D2.4 Validation Plan

This project has received funding from
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Project no. 776348

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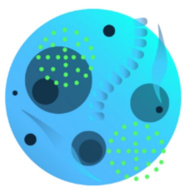
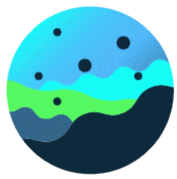
CoastObs Project

CoastObs is an EU H2020 funded project that aims at using satellite remote sensing to monitor coastal water environments and to develop a user-relevant platform that can offer validated products to users including monitoring of seagrass and macroalgae, phytoplankton size classes, primary production, and harmful algae as well as higher level products such as indicators and integration with predictive models.



phytoplankton

seagrass



harmful algal blooms

primary production

To fulfil this mission, we are in dialogue with users from various sectors including dredging companies, aquaculture businesses, national monitoring institutes, among others, in order to create tailored products at highly reduced costs per user that stick to their requirements.

With the synergistic use of Sentinel-3 and Sentinel-2, CoastObs aims at contributing to the sustainability of the Copernicus program and assisting in implementing and further fine-tuning of European Water Quality related directive.

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Partnership

Water Insight BV. (WI)

The University of Stirling (USTIR)

Consiglio Nazionale Delle Ricerche (CNR)

Universite de Nantes (UN)

HZ University of Applied Sciences (HZ)

Universidad de Vigo (UVIGO)

Bio-Littoral (BL)

Geonardo Environmental Technologies Ltd. (GEO)

TABLE OF CONTENTS

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 776348

FIGURES

TABLES

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 776348

Symbols and acronyms

Symbols/acronyms	Description
AERONET	AEROsol Robotic NETwork
AOD	Aerosol Optical Depth
AOPs	Apparent Optical Properties
BL	Bio-Littoral
cal/val	calibration/validation
CDOM	Coloured Dissolved Organic Matter
Chl-*a*	Chlorophyll-*a* concentration
CNR	Consiglio Nazionale Delle Ricerche
CTD	Conductivity, temperature and depth meter
DA	Domoic Acid
DOC	Dissolved organic carbon
EO	Earth Observation
ESA	European Space Agency
GLaSS	Global Lakes Sentinel Services, 7th Framework Programme project
GPS	Global Positioning System
HAB	Harmful Algal Bloom
HR	High Resolution satellite images
HTCO	High Temperature Combustion catalytic Oxidation
HZ	HZ University of Applied Sciences, Netherlands
INFORM	Improved monitoring and forecasting of ecological status of European INland waters by combining Future earth ObseRvation data and Models, 7th Framework Programme project
INTECMAR	Technological Institute for the Control of the Marine Environment of Galicia
IOCCG	International Ocean-Colour Coordinating Group
IOPs	Inherent Optical Properties
ISM	Inorganic Suspended Matter
K	Kappa statistic
L8	Landsat-8

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Symbols/acronyms	**Description**
LIMANDES	Lake Bio-optical Measurements and Matchup Data for Remote Sensing
LV	Lagoon of Venice
MAE	Mean Absolute Error
MSFD	Marine Strategy Framework Directive
NAS	northern Adriatic Sea
NASA	North American Space Agency
OA	Overall Accuracy
OLCI	Ocean and Land Colour Instrument (OLCI) of Sentinel-3
PAR	Photosynthetically Available Radiation
PC	Phycocyanin
PP	Primary Production
PSC	Phytoplankton Size Classes
RMSE	Root Mean Square Error
S	Salinity
S2	Sentinel-2
S3	Sentinel-3
SMA	Seagrass and Macro-algae
SST	Sea Surface Temperature
SVM	Support Vector Machine models
TBD	To Be Defined
TFR	True False Rate
TPR	True Positive Rate
TSM	Total Suspended Matter
TUR	Turbidity
UI	Upwelling index
UN	Universite de Nantes
USTIR	University of Stirling
VIGO	Universidad de Vigo
WFD	Water Framework Directive

Symbols/acronyms	Description
WI	Water Insight
WISP-3	Water Insight SPectrometer with 3 channels
WP	Work Package
WS	Wind speed

Summary

Objective

The overall aim of the CoastObs project is to develop a commercial service platform for user-relevant coastal water monitoring and environmental reporting based on validated Earth Observation and *in situ* optical data. **This deliverable (D2.4, WP2) aims to produce a validation plan, which ensures all products are tested against the requirements defined by each user group.**

The accuracy of the Earth observation products will be assessed using statistical methods based on reference measurements. For the higher-level products, a fitness for purpose analysis will be performed (for example by comparing the classification of a water body according to WFD requirements based on Earth observation data with the classification of the same water body based on laboratory analysis). Moreover, the quality and the utility of the services will be assessed by the user group.

Rationale

Validation is a pivotal part of the CoastObs project and is of particular importance while the EO community prepares for the use of a new generation of Sentinel satellites. The CoastObs consortium had a long record of experience with optical measurements in coastal waters and will be responsible for collection of a comprehensive validation dataset through dedicated field campaigns and integration of the end user community group.

This validation plan is based on the stated and implied user requirements and will specify all activities for accuracy assessment, with emphasis on fitness for purpose analysis of the products, and quality and utility assessment of the services. Besides validation of the products themselves, CoastObs work will also contribute to the validation of Sentinel-2 and Sentinel-3 (S2 and S3) data, including atmospheric and adjacency corrections, using well-calibrated and optically characterised instruments.

Therefore, it is necessary to test and adapt these product algorithms to enhance their applicability in different regions of interest and for the requirements of the users. The products developed within CoastObs will derive from dedicated field campaigns and datasets of relevant measurements available to the partners. To define the accuracy of Earth Observation (EO) data and products and ensure their adequate quality control, all field work will be supported by Water Insight (WI) spectroradiometer systems to collect remote sensing reflectance together with the other parameters of interest, with the objective of connecting algorithms at the field scale to the satellite scale, and - if necessary - to calibrate atmospheric corrections.

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Scope

As the available equipment or selected approach for EO will differ for each partner, this document focuses on description of measurement methods used both in field and in laboratory by the CoastObs consortium. It describes the instrumentation used and the parameters gathered for calibration/validation activities as a background for remote sensing, as well as the dedicated protocols for optical measurements and satellite validation for coastal waters. The scope of the validation plan is to specify all activities for accuracy assessment, emphasise the purpose of analysis of the products, and conduct a quality and utility assessment of the services. After each initial service delivery, fitness for purpose and utility assessments will be carried out to facilitate quick improvements to fit the users' needs. In addition to validation of the products, validation of S2 and S3 data (including atmospheric and adjacency corrections) will be undertaken using our proprietary well-calibrated and optically characterised instrument (WISP-3).

1. Summary of initial user requirements

Initial user requirements for the CoastObs products and service were defined in CoastObs WP2, with content and quality requirements for the CoastObs products and service defined in CoastObs Task 2.2 and the technical and service requirements defined in CoastObs Task 2.3. These were included in the initial user requirements deliverable (D2.2). The initial user data requirements are summarised in Table 1.

Light attenuation (K_d) and the "standard" products chlorophyll-*a* (Chl-*a*), total suspended matter (TSM), turbidity (TUR) and sea surface temperature (SST) were requested by all users, and will therefore have to be validated for all case study areas. The other "standard" products, the innovative and higher level products were only requested by some users, so that here the validation can focus on the specific areas for which the products were requested.

Only three users explicitly stated accuracy requirements (ARPAV requested a general accuracy of 20% over all parameters, whereas the Dutch mussel famers and producer organisation defined accuracies per parameter). Therefore, an iterative process is expected in which the project partners perform an initial validation of the products based on the *in situ* validation data acquired and collated within the project. The results of this validation are then discussed with the users to find out whether they consider the demonstrated accuracy as sufficient. Based on the outcome of this discussion, the next steps are defined: if the users are convinced of the utility of the products and services, a service level agreement is set up for operational service delivery in the second project year. If the users are still doubtful, additional efforts will be made by the project partners to improve and further validate the products during the second project year.

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Table 1 – CoastObs user needs data overview

Site	Chl-*a*	TSM/ TURB/ Kd	CDOM	CPC	SST	SMA presence / status	PSC	Sub-littoral habitat	HAB/ indicator species*	PP	Phyto-plankton bloom phenology	WFD indic-ators	Coastal erosion and accretion	Source identi-fication	Spatial suita-bilty	Additional param-eters
Wadden Sea	S2 (MF, RWS) S3 (MF, RWS)	S2 (MF, POM, RWS) L8 (RWS) S3 (RWS)	S3 (POM, RWS)		L8 (RWS) 1km (RWS)		S3 (MF)		S3 (MF, RWS)				x (RWS)	x (RWS)	x (MF)	
Eastern Scheldt	S2 (MF, RWS) S3 (MF, RWS)	S2 (MF, POM, RWS) L8 (RWS) S3 (RWS)	S3 (POM, RWS)		L8 (RWS) 1km (MF, RWS)		S3 (MF)		S3 (MF, RWS)				x (RWS)	x (RWS)	x (MF)	
Western Scheldt (optional)	S2 (RWS) S3 (RWS)	S2 (RWS) L8 (RWS) S3 (RWS)	S3 (RWS)		L8 (RWS) 1km (RWS)				S3(RWS)				x (RWS)	x (RWS)		
Entire Dutch coast (optional)	S2 (RWS) S3 (RWS)	S2 (RWS) L8 (RWS) S3 (RWS)	S3 (RWS)		L8 (RWS) 1km (RWS)				S3 (RWS)				x (RWS)	x (RWS)		
Bourgneuf Bay & Loire Estuary	S2 (AFB, COREPEM, CRC, SMIDAP) S3 (AFB, COREPEM, CRC, SMIDAP) MODIS	S2 (AFB, COREPEM, CRC, SMIDAP) L8 (COREPEM, CRC, SMIDAP) S3 (AFB,	S3 (AFB)	S3 (SMIDAP)	L8 (AFB,COREPEM, CRC, SMIDA) 1km (AFB, COREPE	S2 (AFB, CRC, COREPEM) L8 (AFB, CRC, COREPEM)			S3 (AFB, CRC)		x (AFB, SMIDAP)	x (SMIDAP)	x (SMIDAP)		x (CRC, SMIDAP)	Maps of bivalve beds (COREPEM, SMIDAP), HR composite colour map

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Site	Chl-*a*	TSM/ TURB/ Kd	CDOM	CPC	SST	SMA presence / status	PSC	Sub-littoral habitat	HAB/ indicator species*	PP	Phyto-plankton bloom phenology	WFD indic-ators	Coastal erosion and accretion	Source identi-fication	Spatial suita-bilty	Additional param-eters
	(COREPEM, CRC, SMIDAP)	COREPEM, CRC, SMIDAP)			M, CRC, SMIDA)											(COREPEM, SMIDAP)
Glénans Archipe-lago	S2 (AFB) S3 (AFB)	S2 (AFB) S3 (AFB)	S3 (AFB)		L8 (AFB) 1km (AFB)	S2 (AFB) L8 (AFB)		S2 (AFB)	S3 (AFB)	S3 (PP)	x(AFB)					
Northern Adriatic coast (or subset thereof)	S2 (ARPAV) S3 (ARPAV) MODIS (ARPAV)	S2 (ARPAV) S3 (ARPAV) L8 (ARPAV)			L8 (ARPAV) 1km (ARPAV)	S2 (ARPAV) L8 (ARPAV)	S3 (ARPAV)	S2 (ARPAV) VHR (ARPAV)	S3 (ARPAV)	S3 (ARPAV)	x (ARPAV)	x (ARPAV)	x (ADB, ARPAV)	x (ARPAV)	x (ARPAV)	Soil moisture (ADB), vegetation stress (ADB)
Galicia	S2 (ARVI, CRMG) S3 (ARVI) MODIS (ARVI)	S2 (CRMG)	S3(CRMG)		L8 (ARVI, CRMG) 1km (ARVI, CRMG)	S2 (CRMG) L8 (CRMG)	S3 (CRMG)		S3 (CRMG)	S3 (ARVI, CRMG)	x (CrMG)					
Mediterr-anean and Black seas		S2 (ISMAR) S3 (ISMAR) L8 (ISMAR)			L8 (ISMAR) 1km (ISMAR)	S2 (ISMAR) L8 (ISMAR)			S3 (ISMAR)							

*HAB species of interest include: *Phaecystis* sp., *Pseudo-nitzchia* sp. *Prorocentrum* sp., *Dinophysis* sp., *Alexandrium* sp. (ostenfeldii), *Gymnodinium Catenatum*

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2. Validation of CoastObs core and innovative products

2.1 CoastObs dedicated sampling effort by region

Dedicated field campaigns will be undertaken on the case study sites: 1) Bourgneuf Bay and Glénan Islands, Atlantic coast (W France), 2) Venice Lagoon and the northern Adriatic coast (Italy), 3) Zeeland coastal waters (Netherlands), and 4) Galician coast (NW Spain). Further details of the sampling effort plan for each region are described in Sections 2.1.1 to 2.1.4 below.

Data will be collected using standard and openly available protocols and subjected to rigorous and fully documented quality assurance procedures and will be compared to the EO-based products. All field campaigns will include the collection of reference R_{rs} observations. These measurements will be supplemented by data available to the project from existing long-term monitoring programmes and instrumented buoys in order to maximise the generation of matchups. LIMNADES (Lake Bio-optical Measurements and Match up data for Remote Sensing) database held and maintained by USTIR will act as a centralised repository for the collected for validation data and will ensure standardisation in data formats and the quality control of the measurements.

2.1.1 France – Coastal Waters

The intertidal case-study site is Bourgneuf bay (2°W, 47°N) a shellfish ecosystem located south of the Loire estuary on the French Atlantic coast. *Zostera noltei* grows as monospecific stands in sandy muddy sediment, stretching out along the shoreline, in areas unoccupied by oyster-farming. Even though the oyster activities do not seem to have a direct impact on seagrass in the Bay, it is a concern for oyster producers because of the close vicinity between this habitat and oyster farming-sites. A joint sampling campaign will be organised by UN and BL in September 2018 for collection of AOP (WISP-3 and TRIOS Ramses) and ground-truthing (seagrass percentage cover and biomass).

The second site is a subtidal *Zostera marina* seagrass bed located in the Glénan archipelago (47° 43′ 01″ N , 4° 00′ 00″ O.) nine miles from the coast in South Brittany. This area of 35 km^2, is characterized by numerous rocky islets and nine small islands, surrounding an enclosed shallow lagoon. The turbidity is low and the archipelago is protected by environmental regulations. A joint sampling campaign will be organised by BL, UN, and CNR in May 2018 for collection of biogeochemical data (Chloroplastic pigments, TSM, CDOM), IOPs (particulate absorption, AC-S and Eco-BB3), AOPs (WISP-3 and TriOS Ramses), seagrass and macro-algae survey. BL will organize a ground-truthing campaign in July/September 2018 to assess the seagrass percentage cover and bottom type. Details of the validation effort in the coastal waters of France are shown in Table 2.

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Table 2 – CoastObs dedicated validation effort in the coastal waters of France

Site ID	Site	Period	Frequency	Number of stations	Map	Satellite sensor	CoastObs partners
[BOUR]	Bourgneuf Bay	10-13 Sep 2018	Daily	3 transects, 10 stations per transects	Figure 1	S2	UN,BL
[GLEN]	Glénan Islands	28-30 May 2018	Daily	12 stations for IOP, AOP	Figure 1	S2	BL,UN, CNR
[GLEN]	Glénan Islands	June/July 2018	3 days	100 stations for ground-truthing	Figure 1	S2	BL

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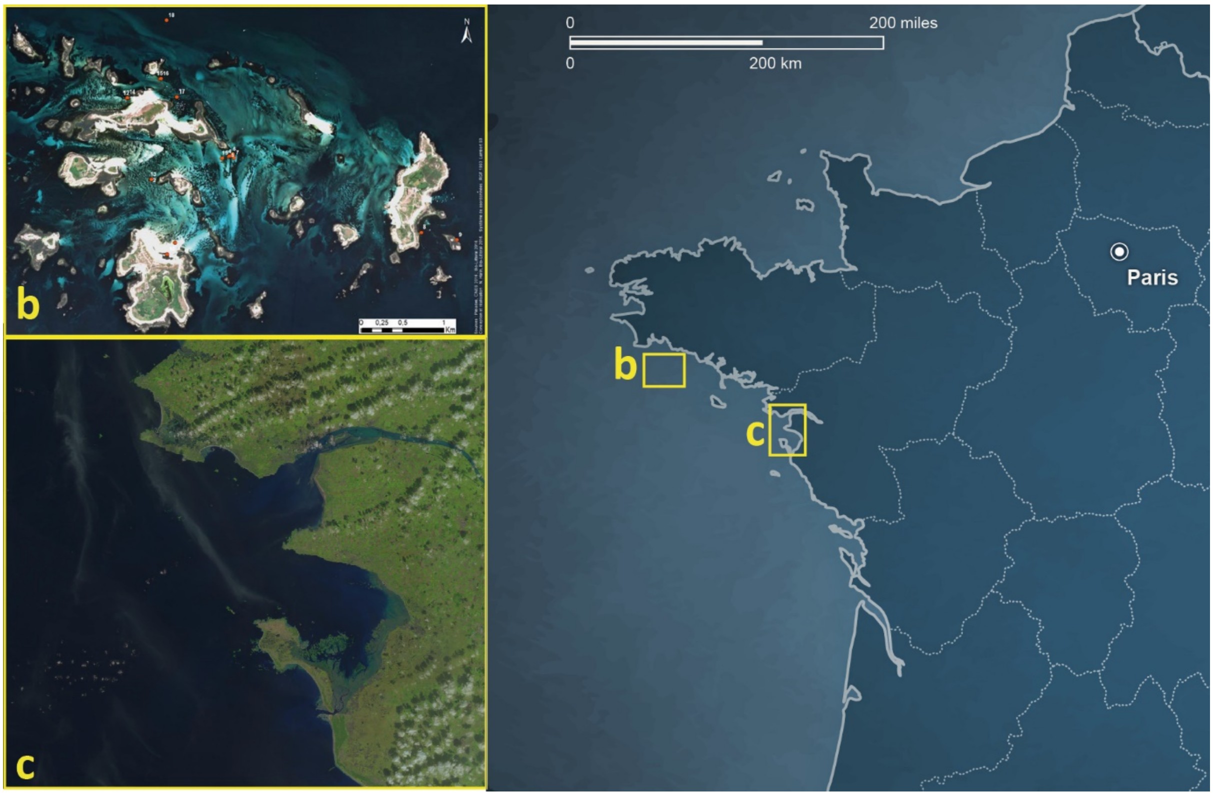

Figure 1 – Sampling sites in the coastal waters of France: (b) Glénan Islands and (c) Bourgneuf Bay and Loire Estuary

2.1.2 Italy – Coastal Waters

The northern Adriatic Sea (NAS) is in the northernmost part of the Mediterranean and is characterized by a shallow depth (averaging 35 m). It receives approximately 20% of the total Mediterranean river run-off, mainly from the Po (the longest river in Italy), and its hydrodynamics are seasonally influenced by meteorological physical forcing (winds and tides). The NAS is also considered to be one of the most productive regions of the generally oligotrophic Mediterranean Sea. The largest phytoplankton blooms occur in its surface layers in late winter and in summer, they occur in the western part of the region. According to Hooker et al. (2004), the area alternates between case 1 and case 2 water types. Case 2 conditions are mainly due to the effects of local winds, which resuspend bottom sediments, and due to the discharge from the Po River and other rivers to the north (Adige, Piave, Tagliamento and Isonzo), which are sources of terrestrial particulate and dissolved matter.

The lagoon of Venice (LV) is a large and shallow coastal lagoon located in the NAS. It has a surface area of ca. 540 km^2 with an average water depth of about 1.1 m and a maximum tidal range of about 1.5 m. It maintains a connection to the NAS through the inlets of Lido,

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Malamocco, and Chioggia, and the exchange of water through the inlets in each tidal cycle is about a third of the total volume of the lagoon. The LV presents a heterogeneous morphology, characterized by a complex pattern of major (navigable) and minor channels, salt marshes, tidal flats and islands. The lagoon has been subject to intense anthropogenic pressures occurred in the 20th, such as the construction of jetties at the inlets and the dredging of the Malamocco–Marghera channel, which shifted the lagoon towards a prevalent erosion, which lead to a negative sedimentary budget. Key ecological impacts include the extensive loss of benthic seagrass cover, areas subject to eutrophication and anoxic crises.

A joint sampling campaign was undertaken by CNR, USTIR and UN in May 2018 for collection of biogeochemical data (Chloroplastic pigments, TSM, CDOM), IOPs (particulate absorption, AC-S and Eco-BB3), AOPs (WISP-3 and TriOS Ramses), seagrass and macro-algae survey, particle size distribution (LISST), phytoplankton abundance and taxonomy, AOT (Microtops) and temperature and depth (CTD). Details of the validation effort in the coastal waters of Italy are shown in Table 3.

Expeditive fieldwork will also be undertaken in the LV to gather data for the purpose of validating CoastObs standard products, including water reflectance and water-quality parameters (turbidity, SST, TSM).

Table 3– CoastObs dedicated validation effort in the coastal waters of Italy

Site ID	Site	Period	Frequency	Number of stations	Map	Satellite sensor	CoastObs partners
[VEN]	Venice Lagoon and Adriatic Coast	3-8 May 2018	Daily	24	Figure 2 (red dots)	S2, S3, Landsat	CNR, USTIR, UN
[VEN]	Venice Lagoon and Adriatic Coast	8-9 May 2018	Daily	16	Figure 2 (green dots)	S2, Landsat	CNR, USTIR, UN
[VEN]	Venice Lagoon and Adriatic Coast	25-29 June 2018	Daily	24	Figure 2 (red dots)	S2, S3, Landsat	USTIR

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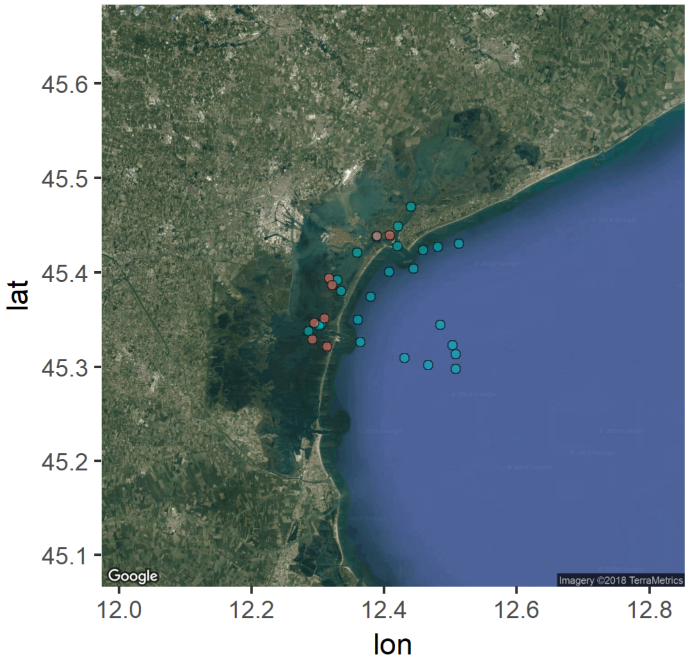

Figure 2 – Sampling locations in the Venice Lagoon and Adriatic Sea, Italy.

2.1.3 Netherlands – Coastal Waters

The study sites in the Netherlands are the Eastern Scheldt and the Wadden Sea. The Eastern Scheldt is an estuary of 350 km^2 located in the Rhine-Meuse-Scheldt delta in the SW of the Netherlands. In 1987 a storm surge barrier has been placed in the mouth of the estuary allowing tidal influence, but the estuary was isolated from river input as well, turning it from a turbid estuary into a sheltered tidal bay. Chlorophyll-*a* concentrations range on average between 2 and 5 mg m^{-3} and TPM from 4 to 10 mg l^{-1}, but values vary spatially (Smaal et al, 2013). Salinity does not change much and typically ranges from 30 to 33 PSU. Oyster and mussel farming cover about 2250 ha of bottom culture plots in the Eastern Scheldt.

The Dutch part of the Wadden Sea in the north of the Netherlands covers 2500 km^2. The Wadden Sea is divided from the North Sea by a range of narrow islands, and in between connected through tidal channels that distribute water through a network of gullies. It has been separated from the freshwater Lake IJssel by a dam. The Wadden Sea is a dynamic and shallow area, and half of it consists of intertidal flats, creating a turbid environment. Salinity ranges from 30 PSU close to the North Sea to 15 PSU close to freshwater discharge points from Lake IJssel. The western part of the Wadden Sea has 7700 ha of bottom culture plots designated for mussel farming.

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Monthly sampling will be undertaken by HZ in both Eastern Scheldt and Wadden Sea for PSC with accompanying WISP measurements in the Eastern Scheldt and continuous data collection (Water temperature, turbidity, Chl-*a*) by means of fixed dataloggers from April to October in 2018 and 2019. Details of the validation effort in the Netherlands are shown in Table 4.

Table 4 – CoastObs dedicated validation effort in the coastal waters of Netherlands

Site ID	Site	Period	Frequency	Number of stations	Map	Satellite sensor	CoastObs partners
[WAD]	Wadden Sea	April – Oct 2018 + 2019	Monthly	12	Figure 3	S2/3	HZ
[OS]	Eastern Scheldt	April – Oct 2018 + 2019	Monthly	12	Figure 3	S2/3	HZ

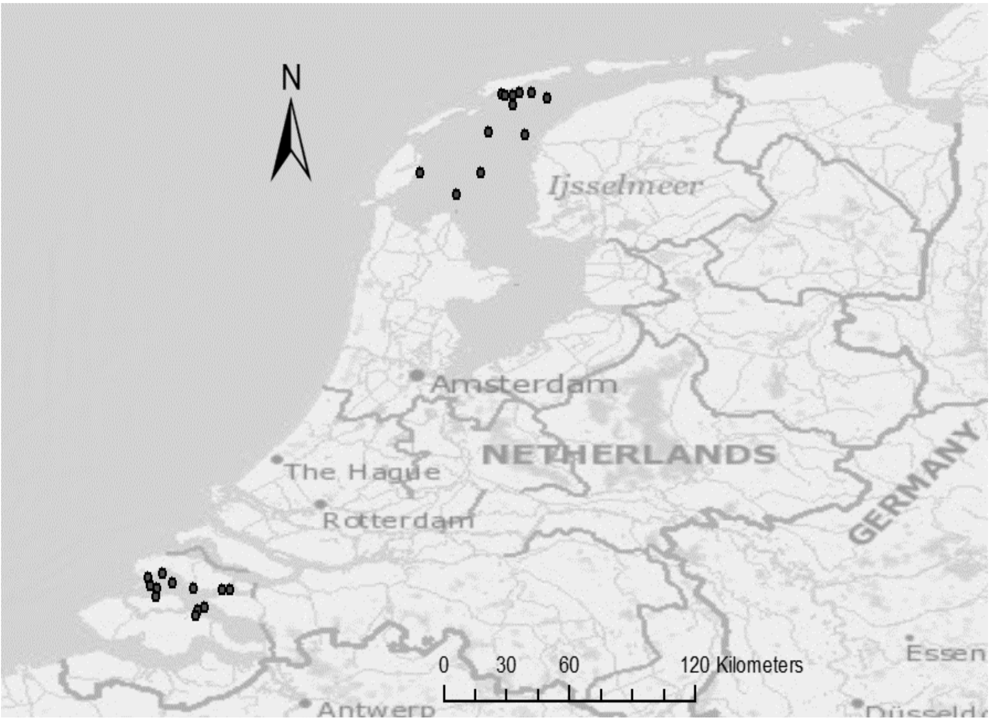

Figure 3 – Sampling locations in the Wadden Sea and Eastern Scheldt, Netherlands

2.1.4 Spain – Coastal waters

The Galician rias are V-like embayments along the northern boundary of the NW Africa upwelling system, formed by sunken river valleys flooded by the sea. These ecosystems are strongly influenced by oceanic conditions on the adjacent continental shelf. The rias Baixas

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constitute the southern part of the Galician rias. They are formed by four large coastal embayments, from north to south: Muros y Noya, Arousa, Pontevedra and Vigo, all oriented in a SW–NE direction and characterized by strong tides. Surface area covers approximately 600 km^2 and water depths range from 5 to 60 m. The ria de Vigo is the longest of the rias whereas the ria de Arousa is the widest. Rias vary in width from 1-3 km in their inner part to 8-12 km in their external part. The main freshwater inputs in the rias are by rivers located in innermost part of the rias. In these highly primary productive upwelling estuarine systems transient increases of phytoplankton abundance, referred to as blooms, are a frequent phenomenon occurring mainly between early spring and late autumn. Phytoplanktonic blooms or ''red tides'' as they were formally called, were mentioned for the first time in the Galician rias in 1918 by Sobrino. Sporadically, some phytoplankton blooms in the Galician rias are perceived as harmful with direct and indirect impacts to the mussel production industry, which constitutes an important economic activity in the area. Harmful algal events in the area are a well-documented phenomenon. Several studies since the 1950s referred to them and in general to phytoplankton ecology particularizing favourable conditions to the development of HABs, their origin, dynamic, distribution and toxicity.

Ten sampling campaigns will be undertaken by UVIGO from June – September 2018 at 12 stations in Ria de Vigo, Galicia (Figure 4). A joint sampling campaign will also be undertaken by USTIR and UVIGO in July 2018, including daily collection of biogeochemical data (Chloroplastic pigments, TSM, CDOM), IOPs (particulate absorption, AC-S and Eco-BB3), AOPs (WISP-3 and TriOS Ramses), particle size distribution (LISST), phytoplankton abundance and taxonomy, AOT (Microtops) and temperature and depth (CTD). Details of the validation effort in the coastal waters of Spain are shown in Table 5.

Table 5 – CoastObs dedicated validation effort in the coastal waters of Spain

Site ID	Site	Period	Frequency	Number of stations	Map	Satellite sensor	CoastObs partners
[VIGO]	Ria de Vigo	June-September 2018	10/year	12	Figure 4	S2/S3	UVIGO
[VIGO]	Ria de Vigo	2-13 July 2018	Daily	12	Figure 4	S2/S3	USTIR, UVIGO

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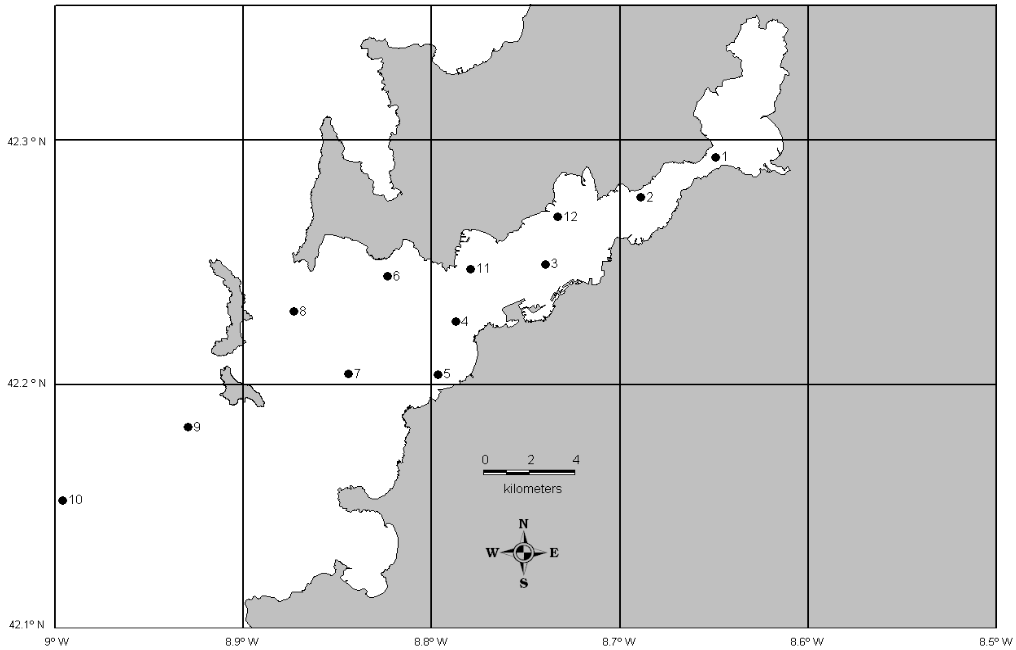

Figure 4 – Sampling locations in Ria de Vigo, Galicia, Spain.

3. Methods and protocols

In order to validate satellite remote sensing products, *in situ* measurements of biogeochemical parameters and the apparent and inherent optical properties are required. The validation activities performed by CoastObs consortium will follow standard protocols with some modifications related to the specifics of the investigated water body. The most commonly implemented protocols for ocean optics are as follows:

- IOCCG (2017). Inherent Optical Property Measurements and Protocols: Absorption Coefficient, available at http://ioccg.org/wp-content/uploads/2015/10/absorption_protocol_forcommunitydistribution-sept2017-2.pdf
- IOCCG (2000). Remote Sensing of Ocean Colour in Coastal, and Other Optically-Complex, Waters. Sathyendranath, S. (ed.), Reports of the International Ocean-Colour Coordinating Group, No. 3, IOCCG, Dartmouth, Canada.
- NASA/TM (2004), Ocean Optics Protocols for Satellite Ocean Color Sensor Validation, Revision 5 Volume VI, Part 2: Special Topics in Ocean Optics Protocols.
- NASA/TM (2003), Ocean Optics Protocols For Satellite Ocean Color Sensor Validation, Revision 4, Volume I: Introduction, Background and Conventions. Mueller, J.L., Fargion, G.S., and McClain, C.R. (Eds). NASA/TM-2003-21621/Rev-Vol I

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- NASA/TM (2003), Ocean Optics Protocols For Satellite Ocean Color Sensor Validation, Revision 4, Volume III: Radiometric Measurements and Data Analysis Protocols. Mueller, J.L., Fargion, G.S., and McClain, C.R. (Eds). NASA/TM-2003-21621/Rev-Vol III
- NASA/TM (2002), Ocean Optics Protocols For Satellite Ocean Color Sensor Validation, Revision 4, Volume IV: Inherent Optical Properties: Instruments, Characterizations, Field Measurements and Data Analysis Protocols, NASA/TM-2003-211621/Rev4-Vol.IV
- NASA/TM (2000) 209966, Ocean Optics Protocols for Satellite Ocean Color Sensor Validation, Revision 2.
- Tilstone, G. and Martinez-Vicente V. (2012). Protocols for the Validation of Ocean Colour Satellite data in Case 2 European Waters. IESCA satellite validation protocols 07-027-FR-ISECA. Plymouth Marine Laboratory, UK.

Additionally, CNR and WI describe their protocols for calibration/validation (cal/val) activities that were presented in the GLaSS Technical Report (2015):

- CNR (Italy): CNR-IREA 2014. Cal-val protocol used at CNR-IREA: quantities, instruments and methods, 5 pg.
- WI (Netherlands): 1) Pasterkamp, R., S.W.M. Peters, M. Laanen 2001. Measurement protocol for the determination of specific inherent optical properties of natural surface water. Institute for Institute for Environmental Studies, Vrije University Report W01/15, 38 pg. 2) Water Insight B.V. WISP-3 user guide. Version 1.2. the Netherlands, 25 pg.

3.1 Core biogeochemical parameters

Water samples for biogeochemical parameters will be collected, analysed and processed according to the CoastObs consortium-standard protocols during the validation campaigns to provide validation data for the EO-based physical and biogeochemical products. Each CoastObs partner has provided the list of biogeochemical parameters that will be measured in Table 6, and descriptions of each analytical method are described below.

3.1.1 Chlorophyll-*a* (Chl-*a*)

Chlorophyll-*a* (Chl-*a*) is the main photosynthetically active pigment of phytoplankton and is therefore commonly used as a proxy for phytoplankton biomass in the water. In a number of countries, Chl-*a* is a water quality indicator of eutrophication with respect to the Water Framework Directive (2000/60/EC) and Marine Strategy Framework Directive (2008/56/EC), therefore it is a vital water quality parameter to include for validation campaigns.

However, the methods for analysis of Chl-*a* concentration are highly variable (GLaSS Technical Report, 2015), with different approaches implementing a range of filters, solvents and wavelengths used for absorbance readings. A detailed description of appropriate selection of approaches for oceanic and coastal systems can be found in *Phytoplankton Pigments in Oceanography, Guidelines to Modern Methods* edited by Jeffery S.W et al. (2005). Chl-*a* concentration will be determined using spectrophotometry by majority of CoastObs partners, but using different calculation approaches, while the high performance liquid chromatography (HPLC) method will be employed by USTIR. Intercomparison of both methods will be undertaken to ensure consistency between the methods as part of the CoastObs project.

3.1.2 Phycocyanin (PC)

Phycocyanin (PC) is an accessory pigment present in cyanobacteria with a diagnostic absorption peak at ~620 nm (full-width-half-maximum of ~75 nm). In the majority of CoastObs study sites, severe cyanobacteria blooms are frequent and therefore of great interest for the users. Furthermore, WHO have established a guideline value for cyanobacteria <100,000 cells/ml for a moderate health alert in recreational waters (WHO, 2003), thus EO estimates of phycocyanin are a vital step towards ensuring safe water quality. The algorithms for PC estimation will therefore be validated with *in situ* collected measurements. The concentration of PC in cyanobacteria will be determined by USTIR according to Horváth et al. (2013), which is a modification of that by Sarada et al. (1999) using the spectrophotometric equations of Bennett and Bogorad (1973).

3.1.3 Total Suspended Matter (TSM)

Total suspended matter (TSM), or suspended particulate matter (SPM), typically originates from terrestrial and river runoff or wind-driven re-suspension of sediments in shallow waters. As TSM represents all suspended particulates, it is a broad ranging water quality indicator that represents both organic and inorganic matter from both internal and external sources. All CoastObs partners are using the same gravimetric method and will be separating organic (OSM) and inorganic suspended matter (ISM) fractions by combusting a pre-weighted filter. The main differences between partner methods are the filters used for the collection of particulate matter and the combustion temperature measurement of OSM/ISM (GLaSS Technical Report, 2015).

3.1.4 Turbidity

Turbidity is a measure of scattering and is directly related to the concentration of TSM in the water column. Turbidity will be measured by USTIR with a turbidity meter according ISO 7027. CNR will use two backscattering optical sensor (Seapoint turbidity meter, operating at 880 nm and ECO Triplet Fluorometer and Backscattering Sensor, operating at 532 nm).

Secchi Depth (Sz, m) is also an indicator of water turbidity, and will be measured using a Secchi disk.

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3.1.5 Dissolved Organic Carbon (DOC)

Dissolved Organic Carbon (DOC) is the sum of organically bound carbon present in water and is regularly measured in monitoring programs. This is routinely analysed by High Temperature Combustion catalytic Oxidation (HTCO). Water samples will be filtered through precombusted 0.7 um GF/F filters, then measured by thermal catalysis at 950C in a High Total Organic Carbon instrument (e.g. Elementar Analysensysteme GmbH Germany) equipped with a platinum catalyst cartridge using synthetic air as the carrier gas.

Table 6 – List of biogeochemical parameters and analysis method

Parameter	BL	CNR	HZ	UN	USTIR	UVIGO
Chl-*a*	Samples will be analysed by USTIR	Chla-fluorescence [5]	Chla-fluorescence [5]	Samples will be analysed by USTIR	High Performance Liquid Chromatography, adapted from [1,4]	Samples will be analysed by USTIR
PC	-	-	-	-	Spectrophotometric, adapted from [2]	-
TSM	Gravimetrically at 10^{-4} accuracy electrobalance using GF/F filters.	Gravimetrically at 10^{-4} accuracy electrobalance using GF/F filters.	-	Gravimetrically at 10^{-4} accuracy electrobalance using GF/F filters.	Gravimetrically at 10^{-4} accuracy electrobalance using GF/F filters.	Samples will be analysed by USTIR
ISM	-	Following TSM gravimetric analysis, combustion at 450°C to remove organic material.	-	-	Following TSM gravimetric analysis, combustion at 450°C to remove organic material.	Samples will be analysed by USTIR
Turbidity	Turbidimeter portable [6]	Turbidmeter [7,8]	Infrared back-scattering sensor - FTU [5]	Turbidimeter portable [6]	Turbidimeter [3]	-
DOC	-	-	-	-	High temperature combustion catalytic oxidation	-

[1] Van Heukelem, L. and C.S. Thomas, 2001. Computer-assisted high-performance liquid chromatography method development with applications to the isolation and analysis of phytoplankton pigments. J. Crom. A. 910:31-49.

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[2] Horváth H., Kovács A.W., Riddick C., Présing, M., 2013. Extraction methods for phycocyanin determination in freshwater filamentous cyanobacteria and their application in a shallow lake, European Journal of Phycology, 48(3), 278-286.
[3] ISO 7027-1:2016, Water quality -- Determination of turbidity -- Part 1: Quantitative methods.
[4] Zapata, M., Rodríguez, F. and Garrido, J.L. (2004) Separation of chlorophylls and carotenoids from marine phytoplankton: a new HPLC method using a reversed phase C8 and pyridine containing mobile phases. Marine Ecology Progress Series: 195, 29–45.
[5] JFE Advantech INFINITY SERIES DATA LOGGER Chlorophyll a & turbidity https://www.jfe-advantech.co.jp/eng/ocean/infinity/infinity-clw.html
[6] Hach 2100Q Portable Turbidity Meter
[7] WetLabs ECO 3-Measurement Sensor (Triplet) User's Guide. http://www.seabird.com/eco-triplet-fluorometer-and-backscattering-sensor
[8] Seapoint Turbidity Meter: User Manual. http://www.seapoint.com/stm.htm

3.2 Optical Properties

Apparent optical properties (AOPs) are those which are dependent upon the ambient light environment and include remote sensing reflectance ($R_{rs}(\lambda)$), upwelling radiance (L_u), sky radiance (L_{sky}), downwelling irradiance (E_d) and Secchi Depth (S_Z). The inherent optical properties (IOPs) are those which are independent of ambient light and vary depending on the quantity and quality of the optically active constituents in the water column. These include the absorption coefficient of coloured dissolved organic matter ($a_{CDOM}(\lambda)$), absorption coefficient of non-algal particles ($a_{NAP}(\lambda)$), absorption coefficient of phytoplankton ($a_{ph}(\lambda)$), total attenuation coefficient ($c(z, \lambda)$), total absorption coefficient ($a(\lambda)$), particulate scattering coefficient ($b_p(z, \lambda)$) and particulate backscattering coefficient ($b_{bp}(z, \lambda)$). The AOPs will be used to validate the atmospheric correction of the satellite data (S2, S3), while IOPs will be input for the bio-optical inversion models to generate biogeochemical products. All data will be measured either in the laboratory or *in situ*, according to the methods outlined below and shown in Table 7.

3.2.1 Apparent Optical Properties (AOPs)

A series of TriOS Ramses radiometers, comprising three hyperspectral radiometers, will also be arranged to measure the upwelling radiance (L_u), sky radiance (L_{sky}) and downwelling irradiance (E_d). These measurements can also calculate the radiance reflectance ratios (L_u/E_d) or remote sensing reflectance (R_{rs}). CNR will also use two TriOS Ramses hyperspectral radiometers for measuring in-water AOPs, which rely on subsurface fixed-depth profiles of upwelling radiance $L_u(z, \lambda, t)$ and downwelling irradiance $E_d(z, \lambda, t)$ at depth z (multiple depths typically between 1 and 10 m), wavelength λ and time t. The above-water downward irradiance $E_d(0^+, \lambda, t)$ is also measured to complement the in-water data. These latter data are used to extrapolate to 0^- (i.e. just below the water surface), the radiometric quantities which cannot be directly measured because of wave perturbations.

AOP measurements will also be undertaken with a WISP-3. The WISP-3 is a hand-held optical instrument which contains three Ocean Optics JAZ radiometers, to measure downwelling

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irradiance (E_d), downwelling radiance (L_d) and upwelling radiance (L_u), from which it derives R_{rs}. WISP-3 instruments can be deployed with Gershun tubes with a 3° field of view (FOV) or with a collimating lens. The collimating lenses have a FOV of 2.8° however they capture more light than the Gershun tubes, which leads to a higher signal-to-noise ratio of the measurements using this method. All details of the WISP-3 method can be found in the GLaSS Technical Report (2015).

Mobley (1999) describes the measurements protocol for above-water reflectance measurements, which applies to the TriOS Ramses. Briefly, the measurement angle relative to the sun should at least be 90°, although closer to 135° is optimal. Angles < 90° (towards the sun) and ~180° (opposite to the sun) should absolutely be avoided. If the sky is fully overcast and shadows are not visible, the angle is less critical but measuring towards the position of the sun is still not advised. L_d and L_u should be measured at 42° relative to the zenith and the nadir, and therefore it is required to keep the Ramses instruments level during measurements.

3.2.2 Inherent Optical Properties (IOPs)

Absorption Coefficient of Coloured Dissolved Organic Matter (a_{CDOM} (λ))

Coloured Dissolved Organic Matter (CDOM), also known as humic substances, yellow substances, gelbstoff or gilvin, is a mixture of compounds that are products of plant and animal decomposition. The determination method for the absorption coefficient of CDOM (a_{CDOM}) involves the measurement of filtered water (mainly using nucleopore filters with pore size of 0.22µm) at one or more wavelengths, or the entire spectrum of the filtered sample from the near UV throughout the visible spectrum. The most frequently used wavelength is 440 nm, with a correction for scattering at 750 nm.

Particulate absorption coefficients

Total particle absorption (a_p) is comprised of non-algal absorption (a_{NAP}) and phytoplankton absorption (a_{ph}) coefficients. The standard method for a determination of *in vivo* particle absorption is by light transmission measurement of aquatic particles retained on a filter pad. The analysis consists of measuring the fraction of a light beam passing through particles retained on a filter. Absorption by particles a_p(λ) and bleached particles a_{NAP}(λ) will be measured by CoastObs partners in the laboratory using a dual-beam spectrophotometer equipped with integrating sphere, according to the method of Tassan and Ferrari (1995) with some modifications of extraction solvent (GLaSS Technical Report, 2015), following the IOCCG protocols for measurement of absorption coefficients (IOCCG, 2017).

In situ *IOP measurements*

Total absorption (a(λ)) and attenuation (c(λ)) coefficients will be measured *in situ* using a WETLabs absorption-attenuation meter (AC-S) with continuous spectra in 400-730 nm (GLaSS Technical Report, 2015). The scattering coefficient (b(λ)) will be calculated by simple subtraction ($c(\lambda)-a(\lambda) = b(\lambda)$).

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research and innovation programme under grant agreement No 776348

Backscattering ($b_b(\lambda)$) will be measured *in situ* using a WETLabs ECO-BB3, according to the GLaSS Technical Report (2015) and the WETLabs User Guide.

Table 7 – List of apparent and inherent optical properties and measurement plan

Parameter	BL	CNR	HZ	UN	USTIR	UVIGO
Remote sensing reflectance $R_{rs}(\lambda, 0^+)$	TriOS Ramses and WISP-3	TriOS Ramses and WISP-3	WISP-3	TriOS Ramses and WISP-3	TriOS Ramses	TriOS Ramses and WISP-3
Upwelling radiance $L_u(\lambda, 0+)$	TriOS Ramses and WISP-3	TriOS Ramses and WISP-3	WISP-3	TriOS Ramses and WISP-3	TriOS Ramses	TriOS Ramses and WISP-3
Sky radiance L_{sky} (λ, 0+)	TriOS Ramses and WISP-3	TriOS Ramses and WISP-3	WISP-3	TriOS Ramses and WISP-3	TriOS Ramses	TriOS Ramses and WISP-3
Downwelling irradiance $E_d(\lambda, 0+)$	TriOS Ramses and WISP-3	TriOS Ramses and WISP-3	WISP-3	TriOS Ramses and WISP-3	TriOS Ramses	TriOS Ramses and WISP-3
Secchi Depth (S_Z)	Secchi disk	Secchi disk	Secchi disk	Secchi disk	Secchi disk	Secchi disk
CDOM absorption coefficient $a_{CDOM}(\lambda)$	Samples will be analysed by USTIR	CDOM-fluorescence [7]		Samples will be analysed by USTIR	Spectrophotometric (235-800 nm) (modified from Mitchell et al 2003 and using traceable standards)	Samples will be analysed by USTIR
Non-algal particulate absorption $a_{NAP}(\lambda)$	Samples will be analysed by USTIR	Spectrophotometric [1]	Samples will be analysed by USTIR	Samples will be analysed by USTIR	Spectrophotometric [1,2] (inside the sphere)	Samples will be analysed by USTIR
Phytoplankton absorption coefficient $a_{ph}(\lambda)$	Samples will be analysed by USTIR	Spectrophotometric [1]	Samples will be analysed by USTIR	Samples will be analysed by USTIR	Spectrophotometric [1,2] (inside the sphere)	Samples will be analysed by USTIR
Beam attenuation coefficient *c* (z,λ)	-	WETLabs AC-9 [3]	-	-	WETLabs AC-S [3]	WETLabs AC-S [3]
Absorption coefficient *a* (z,λ)	-	WETLabs AC-9 [3]	-	-	WETLabs AC-S [3]; Trios OSCAR for very turbid	WETLabs AC-S [3]
Particulate scattering coefficient b_p (z,λ)	-	WETLabs AC-9 [3]	-	-	WETLabs AC-S [3]	WETLabs AC-S [3]

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Parameter	BL	CNR	HZ	UN	USTIR	UVIGO
Particulate backscattering coefficient b_{bp} (z,λ)	-	HOBI labs HydroScat-6 [5]	-	-	WETLabs BB3 [4]	-

[1] Tassan S., and Ferrari G.M., 1995. An alternative approach to absorption measurements of aquatic particles retained on filters. Limnol. Oceanogr. 40: 1358-1368.
[2] IOCCG (2017). Inherent Optical Property Measurements and Protocols: Absorption Coefficient, available at http://ioccg.org/wp-content/uploads/2015/10/absorption_protocol_forcommunitydistribution-sept2017-2.pdf
[3] WETLabs, Sea Bird Scientific. *ac protocol document.* (http://www.seabird.com/sites/default/files/documents/manual-acprotq.pdf)
[4] WETLabs, Sea Bird Scientific. *Scattering meter: ECO-BB9 Users Guide.* (http://www.seabird.com/sites/default/files/documents/manual-bb9-M.pdf)
[5] HOBI Labs HydroScat-6 Spectral Backscattering Sensor & Fluorometer: User's Manual, Revision J http://www.hobilabs.com/cmsitems/attachments/3/HS6ManualRevJ-2010-8a.pdf

3.3 Atmospheric Correction

All satellite data will undergo atmospheric correction, and the atmospheric correction used will be validated with *in situ* reflectance data (e.g. Figure 5). Microtops or AERONET instruments will provide AOD data, which are required for use in atmospheric correction models. Sentinel-3 OLCI data will be atmospherically corrected using MEG28.1, FUB-WeW, C2R, CoastColour or Polymer, while Sentinel-2 or Landsat 8 data will be corrected with Polymer, C2RCC, Acolite, iCOR, l2gen and Sen2Cor. Results will be assessed using the metrics for quantitative data, as described in Section 7.

In stations located in the intertidal region of the Bourgneuf Bay, images collected during the low tide will be used, with exposed vegetation or with negligible water coverage. In this case, the data will be acquired in L2 of processing, which have already passed through standard atmospheric correction routines.

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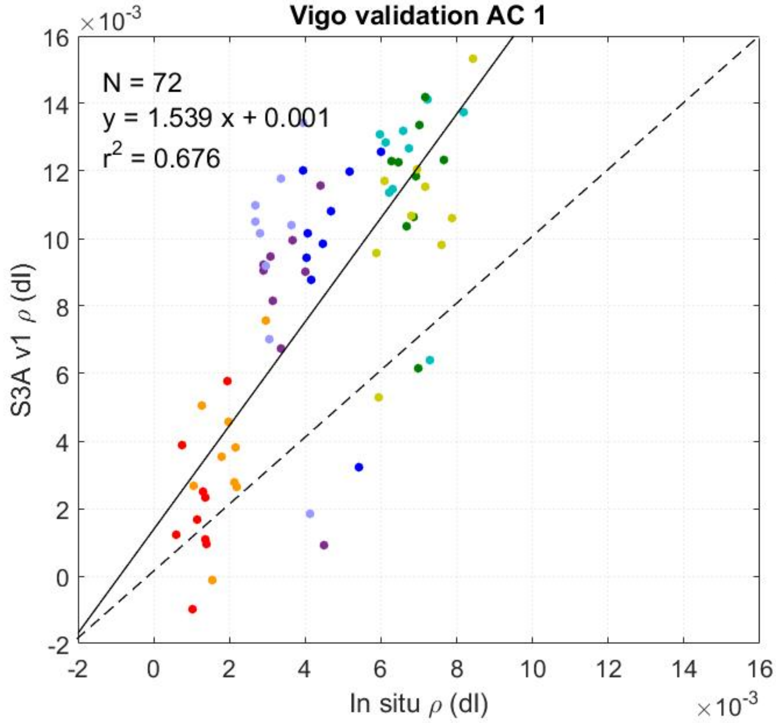

Figure 5 – Example of validation plots for atmospherically corrected Sentinel-3A reflectance data (y-axis) using *in situ* reflectance data (x-axis).

3.4 Metadata

Metadata are required both for corrections of optical measurements (e.g. temperature and salinity corrections for the AC-S absorption measurements), as well as for atmospheric correction of the satellite data (e.g. AOD). The metadata requirements and methods are outlined in Table 8.

Table 8 – List of metadata parameters and instruments

Parameter	BL	CNR	HZ	UN	USTIR	UVIGO
Sea Surface Temperature (SST)	NKE CTD	IDRONAUT and Sea-bird CTD	[OS] YSI multimeter	NKE CTD	Sea-bird CTD	Sea-bird CTD
Salinity (S)	NKE CTD	IDRONAUT and Sea-bird CTD	[OS] YSI multimeter	NKE CTD	Sea-bird CTD	Sea-bird CTD
Wind Speed (WS)	Hand Anemometer	Hand Anemometer or weather-stations	Hand Anemometer	Hand Anemometer	Hand Anemometer	Hand Anemometer
Upwelling Index (UI)	-	-	-	-	According to [1]	According to [1]
Aerosol Optical	-	AERONET data at Acqua Alta	-	-	Microtops from a stable	Microtops from a stable

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Parameter	BL	CNR	HZ	UN	USTIR	UVIGO
Depth, (AOD, τ_a, λ)		Oceanographic Platform [2]			platform. Data are reprocessed and corrected by NASA.	platform. Data are reprocessed and corrected by NASA.
GPS Location (Latitude, Longitude)	+	+	+	+	+	+

[1] Bakun, A., 1990. Global climate change and intensification of coastal ocean upwelling. *Science*, 247(4939): 198-201.
[2] Aeronet: Aerosol Robotic Network.
https://aeronet.gsfc.nasa.gov/cgi-bin/data_display_aod_v3?site=Venise&nachal=2&level=3&place_code=10

3.5 Innovative (and Supplementary) Products

3.5.1 Seagrass and Macro-Algae (SMA)

EO standard products will provide seagrass and macroalgae percentage cover and beds extent while the innovative products will be related to species composition, biomass spatial distribution and epiphyte cover. Multispectral imagery has been successfully used to detect temporal changes of seagrass beds (Dekker et al., 2005; Phinn et al. 2008), and is adapted to assess the areal extent of large intertidal meadows (Barillé et al. 2010). Deeper insight has been obtained using hyperspectral airborne remote sensing (Fyfe, 2003; Valle et al. 2015) using either empirical approaches or more sophisticated semi-analytical algorithms. However, algorithms associated to hyperspectral data are in general complex due to high computational requirements, and not automated. For intertidal beds, simple algorithms based on various vegetation indices and classification techniques can be a cost effective way to retrieve seagrass beds areal extent and biomass (Bargain et al. 2012, 2013). An adaptation of these algorithms is required for S2 with a robust field validation. Spatial resolution will probably set a limit to the detection of small and fragmented seagrass beds, and this remains to be tested. Due to the high spatial variability in the intertidal and shallow subtidal zones, VHR satellite data from the Copernicus Data Warehouse will be used for seagrass and macroalgae habitat mapping. These data will be used as a benchmark to assess whether the spatial resolution of S2 is sufficient to retrieve seagrass extent and biomass to an acceptable level of accuracy. Based on the results of this benchmark, also a hybrid approach using both S2 for the higher temporal resolution and VHR data for the higher spatial resolution could be pursued further. Seagrass beds may also be monitored using *in situ* reflectance data obtained with handheld spectro-radiometers. There is challenge to show that as a non-intrusive technique field radiometry can become a routine and efficient methodology to sample and quantify seagrass biomass, pigment composition, and epiphyte cover. Laboratory and field measurements will be done to develop relevant algorithms.

For subtidal beds the feasibility of accurately mapping seagrass cover will be tested adapting the processing chain implemented in ESA's SNAP processor by CNR for Sentinel2-MSI data for shallow water mapping in coral reef environments. Processing chains for shallow water mapping from space can be based on classification techniques and on semi-analytical model inversions. Both approaches will be tested to determine the most accurate algorithm.

3.5.2 Phytoplankton size classes (PSC)

Phytoplankton size classes (PSC) can identify phytoplankton functional type. Each class represents a threshold in the continuum of phytoplankton size fractions from 0.2 μm to 200 μm. The detailed plankton size classification proposed by Sieburth et al. (1978) is generally summarised into three autotrophic categories: picoplankton (0.2-2 μm), nanoplankton (2-20 μm) and microplankton (20-200 μm) (Hirata et al., 2008; Brewin et al., 2010; Devred et al., 2011). The physical and chemical traits of species classified within each size class may differ (Nair et al., 2008), however their optical properties are likely to be similar due to the effect of cell size on the absorption and scattering properties of particles (Morel & Bricaud, 1981; Stramski & Mobley, 1997). Most of the PSC retrieval algorithms are based on abundance (e.g. Brewin et al. 2010), radiance (e.g. Li et al. 2013) or absorption (e.g. Roy et al. 2013), however these approaches are often globally focused and often lack detail on their uncertainties and strengths. Time series data of coincident *in situ* AOP, IOP and phytoplankton characteristics are rare but very essential for testing the detection capabilities of PSC algorithms. PSC algorithms will be calibrated for operational use in local circumstances.

PSC will be analysed using HPLC (USTIR) for analysis of indicator pigments Fucoxanthin, Peridinin, 19'-hexanoyloxyfucoxanthin, 19'-butanoyloxyfucoxanthin, Alloxanthin, Chlorophyll-*b* and Zeaxanthin. Chlorophyll-*a* and particulate absorption measurements will also be fractionated, by filtration through 20 μm nylon filters then 2 μm GF and 0.3 μm GF. *In situ* AC-S measurements will also be filtered through 198 μm, 20 μm, 2 μm, 1 μm and 0.2 μm filters for collection of fractionated absorption measurements. Microscopy data will also supplement the HPLC and fractionated filtration data, with phytoplankton enumeration and identification following the method of **Utermöhl** (1958).

3.5.3 Primary Production (PP)

Algorithms for the estimation of phytoplankton primary production (PP) from satellite data have been widely tested and validated in open oceans (Smyth et al. 2005), shelf seas (Tilstone et al. 2005) and coastal waters (Barnes et al. 2014). These range from simple empirical approaches that model PP as a function of the near surface Chl-*a* (e.g. Behrenfeld et al. 1998), depth-integrated models that account for variability in chlorophyll-specific assimilation

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efficiency for carbon fixation (e.g. Vertically Generalized Production Model (VGPM); Behrenfeld and Falkowski, 1997) and in some cases its dependency on temperature (e.g. Eppley et al. 1972), to more complex models that estimate PP as a function of wavelength (Wavelength Resolved Model (WRM); Morel, 1991). These models typically output an estimate of the daily phytoplankton carbon fixation (in mg C) within the euphotic zone per unit of water surface area.

Most algorithms model PP as a function of the Chl-*a*, however more recent approaches based on phytoplankton absorption (Barnes et al. 2014) or phytoplankton carbon (Behrenfeld et al. 2005; Westberry et al. 2008) have been developed to reduce model uncertainties due to variability in chlorophyll-specific rates of primary production. Of these algorithms, the most robust and accurate methods that have proven operational capability (e.g. the VGPM model in the Dutch Wadden Sea; Woldegiorgis, 2012) will be adapted to S3 through refined parameterisations and calibrations.

Marine PP is most commonly measured by the ^{14}C method and this will be implemented for CoastObs (Steemann Nielsen, 1952), with the method adapted from the INFORM project (INFORM, 2017). Samples will be labelled with a known amount of 14-C-bicarbonate. After incubation, carbon fixation is quantified by liquid scintillation counting to detect ^{14}C in organic form. Dissolved and particulate organic carbon can be quantified after acidification to remove the inorganic fraction. PP analysis will be measured by USTIR using a 6 x 15 chamber photosynthetron (irradiance 0-2500 μmol m^{-2} s^{-1}, temperature 5-35°C).

3.5.4 Harmful algae blooms and indicator species (HABs)

Spanish mussel culture takes place almost exclusively in the Galicia Rías (total production oscillates around 200,000 tons per year). The high productivity of the Galician coast is a consequence of its western oceanic boundary together with the seasonal northerly winds, generating strong upwelling of rich nutrient cold waters in the period from May to September. These waters rise up to the photic zone within the Rías, reaching the surface in the most intense upwelling and supplying the nutrients required for aquiculture. Episodic Harmful Algal Blooms (HABs) in Galician coastal areas result in mass ecosystem dysfunction, risks to public health, and enormous economic losses to the mussel industry. Ocean color measurements from space have been proved useful in obtaining information about the abundance of phytoplankton, including some toxic species. The Remote Sensing Laboratory work in Galicia has made use of MERIS images (ESA ENVISAT-AO 623 project) and field data obtained from the monitoring program of the Galician Centre for Quality Control of Marine Environment (CCMM). Since MERIS has a high spectral and radiometric resolution, the utilization of supervised classification techniques allows monitoring of the toxic blooms by using full resolution (FR) products.

The Galician rias are V-like embayments along the northern boundary of the northwest Africa upwelling system formed by sunken river valleys flooded by the sea, whose ecosystems are

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strongly influenced by oceanic conditions on the adjacent continental shelf. The rias Baixas constitute the southern part of the Galician rias. They are formed by four large coastal embayments, from north to south: Muros y Noya, Arousa, Pontevedra and Vigo, all oriented in a SW–NE direction, and are characterized by strong tides.

The surface area covers approximately 600 km^2 and water depths range from 5 to 60 m. *Pseudo-nitzschia* blooms, which are sporadically associated with short-term domoic acid (DA) outbreaks (Trainer et al., 2010), are a frequent phenomenon along the northern boundary of the Iberian-Canary current upwelling system. Most of the studies in this system are focused on the Galician rias, one of the most intensive areas of mussel production in the world. Harmful algal blooms (HABs) in this area are a well-documented phenomenon. Several studies since the 1950s referred to Galician rias specific favourable conditions to the development of HABs, their origin, dynamic, distribution and toxicity levels (Margalef, 1956; Tilstone et al., 1994; Figueiras et al., 1994; GEOHAB, 2005).

There is considerable interest in the study of *Pseudo-nitzschia* and the detection of DA in the Galician rias due to the economic and social importance of the extensive culture of mussels in this region and human health concerns. As part of a routine monitoring programme, the Technological Institute for the Control of the Marine Environment of Galicia (INTECMAR) has organized sampling campaigns on a weekly basis in the Galician rias where, among other water parameters, the *Pseudo-nitzschia* spp. abundance and the biotoxins in mussels and other molluscs are recorded. In this study, near twenty years of *Pseudo-nitzschia* spp. abundance and associated meteorological and oceanographic data will be used to develop and validate support vector machine (SVM) models for the prediction of these diatoms. SVM were used to identify presence/below low detection limit, bloom/no bloom conditions of *Pseudo-nitzschia* spp. and finally to predict blooms due to these diatoms in the coastal systems of the Galician rias. Regarding the presence/below low detection limit, bloom/no bloom models the best results in the validation dataset were achieved using all the variables: ria code, day of the year, temperature, salinity, upwelling indices and bloom occurrence in previous weeks.

The frequency, duration and intensity of algal blooms are directly related to a wide range of biological, chemical and physical factors. Relationships between all these factors are complex and difficult to establish. The aim of this work is the establishment of a reliable model in order to explain the main causes of the red tides behaviour along the Galician coast. Data used in the study are:

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- 20 year series of *in situ* data (*Pseudo-nitzschia* spp. cells concentration, temperature, salinity, oxygen, pH, etc) provided by INTECMAR. All data were sampled in selected points placed along the Galician coastline.
- Meteorological data (sea surface pressure maps) from where upwelling indexes were calculated using Bakun (1990) methodology provided by Meteogalicia. This index gives us an idea about the amount of upwelled water along the coast. Positive values are, in general, the result of equatorward wind stress. Negative values imply downwelling, the onshore advection of surface waters accompanied by a downward displacement of water.
- 20 year series of Zone closures mussel production by detection of toxins in molluscs produced by HABs provided by The Regulatory Council of Mussel from Galicia.

As the foundation of the aquatic food chain, phytoplankton is an integral part of the ecosystem, affecting trophic dynamics, nutrient cycling, habitat condition, light availability and fisheries resources. Phytoplankton serves as an indicator of trophic status of a waterbody (including effects of eutrophication) and therefore is monitored worldwide. The inverted microscopy method will be used to identify phytoplankton species, quantify phytoplankton abundance and calculate biovolume, according to Utermöhl (1958) and HELCOM COMBINE (2015).

Table 9 – Supplementary data products to be produced from each CoastObs sampling campaign

Product	France	Italy	Netherlands	Spain
SMA	✔	✔		
PSC			✔	✔
PP				✔
HABs				✔

Table 10 – Methods for innovative data products to be produced by each CoastObs partner (See parameter list and units in Table 12)

Parameter	BL	CNR	HZ	UN	USTIR	UVIGO
Macrophyte species	Monitoring surveys	Monitoring surveys	-	Monitoring surveys	-	-
Macrophyte spatial coverage	Photo quadrats	Monitoring surveys	-	Photo quadrats	-	-
PHYTO	-	Samples will be analysed by USTIR	If needed : hematocytometer cell counts are possible	-	-	Inverted microscopy [1]

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Parameter	BL	CNR	HZ	UN	USTIR	UVIGO
PHYTO_BIO	-	Samples will be analysed by USTIR	-	-	-	Inverted microscopy [1]
Fuco	Samples will be analysed by USTIR	Samples will be analysed by USTIR	Samples will be analysed by USTIR	Samples will be analysed by USTIR	High Performance Liquid Chromatography adapted from [2]	Samples will be analysed by USTIR
Peri	Samples will be analysed by USTIR	Samples will be analysed by USTIR	Samples will be analysed by USTIR	Samples will be analysed by USTIR	High Performance Liquid Chromatography adapted from [2]	Samples will be analysed by USTIR
Hex-Fuco	Samples will be analysed by USTIR	Samples will be analysed by USTIR	Samples will be analysed by USTIR	Samples will be analysed by USTIR	High Performance Liquid Chromatography adapted from [2]	Samples will be analysed by USTIR
But-Fuco	Samples will be analysed by USTIR	Samples will be analysed by USTIR	Samples will be analysed by USTIR	Samples will be analysed by USTIR	High Performance Liquid Chromatography adapted from [2]	Samples will be analysed by USTIR
Allo	Samples will be analysed by USTIR	Samples will be analysed by USTIR	Samples will be analysed by USTIR	Samples will be analysed by USTIR	High Performance Liquid Chromatography adapted from [2]	Samples will be analysed by USTIR
Chl-*b*	Samples will be analysed by USTIR	Samples will be analysed by USTIR	Samples will be analysed by USTIR	Samples will be analysed by USTIR	High Performance Liquid Chromatography adapted from [2]	Samples will be analysed by USTIR
Zea	Samples will be analysed by USTIR	Samples will be analysed by USTIR	Samples will be analysed by USTIR	Samples will be analysed by USTIR	High Performance Liquid Chromatography adapted from [2]	Samples will be analysed by USTIR
PP	-	-	-	-	^{14}C photosynthesis-irradiance (PE) incubations [3]	-
PAR	-	-	-	-	Li-COR LI-193-R spherical underwater quantum sensor	-
Chl_0.3µm	-	Samples will be analysed by USTIR	Samples will be analysed by USTIR	-	High Performance Liquid Chromatography adapted from [2] using a 0.3 µm GF filter	Samples will be analysed by USTIR
Chl_2µm	-	Samples will be analysed by USTIR	Samples will be analysed by USTIR	-	High Performance Liquid Chromatography adapted from [2] using a 2 µm GF filter	Samples will be analysed by USTIR

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Parameter	BL	CNR	HZ	UN	USTIR	UVIGO
Chl_20μm	-	Samples will be analysed by USTIR	Samples will be analysed by USTIR	-	High Performance Liquid Chromatography adapted from [1] using a 2 mm GF filter	Samples will be analysed by USTIR
a_{NAP}(λ)_0.3μm	-	-	-	-	Spectrophotometric [4] (inside the sphere)	Samples will be analysed by USTIR
a_{NAP}(λ)_2μm	-	-	-	-	Spectrophotometric [4] (inside the sphere)	Samples will be analysed by USTIR
a_{NAP}(λ)_20μm	-	-	-	-	Spectrophotometric [4] (inside the sphere)	Samples will be analysed by USTIR
a_{ph}(λ)_0.3μm	-	-	-	-	Spectrophotometric [4] (inside the sphere)	Samples will be analysed by USTIR
a_{ph}(λ)_2μm	-	-	-	-	Spectrophotometric [4] (inside the sphere)	Samples will be analysed by USTIR

[1] Utermöhl (1958) and HELCOM COMBINE (2015).
[2] Van Heukelem, L. and C.S. Thomas, 2001. Computer-assisted high-performance liquid chromatography method development with applications to the isolation and analysis of phytoplankton pigments. *J. Crom. A.* 910:31-49.
[3] Method as in INFORM D 5.15 (2017)
[4] Tassan S., and Ferrari G.M., 1995. An alternative approach to absorption measurements of aquatic particles retained on filters. Limnol. Oceanogr. 40: 1358-1368.

4. Other data sources for validation

Other databases or historical data which will be used as sources of validation for the satellite data are shown in Table 11.

Table 11 – Details of other data sources for validation

Parameter/ product	Site	Period	No. of data points	Format	Licence to use within CoastObs	Reference / link
Chl-*a*	Rias Baixas, Spain	2007-2010	~80	.csv	Spyrakos 2011, PhD thesis	Data from PhD thesis
Monitoring Data	Rias Baixas, Spain	1992-2000/ 2002-2012	3428/ 1810	.csv	UVIGO and INTECMAR	-
Zone closures mussel production	Rias Baixas, Spain	1993-2010	5475	.csv	The Regulatory Council of	-

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Parameter/ product	Site	Period	No. of data points	Format	Licence to use within CoastObs	Reference / link
					Mussel from Galicia	
Upwelling Index	Rias Baixas, Spain	1967-2018	18.615	.csv	Meteogalicia	-
Monitoring data Chl-*a* and Water temperature	Eastern Scheldt, NL	2014-2017		.csv	HZ	-
MN148	Black Sea	2016	25 stations, 5 depths	.csv	USTIR	-
VG2016	Ria de Vigo	2016	22 Stations	.csv	USTIR/UVIGO	-
Chl-*a*, TSM, Kd, SD, T	Dutch coastal waters including Wadden Sea and Eastern Scheldt	1997-2018	Up to 50 stations (variable per parameter and time period)	.csv	Public data	Dutch national monitoring programme MWTL (live.waterbase.nl)
Algae species counts	Dutch coastal waters including Wadden Sea (additional data can be requested)	2002-2013 (additional data can be requested)	Up to 20 stations	.csv	Public data	Dutch national monitoring programme MWTL (available upon request)
AOPs, IOPs, CTD, Chl-*a*, TSM, ISM, CDOM concentrations	Northern Adriatic Sea	Oceanographic cruises 2012-2015	~80	.csv	Pending	-
TSM, ISM, Turbidity, CTD, Secchi Disk	Lagoon of Venice	Expeditive surveys	~80	.xls	Yes	-

5. *In situ* data formats

For consistency among the dedicated sampling campaigns, all data will be collected in the formats and units as shown in Table 12.

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Table 12 – *In situ* data formats and units for CoastObs

Header	Description and units
CoastObs ID	String, "CoastObs_ID" CO_ID_XXXX_IIII ID: country ID (FR, IT, NL, ES) XXXX: SITE ID (same as table xx) IIII: Sample ID (unique number)
Latitude	Decimal degrees, North is positive
Longitude	Decimal degrees, East is positive
Date	UTC time standard, (YYYY-MM-DD HH:MM:SS)
Sampling_Depth	Depth of the measurements (m)
SZ	Secchi disk depth (m)
chla_SPEC	Chlorophyll a concentration determined by spectrophotometric methods (mg m^{-3})
chla_HPLC	Chlorophyll a concentration determined using HPLC-based methods (mg m^{-3})
chla_FLUO	Fluorometrically determined Chlorophyll a after extraction (mg m^{-3}). Note HZ dataloggers will use non-analytical fluorecence method.
TSM	Total suspended matter or suspended particulate material (mg L^{-1})
ISM	inorganic part of TSM (mg L^{-1})
Turb.	Turbidity (NTU or FTU)
DOC	Dissolved organic carbon (mg L^{-1})
POC	Particulate organic carbon (mg L^{-1})
Rrs	Remote Sensing Reflectance (sr^{-1})
L_u	Upwelling radiance (sr m^2 nm)
L_{sky}	Sky radiance (sr m^2 nm)
E_d	Sun irradiance (m^2 nm)
SD	Secchi disk depth (m)
$a_{CDOM}(\lambda)$	spectral coloured dissolved organic material absorption coefficient (m^{-1})
$a_{NAP}(\lambda)$	spectral non-algal material absorption coefficient (m^{-1})
$a_{ph}(\lambda)$	spectral phytoplankton absorption coefficient (m^{-1})
c (z,λ)	Beam attenuation (m^{-1})
a (z,λ)	Total absorption (m^{-1})
b_p (z,λ)	particulate optical scattering coefficient (m^{-1})
b_{bp} (z,λ)	particulate optical backscattering coefficient (m^{-1})
SST	Sea surface temperature (°C)
S	Salinity (PSU)
WS	Wind speed (m s^{-1})
UI	Upwelling index (m^3 s^{-1} km^{-1})
AOD(λ)	Aerosol Optical Depth
Macrophyte species	According to taxonomical standards
Macrophyte spatial coverage	Percentage cover (%) and seagrass bed areal extent (ha or m^2)
PHYTO	Phytoplankton abundance, cell L^{-1} for species or different major phytoplankton groups
PHYTO_BIO	Phytoplankton biovolume, mg L^{-1} for species or different major phytoplankton groups
Fuco	Fucoxanthin (mg m^{-3} or area)
Peri	Peridinin (mg m^{-3} or area)
Hex-Fuco	19′-hexanoyloxyfucoxanthin (mg m^{-3} or area)
But-Fuco	19′-butanoyloxyfucoxanthin (mg m^{-3} or area)
Allo	Alloxanthin (mg m^{-3} or area)
Chl-*b*	Chlorophyll-b (mg m^{-3} or area)

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Header	Description and units
Zea	Zeaxanthin (mg m^{-3} or area)
PP	Primary production (mg C m^{-3} h^{-1}) at depth *z*
PAR	Photosynthetically available radiation, μE s^{-1}
Chl_0.3μm	chlorophyll *a* concentration for a sample filtered through a GF 0.3 μm filter (mg m^{-3})
Chl_2μm	chlorophyll *a* concentration for a sample filtered through a GF 2 μm filter (mg m^{-3})
Chl_20μm	chlorophyll *a* concentration for a sample filtered through a Nucleopore 20 μm filter (mg m^{-3})
$a_{NAP}(\lambda)$_0.3μm	spectral non-algal material absorption coefficient concentration for a sample filtered through a GF 0.3 μm filter (m^{-1})
$a_{NAP}(\lambda)$_2μm	spectral non-algal material absorption coefficient concentration for a sample filtered through a GF 2 μm filter (m^{-1})
$a_{NAP}(\lambda)$_20μm	spectral non-algal material absorption coefficient concentration for a sample filtered through a Nucleopore 20 μm filter and then resuspended to a GF filter (m^{-1})
$a_{ph}(\lambda)$_0.3μm	spectral algal material absorption coefficient concentration for a sample filtered through a GF 0.3 μm filter (m^{-1})
$a_{ph}(\lambda)$_2μm	spectral algal material absorption coefficient concentration for a sample filtered through a GF 2 μm filter (m^{-1})
$a_{ph}(\lambda)$_20μm	spectral algal material absorption coefficient concentration for a sample filtered through a Nucleopore 20 μm filter and then resuspended to a GF filter (m^{-1})

6. Data Management

The guidelines for data management in CoastObs are detailed in D2.3 – Data Management Plan. For the *in situ* data collected by the project partners, the principle is that they are fully shared within the project as they become available. They will be shared in the project Dropbox; should that become a problem with respect to size, sharing will be organised via an FTP server hosted by WI. The collected *in situ* data will also be made publicly available following the FAIR data principles via suitable community specific (e.g. LIMNADES) and/or general purpose (e.g. ZENODO) data repositories. The timeline of publication will be discussed at the Management Board meeting after the end of each reporting period.

For additional validation data collected from the users or external sources, usage rights and conditions are determined by the data owners. If they permit it, the data will be shared internally in the same way as the project's own data. Externally collected data will not be shared outside the consortium.

Table 13 – Data sharing and storage for CoastObs

Data Type	Source	Owner	Storage	Internal Sharing	External Sharing
CoastObs *in situ* data	Own Collection	Partners involved in collecting and	Dropbox or FTP for spectral	Yes	Yes, via ZENODO or

Data Type	Source	Owner	Storage	Internal Sharing	External Sharing
		processing the samples/data	measurements : WISPweb		dedicated repository
User in situ data / data from external sources	CoastObs users/ various sources (national monitoring networks, other researchers)	Original data owner		If permitted by data owner	No

7. CoastObs Products – Quality Requirements and Criteria

All CoastObs products will be validated with *in situ* data and goodness of fit will be assessed using a range of statistical methods. Validation and uncertainty assessment is a crucial requirement for a satellite data product and methods will consider those metrics most suited to the data type, whether quantitative or qualitative. EO data derived from an aquatic environment is usually quantitative (e.g. Chl-*a*), and this can often be transformed into qualitative information (e.g. presence/absence of HABs).

7.1 Quantitative Data Assessment

Performance assessment of quantitative data for ocean colour remote sensing is often based on mean squared errors, including the coefficient of determination (r^2), root mean squared error (RMSE) and the regression slope (Seegers et al., 2018; Table 14).

RMSE is defined as:

$$\boldsymbol{RMSE} = \sqrt{\frac{\sum_{i=1}^{n}(M_i - O_i)^2}{n}} \qquad (1)$$

where *M, O* and *n* represent the modelled value, observed value and number of samples, respectively. Therefore, RMSE varies with the average error and variability in the error magnitudes, as well as sample size (*n*), indicating its sensitivity to dataset distribution type and presence of outliers (Chai and Draxler, 2014). RMSE is most appropriate for Gaussian distributions without outliers, thus this metric is not always suitable for validation of EO datasets. Nevertheless, RMSE is one of the most commonly reported measures of accuracy in literature for EO datasets, therefore for legacy purposes it is useful to retain as part of a suite of error metrics.

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Table 14 – Measurements used to assess algorithm performance for quantitative data (from Seegers et al, 2018).

Measurement	Frequently Used Metrics	Why or Why Not for Ocean Color	Notes
Accuracy	RMSE	• Distribution sensitive (assumes Gaussian) • Often misinterpreted to be a simple estimate of average error • No consistent relationship with average error magnitudes	Other Sum of Squares based measures have same problems, such as standard deviation, standard error.
Goodness of fit	r^2	• Can be misinterpreted if not given in context, because it lacks a response to bias and is sensitive to outliers • Can misrepresent error when the range is small • Can overstate variable relationships even with apparently random error	
	Slope	• Can be misinterpreted, by reporting a good value for strongly-biased, low-precision models. • Leverages (biased errors on either end) produce meaningless slopes • Cannot address non-linear error • Can allow tuning of a model to fit a particular region	Common least squares regression gives biased slope when the x variables contain errors [9]
	Suggested Metrics		
Bias	Bias	• Quantifies the average difference between this estimator and expected value • Estimates systematic error	Often based on mean, however median error can also be used if a more robust metric is needed
Accuracy	MAE	• Does not amplify outliers • Accurately reflects error magnitude	Compared to mean, median absolute estimates are less sensitive to outliers. Similar metrics include mean/ median absolute percent error
	New Approaches		
Point by point accuracy	% wins (Residuals)	• Considers model failures • Provides consistent head-to-head comparison of algorithms	Pairwise comparison Decision support metric
Temporal stability	CV Intra-pixel	• Estimates imagery pixel stability. • Estimates algorithm spatial and temporal performance. • Does not require satellite-to-*in situ* match-ups	

The relationship between EO data and *in situ* values is often illustrated by a scatterplot to assess goodness of fit (Willmott, 1982). A diagonal line on the scatterplot indicates a perfect prediction (1:1), where regression slope (*a*) is 1 and intercept (*b*) is 0 (Figure 6). The coefficient of determination (r^2) is defined as the proportion of the variance in the dependent variable that is predictable from the independent variable(s). The value of r^2 thus varies between 0 and 1, with 1 indicating a perfect prediction. However, r^2 is sensitive to outliers, inconsistently interpretable across datasets and has a tendency to overstate a variable relationship (Seegers et al., 2018). Similarly, the slope of a least-squares linear regression between estimated and *in*

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situ parameters is also particularly sensitive to outliers. While the r^2 and the regression slope do not provide a complete assessment of algorithm performance, they can be useful metrics for validation exercises if interpreted cautiously and used in combination with other error metrics.

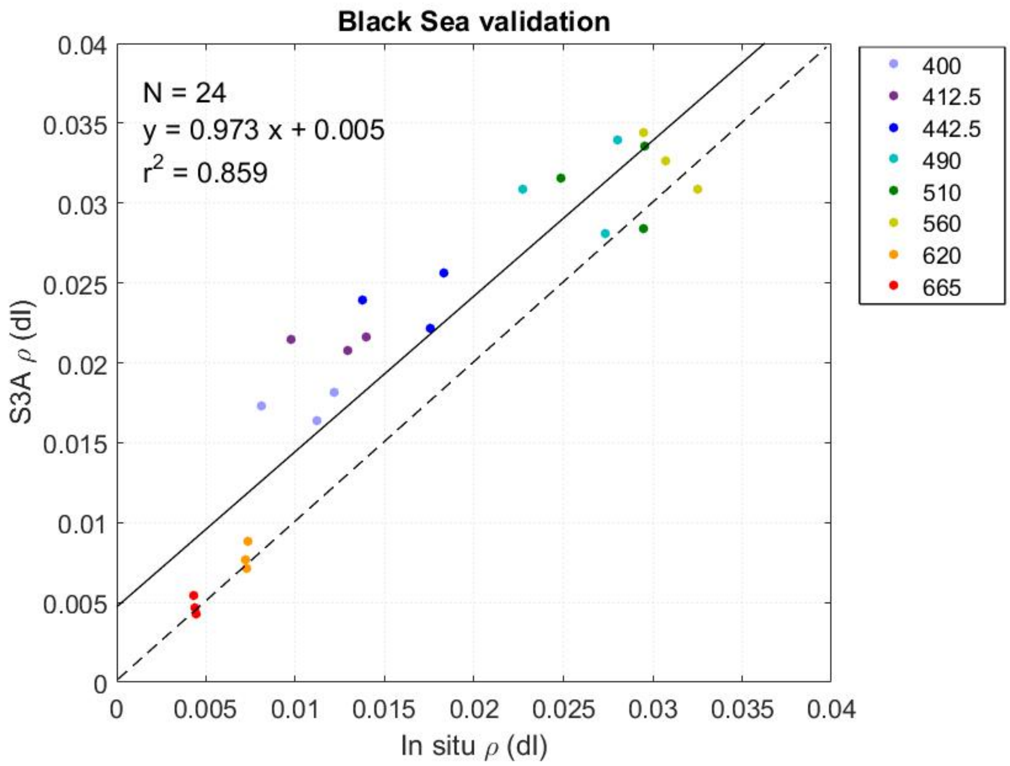

Figure 6 – Example of a scatterplot between Sentinel-3A and *in situ* water leaving reflectance (ρ) in the Black Sea (6-12th May 2016). Dashed line indicates 1:1 prediction.

Metrics based on simple deviations, including bias and mean absolute error (MAE), are considered more robust for assessment of quantitative data retrieved from remote sensing data (Seegers et al., 2018). These metrics are defined, respectively, as:

$$\boldsymbol{Bias} = \frac{\sum_{i=1}^{n} M_i - O_i}{n} \qquad (2)$$

$$\boldsymbol{MAE} = \frac{\sum_{i=1}^{n} |M_i - O_i|}{n} \qquad (3)$$

where *M, O* and *n* represent the modelled value, observed value and number of samples, respectively. Bias provides an assessment of the systematic direction of the error, either as over- or under-estimating the prediction on average (Walther and Moore, 2005). MAE is a measure of accuracy and is less sensitive to outliers (as compared to RMSE), therefore MAE is appropriate for data from non-Gaussian distributions (Seegers et al., 2018).

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7.2 Qualitative Data Assessment

Models for qualitative data, or classification data, are commonly assessed using the overall accuracy (OA), percentage of samples that are correctly classified, the individual accuracy for each class and the kappa statistic (Landis and Koch, 1977). The kappa statistic assesses the classification agreement by removal of the chance effect (Gonzalez Vilas et al., 2014).

More specifically, when data is dichotomous or binomial (e.g. presence/absence of HABs), the accuracy of a model prediction can be summarised in a confusion or error matrix (Table 15; Fielding and Bell, 1997).

Table 15 - A confusion matrix indicating instances of true positives (TP), true negatives (TN), false positives (FP) and false negatives (FN).

		Actual Class (*in situ* data)	
		Present	Absent
Predicted Class (EO data)	Present	*TP*	*FP*
	Absent	*FN*	*TN*

Several useful error metrics for assessment of qualitative data can be derived from a confusion matrix. The **kappa statistic (*K*)** ranges from 0 to 1, and for 2-class classification this is calculated as:

$$K = \frac{OA - CA}{1 - CA} \quad (4)$$

where *OA* is the **overall accuracy** or overall agreement, and *CA* is the hypothetical probability of chance agreement, defined respectively as:

$$OA = \frac{(TP + TN)}{n} \quad (5)$$

$$CA = \frac{(TP \times TN) + (FP \times FN)}{n^2} \quad (6)$$

where *TP* is the number of true positives, *TN* is the number of true negatives, *FP* is the number of false positives, *FN* is the number of false negatives and *n* is the total number of observations.

Based on the confusion matrix, the **true false rate (TFR),** or specificity, is defined as:

$$TFR = \frac{TN}{FP + TN} \quad (7)$$

while the **true positive rate (TPR),** or sensitivity, is defined as:

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$$TPR = \frac{TP}{TP+FN}. \qquad (8)$$

7.3 Error metrics and methods to be used

A single index is unlikely to adequately describe model performance, therefore an array of complementary measures will be reported for the purposes of the users. Upon consideration of the range of accuracy/uncertainty metrics, those have been selected that have few assumptions and are most applicable for the validation of EO data within the CoastObs project.

The error measures for **quantitative data** will include:

- Intercept (*b*) and slope (*a*) of a regression line of a scatterplot of EO retrieved data vs. *in situ* or laboratory measured data (with a 1:1 prediction line; e.g. Figure 6)
- Root mean square error (RMSE)
- Mean absolute error (MAE)
- Bias

Where appropriate, data will be log-transformed prior to calculation of error metrics (including RMSE, Bias and MAE), particularly for parameters where data span multiple orders of magnitude and the uncertainty varies proportionally with data values (e.g. Chl-*a*). Seegers et al. (2018) also recommend back-transformation (i.e. converting statistics back out of $\log_{10}$ space) prior to interpretation in order to minimise the possibility of misinterpretation of the reported error. For clarity, back-transformation will also be applied for the assessment of CoastObs algorithm performance and presentation of errors to the users.

The error measures for **qualitative data** will include:

- True false rate (TFR)
- True positive rate (TPR)
- Overall accuracy (OA)
- Kappa statistic (*K*)

We will ultimately aim to achieve product accuracy to the satisfaction of the users and their requirements, and this will be an iterative process, if required.

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