products (Chl and Rhow) is computed.

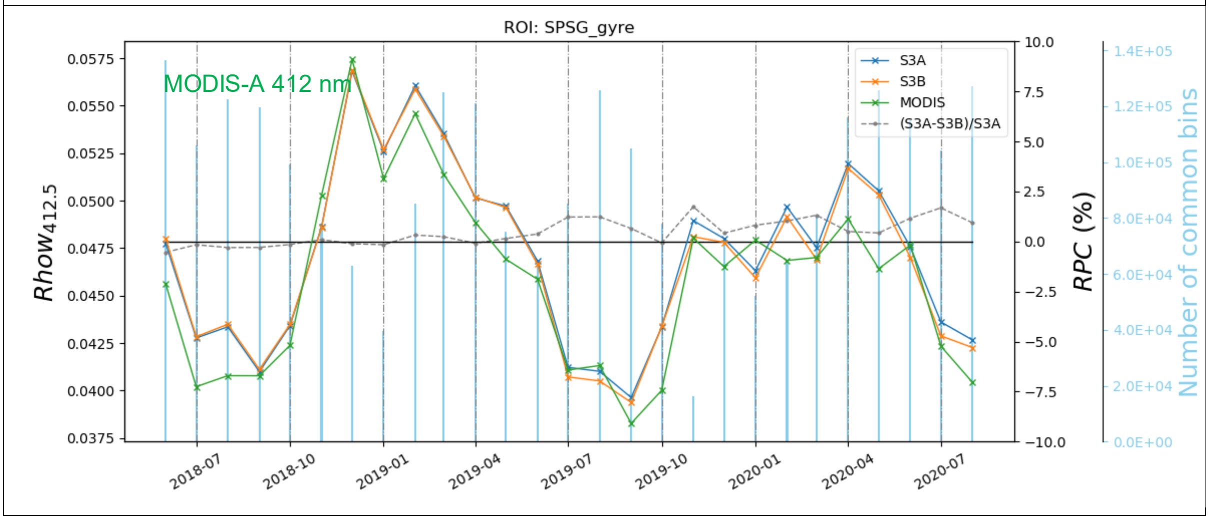
The applied datasets and methodology are described in sections 4.1.1, 4.1.3, 4.2.2. On the plots, grey dashed-lines denote Relative Percentage Change (RPC):

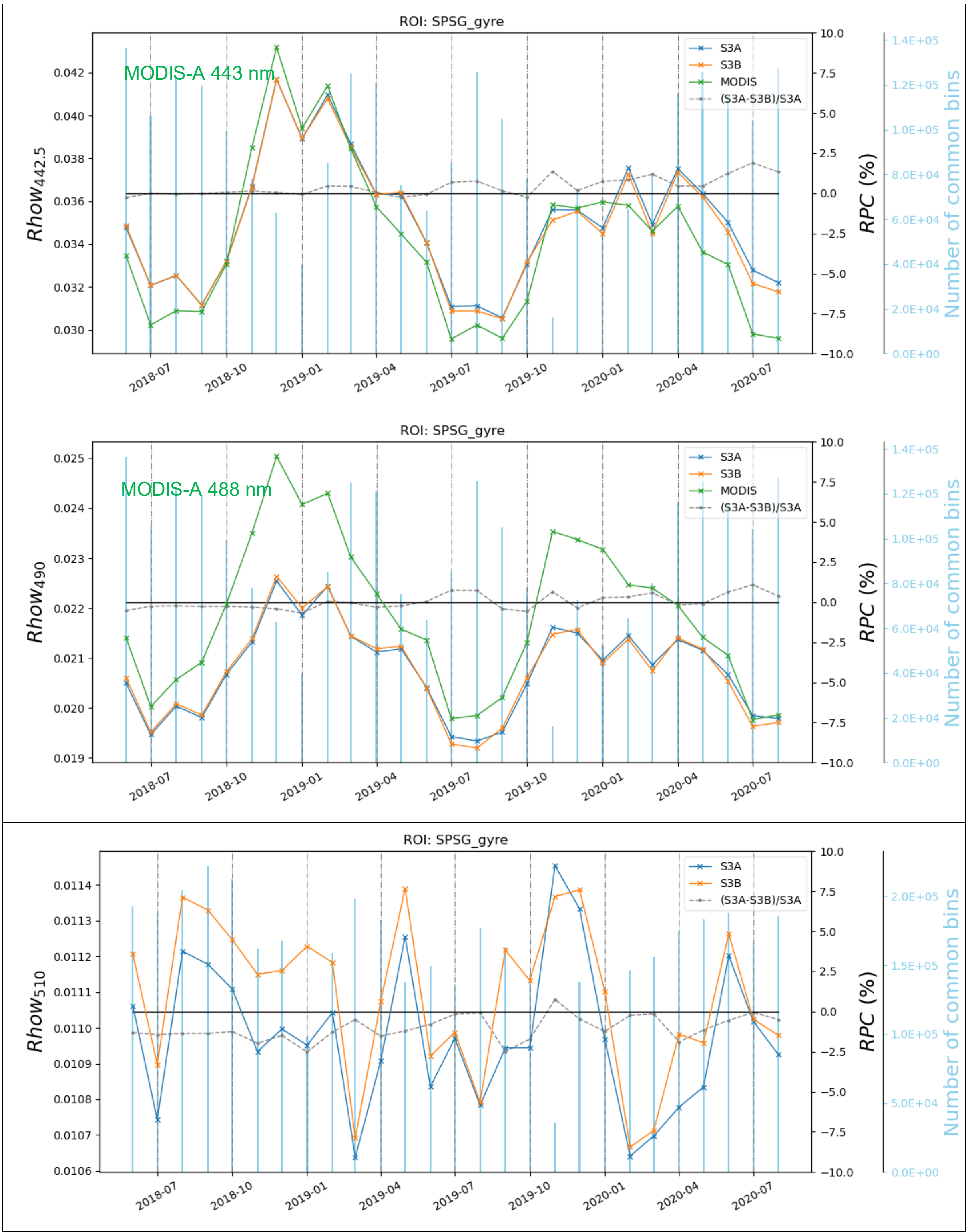
$$RPC = \frac{S3A - S3B}{S3A} * 100$$

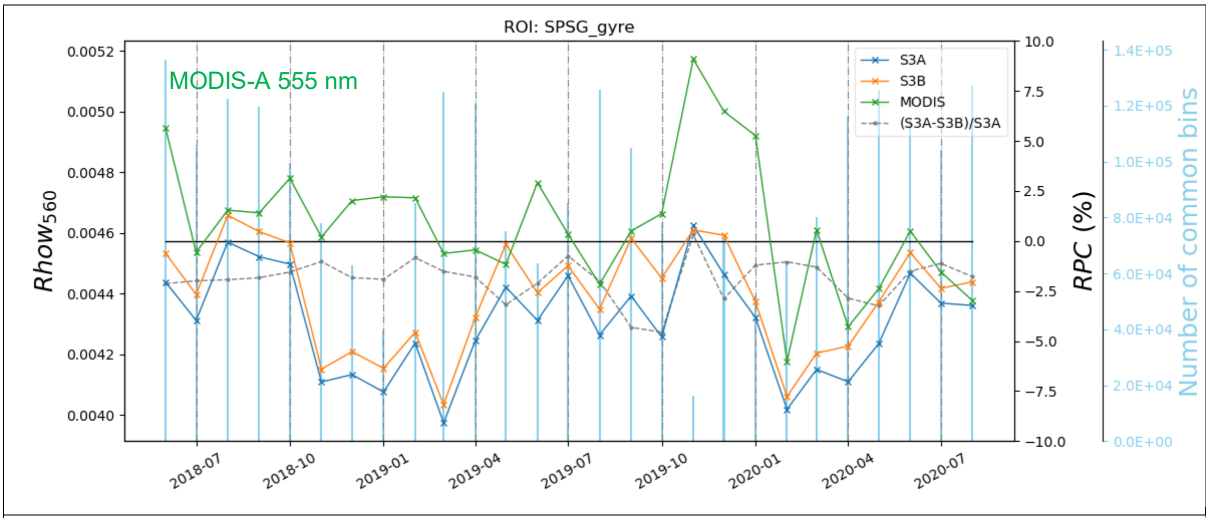
The blue barplot provides the numbers of common bins between OLCI-A and OLCI-B, and MODIS, when relevant.

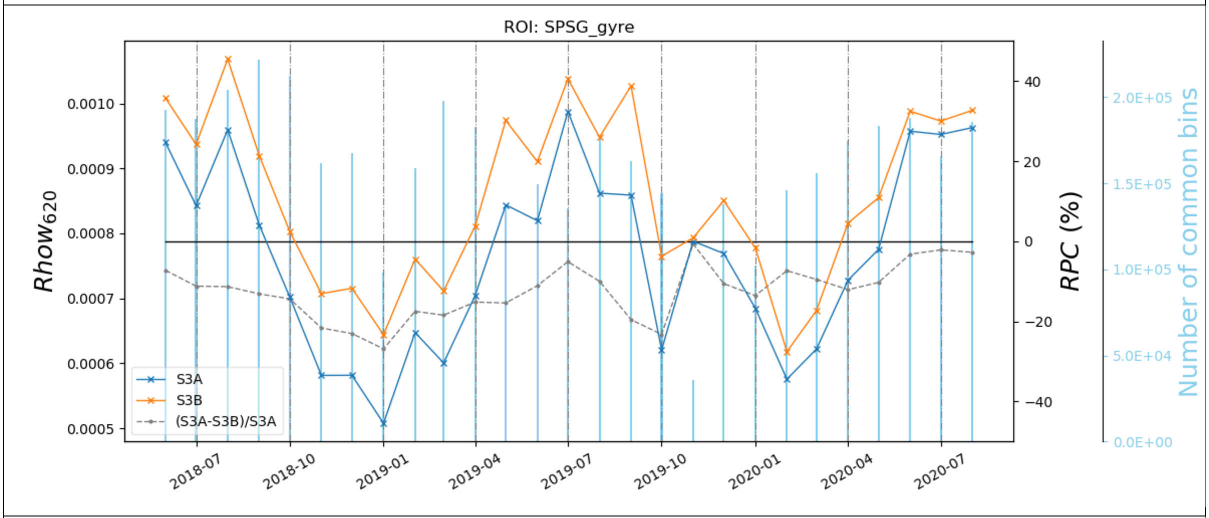
Particularly interesting is the time period June to October 2018 when Sentinel-3B flew in tandem with Sentinel-3A, 30 seconds apart (RD-12). In this period, the ground coverage between OLCI-A and OLCI-B was almost identical, allowing exact inter-comparisons between mission products.

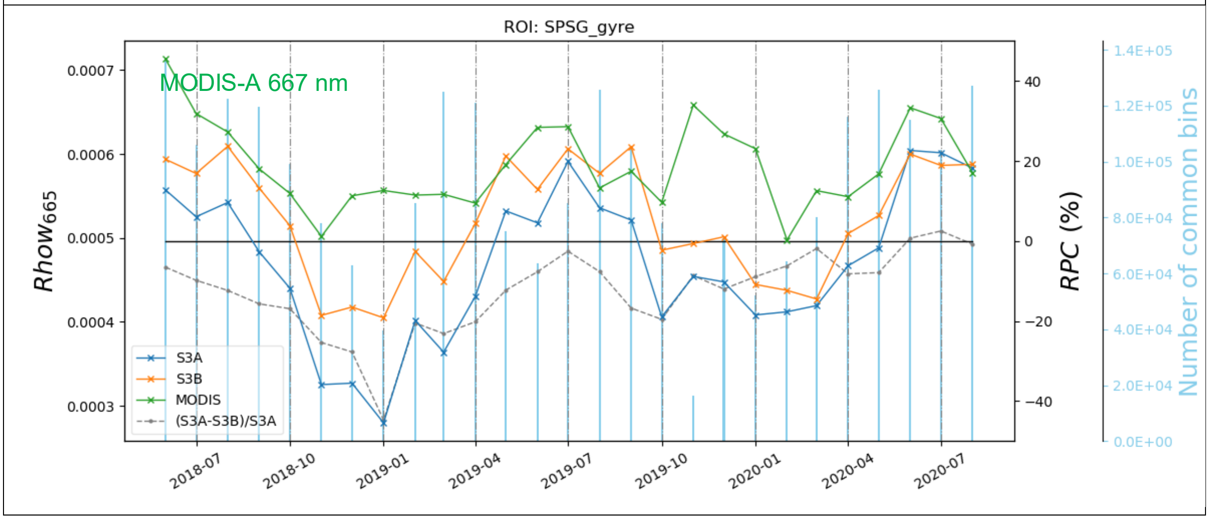





ROI: SPSG_gyre
MODIS-A 443 nm
S3A
S3B
MODIS
(S3A-S3B)/S3A
Rhow442.5
RPC (%)
Number of common bins
ROI: SPSG_gyre
MODIS-A 488 nm
S3A
S3B
MODIS
(S3A-S3B)/S3A
Rhow490
RPC (%)
Number of common bins
ROI: SPSG_gyre
S3A
S3B
(S3A-S3B)/S3A
Rhow510
RPC (%)
Number of common bins
2018-07
2018-10
2019-01
2019-04
2019-07
2019-10
2020-01
2020-04
2020-07


ROI: SPSG_gyre
MODIS-A 555 nm
S3A
S3B
MODIS
(S3A-S3B)/S3A
Rhow560
RPC (%)
Number of common bins


ROI: SPSG_gyre
S3A
S3B
(S3A-S3B)/S3A
Rhow620
RPC (%)
Number of common bins


ROI: SPSG_gyre
MODIS-A 667 nm
S3A
S3B
MODIS
(S3A-S3B)/S3A
Rhow665
RPC (%)
Number of common bins

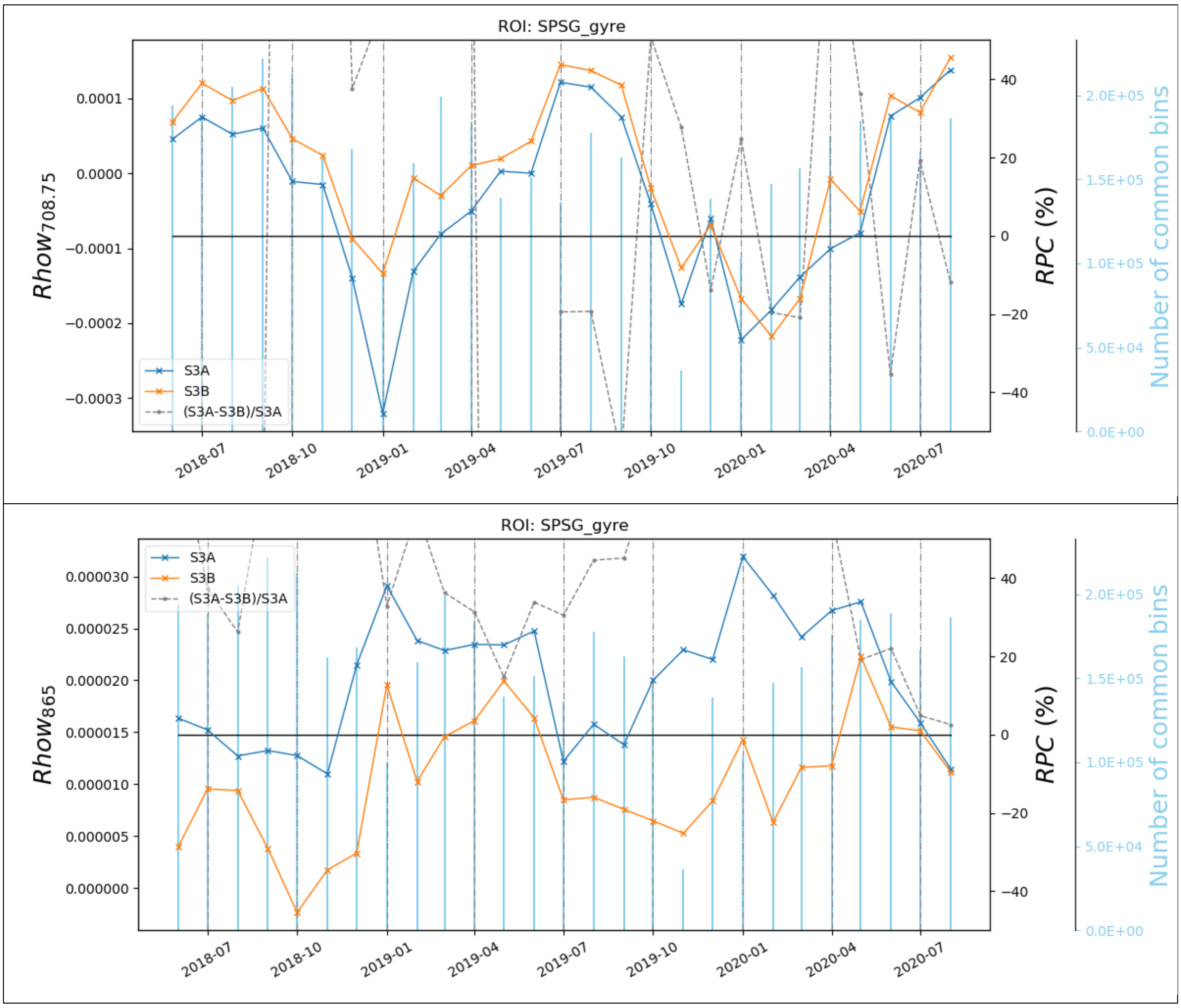


Figure 10: SPG time series inter-comparison between OLCI-A, OLCI-B and MODIS-Aqua

5.3 Water reflectance validations with in situ AERONET-OC

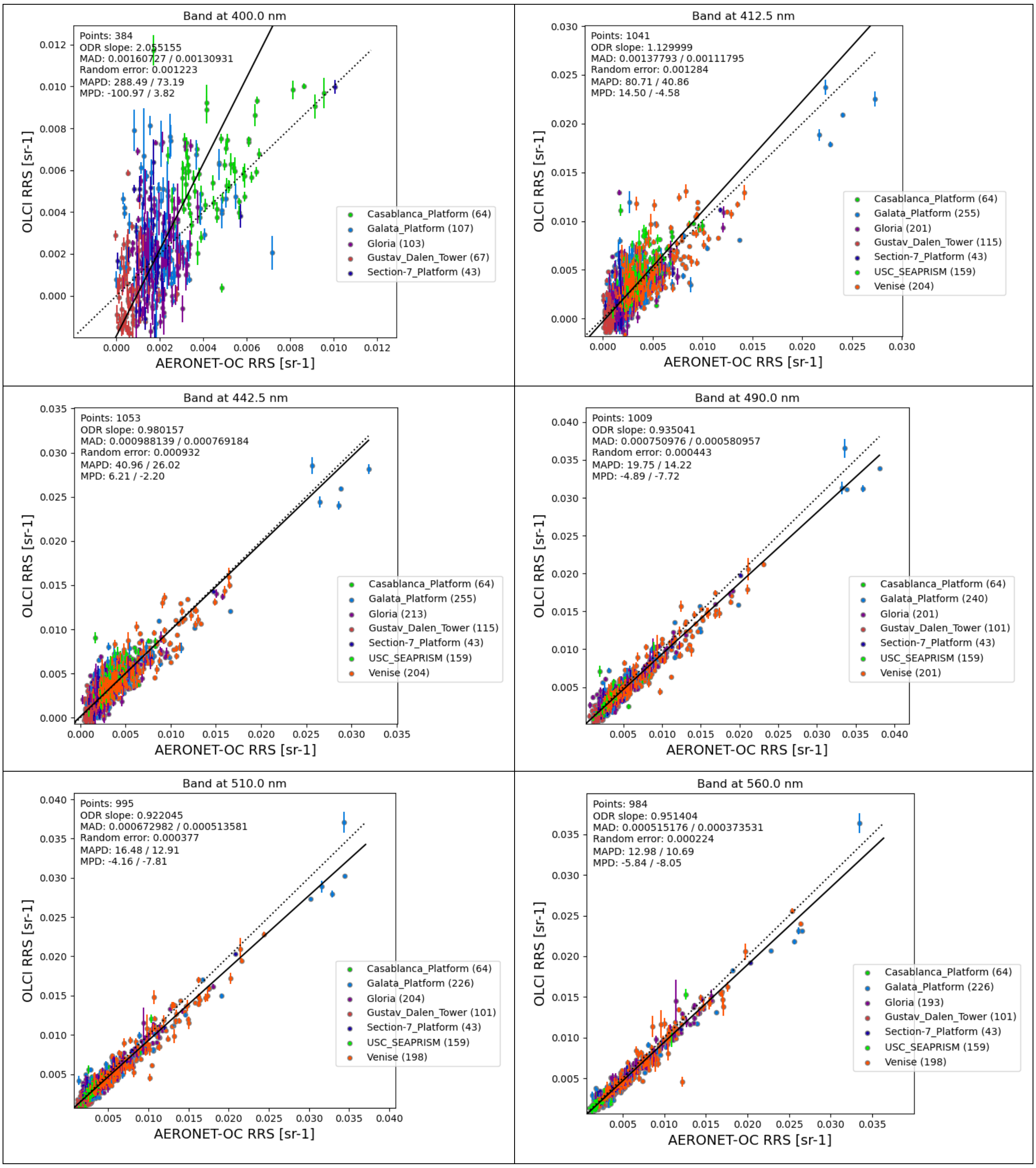
AERONET-OC radiometric measurements constitute the major OLCI operational in situ validation source of fiducial quality (RD-36, RD-37). AERONET-OC validations provide an independent evaluation of OLCI-A and OLCI-B product uncertainties.

It is important to repeat that AERONET-OC sites are set in coastal locations and frequently in complex waters. Out of the seven sites used in the validations below, only Casablanca Platform is located in oligotrophic-mesotrophic waters. Venise location is in moderately sediment-dominated waters, Gloria is in coloured dissolved organic matter (CDOM) and sediment-dominated waters, and Gustav Dalen is in highly CDOM-dominated waters.

Therefore, the results of the following validations reflect OLCI algorithm performance in those specific water regimes and not in open oceanic waters.

The applied datasets and methodology are described in sections 4.1.1, 4.1.2.2, 4.2.1.

5.3.1 OLCI-A validations



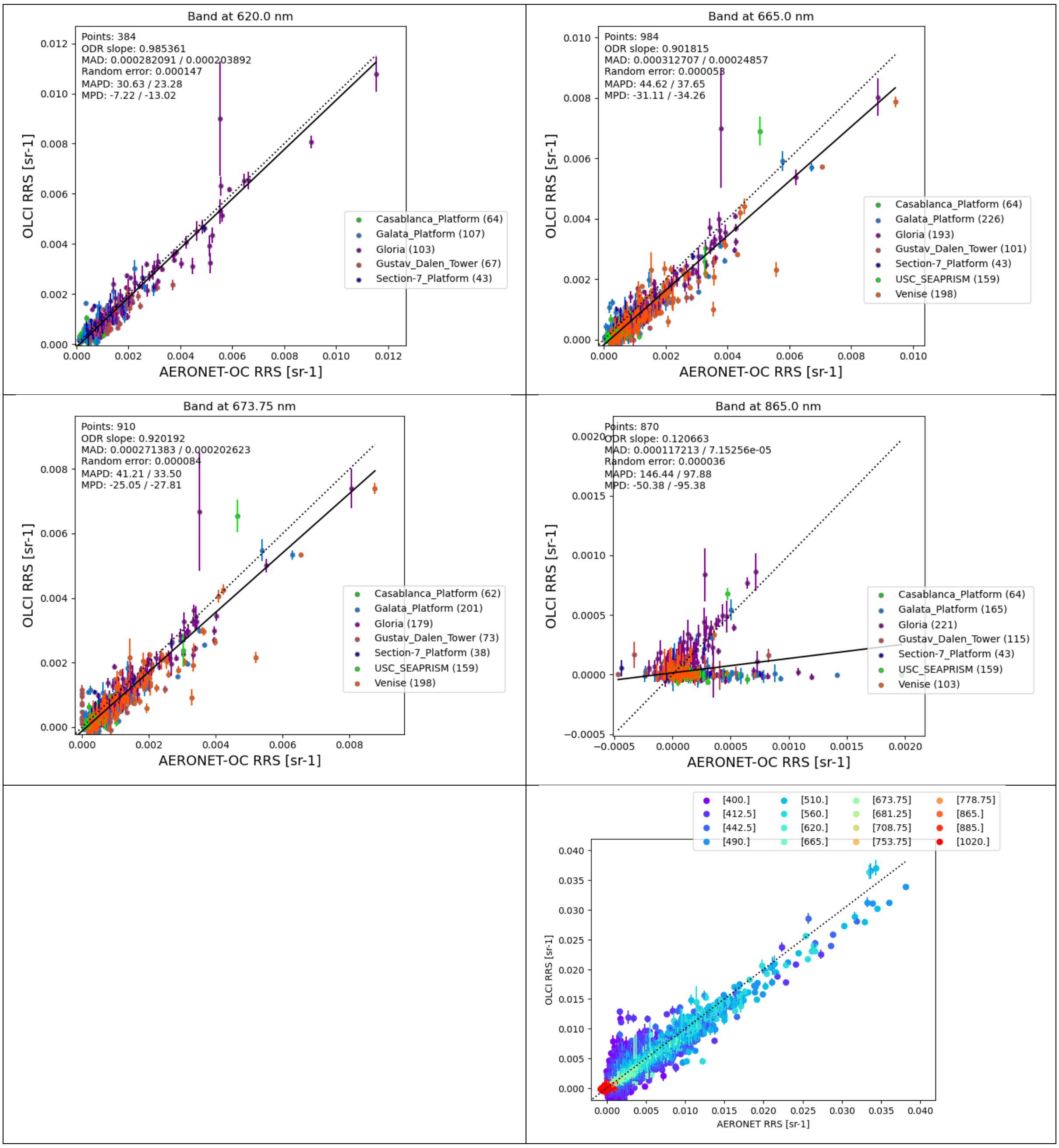
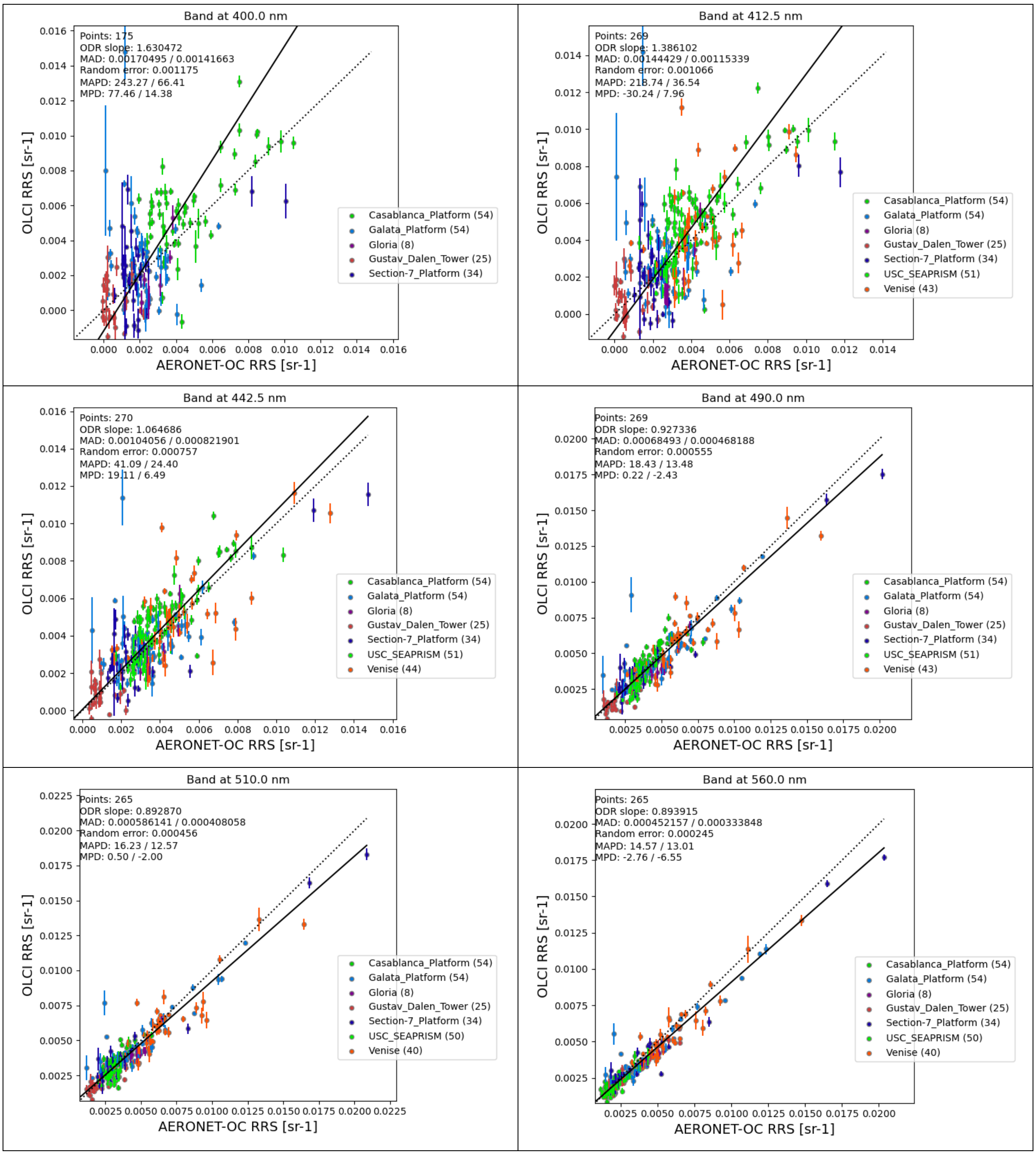


Figure 11: OLCI-A - AERONET-OC match-ups

Wavelength	*400*	*412.5*	*442.5*	*490*	*510*	*560*	*620*	*665*
Median %D	3.82	-4.58	-2.20	-7.72	-7.81	-8.05	-13.02	-34.26
Wavelength	*673.75*	*681.25*	*708.75*	*753.75*	*778.75*	*865*	*885*	*1020*
Median %D	-27.81	-	-	-	-68.39	-95.38	-	-58.14

Table 7: Median percentage difference between AERONET-OC in situ measurements and OLCI-A Rrs at all available AERONET-OC wavelengths

5.3.2 OLCI-B validations



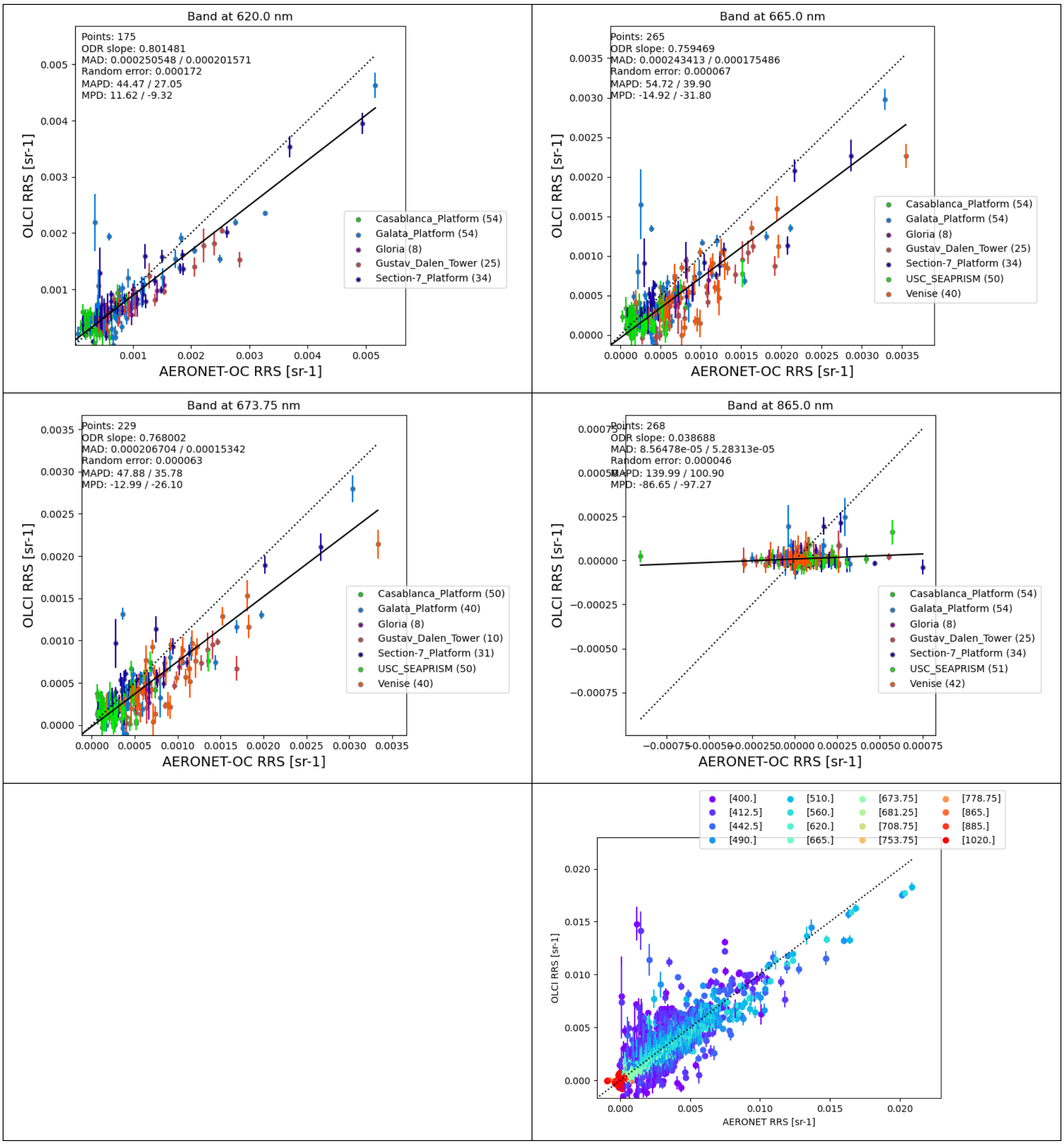


Figure 12: OLCI-B - AERONET-OC match-ups

Wavelength	*400*	*412.5*	*442.5*	*490*	*510*	*560*	*620*	*665*
Median %D	14.38	7.96	6.49	-2.43	-2.00	-6.55	-9.32	-31.80
Wavelength	***673.75***	***681.25***	***708.75***	***753.75***	***778.75***	***865***	***885***	***1020***
Median %D	-26.10	-	-	-	-78.87	-97.27	-	-92.92

Table 8: Median percentage difference between AERONET-OC in situ measurements and OLCI-B Rrs at all available AERONET-OC wavelengths

5.4 Water reflectance validations with mission inter-comparisons

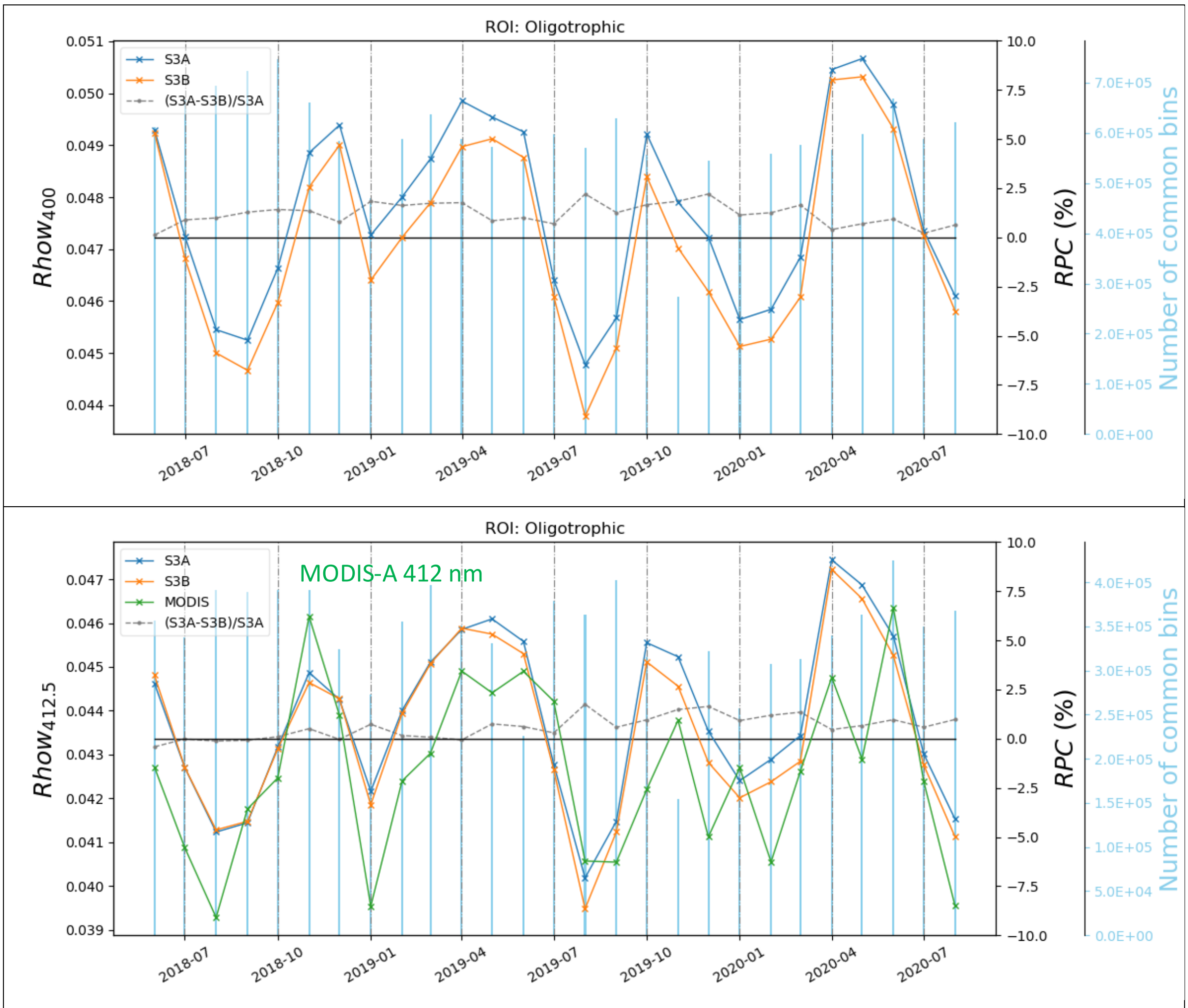
Inter-comparisons of mission time series allow for a large-scale global analysis of OLCI products and validation of multi-mission consistency and stability. The comparisons are performed with L3 time series covering four first days of each month with common bins between OLCI-A and OLCI-B, as well as between OLCI-A, -B, and MODIS-Aqua, when corresponding MODIS bands are available. The analyses are stratified across oligotrophic, mesotrophic and eutrophic waters to identify processor behaviour separately across water regimes of different complexity.

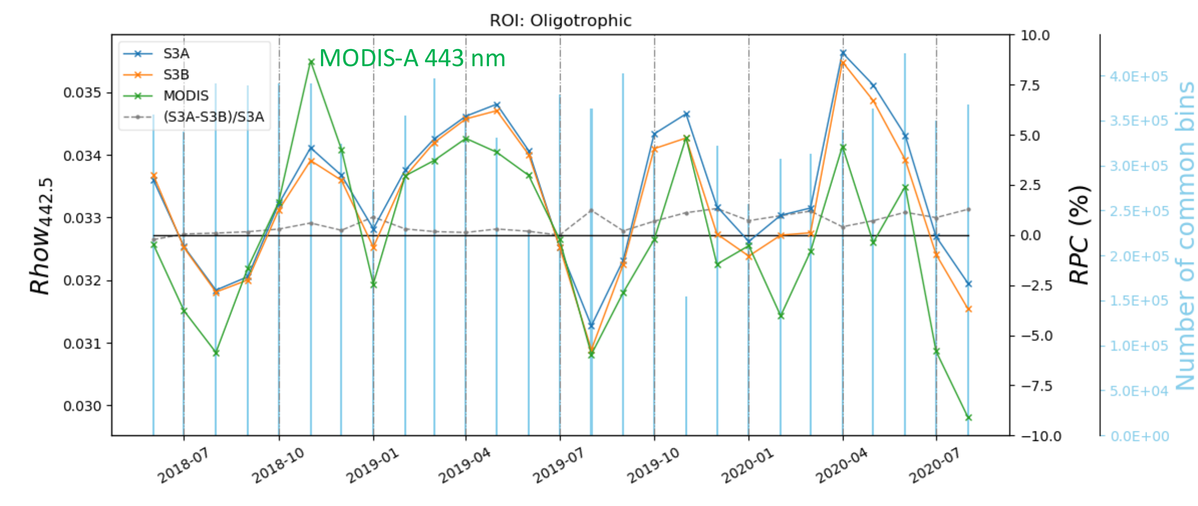
It should be noted that MODIS spectral bands are different from OLCI's and the differences in radiometric products are expected and should be different at different water trophic levels.

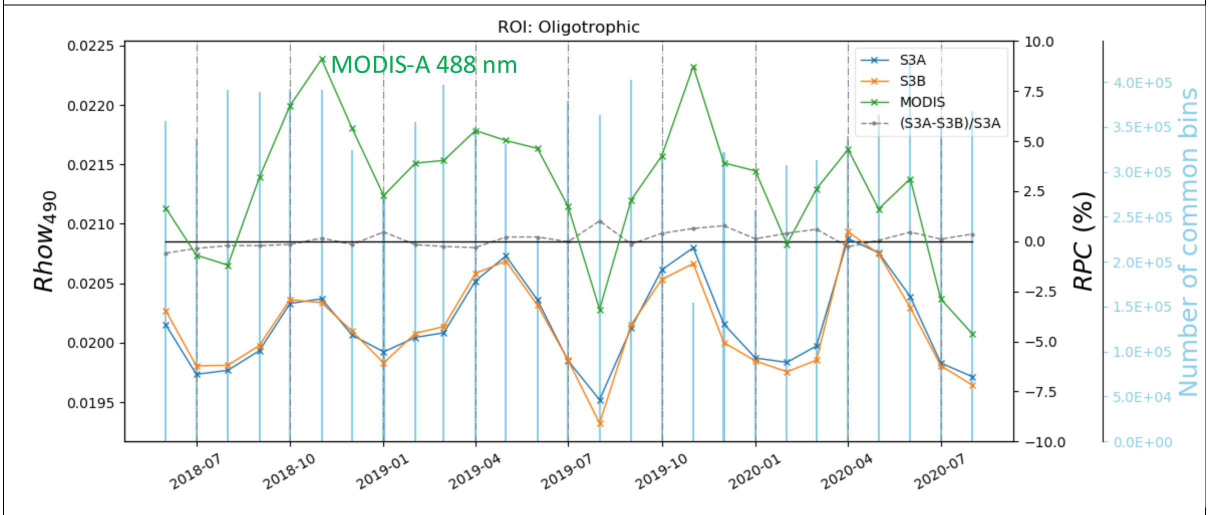
The time period June to October 2018 of Sentinel-3A and -3B tandem phase allows for almost exact inter-comparison between OLCI-A and -B products because the two instruments are covering the same ground track 30 seconds apart (RD-12).

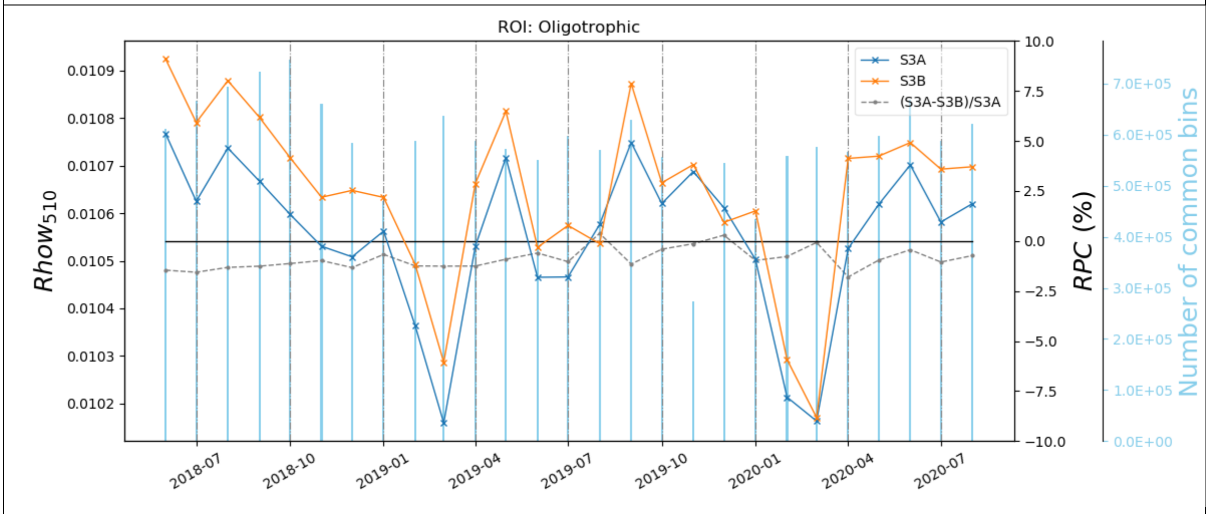
The applied datasets and methodology are described in sections 4.1.1, 4.1.3, 4.2.2.

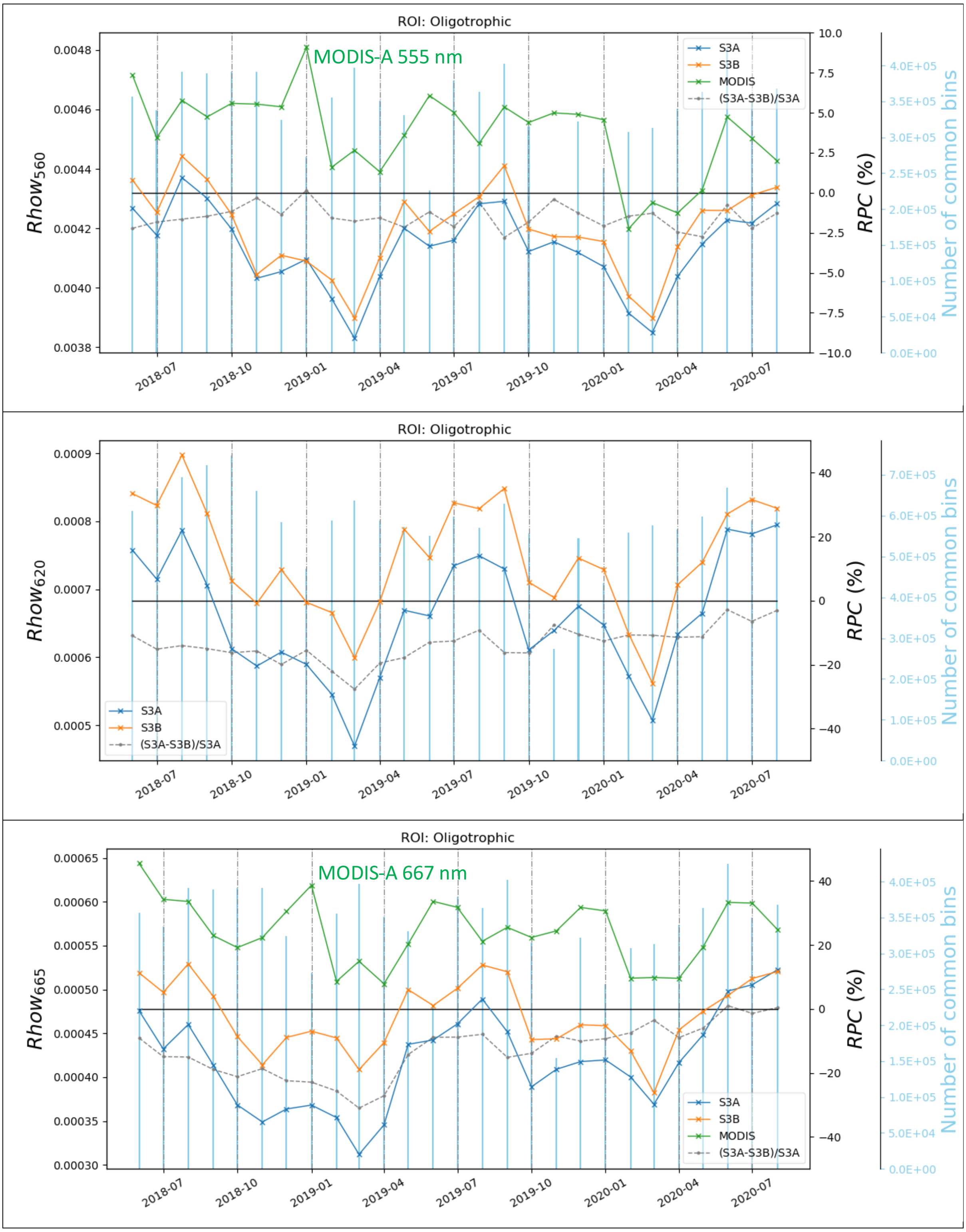
5.4.1 Oligotrophic waters




ROI: Oligotrophic
MODIS-A 443 nm
S3A
S3B
MODIS
(S3A-S3B)/S3A
$Rhow_{442.5}$
RPC (%)
Number of common bins


ROI: Oligotrophic
MODIS-A 488 nm
S3A
S3B
MODIS
(S3A-S3B)/S3A
$Rhow_{490}$
RPC (%)
Number of common bins


ROI: Oligotrophic
S3A
S3B
(S3A-S3B)/S3A
$Rhow_{510}$
RPC (%)
Number of common bins


ROI: Oligotrophic
MODIS-A 555 nm
S3A
S3B
MODIS
(S3A-S3B)/S3A
Rhow560
RPC (%)
Number of common bins
ROI: Oligotrophic
S3A
S3B
(S3A-S3B)/S3A
Rhow620
RPC (%)
Number of common bins
ROI: Oligotrophic
MODIS-A 667 nm
S3A
S3B
MODIS
(S3A-S3B)/S3A
Rhow665
RPC (%)
Number of common bins

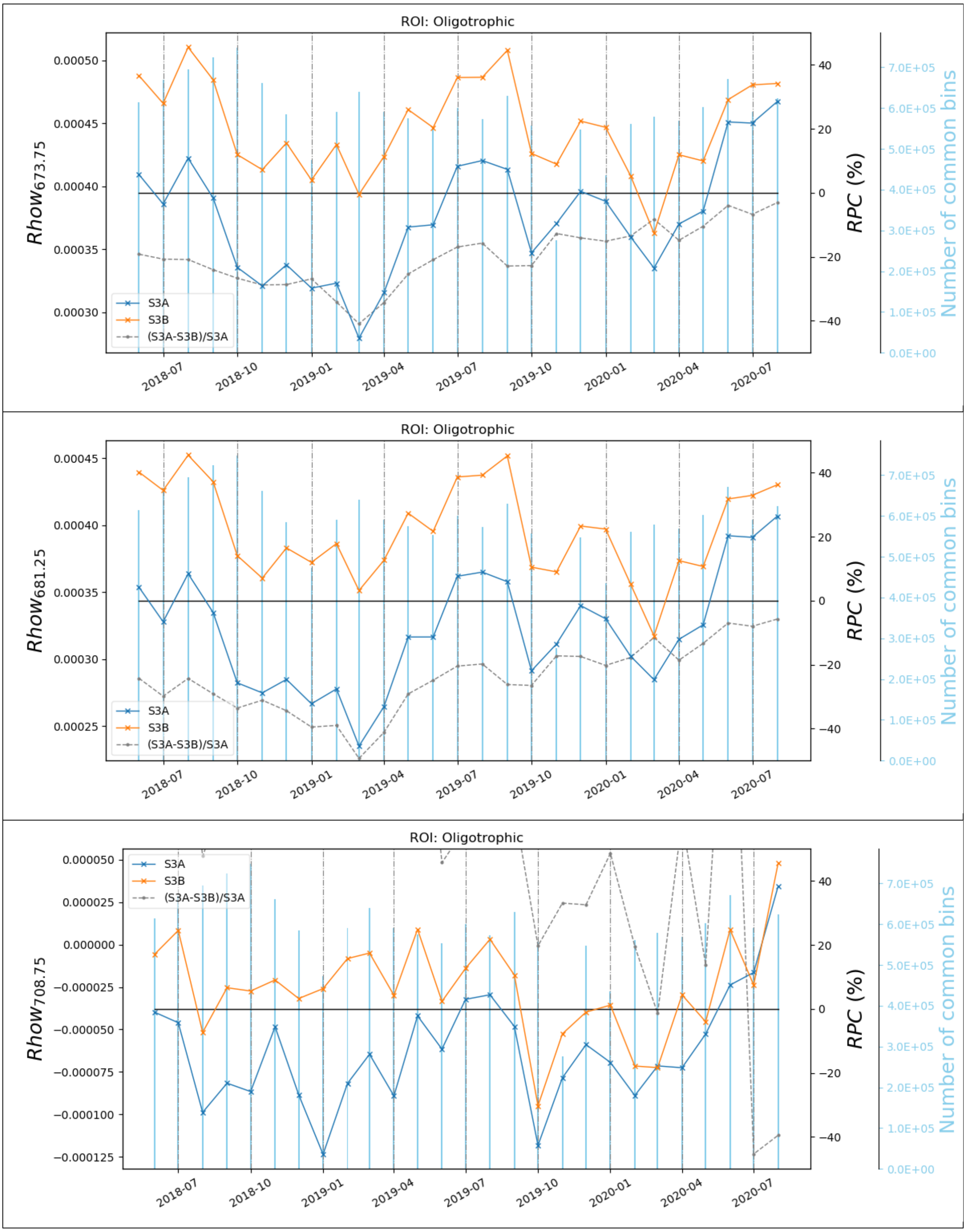
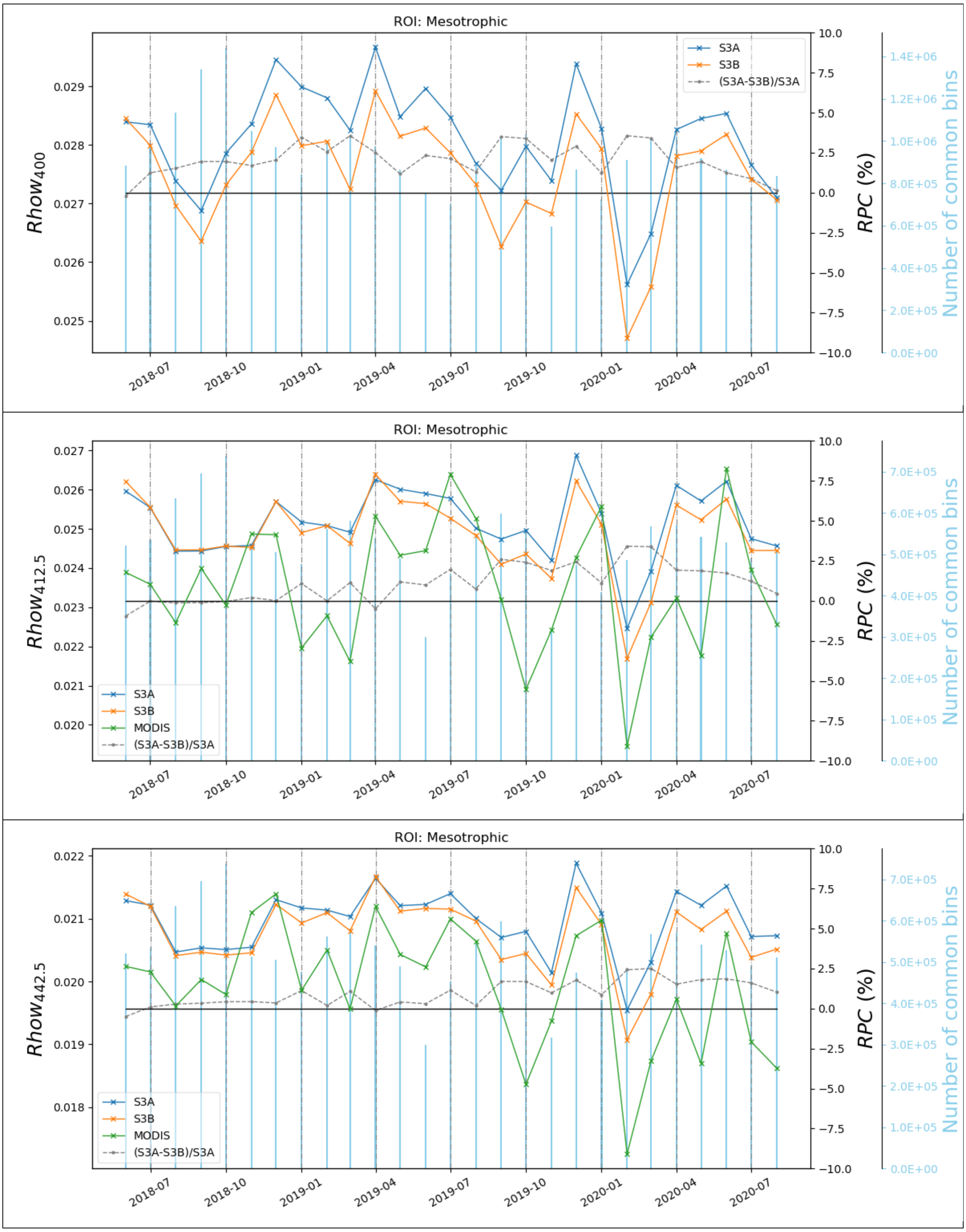
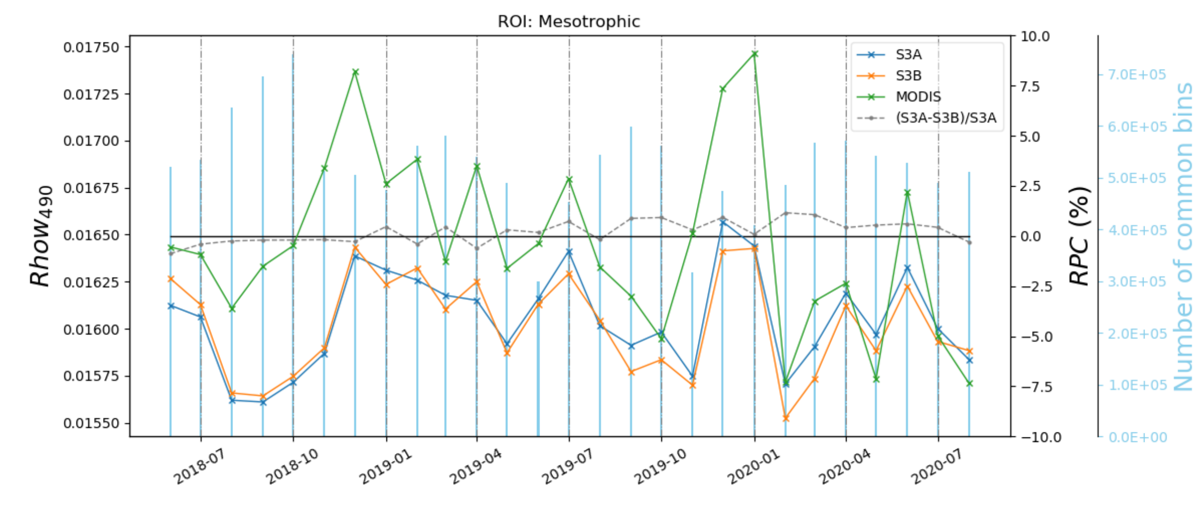
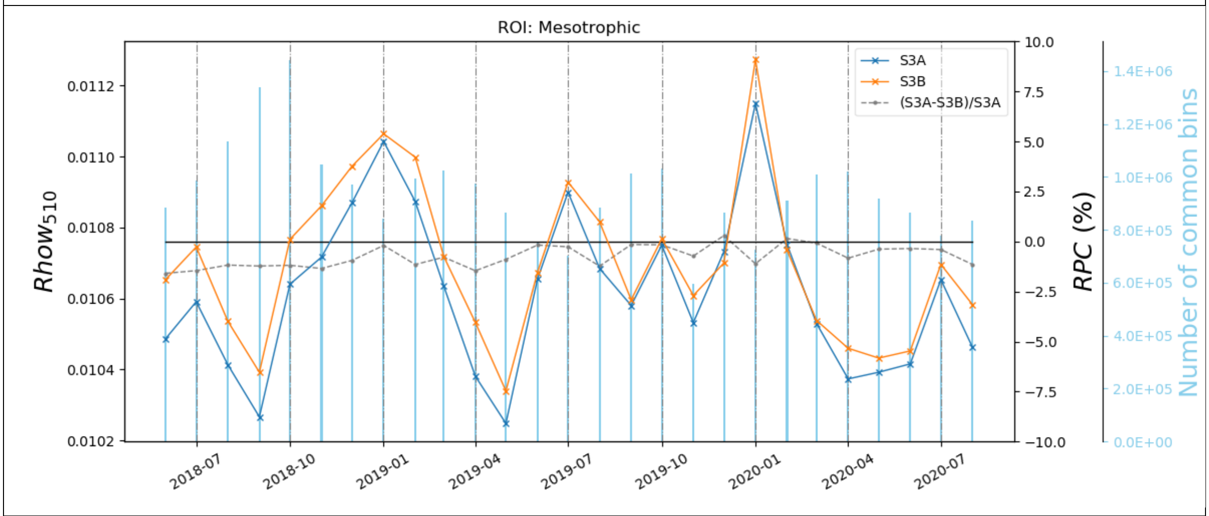


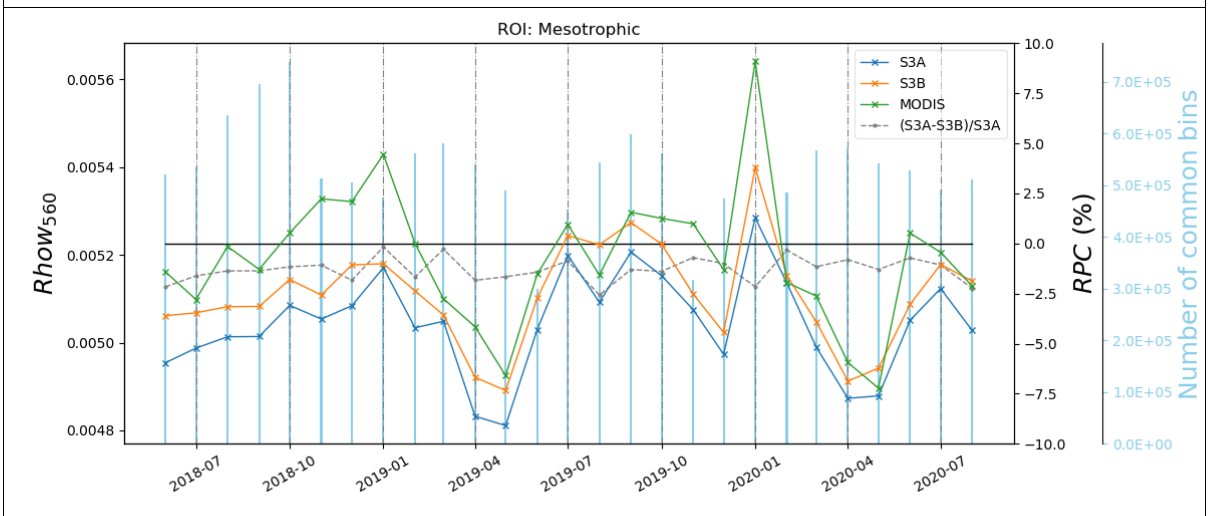
Figure 13: Oligotrophic-waters time series comparison between OLCI-A, OLCI-B and MODIS-Aqua

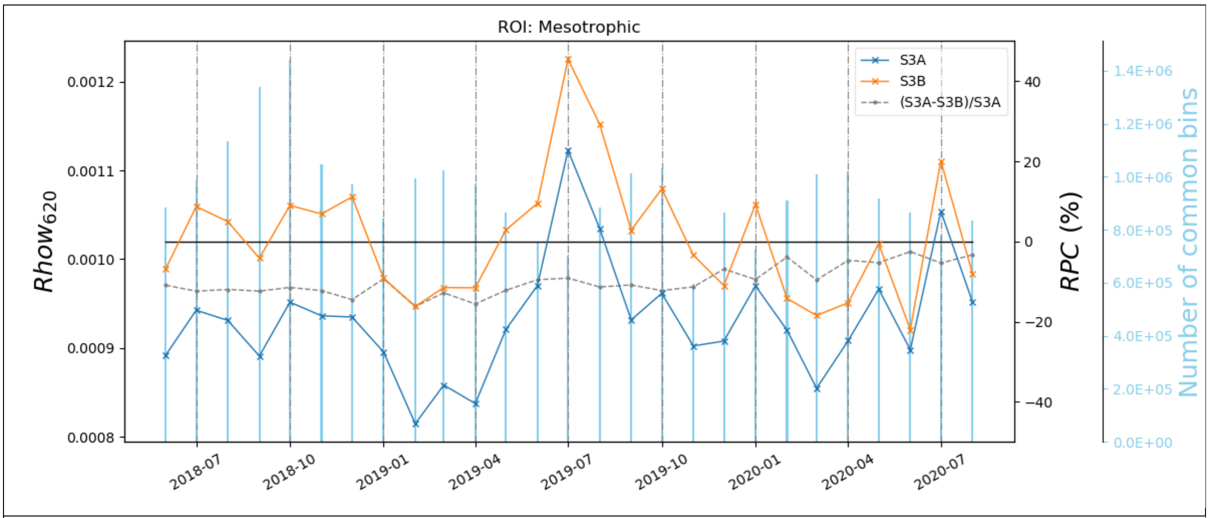
5.4.2 Mesotrophic waters

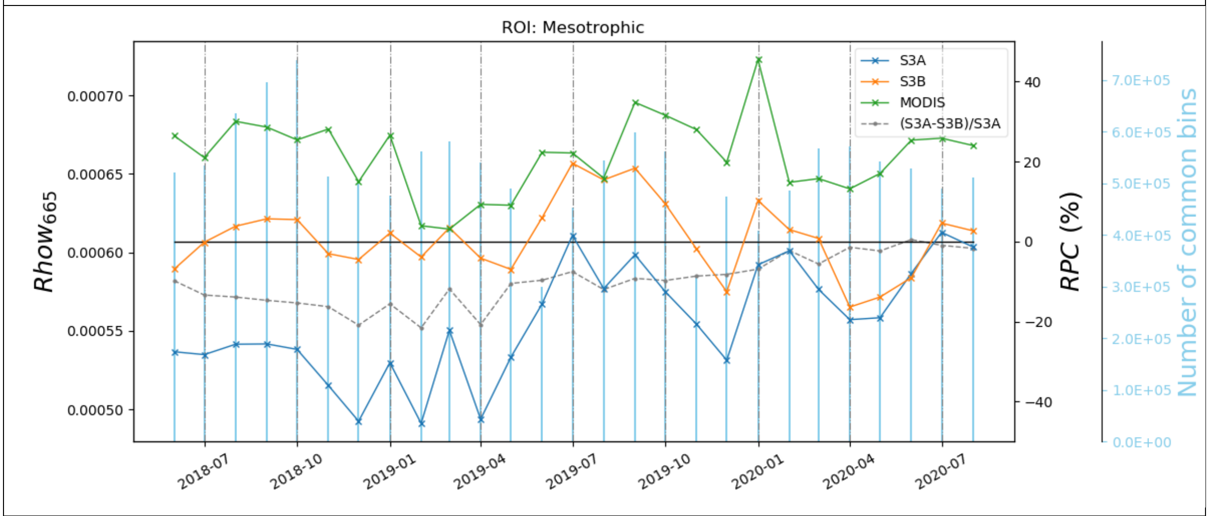



ROI: Mesotrophic
S3A
S3B
MODIS
(S3A-S3B)/S3A
$Rhow_{490}$
RPC (%)
Number of common bins
0.01750
0.01725
0.01700
0.01675
0.01650
0.01625
0.01600
0.01575
0.01550
10.0
7.5
5.0
2.5
0.0
−2.5
−5.0
−7.5
−10.0
7.0E+05
6.0E+05
5.0E+05
4.0E+05
3.0E+05
2.0E+05
1.0E+05
0.0E+00
2018-07
2018-10
2019-01
2019-04
2019-07
2019-10
2020-01
2020-04
2020-07


ROI: Mesotrophic
S3A
S3B
(S3A-S3B)/S3A
$Rhow_{510}$
RPC (%)
Number of common bins
0.0112
0.0110
0.0108
0.0106
0.0104
0.0102
10.0
7.5
5.0
2.5
0.0
−2.5
−5.0
−7.5
−10.0
1.4E+06
1.2E+06
1.0E+06
8.0E+05
6.0E+05
4.0E+05
2.0E+05
0.0E+00
2018-07
2018-10
2019-01
2019-04
2019-07
2019-10
2020-01
2020-04
2020-07


ROI: Mesotrophic
S3A
S3B
MODIS
(S3A-S3B)/S3A
$Rhow_{560}$
RPC (%)
Number of common bins
0.0056
0.0054
0.0052
0.0050
0.0048
10.0
7.5
5.0
2.5
0.0
−2.5
−5.0
−7.5
−10.0
7.0E+05
6.0E+05
5.0E+05
4.0E+05
3.0E+05
2.0E+05
1.0E+05
0.0E+00
2018-07
2018-10
2019-01
2019-04
2019-07
2019-10
2020-01
2020-04
2020-07


ROI: Mesotrophic
S3A
S3B
(S3A-S3B)/S3A
$Rhow_{620}$
RPC (%)
Number of common bins


ROI: Mesotrophic
S3A
S3B
MODIS
(S3A-S3B)/S3A
$Rhow_{665}$
RPC (%)
Number of common bins

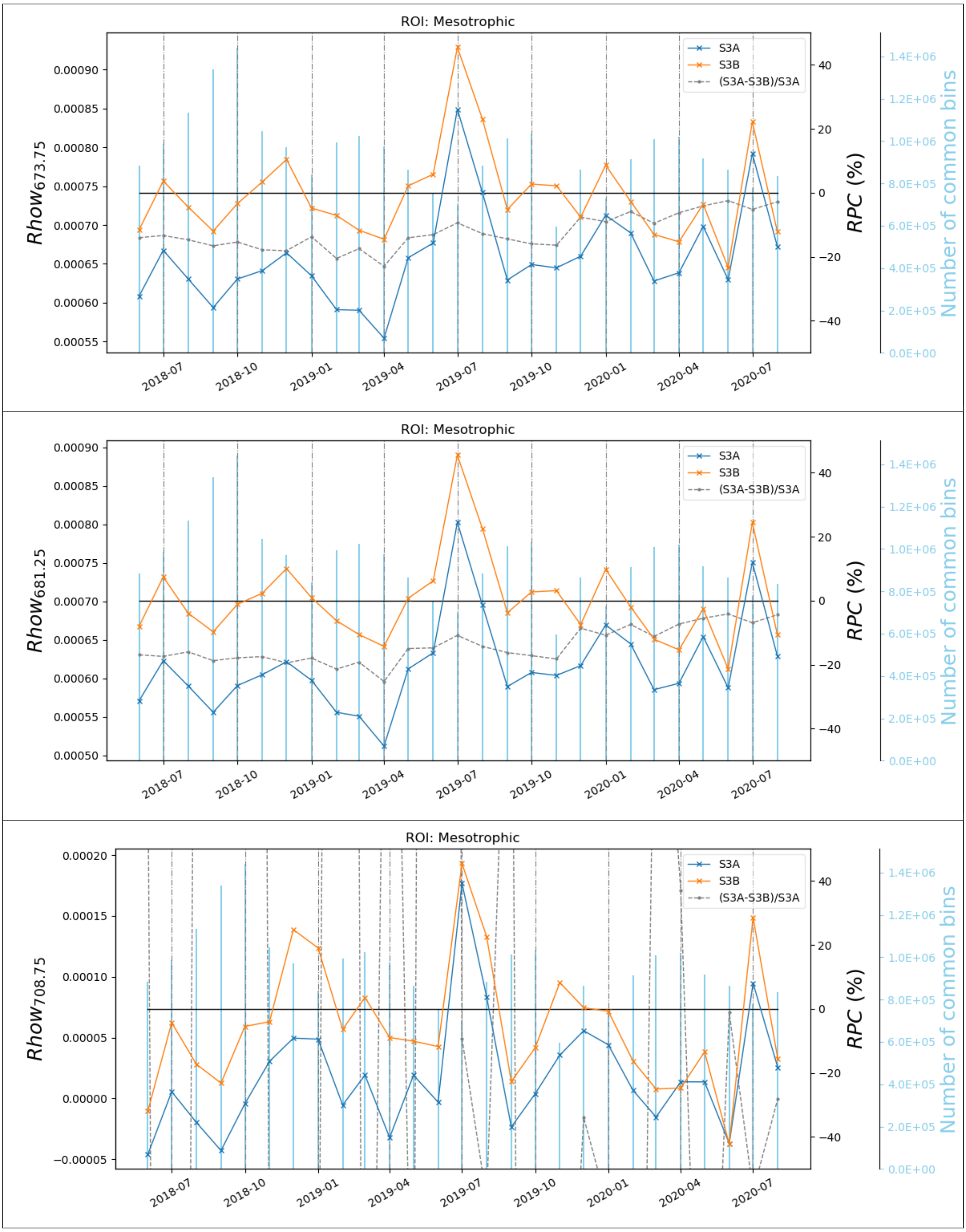
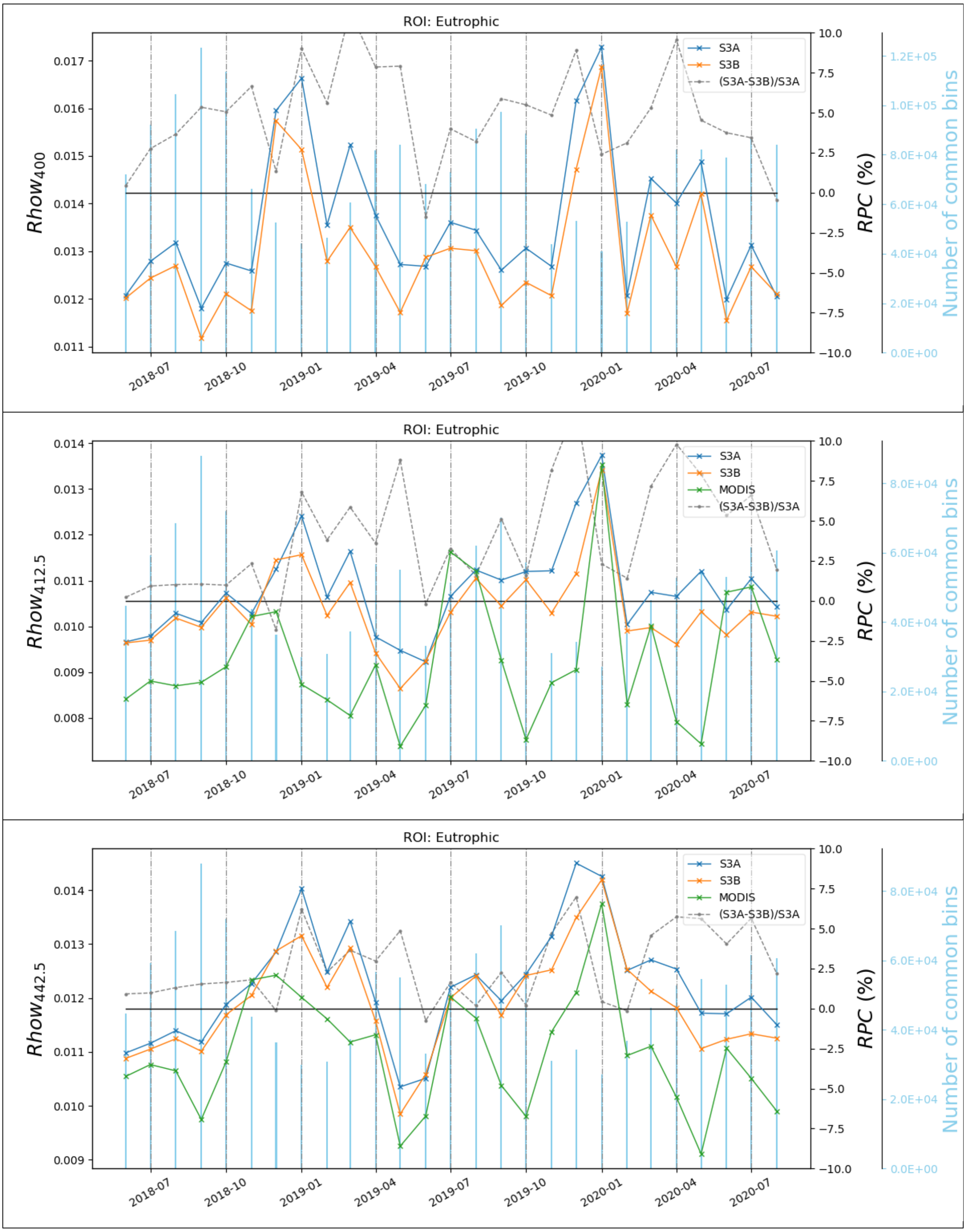
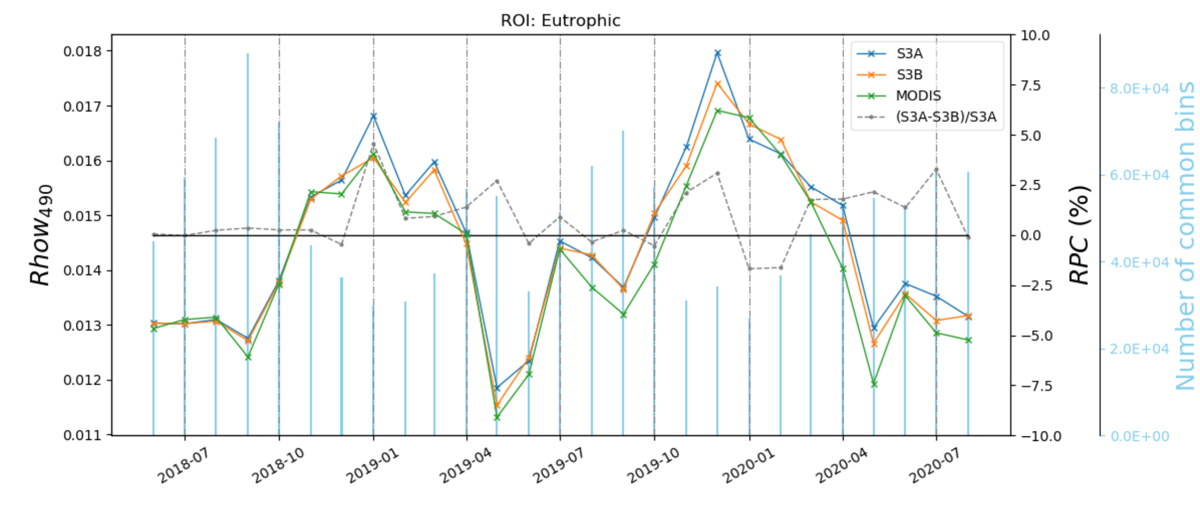
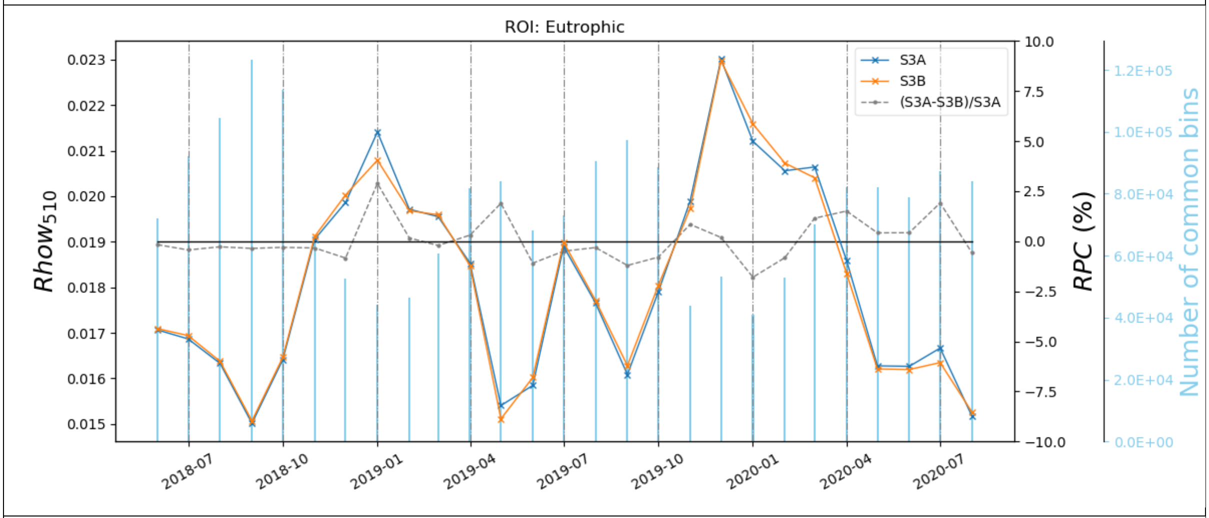


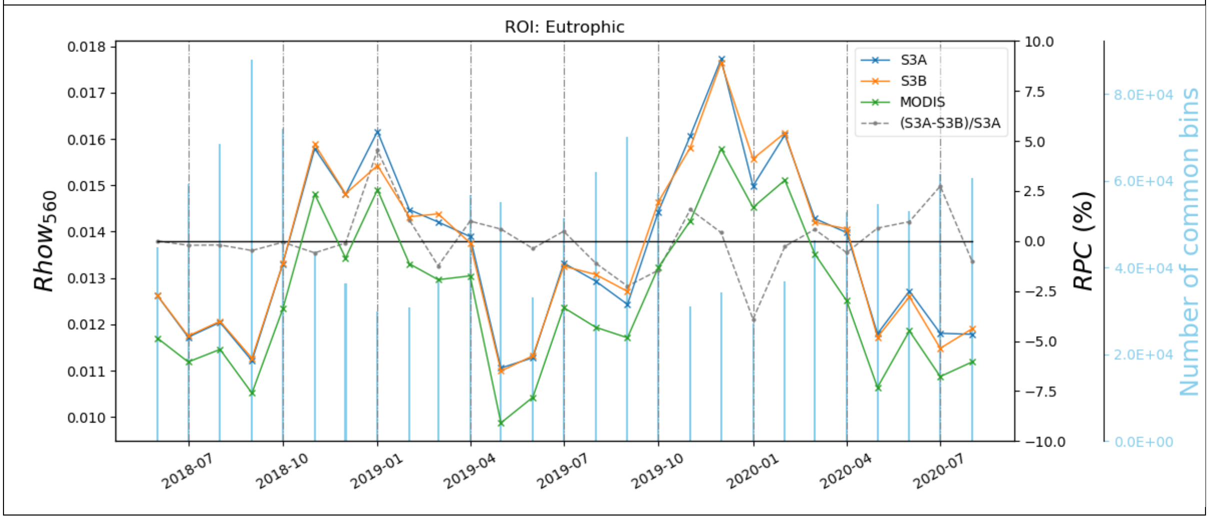
Figure 14: Mesotrophic-waters time series comparison between OLCI-A, OLCI-B and MODIS-Aqua

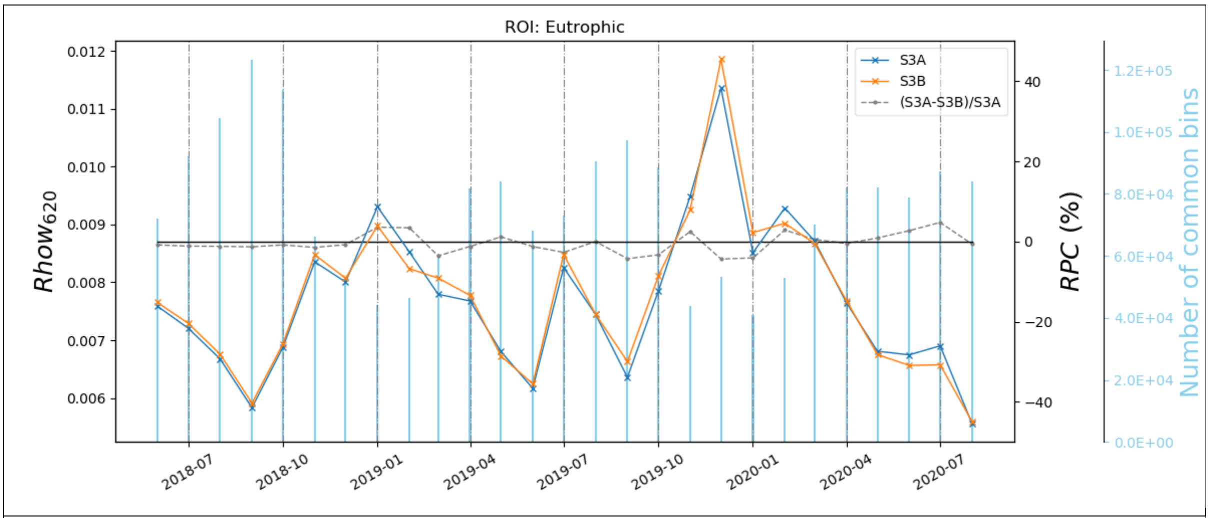
5.4.3 Eutrophic waters

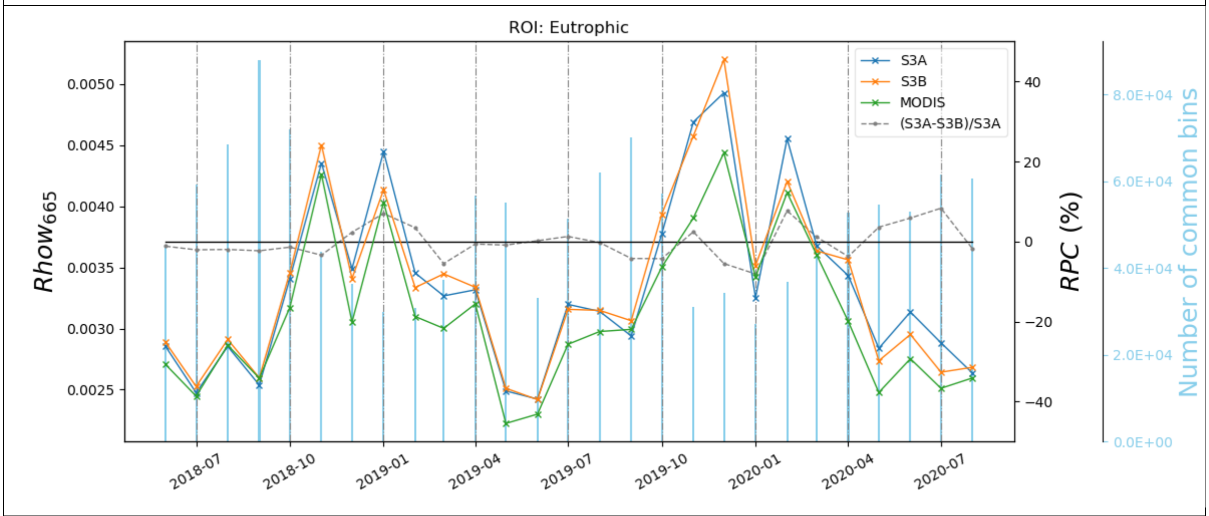



ROI: Eutrophic
S3A
S3B
MODIS
(S3A-S3B)/S3A
$Rhow_{490}$
RPC (%)
Number of common bins


ROI: Eutrophic
S3A
S3B
(S3A-S3B)/S3A
$Rhow_{510}$
RPC (%)
Number of common bins


ROI: Eutrophic
S3A
S3B
MODIS
(S3A-S3B)/S3A
$Rhow_{560}$
RPC (%)
Number of common bins


ROI: Eutrophic
S3A
S3B
(S3A-S3B)/S3A
$Rhow_{620}$
RPC (%)
Number of common bins


ROI: Eutrophic
S3A
S3B
MODIS
(S3A-S3B)/S3A
$Rhow_{665}$
RPC (%)
Number of common bins

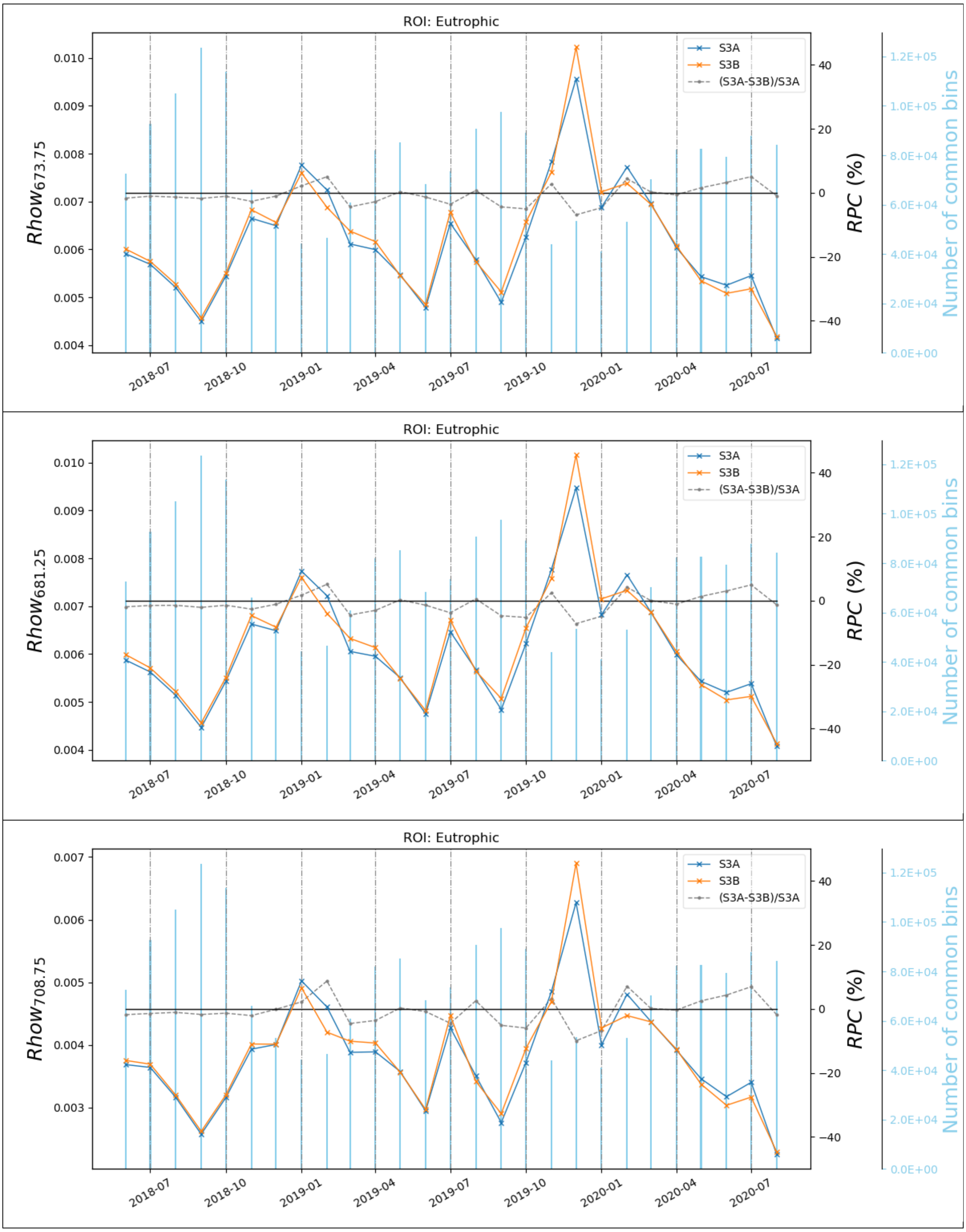


Figure 15: Eutrophic-waters time series comparison between OLCI-A, OLCI-B and MODIS-Aqua

5.5 Validations of algal pigment concentrations with in situ measurements

Algal pigment concentration is a major OLCI water bio-optical product and its validation is fundamental. Nevertheless, publicly available chlorophyll measurements are sparse. Presented below results encompass PML validations from AMT cruise data (see section 4.1.2.4) and EUMETSAT's validations using NASA's SeaBASS in situ records.

The applied datasets and methodology are described in sections 4.1.1, 4.1.2.3, 4.1.2.4, 4.2.1.

5.5.1 OLCI-A validations

OLCI-A matchups in comparison with AMT data are displayed in Figure 16. The value of AMT measurements is crucial as it allows for OLCI validation in open oceanic waters. The AMT validations cover oligotrophic and mesotrophic waters and show that OLCI achieves the goal of 30% uncertainty requirement in these waters.

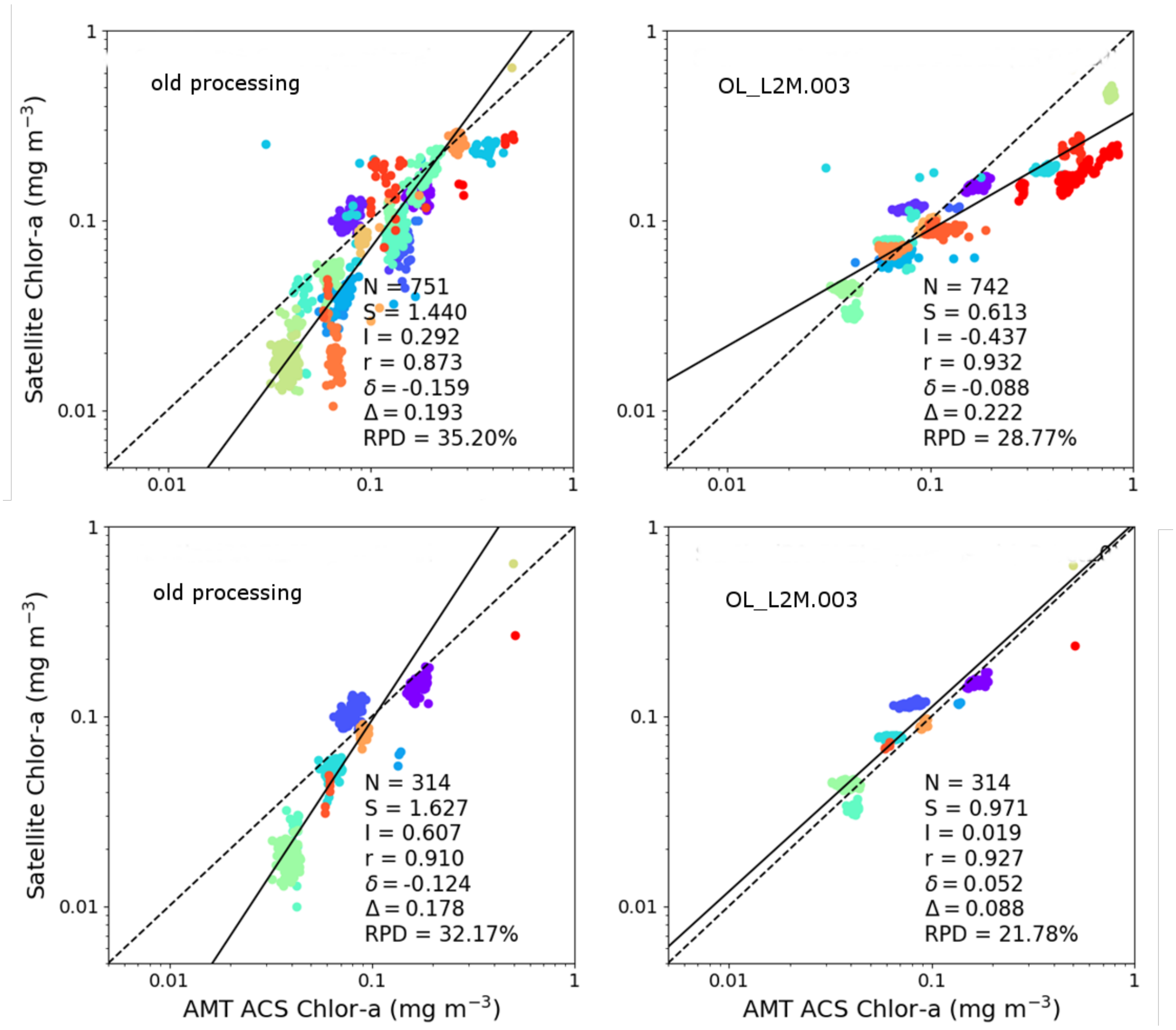


Figure 16: OLCI-A algal pigment concentration matchups with AMT cruise data for old products, left column, and new products OL_L2M.003, right column, where top row results represent all available matchups and bottom row results only the matchups in common between the old and new processors. Image curtesy of Gavin Tilstone and Silvia Pardo, PML.

Figure 17 covers oligotrophic, mesotrophic and eutrophic water validations with NASA's SeaBASS in situ HPLC measurements. Both OLCI Algal Pigment Concentration products are presented, CHL_OC4ME and CHL_NN. The CHL_OC4ME product is approximately within 30% uncertainty. Some overestimation in more eutrophic waters may be possible (the 70% uncertainty requirement applies for case-2 waters).

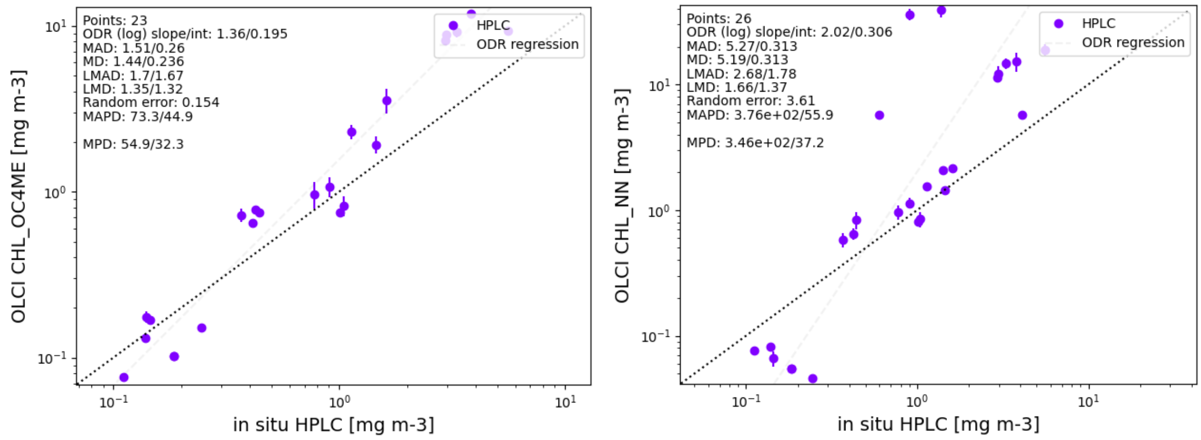


Figure 17: OLCI-A algal pigment concentration matchups with NASA's SeaBASS in situ HPLC measurements for CHL_OC4ME Open Water product, left, and CHL_NN Complex Water product, right.

5.5.2 OLCI-B validations

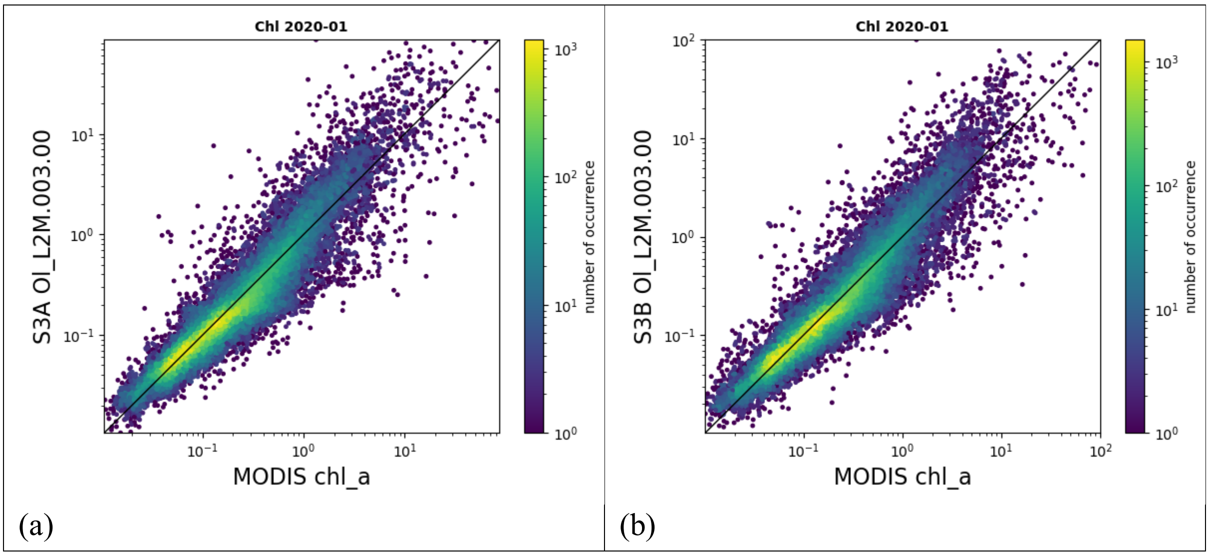
OLCI-B validations with in situ measurements are not yet available due to lack of in situ data.

5.6 Validations of algal pigment concentrations with mission inter-comparisons

OLCI-A and OLCI-B algal pigment concentration L3 datasets are compared with MODIS-Aqua across the full range of chlorophyll and, separately, at three different global water trophic regimes. MODIS provides an independent source of validation for OLCI and allows obtaining large-scale reliable statistics.

The applied datasets and methodology are described in sections 4.1.1, 4.1.3, 4.2.2.

The scatterplots in Figure 18 demonstrate the distribution of OLCI-A and OLCI-B algal pigment concentrations across the full range of chlorophyll in comparison with MODIS-Aqua and the previous processor version (old PB2.43/1.15) that did not have the CI oligotrophic algorithm implemented.



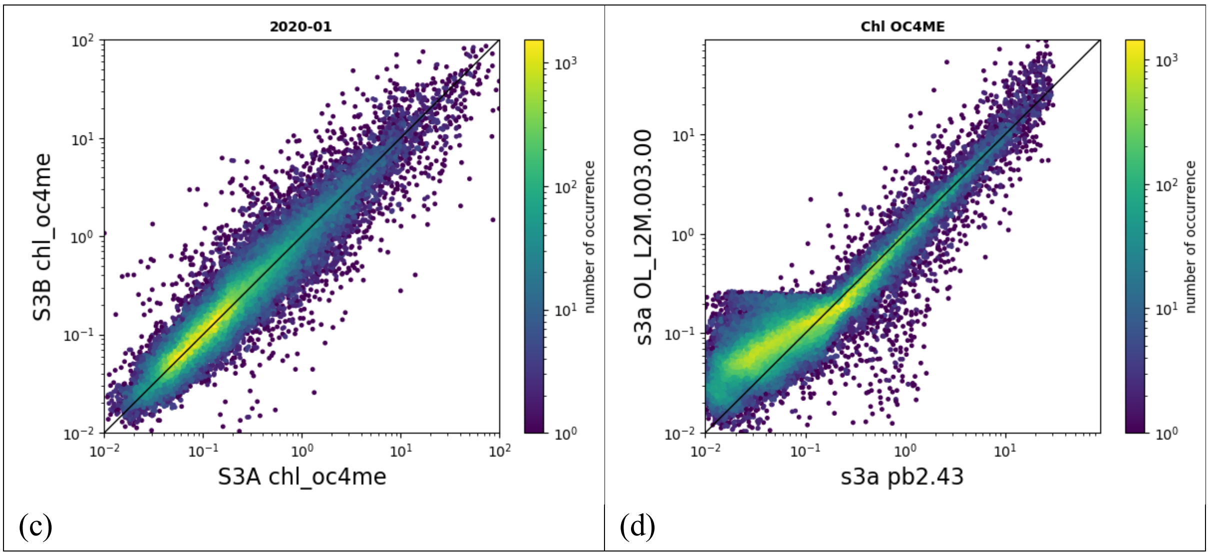


Figure 18: Density plots of Level-3 bin-to-bin comparisons: (a) MODIS-Aqua vs OLCI-A, (b) MODIS-Aqua vs OLCI-B, (c) OLCI-A vs OLCI-B, (d) new OLCI-A OL_L2M.003.00 vs old PB2.43/1.15.

In Figure 19, Figure 20, and Figure 21, OLCI-A and OLCI-B algal pigment concentration L3 time series are compared with MODIS-Aqua across three different global water trophic regimes. MODIS provides an independent source of validation for OLCI and allow obtaining large-scale reliable statistics.

5.6.1 Oligotrophic waters

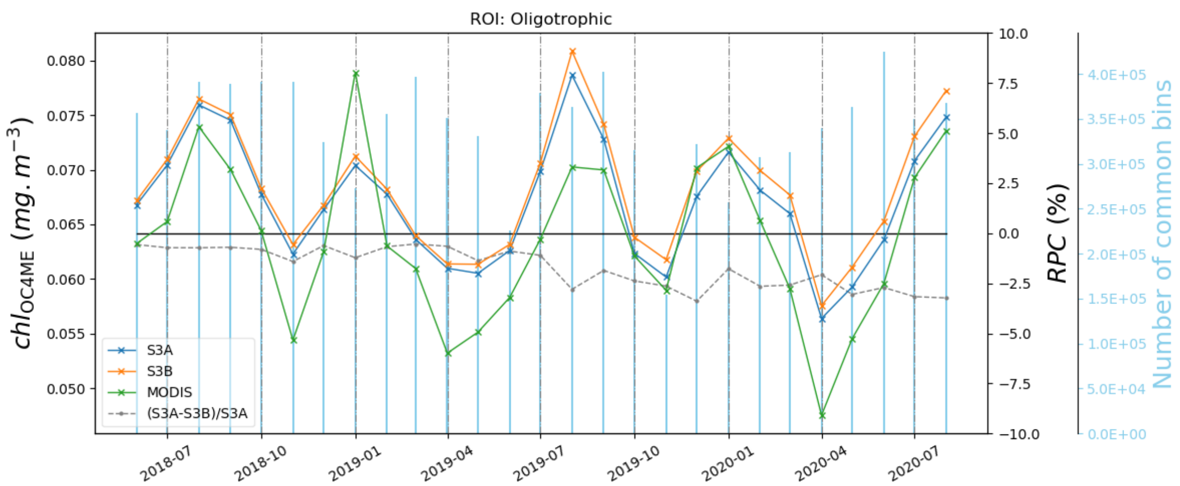


Figure 19: Oligotrophic waters Chlorophyll time series comparison

5.6.2 Mesotrophic waters

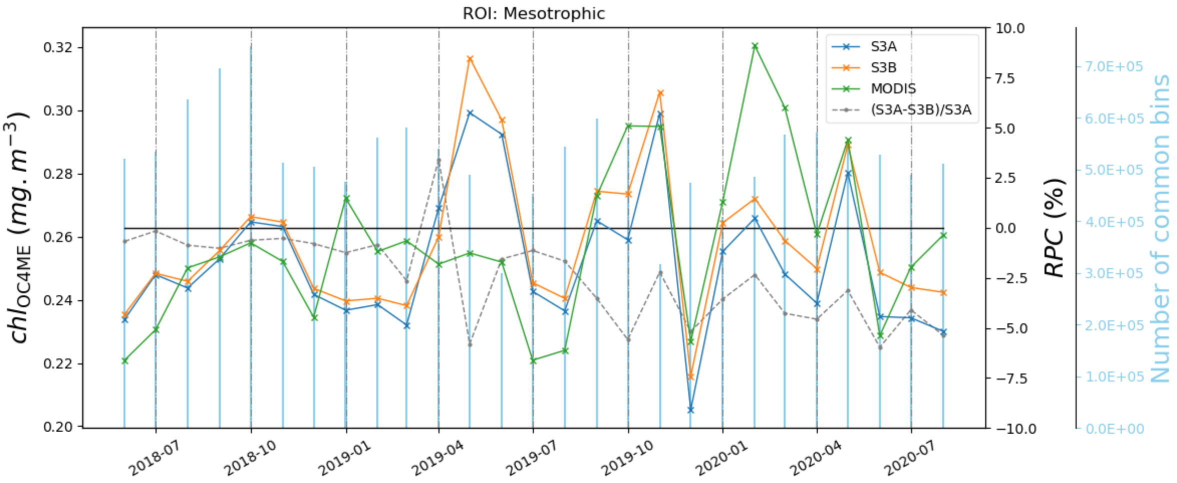


Figure 20: Mesotrophic waters Chlorophyll time series comparison

5.6.3 Eutrophic waters

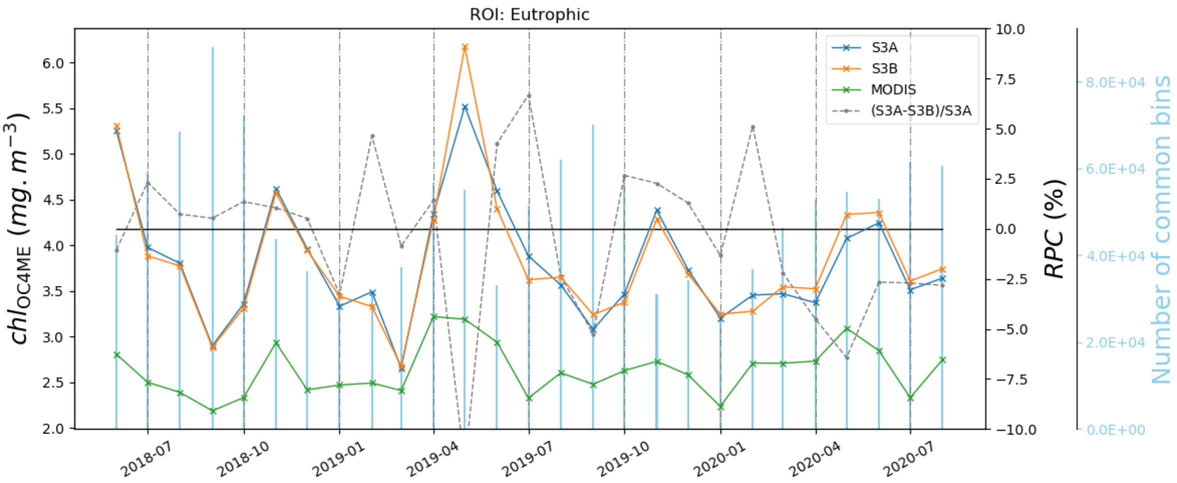


Figure 21: Eutrophic waters Chlorophyll time series comparison

5.7 Validations of Total Suspended Matter product

5.7.1 TSM validations with in situ measurements

Figure 22 shows OLCI-A validations with Cefas smart buoy turbidity measurements. Cefas datasets are described in section 4.1.2.5. As the NN retrieves the IOP parameters and converts them to concentrations (see section 3.3.1), the figure shows the previously used $b_{b,total}$ to TSM conversion result, the result from the previous NNv1, and the current NNv2 and TSM conversion used in Collection OL_L2M.003.

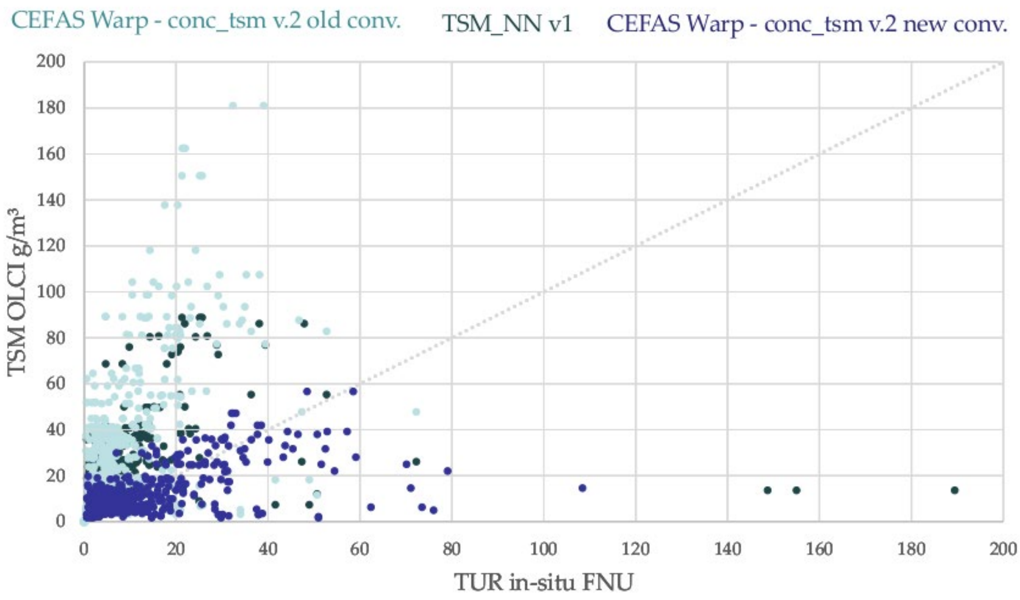


Figure 22: OLCI-A Total Suspended Matter matchups with Cefas smart buoy turbidity measurements for the old $b_{b,total}$ to TSM conversion, in light blue, for the previous NNv1 retrieval, in black, and for the new NNv2 and $b_{b,total}$ to TSM conversion in OL_L2M.003, in dark blue. Image curtesy of Carole Lebreton and Carsten Brockmann, Brockmann Consult, GmbH.

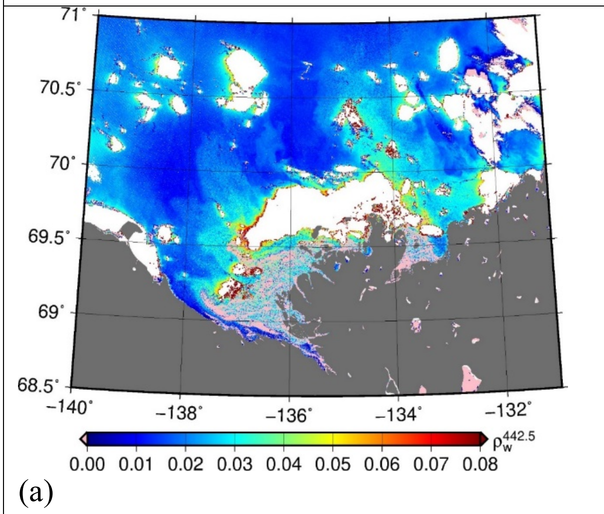
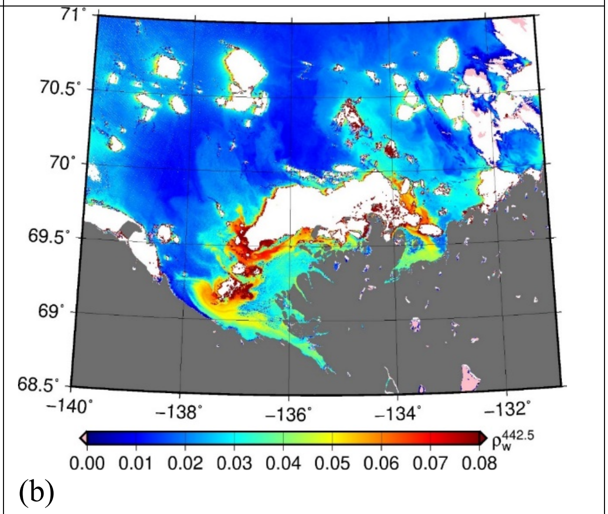
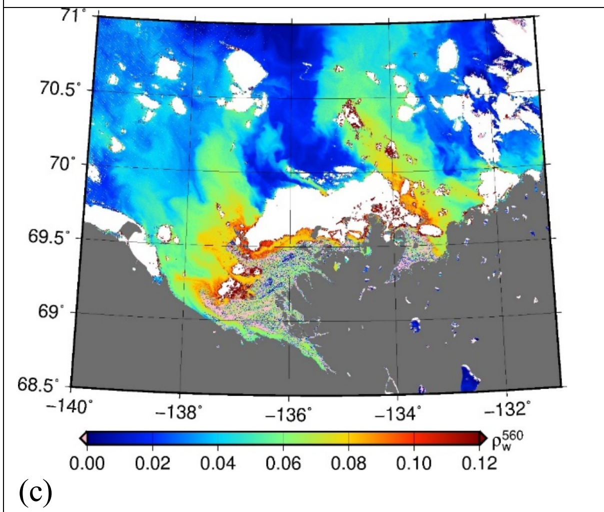
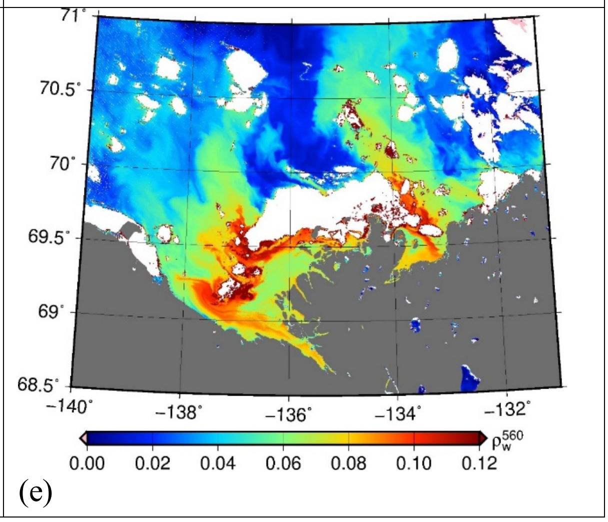
6 COLLECTION OL_L2M.003 INTER-COMPARISONS WITH THE PREVIOUS PROCESSING BASELINE

The results in this section document inter-comparisons with the previous OLCI L2 Marine processing and demonstrate improvements and changes brought by Collection OL_L2M.003. The L2 Marine previous processing went into operations in November 2017. Only a minor update to this baseline occurred in 2019, at the time of OLCI-B operational release, as OLCI-B OC-SVC gains were set to 1 (no SVC applied for OLCI-B) in addition to the OC-SVC gains for OLCI-A implemented with the 2017.

The operational processing baseline previous to Collection OL_L2M.003 was PB2.43/1.15 and this label is used in the following inter-comparisons.

6.1 High level overview of OLCI-A and -B Ocean Colour product improvements in complex waters

Two figures below illustrate improvements brought in Collection OL_L2M.003 compared to the previous processing baseline PB2.43/1.15. Collection OL_L2M.003 product retrievals are smoothly extending close to the coast in very turbid waters and provide realistic values.

PB2.43/1.15	OL_L2M.003
 (a)	 (b)
 (c)	 (e)

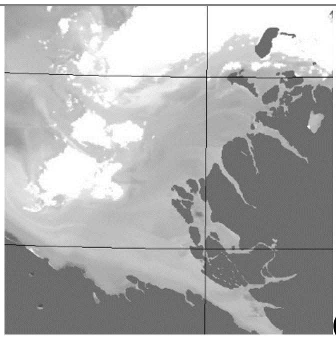
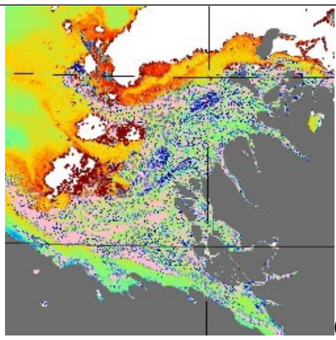
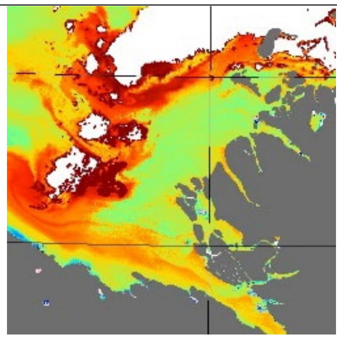
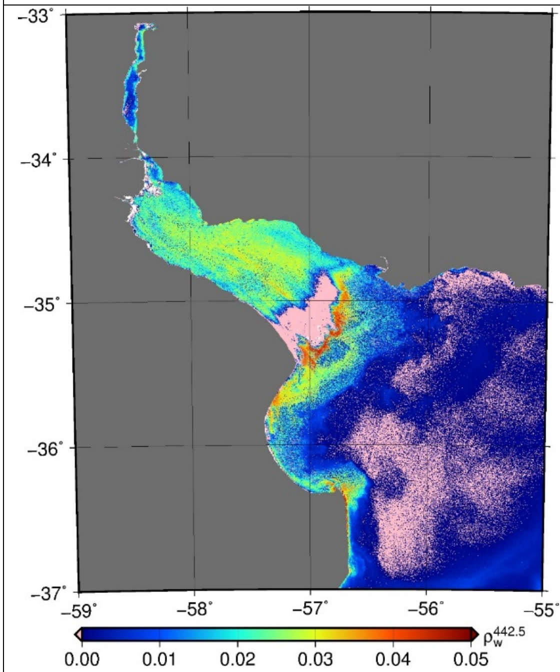
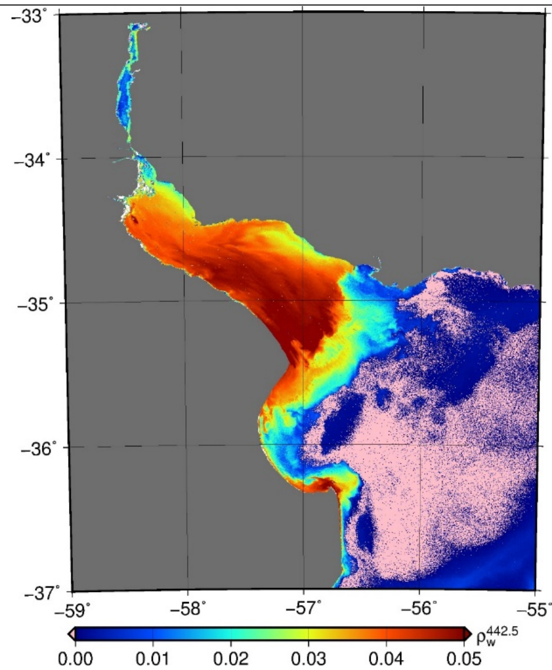
Radiance 560 nm	ρ_w^{560} PB2.43/1.15	ρ_w^{560} OL_L2M.003.00
 (f)	 (g)	 (h)

Figure 23: Mackenzie River estuary comparison between PB2.43/1.15 and OL_L2M.003

PB2.43/1.15	OL_L2M.003
 (a)	 (b)

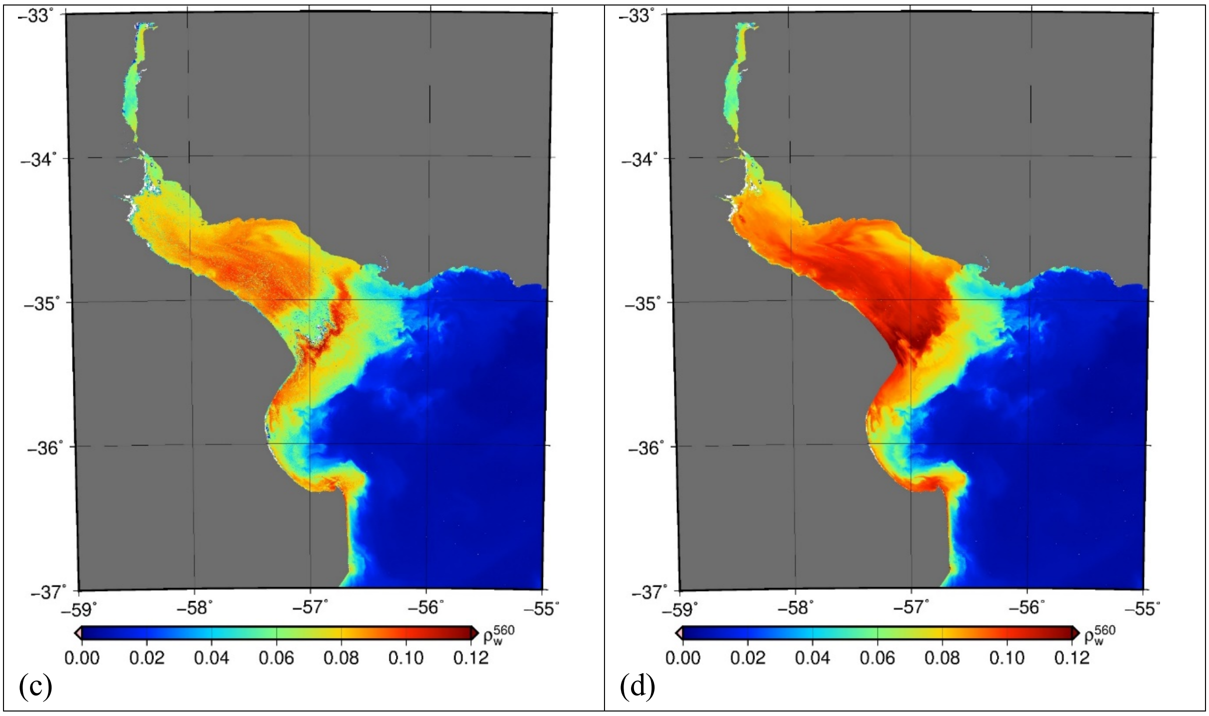
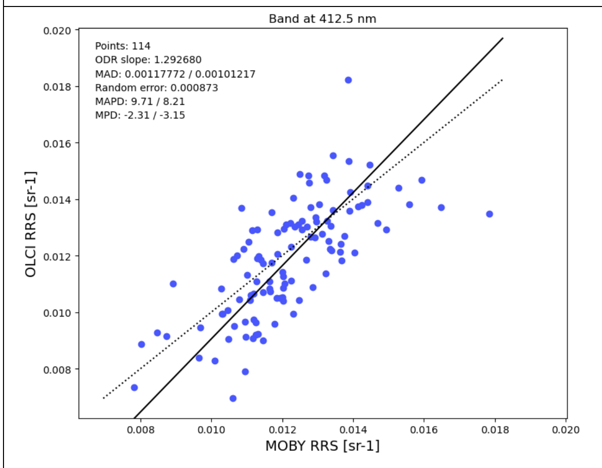
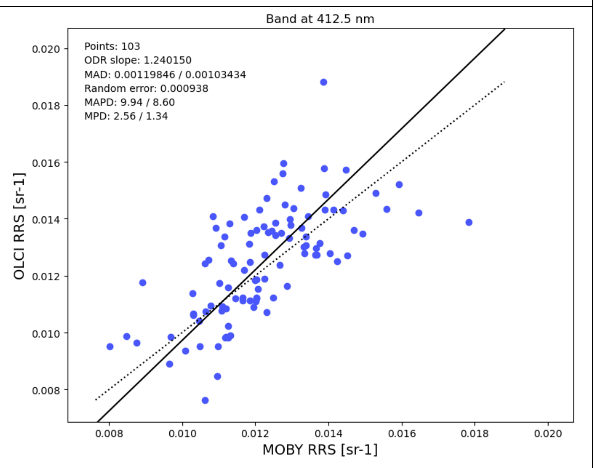


Figure 24: Rio de la Plata highly turbid waters, comparison between PB2.43/1.15 and OL_L2M.003

6.2 Inter-comparisons of SVC gain performance

6.2.1 Verification with MOBY in situ radiometric measurements

6.2.1.1 OLCI-A matchup inter-comparison

PB2.43/1.15	OL_L2M.003.00
	

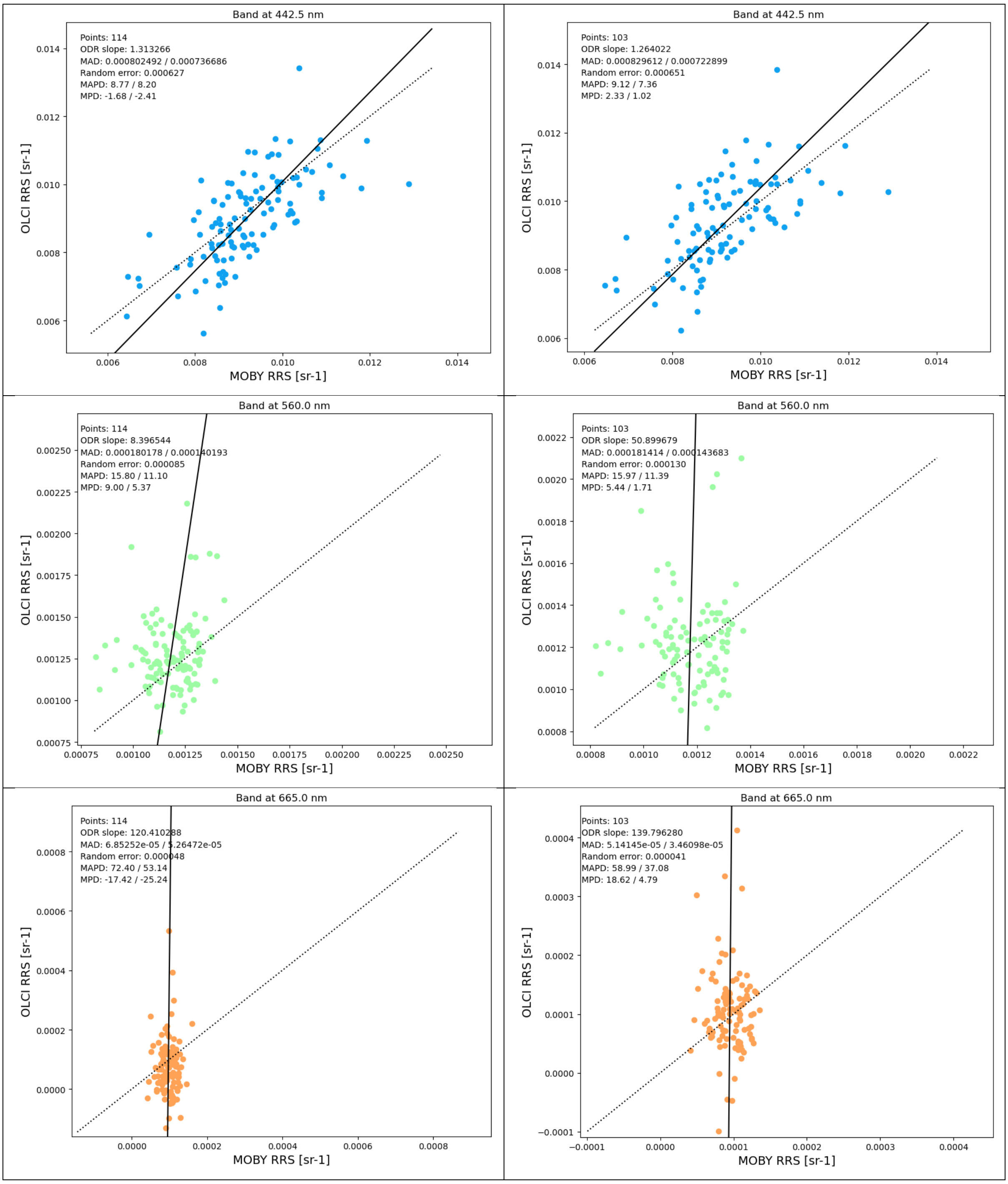
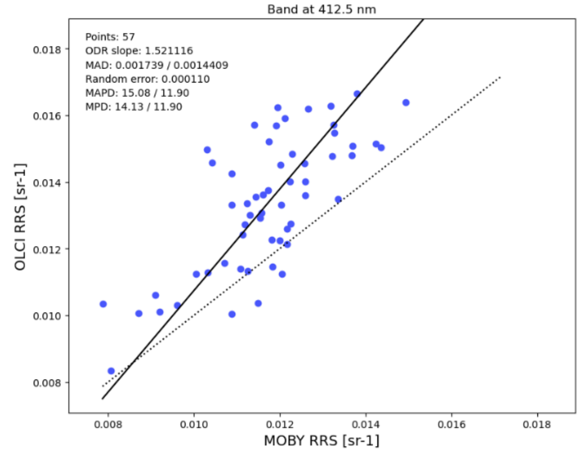


Figure 25: OLCI-A MOBY matchup inter-comparisons for the previous operational PB2.43/1.15 and Collection OL_L2M.003

6.2.1.2 OLCI-B matchup inter-comparison

For OLCI-B, because there were no OC-SVC gains available in the previous PB2.43/1.15, the inter-comparisons in Figure 26 show clear bad performance of OLCI-B in matchups with MOBY. This result emphasizes the criticality of Ocean Colour System Vicarious Calibration.

<table>
<tr><th>PB2.43/1.15</th><th>OL_L2M.003.00</th></tr>
<tr><td>


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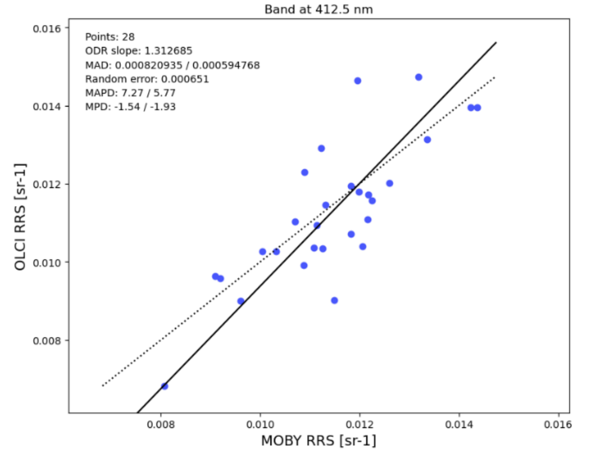

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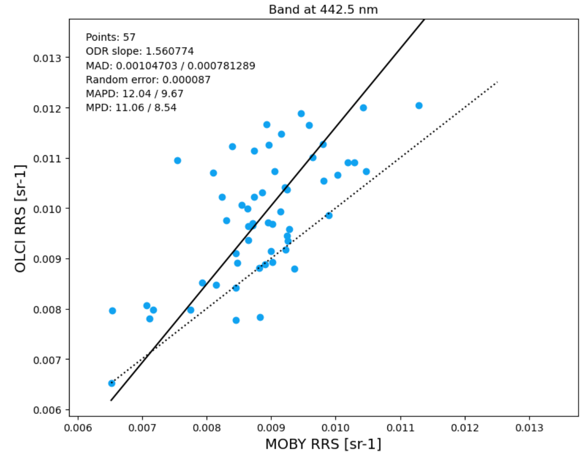

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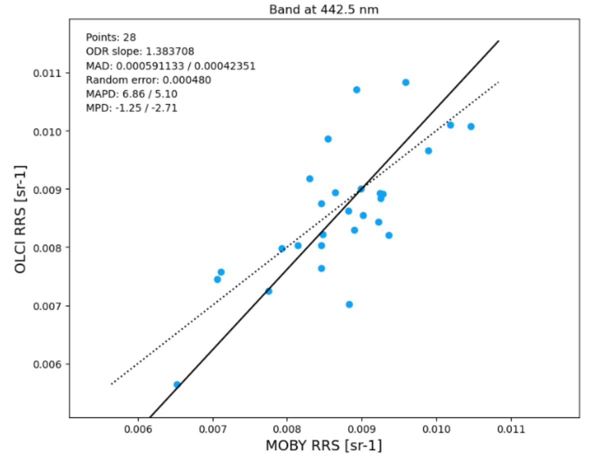

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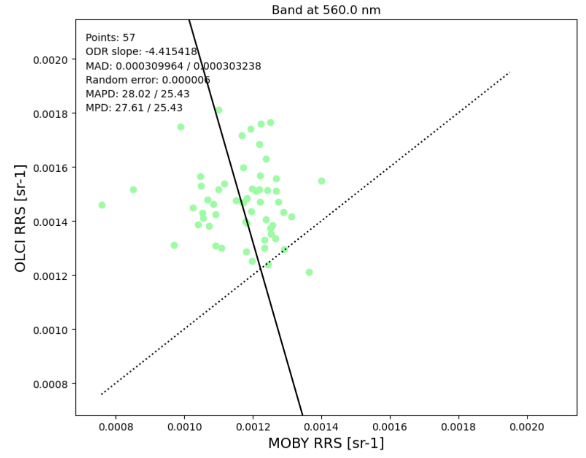

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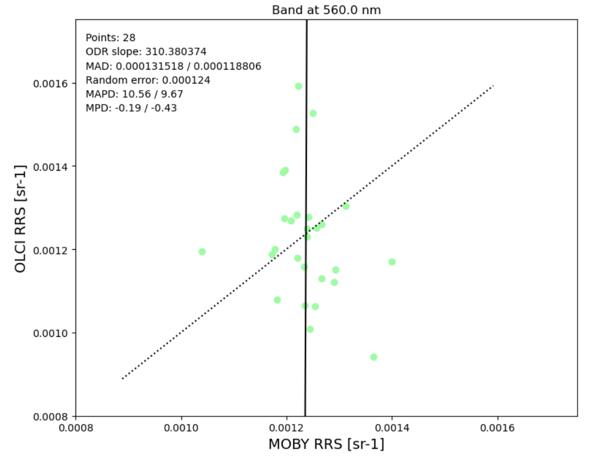

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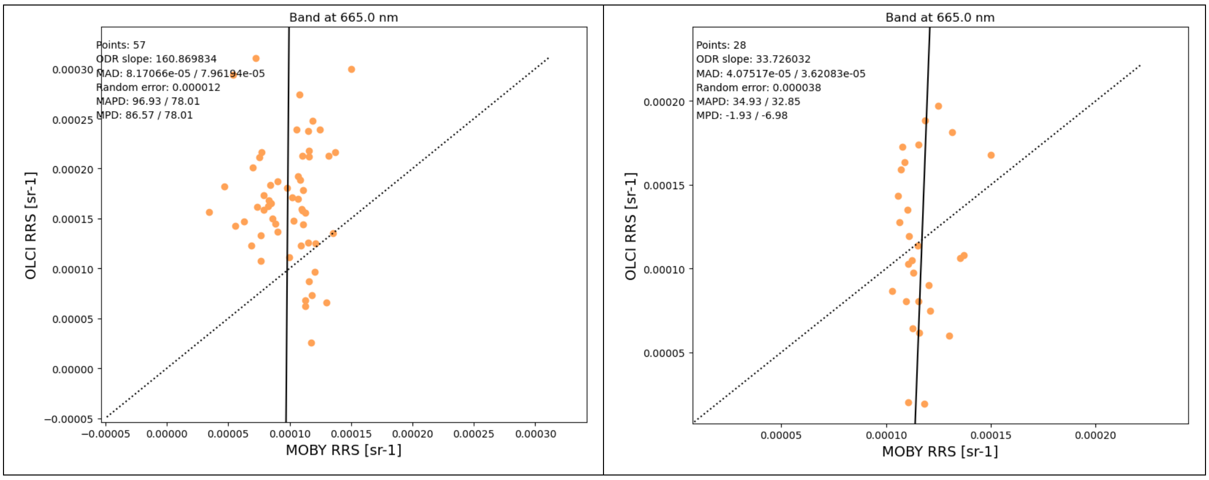


Figure 26: OLCI-B MOBY matchup inter-comparisons for the previous operational PB2.43/1.15 and Collection OL_L2M.003

6.2.2 Inter-comparison with mission time series over the South Pacific Gyre

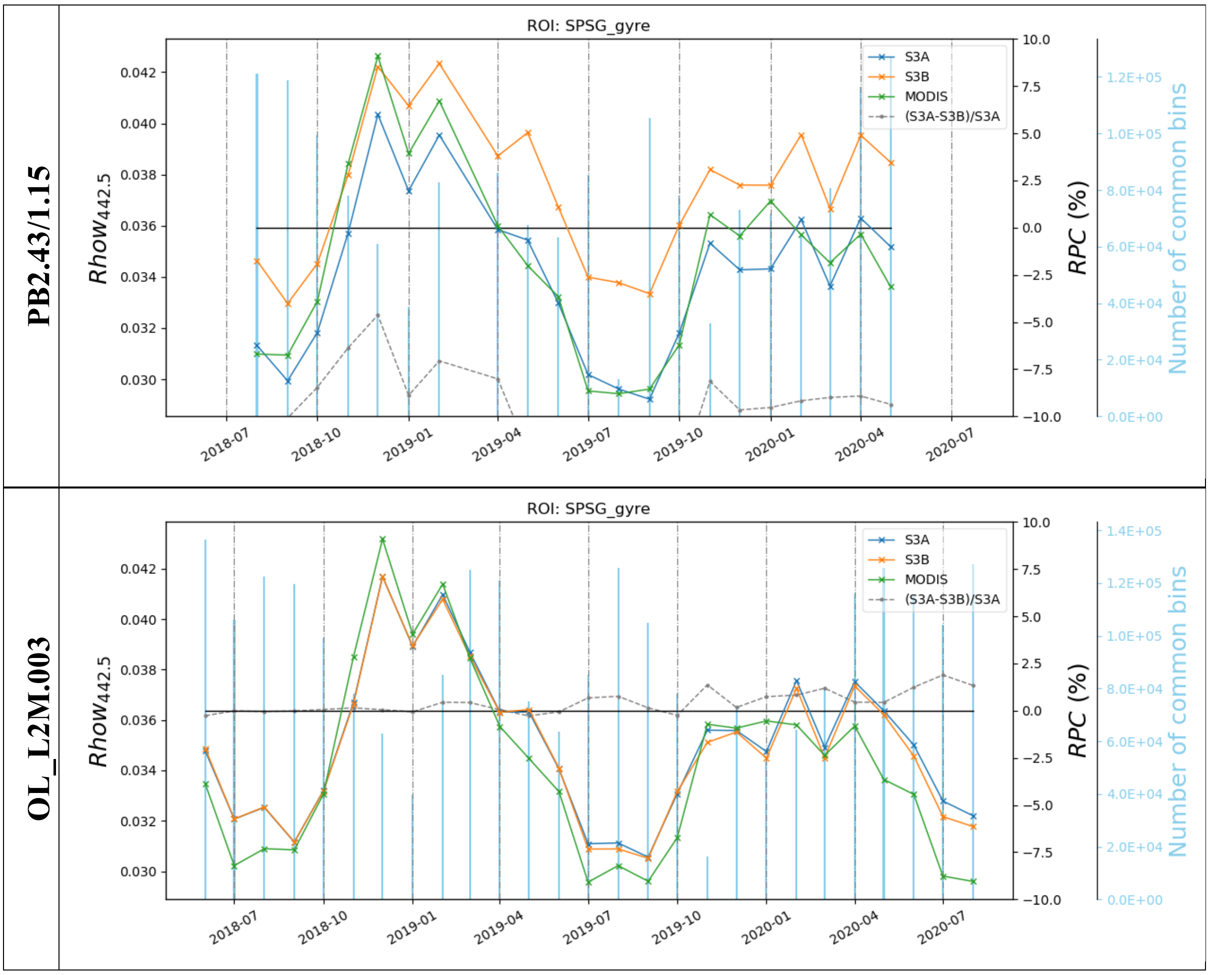


Figure 27: Rhow 442.5 time series comparison for the previous operational PB2.43/1.15 and Collection OL_L2M.003

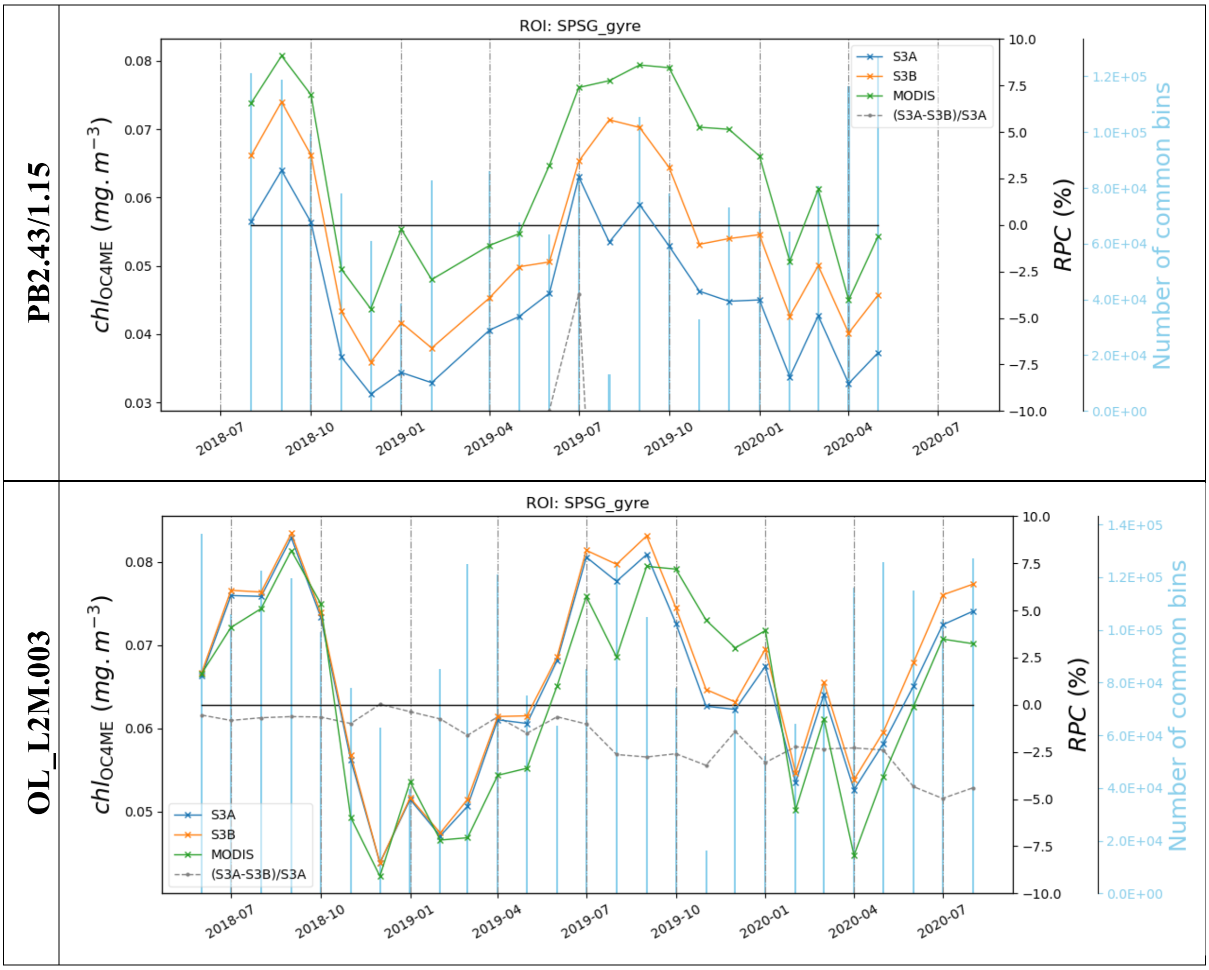
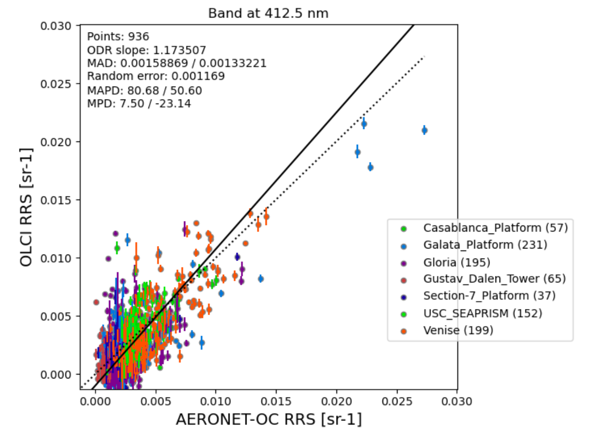


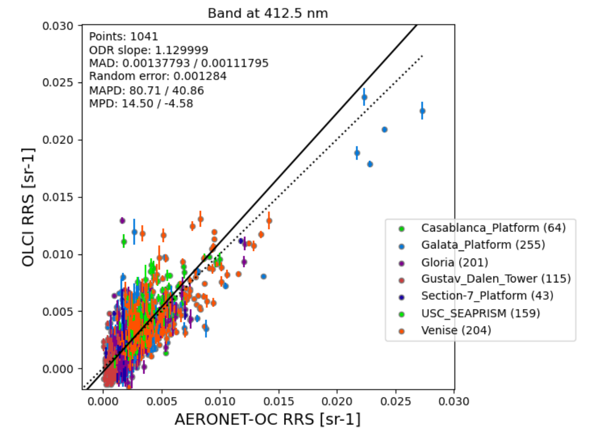
Figure 28: Chlorophyll time series comparison for the previous operational PB2.43/1.15 and Collection OL_L2M.003

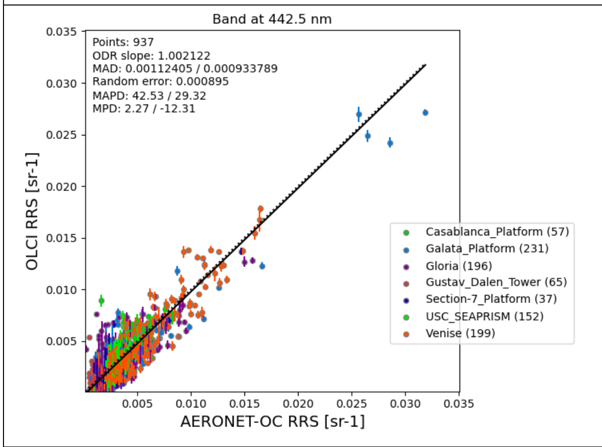
6.3 Water reflectance validation inter-comparisons with in situ AERONET-OC

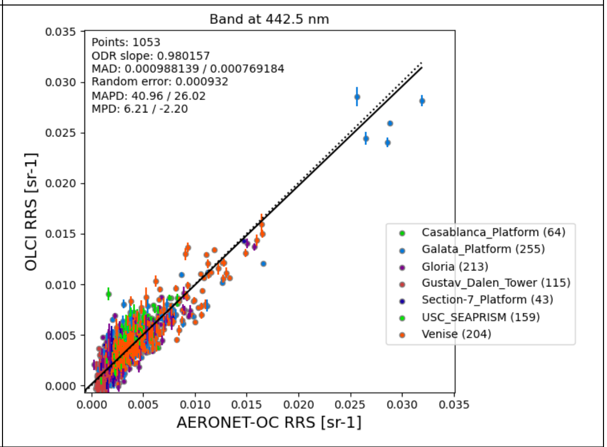
6.3.1 OLCI-A validation inter-comparisons

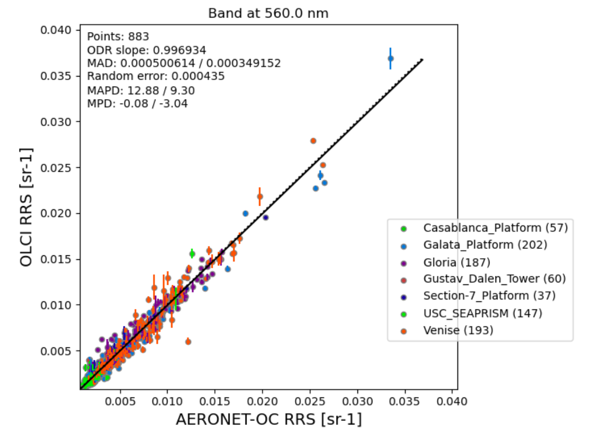
PB2.43/1.15	OL_L2M.003.00

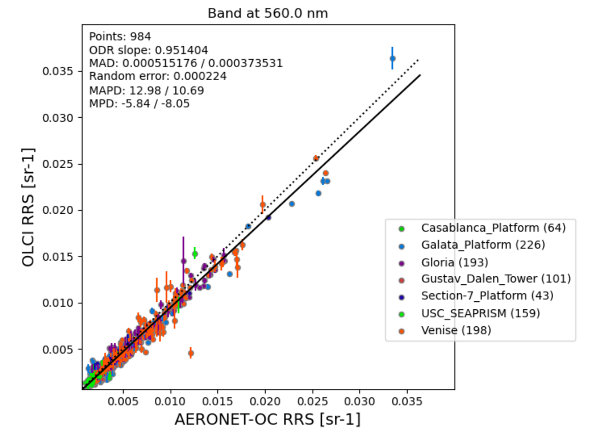












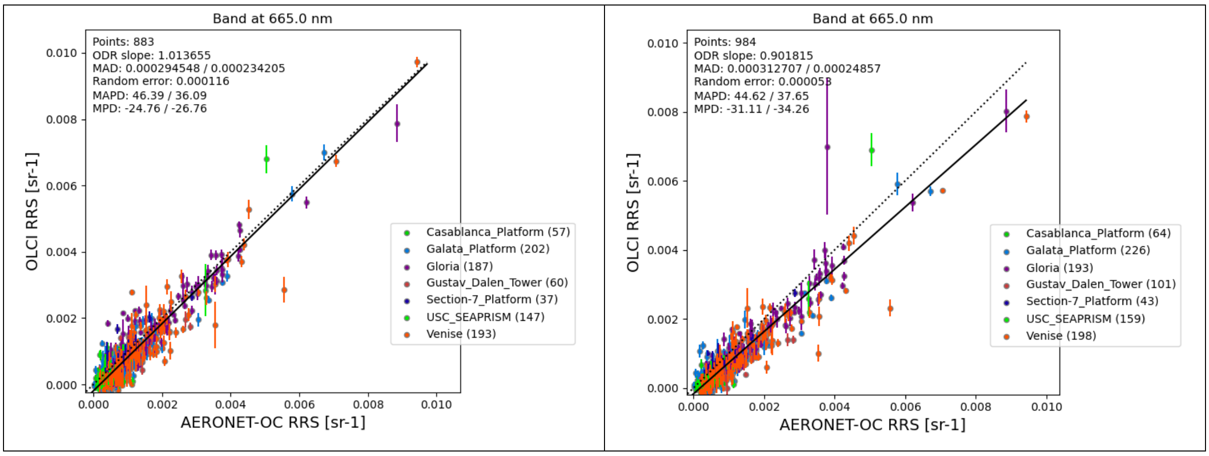
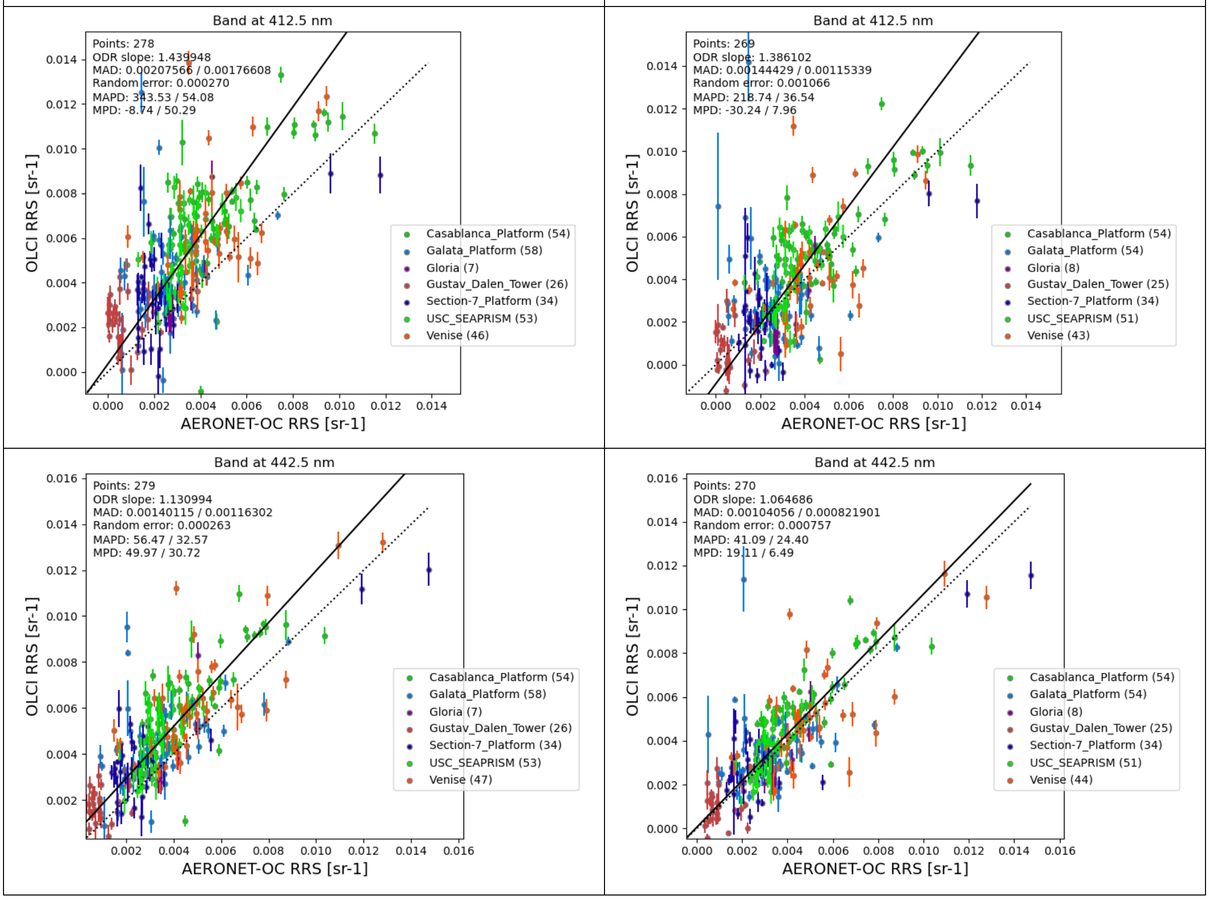


Figure 29: OLCI-A AERONET-OC matchup inter-comparisons for the previous operational PB2.43/1.15 and Collection OL_L2M.003

6.3.2 OLCI-B matchups inter-comparisons

PB2.43/1.15	OL_L2M.003.00



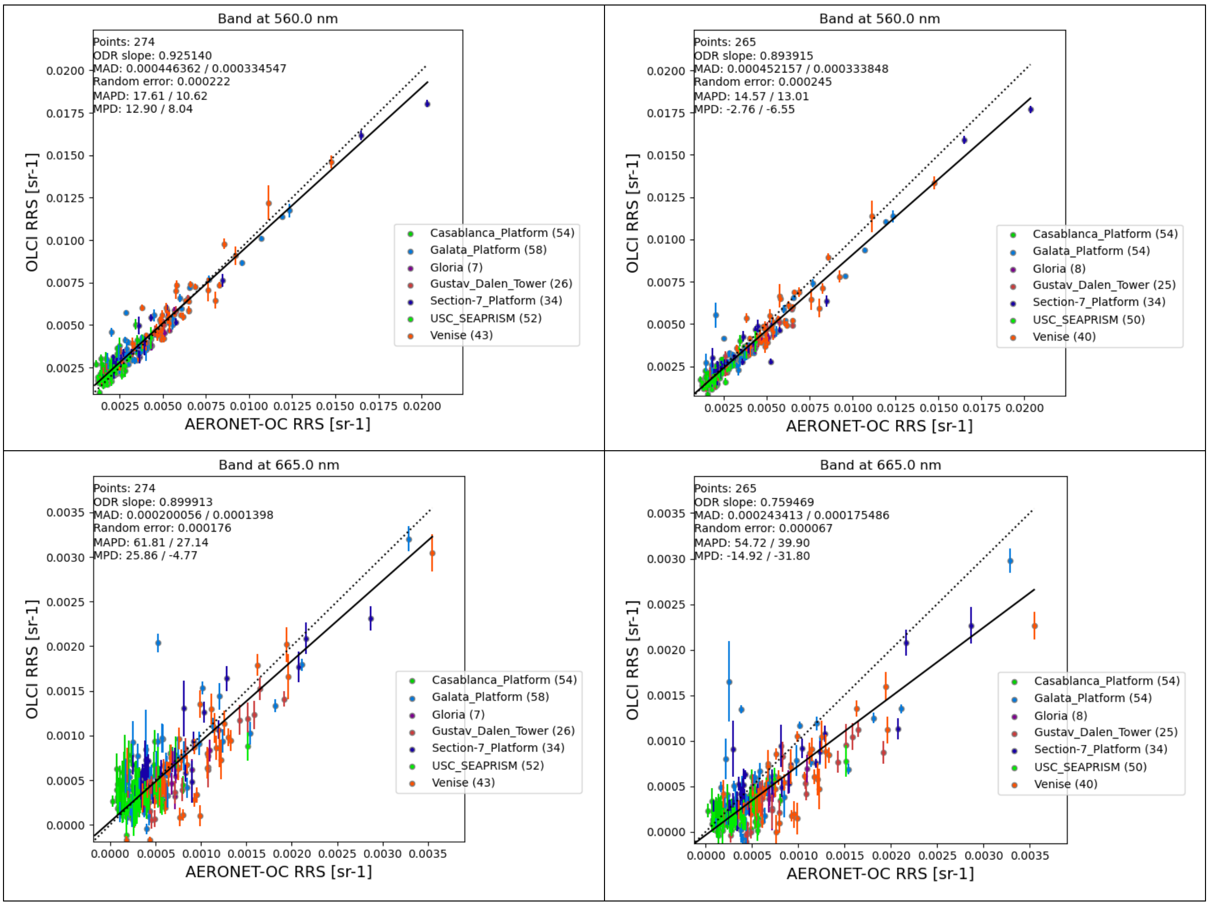
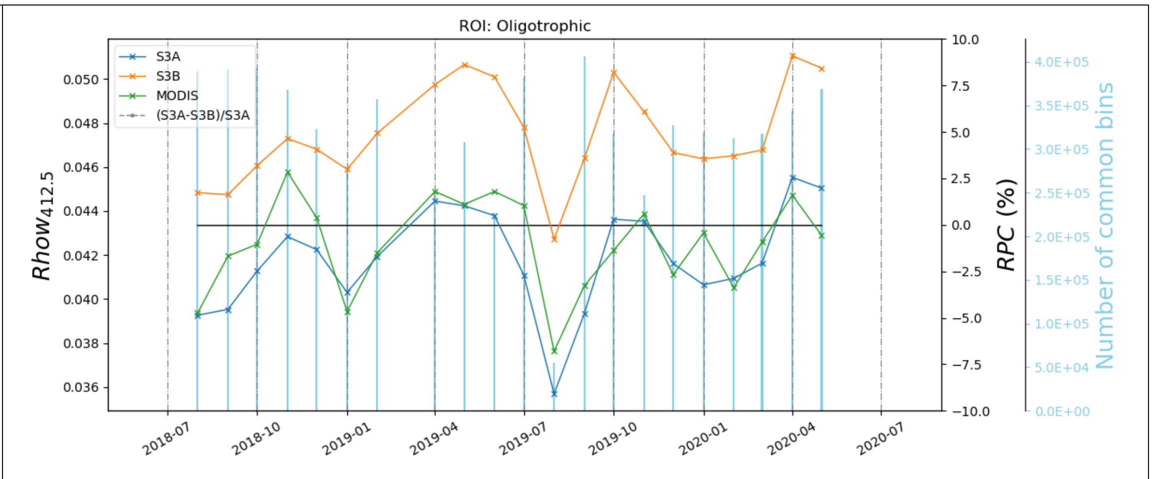


Figure 30: OLCI-B AERONET-OC matchup inter-comparisons for the previous operational PB2.43/1.15 and Collection OL_L2M.003

6.4 Water reflectance validation inter-comparisons across missions

6.4.1 Oligotrophic waters

PB2.43/1.15



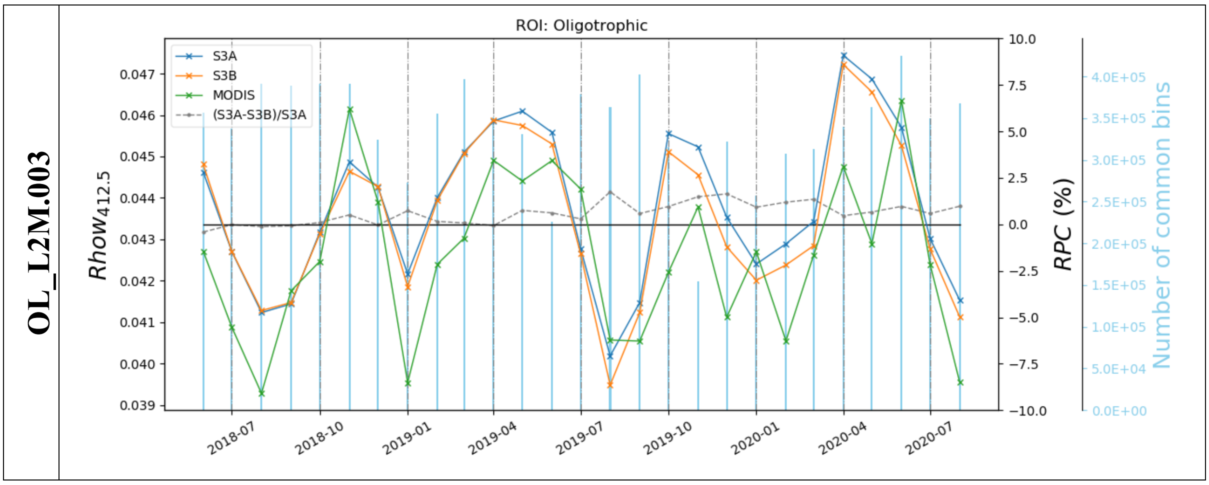


Figure 31: Rhow412.5 Oligotrophic waters - PB2.43/1.15 vs OL_L2M.003 inter-comparison

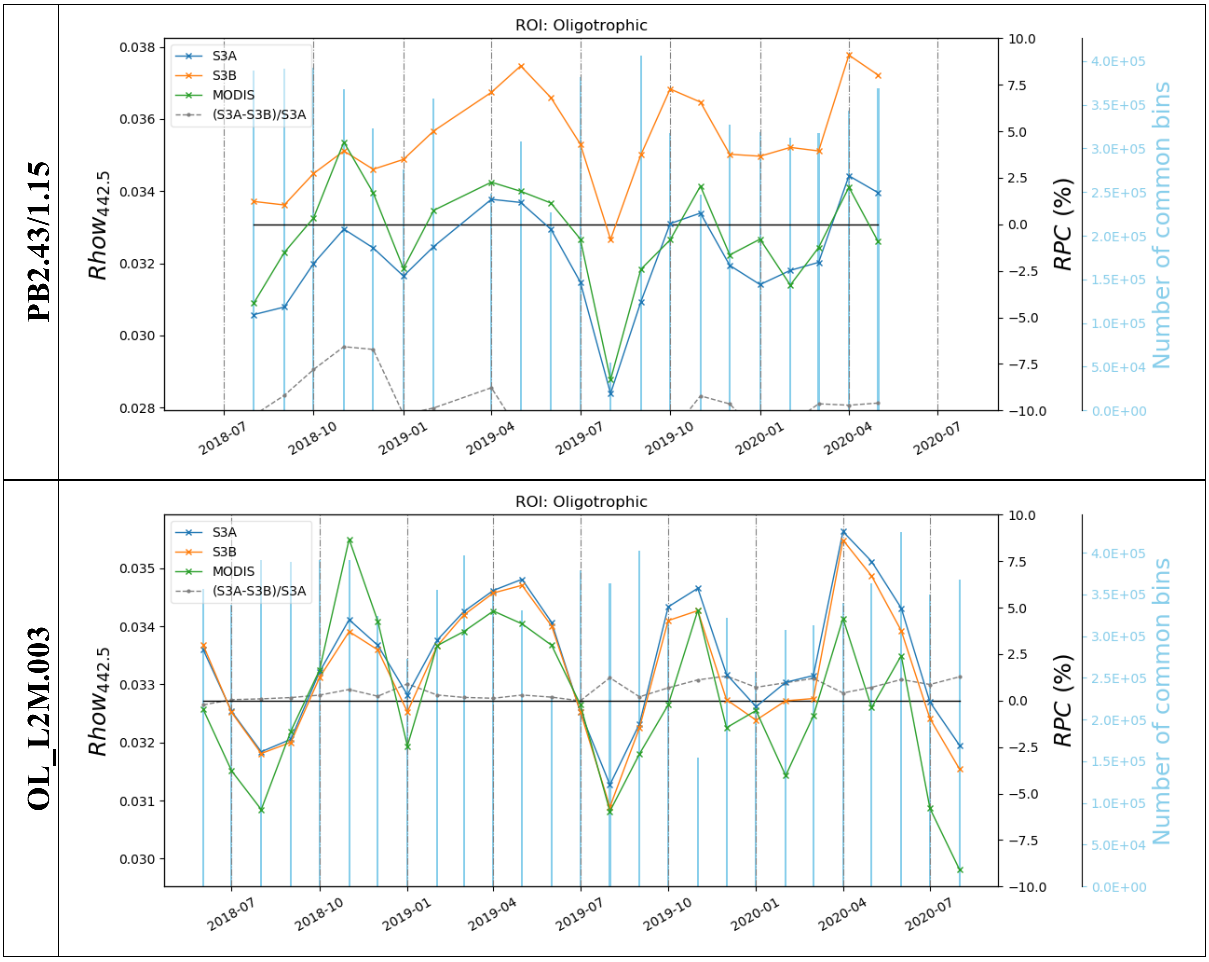
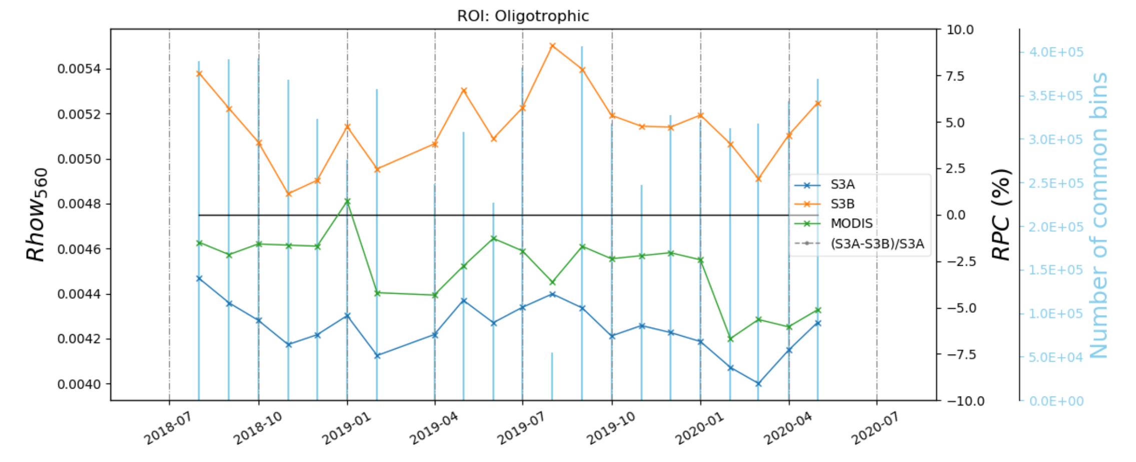


Figure 32: Rhow442.5 Oligotrophic waters - PB2.43/1.15 vs OL_L2M.003 inter-comparison

PB2.43/1.15



OL_L2M.003

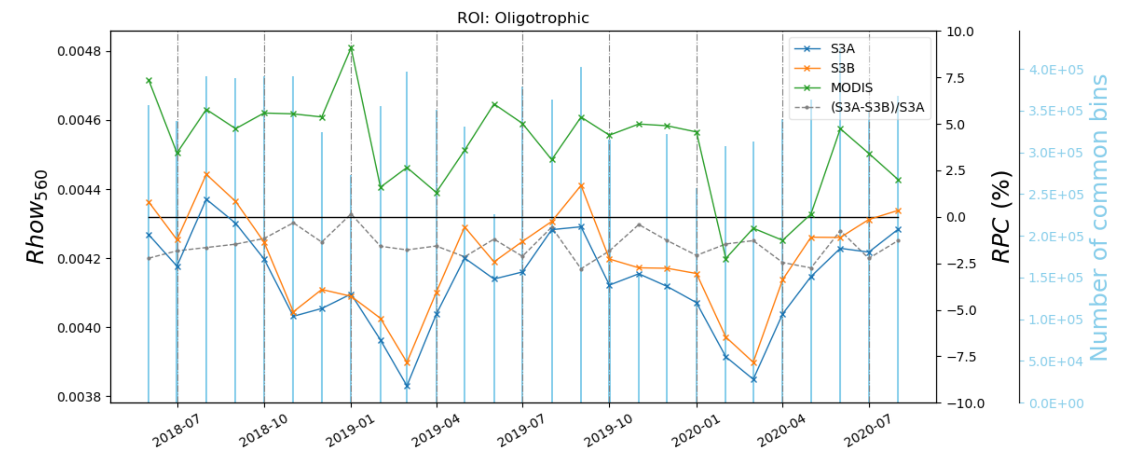
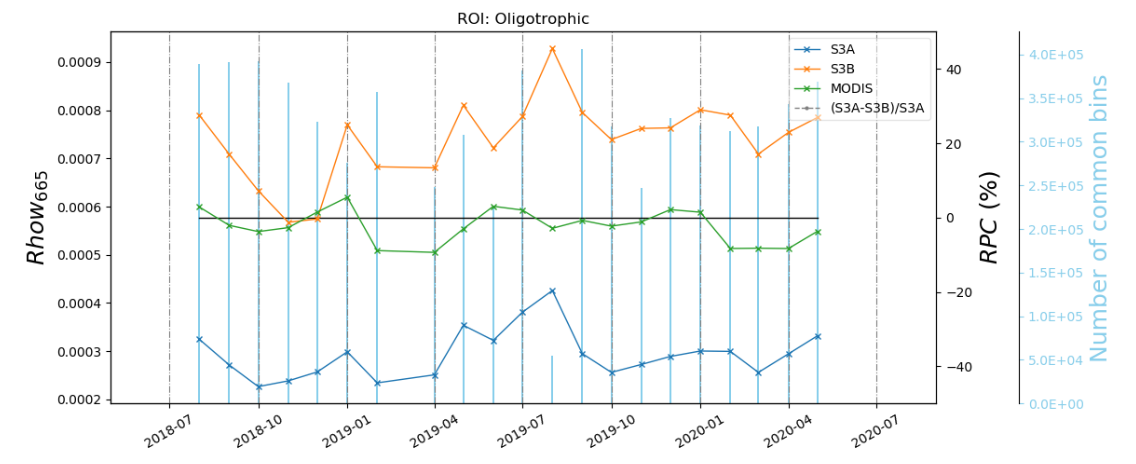


Figure 33: Rhow560 Oligotrophic waters - PB2.43/1.15 vs OL_L2M.003 inter-comparison

PB2.43/1.15



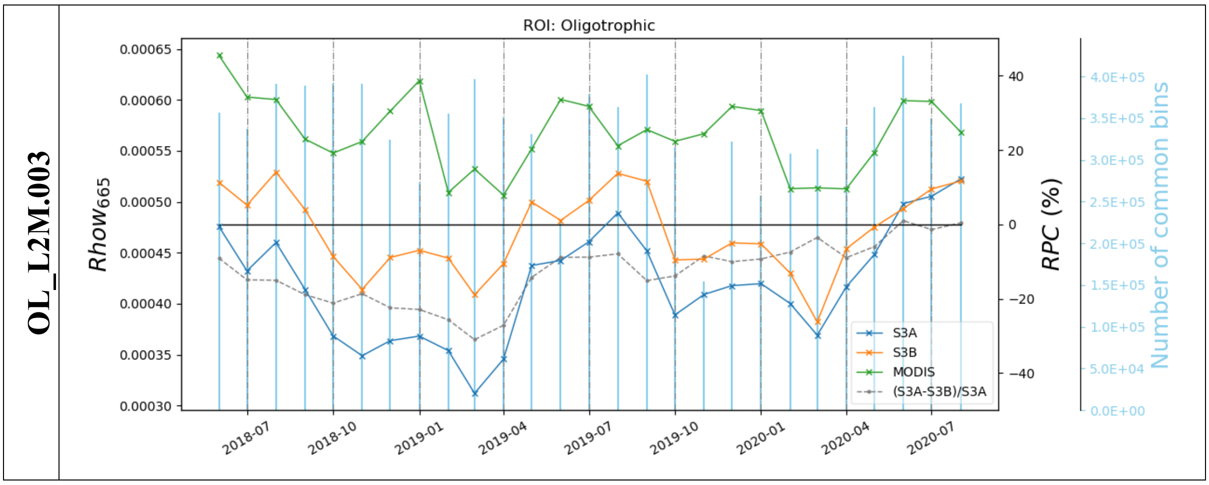


Figure 34: Rhow665 Oligotrophic waters - PB2.43/1.15 vs OL_L2M.003 inter-comparison

6.4.2 Mesotrophic waters

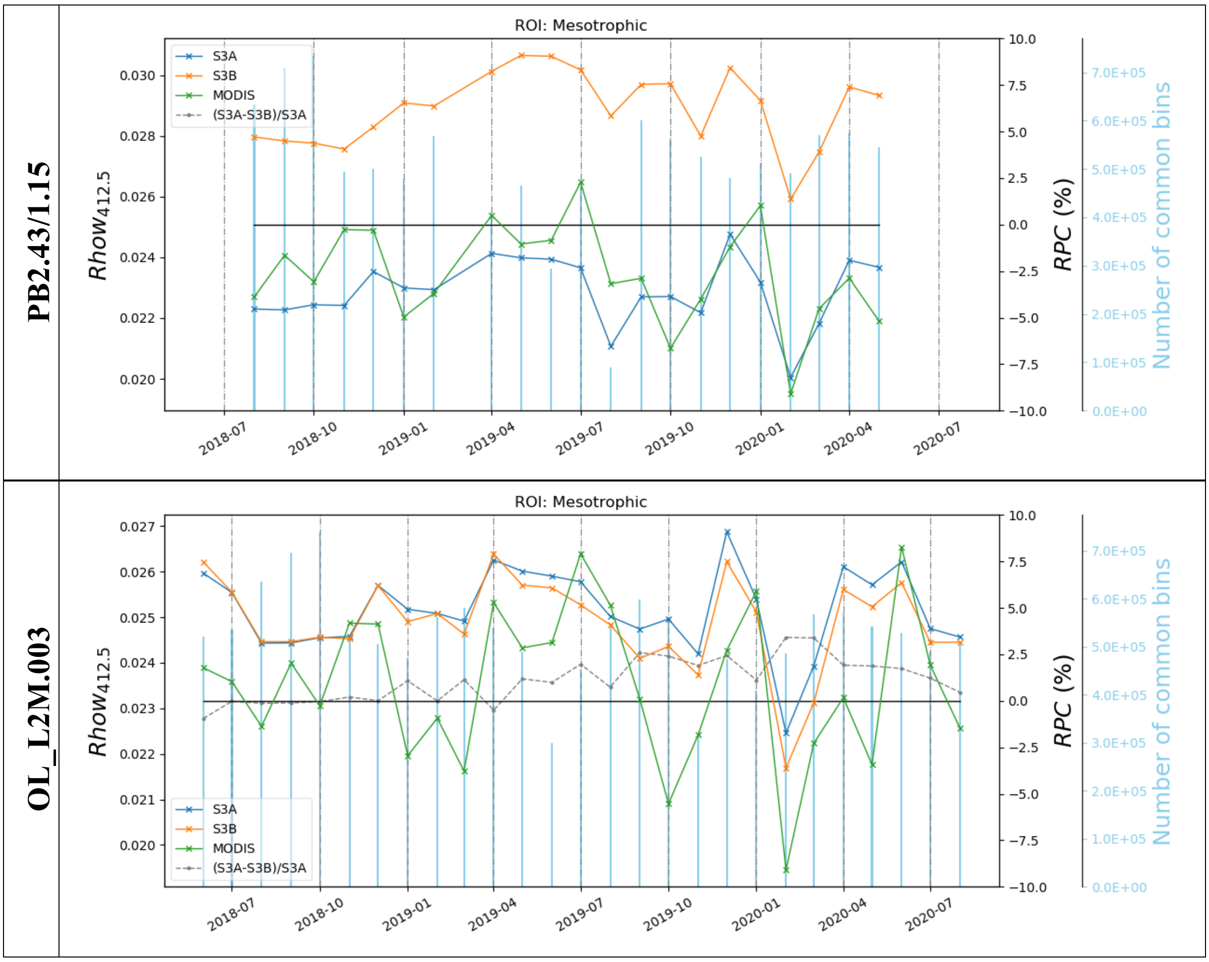
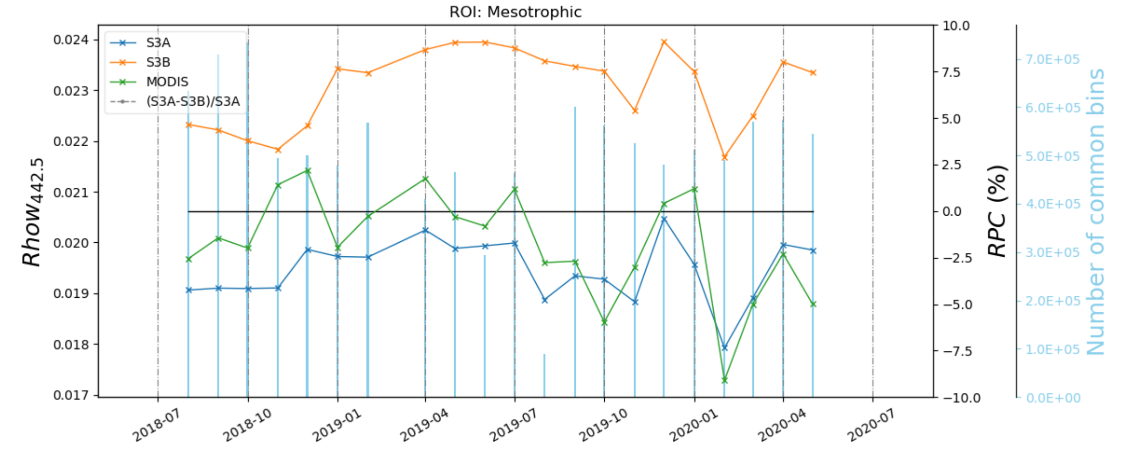


Figure 35: Rhow412.5 Mesotrophic waters - PB2.43/1.15 vs OL_L2M.003 inter-comparison

PB2.43/1.15



OL_L2M.003

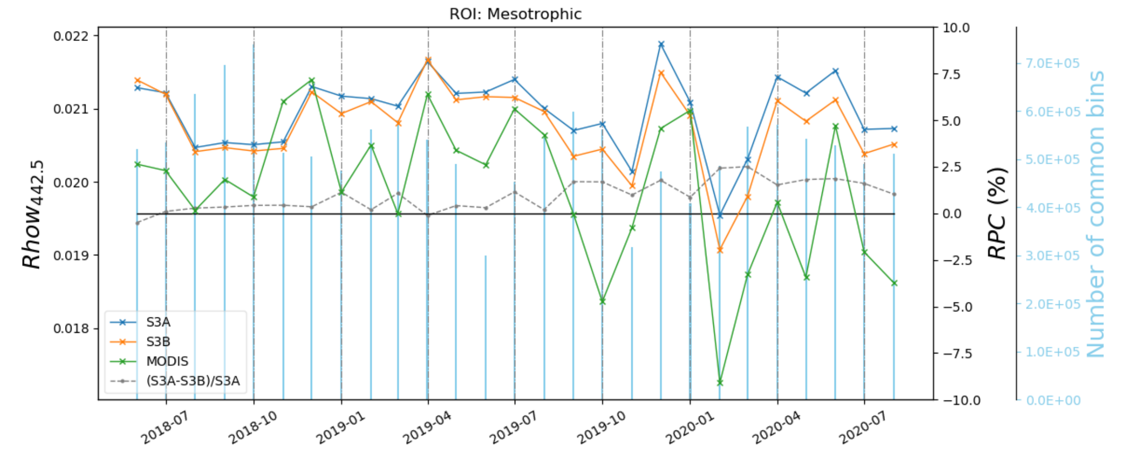
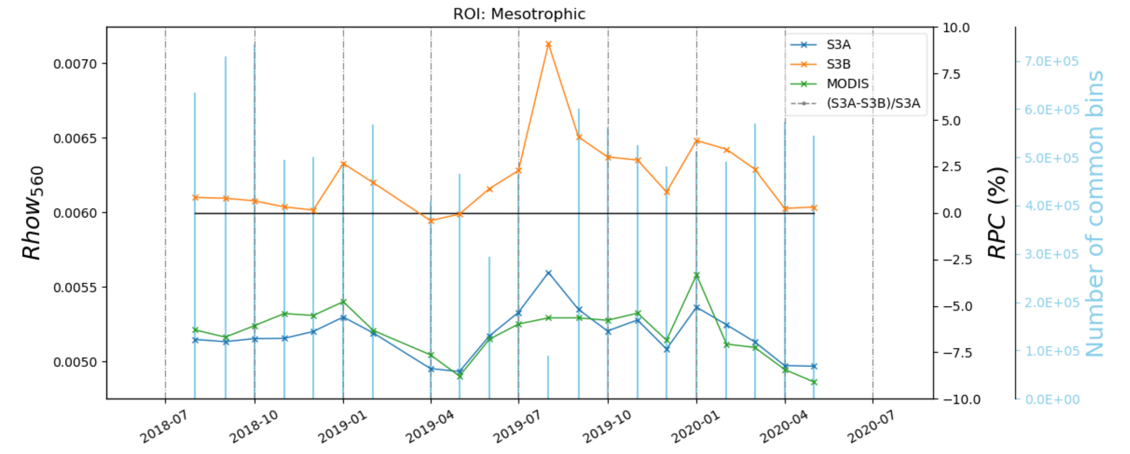


Figure 36: Rhow442.5 Mesotrophic waters - PB2.43/1.15 vs OL_L2M.003 inter-comparison

PB2.43/1.15



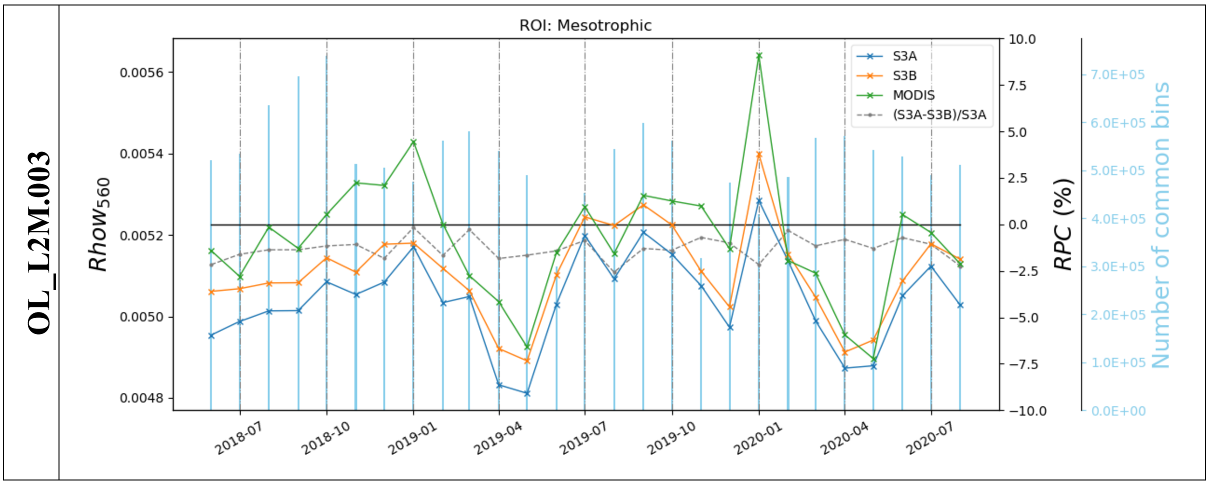


Figure 37: Rhow560 Mesotrophic waters - PB2.43/1.15 vs OL_L2M.003 inter-comparison

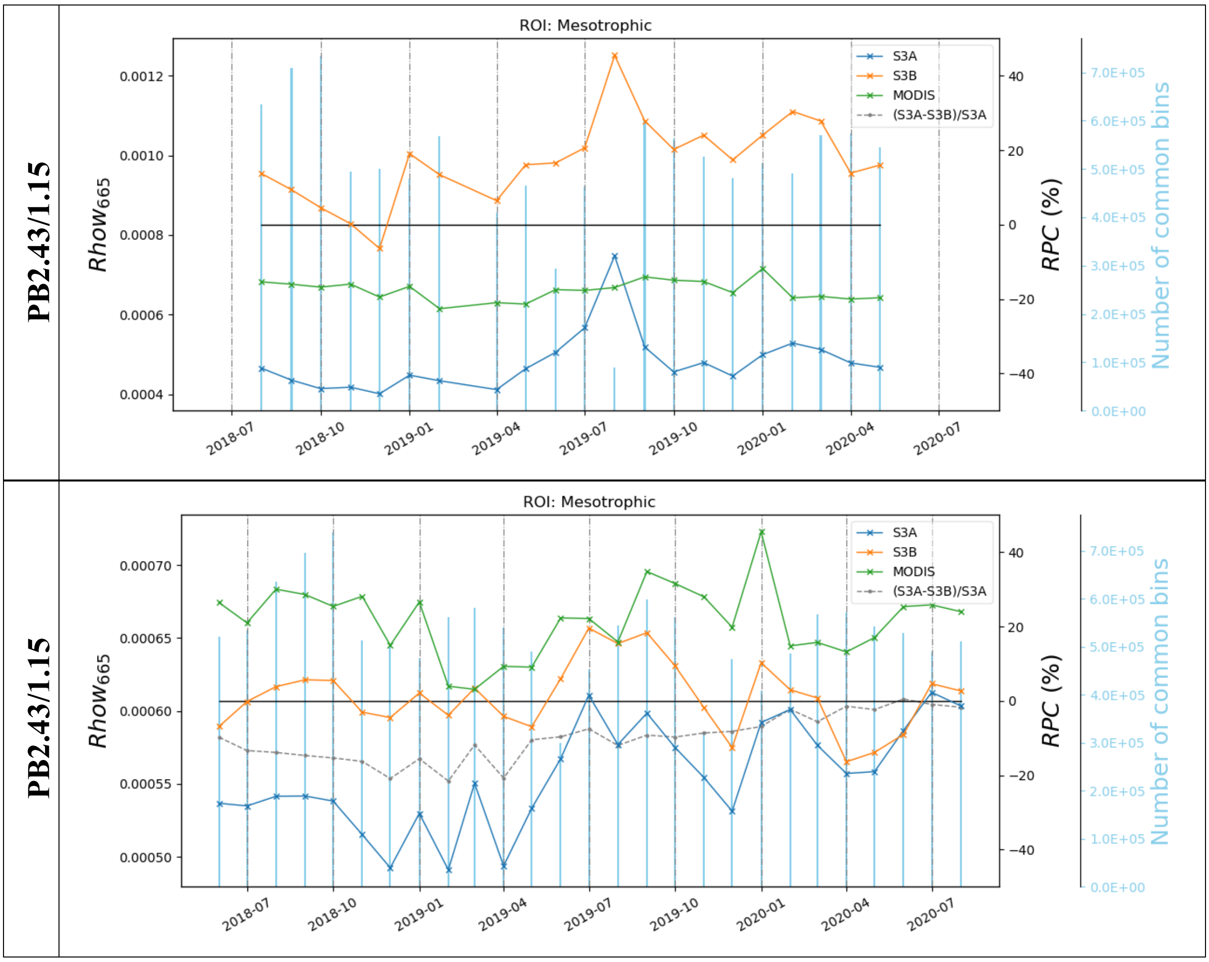
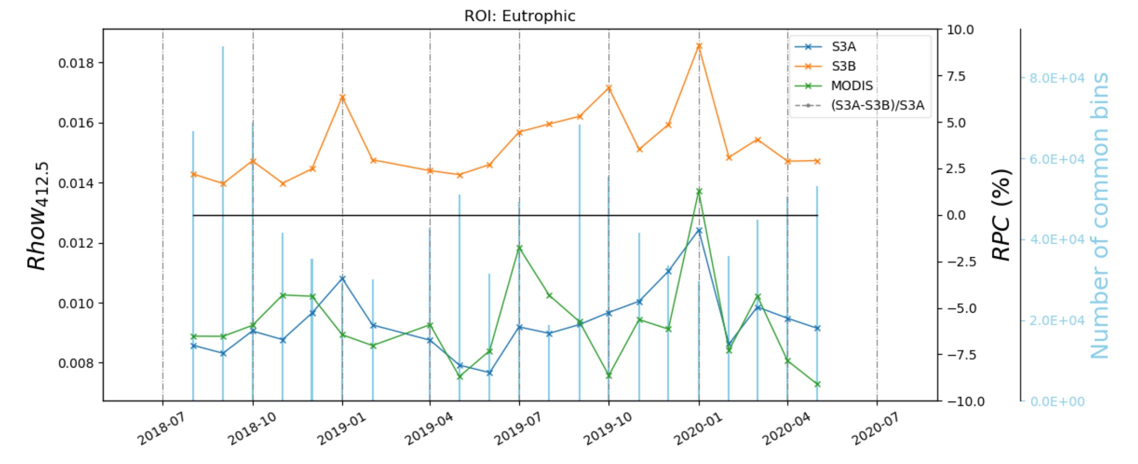


Figure 38: Rhow665 Mesotrophic waters - PB2.43/1.15 vs OL_L2M.003 inter-comparison

6.4.3 Eutrophic waters

PB2.43/1.15



OL_L2M.003

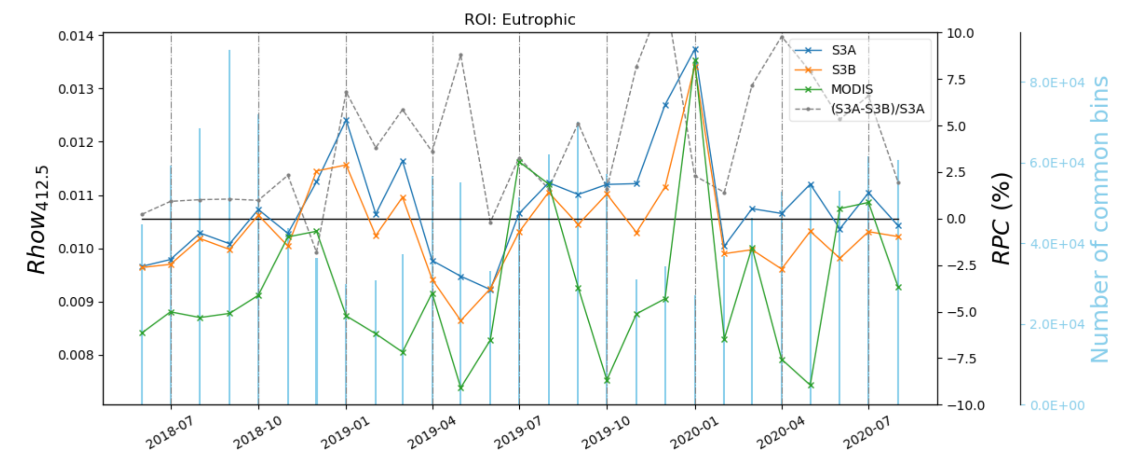
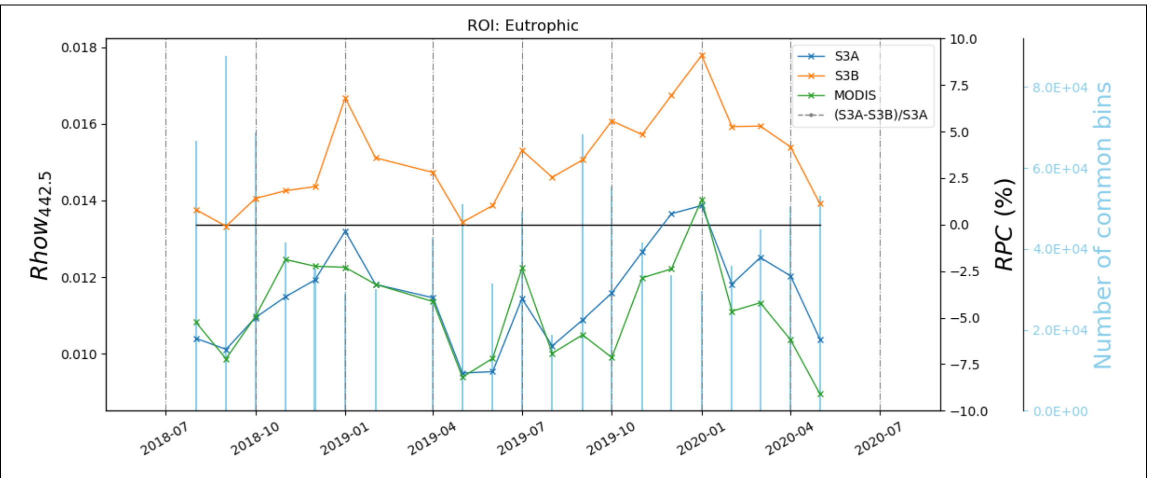


Figure 39: Rhow412.5 Eutrophic waters - PB2.43/1.15 vs OL_L2M.003 inter-comparison

PB2.43/1.15



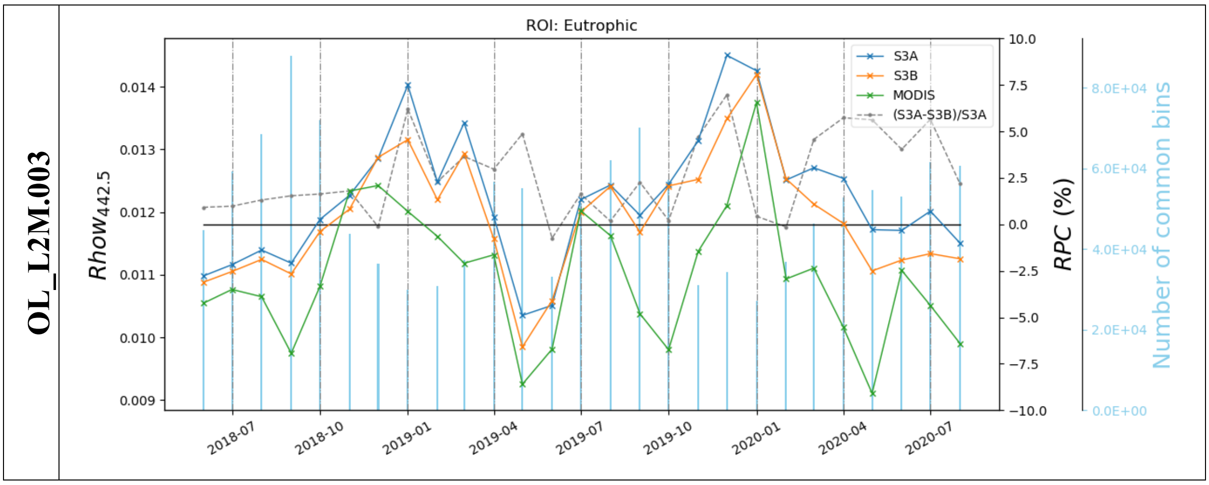


Figure 40: Rhow442.5 Eutrophic waters - PB2.43/1.15 vs OL_L2M.003 inter-comparison

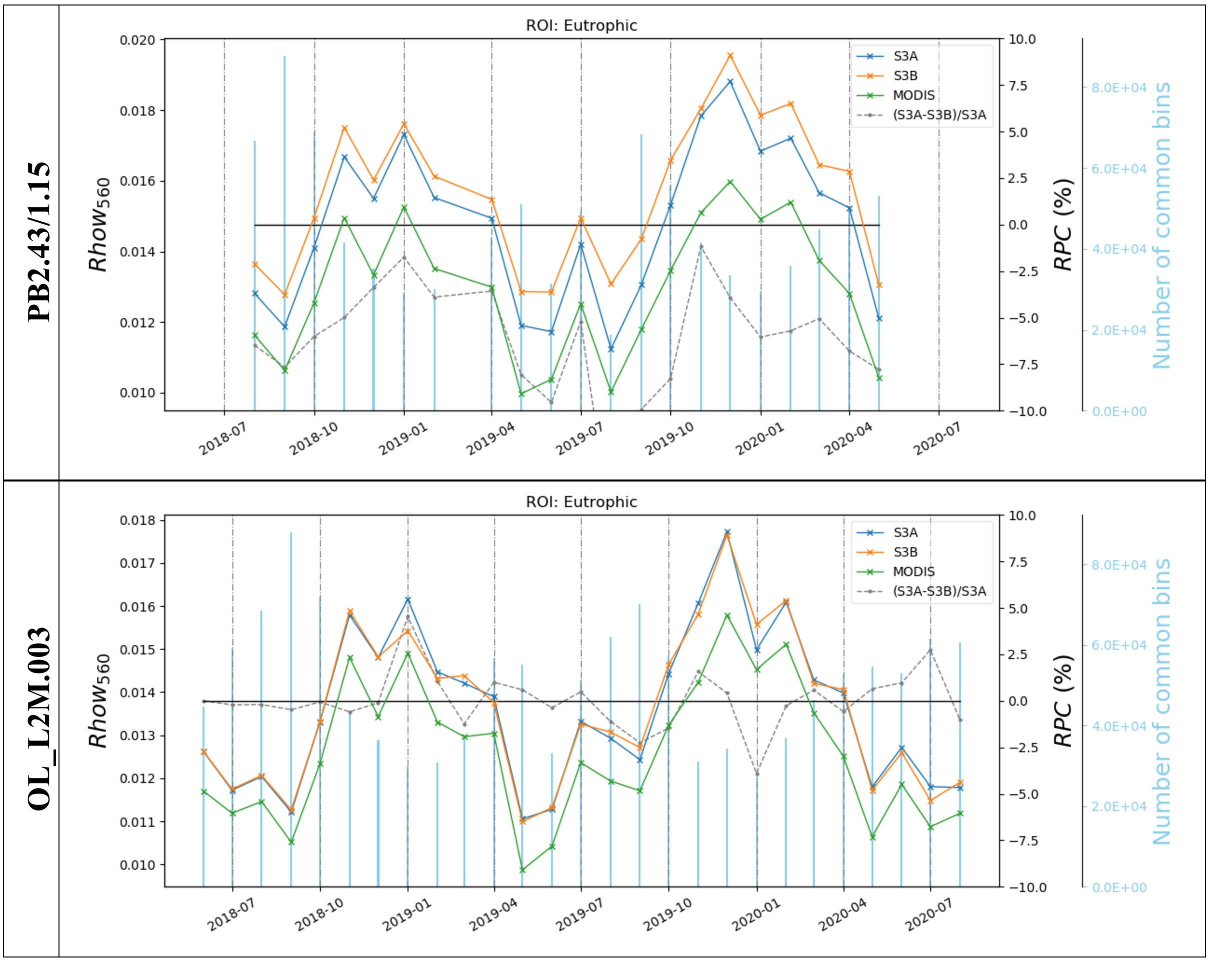


Figure 41: Rhow560 Eutrophic waters - PB2.43/1.15 vs OL_L2M.003 inter-comparison

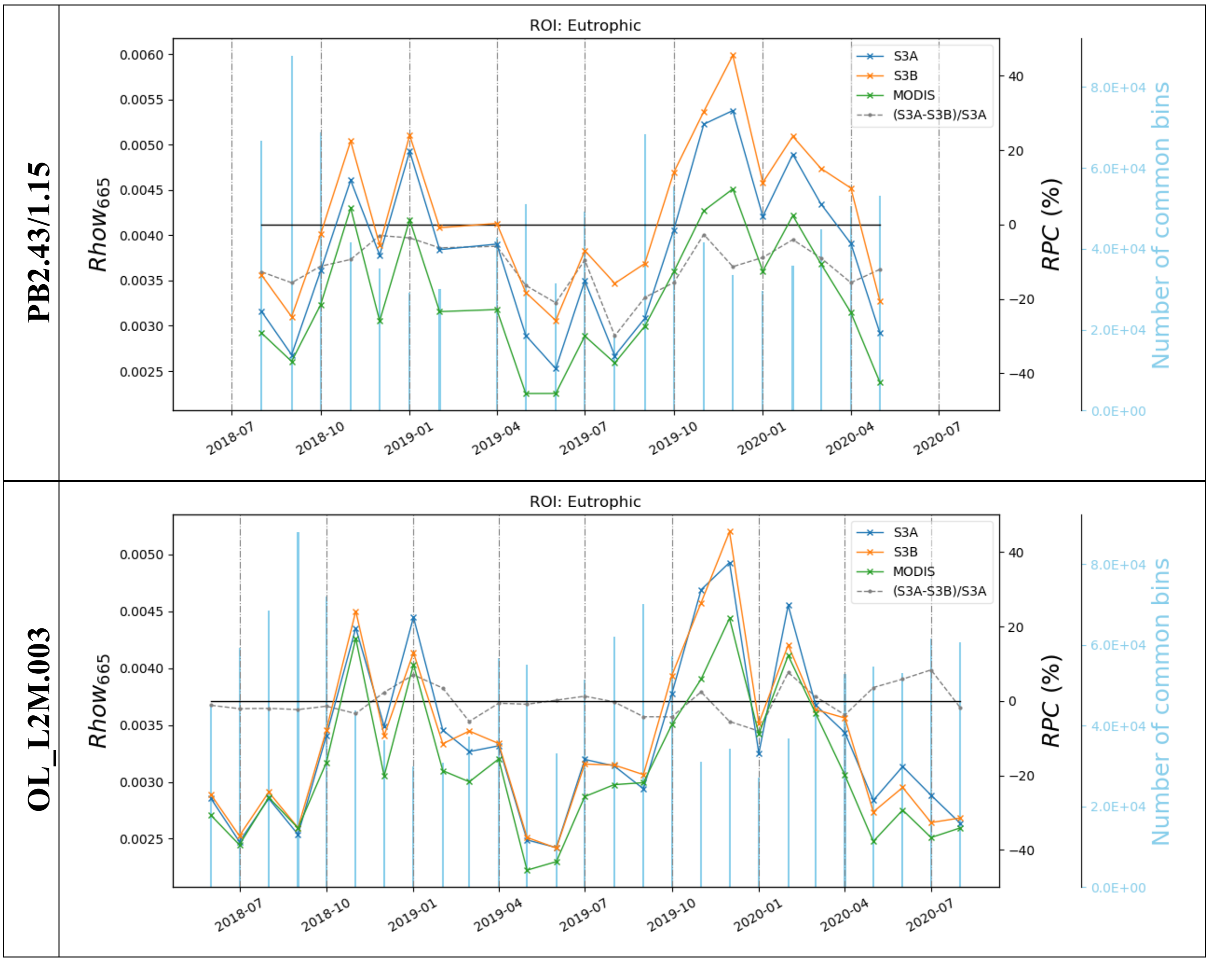


Figure 42: Rhow665 Eutrophic waters - PB2.43/1.15 vs OL_L2M.003 inter-comparison

6.5 TSM_NN product range improvement

Collection OL_L2M.003.01 introduces the updated validity range of the TSM_NN product, which is not anymore cut-off at 100 g/m^3, but can go up to 400 g/m^3, as explained in section 3.3.2.

This is illustrated in Figure 43 below, with scenes including extremely turbid estuarine waters of Rio de la Plata and Mackenzie River.

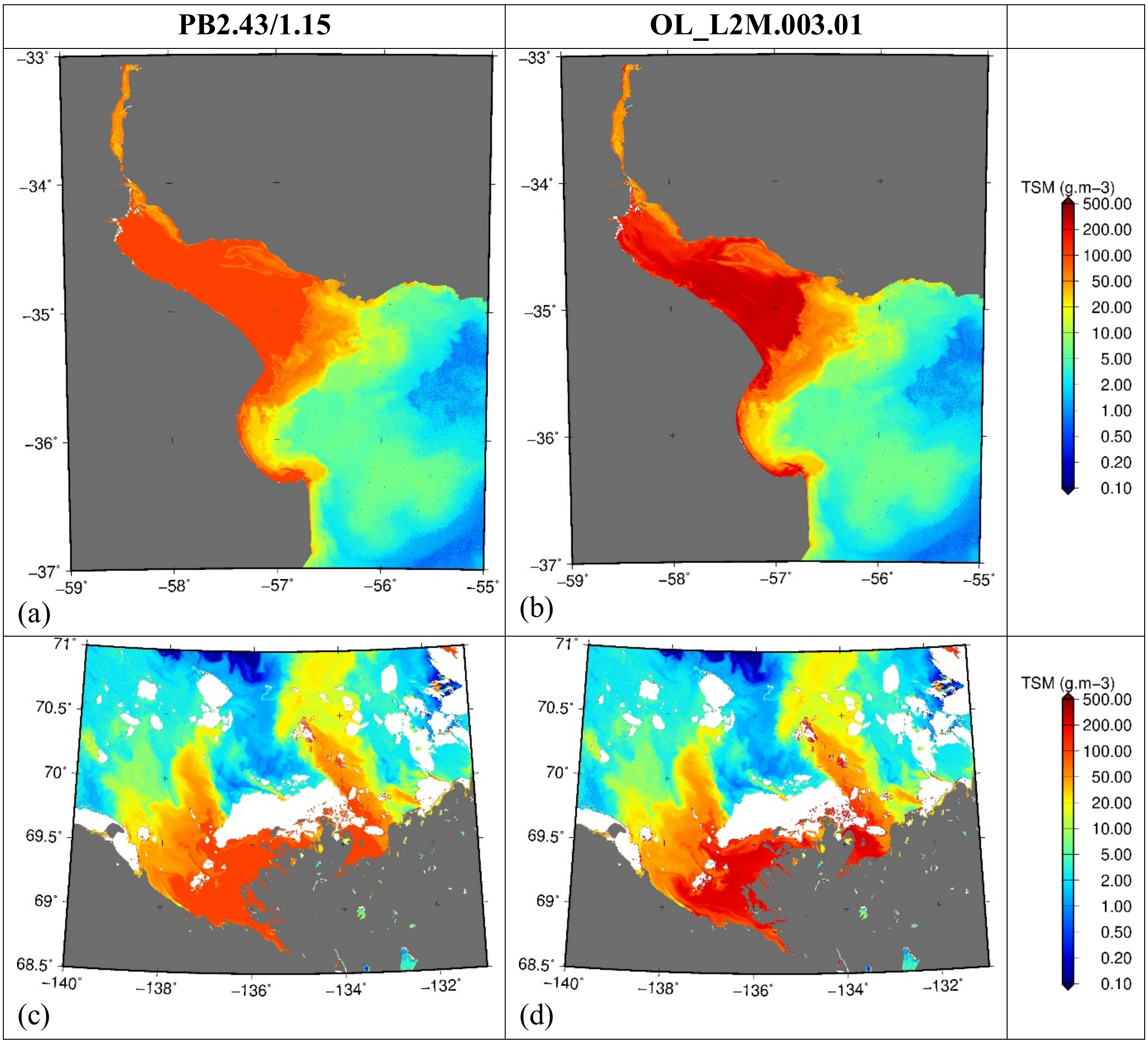


Figure 43: OL_L2M.003.01 TSM validity range comparison with previous version

7 SUMMARY OF BASELINE COLLECTION OL_L2M.003 STATUS AND FUTURE DEVELOPMENT

7.1 Summary of OLCI Collection OL_L2M.003 validation results

Collection OL_L2M.003 algorithm updates follow EUMETSAT's Ocean Colour Marine Roadmap and recommendations from Sentinel-3 OLCI/SYN Quality Working Group and Sentinel-3 Validation Team.

Collection OL_L2M.003 demonstrates

- high consistency between OLCI-A and OLCI-B Ocean Colour products
- oligotrophic algal pigment concentration within mission requirements
- improved coastal retrievals
- reduced «salt and pepper» noise

New OC-SVC gains ensure traceable and harmonised SVC strategy for OLCI-A and -B. OC-SVC produces an excellent agreement between the missions, despite the gains were derived fully independently for both instruments. This consistency opens new capabilities to use both OLCI missions together and merging their data.

New OC-SVC gains provide notable reduction of positive biases in OLCI-B radiometry. The OC-SVC gains have a significant impact in the blue bands where a more accurate spectral shape is now retrieved in comparison with in situ measurements. OLCI also shows a good agreement with MODIS-Aqua, with differences explained by spectral bands differences.

The updated Bright Pixel Correction eliminates frequent failures of the previous BPC. It reduces salt-and-pepper noise in products and improves coverage of coastal retrievals, particularly allowing for better retrievals in the most turbid cases, not achieved to date.

The new Chlorophyll Index algorithm introduced for application in low-chlorophyll oligotrophic waters has a significant impact on reducing biases in open ocean chlorophyll retrievals and allows OLCI algal pigment concentration product to reach mission requirements.

Cloud flagging improvements eliminate many cloud omissions and the need to apply other flags to compensate for cloud flagging failure. Thanks to the cloud flagging update, the ANNOT flags are now removed from the list of recommended flags following numerous user proposals.

NNv2 provides an important improvement in the three bio-optical products, particularly in TSM_NN and chl_NN. The NNv2 results are not included in this report but available online from S3VT#6 meeting Web site to S3VT members (RD-33). The extended range of TSM_NN enables retrievals in waters heavily dominated by sediments.

OLCI Collection OL_L2M.003 has achieved much progress, but there is still room for improvements. Large uncertainties are still present in more complex waters, particularly in waters with coloured dissolved organic matter (CDOM) contribution. There are problems with the standard atmospheric correction (BAC), which are apparent from issues with aerosol Ångström (restrictive limit of 1.6 value), residual noise in products, and degraded complex water retrievals.

S3 OLCI/SYN QWG has issued the following recommendation (R6.16):

QWG recommends for EUMETSAT to go ahead with the operational release of the new OLCI L2 Marine processor and with the L2 OLCI-A and -B full mission reprocessing, as the product improvements highly justify this.

7.2 OLCI performance requirements validation status

OLCI Marine product requirements are stated in Sentinel-3 Mission Requirement Document (AD-1) and Sentinel-3 Mission Requirement Traceability Document (AD-2). The goal of OLCI algorithm development and product validation activities is to achieve these requirements.

S3 OLCI/SYN QWG has issued a recommendation (R5.18) that OLCI marine product status with respect to the requirements should be accompanied with guidance on the interpretation of these requirements. The aim is to facilitate understanding for mission fulfilment of its performance numbers.

S3 OLCI/SYN QWG recommendation (R5.18):

2. Provide a reader guide to the Requirement tables – to correctly interpret the values with understanding that they are not realistic in some water types.

Performance of Ocean Colour algorithms depends on the optical complexity of water and atmosphere. In water, the uncertainty is modulated by types and concentrations of absorbing and backscattering constituents, such as coloured dissolved matter, phytoplankton, and sediments. Water reflectance spectra change with these types and concentrations. The smallest uncertainty is associated with open oceanic waters dominated by low phytoplankton concentrations and by coloured matter correlated with phytoplankton (case 1). These open oceanic waters compose the majority of the global ocean.

Coastal and inland waters (case 2) are associated with highest retrieval uncertainty because of their optical complexity. Water reflectance signal can vary vastly in these waters and so their natural standard uncertainty. For example for three AERONET-OC sites: at Venise the standard uncertainty is about 0.038 in radiance [mW cm^{-2} sr^{-1} µm^{-1}] corresponding to 5.3% of the water signal, at Helsinki Lighthouse the standard uncertainty is 0.016 [mW cm^{-2} sr^{-1} µm^{-1}] that corresponds to 27.4% of the signal, and at Gustav Dalen Tower the standard uncertainty is 0.018 [mW cm^{-2} sr^{-1} µm^{-1}] that corresponds to 16.3% of the signal (due to large absorption by CDOM). OLCI water-leaving radiance/reflectance requirement is defined as <5% uncertainty. However, most of OLCI validations are performed in coastal waters.

Additional uncertainties are also associated with the in situ measurements themselves, both radiometric and bio-optical, which constitute the ground truth for demonstrating fulfilment of the requirements. The uncertainties are included in in-situ instrument calibration, measurement protocol followed in the field, and processing of in situ data. For example, chlorophyll concentration cannot be obtained in a laboratory at an uncertainty better than 15% and the uncertainties significantly increase in the field. OLCI chlorophyll requirement is defined as <30% uncertainty.

The requirements do not specify product temporal stability, consistency of coverage across scenes and noisiness of retrievals, which are also important for users.

Table 9 presents a summary validation status of OLCI L2 Ocean Colour products referenced to S3 Mission Requirements.

Following the S3 OLCI/SYN recommendation and the discussion above, users are advised to consider these requirements as OLCI target values, which depend on retrieval complexity and may not be realistic in some waters.

Performance factor	**Requirement**	**Validation status with PB 2.43/1.15**		**Validation status with OL_L2M.003**		**Notes**
	Threshold, [goal][1]	**OLCI-A**	**OLCI-B**	**OLCI-A**	**OLCI-B**	
Marine reflectance@442nm	5.10^{-4}	Not Compliant 9.10^{-4}	Not Compliant 11.10^{-4}	Not Compliant 7.10^{-4}	Not Compliant 8.10^{-4}	Validation numbers are for coastal AERONET-OC sites with higher optical complexity. Open ocean inter-comparisons with MODIS-Aqua indicate < 5.10^{-4}.
Water-leaving radiance / reflectance	<5%	Partly Compliant <5% 490-560nm	Not compliant	Partly Compliant <5% 400-442nm <8% 490-560nm	Partly Compliant <5% 490-510nm <8% 412-560nm	Validation numbers are for coastal AERONET-OC sites with higher optical complexity. Open ocean verifications at MOBY indicate < 5% 400 – 620 nm.
Chlorophyll	<30% [10%]	Partly Compliant (only meso- and eutrophic waters)	Preliminary	Compliant	Compliant	Validations numbers are for in situ matchups mostly in oligotrophic and mesotrophic waters. Mission inter-comparisons with MODIS indicate a potential overestimate in eutrophic waters, but there MRD is 70%.
Photosynthetically Active Radiation	<5%	Preliminary	Preliminary	Preliminary	Preliminary	Lack of in situ validation data
Diffuse attenuation coefficient	<5%	Preliminary	Preliminary	Preliminary	Preliminary	Lack of in situ validation data
Total Suspended Matter	<70% [10%] (case 2 waters) 30% [10%] (case 1 waters)	Preliminary	Preliminary	Preliminary	Preliminary	Lack of in situ validation data S3VT-OC shows TSM improvements

[1] According to (AD-1)

Coloured Dissolved Organic Matter	<70% [10%] (case 2 waters) 50% [10%] (case 1 waters)	Preliminary	Preliminary	Preliminary	Preliminary	Lack of in situ validation data

Table 9 : OLCI L2 Ocean Colour performance Sentinel-3 Mission Requirement fulfilment status

7.3 Open Issues and Future Improvements

OLCI Collection OL_L2M.003 has achieved much progress, but there is room for improvement as indicated before. Known product quality limitations are described in Table 10 below.

Known product quality limitation	**Description**
Remaining biases in Open-Water radiometry and bio-optical products	• Water Reflectance products only partially meet S3 Mission Requirements (section 7.2 based on validation at AERONET-OC sites). • Algal Pigment Concentration product could be further improved (section 5.6, considering the accuracy of bio-optical products is dependent on the quality of Water Reflectance retrievals). Furthermore, the product has an updated range 0.01 to 100 mg/m^3, as OC4ME_FAIL flag now stops masking chlorophyll above 30 mg/m^3 (see section 3.2.3). As explained, the OC4ME algorithm is not designed for high chlorophyll waters, ≥ 10 mg/m^3, and there is evidence that it may produce overestimate. Users are cautioned about higher OC4ME values, validation feedback is welcome. • Open Water products may show potential airmass dependence exhibited as OLCI cross-track or seasonal variability. • The remaining product biases and dependencies are traced to uncertainties in OLCI standard/baseline atmospheric correction (BAC). Improvements in BAC are recommended by OLCI/SYN QWG (R 6.17), including switching to a more robust selection of aerosol models to ensure a broader range and a better discretization of aerosol sampling in the Ångström space.
Reduced quality in coastal and complex-water areas	• Products still exhibit large uncertainties in more complex waters, particularly in absorbing waters with coloured dissolved matter contribution like Baltic Sea and in lakes. • Products may display recurring negative Water Reflectances.
Noise in Open Water products	• Residual noise may be present in Open Water products.
Residual Level-2 flag limitations	• Residual cloud flag limitations may occur over bright surfaces e.g. snow/sands/coastlines/desserts/glint and at camera interfaces. • CLOUD_AMBIGUOUS may flag some coastline pixels and then CLOUD_MARGIN would expand the flagged area (see section 3.4.3.1). • Intertidal or water covered area classification into dry-fallen is not working optimally in Complex Water products.
Biases in Integrated Water Vapour product	• Over land surfaces, there is a systematic overestimation of 9 – 13%, which leads to a bias of 0.9 – 2.0 kg/m^2. Over water, there are larger uncertainties and strong overestimation in the transition from glint to no-glint.
Lack of in situ measurements and preliminary product validation status	• OLCI product quality status is defined through inter-comparisons with ground truth in situ measurements but these measurements are severely limited or lacking for certain products and across different water types. Consequently, none or preliminary product quality status is provided at this time.
Level-2 error product caution	• Level-2 per-pixel error products do not include the uncertainty estimate from Level-1B products because it is not yet available. • Level-2 error products have not been validated.
Anomalies implemented in release OL_L2M.003.01 (Spring 2021)	• Scaling of the TSM_NN product in OL_L2M.003.00 limits TSM values to 100g/m^3 and in OL_L2M.003.01 it is extended to 400g/m^3 following the description in section 3.3.2. • Excessive flagging as CLOUD_AMBIGUOUS of pixels along some coastlines in OL_L2M.003.00 is reduced in FR products in OL_L2M.003.01, as described in section 3.4.3.1.

Table 10 : OLCI L2 Ocean Colour known product quality limitations

To address the known product quality limitations, OLCI L2 Ocean Colour algorithm evolutions are planned towards Collection 4 (OL_L2M.004):

- redevelopment of the standard/baseline atmospheric correction (BAC) will provide the highest impact,
- improvements in flagging and bio-optical products will be investigated,
- Integrated Water Vapour will be separated into a dedicated NRT atmospheric product suite and will undergo algorithmic improvements.

In addition to addressing the product limitations above, the OLCI/SYN QWG and S3VT-OC expressed a need for extending OLCI Ocean Colour products, mainly

- including Inherent Optical Property (IOP) products in OLCI L2 marine product suite (QWG R2.42),
- including Fluorescence product in OLCI L2 marine product suite (QWG R2.42),
- correcting OLCI directional Water Reflectance products with bidirectional reflectance distribution function (BRDF) via an “f /Q correction” that is suited to different water types (S3VT-OC#6, QWG R5.16).

IOP and Fluorescence products have already been developed and are available for user validation in SNAP toolboxes and in source code:

- IOP
    - website: https://www.eumetsat.int/S3-OLCI-IOP
    - GitLab: https://gitlab.eumetsat.int/eumetlab/oceans/ocean-science-studies/olci-iop-processor
    - SNAP toolbox: http://s3vt.skytek.com/group/s3vt-oc/home
- Fluorescence
    - website: https://www.eumetsat.int/S3-OLCI-FLUO
    - SNAP plugin: http://s3vt.skytek.com/group/s3vt-oc/home

The BRDF SNAP plugin is also available, yet based on the Open Ocean water model (RD-41):

- BRDF SNAP plugin: http://s3vt.skytek.com/group/s3vt-oc/home

To follow the user recommendation, the BRDF correction suited to different water types will require a dedicated investigation.

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- S3 OLCI/SYN QWG for critical analyses and formal recommendations.

APPENDIX A DETAILS OF COLLECTION OL_L2M.003 SUBVERSIONS, IPF-OL-2 DEPLOYMENT TIMELINE AND DISTRIBUTION

Collection 3, OL_L2M.003, is a name for the major OLCI L2 Ocean Colour product update starting in February 2021. Small changes are and will be introduced to Collection 3 OLCI processing and will be defined as subversions. This report and this Appendix will be successively updated with new subversion definitions and results.

As of the date of this report, two subversions of OLCI L2 Ocean Colour Collection OL_L2M.003 are available: 3.00 and 3.01, i.e. OL_L2M.003.00 and OL_L2M.003.01. The two subversions are associated with IPF-OL-2 v.07.00 and v.07.01, respectively. However, the subversion 3.01 is not yet submitted to operations. The two subversions are explained in Table 11. The table also shows the release dates and data availability:

Subversions of OLCI L2 Ocean Colour Collection OL_L2M.003	**Subversion processor updates**	**Subversion availability and data distribution**

OL_L2M.003.00
(IPF-OL-2 v.07.00)
	• Scaling of the TSM_NN product still limits TSM values to 100 g/m^3 (see section 3.3.2).
	• Flag re-assignment from CLOUD_AMBIGUOUS to ADJAC to limit cloud misclassification along coastlines is still set to 1 pixel radius in FR products (see section 3.4.3.1).
		• Public release 16 February 2021
		• Operational products available from 16 February 2021 via
		  ○ coda.eumetsat.int,
		  ○ EUMETCast (NRT only),
		  ○ eoportal.eumetsat.int

OL_L2M.003.01
(IPF-OL-2 v.07.01)
	• Scaling of the TSM_NN product now extends TSM values to 400 g/m^3 following the description in section 3.3.2.
	• Flag re-assignment from CLOUD_AMBIGUOUS to ADJAC to limit excessive cloud misclassification along coastlines is now set to 2 pixel radius in FR products (see section 3.4.3.1).
		• Public release March/April 2021
		• Full mission reprocessing OLCI-A+B
		• Operational products available from March/April 2021 via
		  ○ coda.eumetsat.int,
		  ○ EUMETCast (NRT only),
		  ○ eoportal.eumetsat.int
		• Full reprocessed time series from the beginning of OLCI-A and -B missions, respectively, to March/April 2021 available from
		  ○ codarep.eumetsat.int.

Table 11 : OLCI L2 Ocean Colour Collection 3 OL_L2M.003 subversions