PHYTOplankton biomass and diversity Climate Change Initiative (PHYTO-CCI)

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D1.2 Product Specification Document (PSD)

Project led by

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1 Introduction

1.1 Purpose of document

This Product Specification Document (PSD) sets out the details of the phytoplankton biomass and diversity Essential Climate Variables (ECVs) to be developed by the PHYTOplankton biomass and diversity Climate Change Initiative (PHYTO-CCI). The product specifications are based on user requirements and those requirements set out by the Global Climate Observing System (GCOS). The PSD details the specifications for the first version of the PHYTO-CCI dataset, that is only available to the project team and project collaborators. The document will evolve as part of the ECV development process, in which initial ECV products are assessed by the Climate Research Group (CRG) of the PHYTO-CCI team and feedback for improvement is provided.

1.2 Structure

The PSD describes the specification of ocean biosphere ECV products from ocean-colour remote sensing observations, with the targeted ECVs and their requirements provided in Section 2 and information on data format and access provided in Section 3. In Section 4, the product specifications are summarised in a technical summary. References are provided in Section 5 and an example of the expected data structure and metadata is provided in Appendix I.

1.3 Related documents

Documents related to the PHYTO-CCI PSD are the PHYTO-CCI User Requirement Document (URD), the GCOS requirements (WMO, 2022) and the PSD of the Ocean Colour Climate Change Initiative (OC-CCI) (OC-CCI, 2017).

2 Product specification

2.1 Selected ocean biosphere ECV products

Based on results from the user consultation carried out for PHYTO-CCI, and based on requirements set out by GCOS, the following ocean-colour products are targeted for the ocean biosphere ECV:

- *Phytoplankton biomass* will be provided as the weight of carbon per volume, i.e., phytoplankton carbon in mg m^{-3}. We will target the total phytoplankton carbon concentration, and where possible, also provide the carbon content of three phytoplankton size classes, i.e., pico-, nano- and microphytoplankton.

- *Phytoplankton diversity* will be provided as the concentration of pigment types per volume, i.e., specific phytoplankton pigments in mg m^{-3}. We will target eight phytoplankton pigments: 19'-butanoyloxyfucoxanthin, 19'-hexanoyloxyfucoxanthin, alloxanthin, divinyl chlorophyll-a, chlorophyll-b, fucoxanthin, peridinin and zeaxanthin. These pigments are commonly used to derive other phytoplankton biodiversity indicators, including phytoplankton functional types.

Note that chlorophyll-a, the main photosynthetic pigment in phytoplankton, and also a measure of phytoplankton biomass, will not be targeted in PHYTO-CCI, as it is already available through OC-CCI. A summary of the GCOS and user requirements for the selected products is provided in Table 1. The ocean biosphere ECV products will be based on the merged ocean-colour time series of the OC-CCI, with remote sensing reflectances, inherent optical properties and chlorophyll-a as input to the various algorithms of phytoplankton carbon and phytoplankton pigments. An optical water class approach will be followed, where possible, to blend best-performing algorithms into one product.

Table 1. Summary of requirements for the ocean biosphere ECV according to GCOS (WMO, 2022) and users (see PHYTO-CCI User Requirement Document). Requirements for the spatial and temporal resolution, uncertainty (assessed as accuracy and precision among users) and stability (e.g., change in bias over time) are provided at three levels of maturity: the ideal requirement above which no further improvements are needed (G – Goal), an intermediate level at which significant improvements are made (B – Breakthrough), and the minimum requirements to ensure usefulness of the data product (T – Threshold). The values provided by GCOS for phytoplankton biomass and diversity are for in situ *observations, whereas the values from users are provided for ocean-colour remote sensing observations. * Note that for phytoplankton diversity the values for the horizontal resolution provided in the table are for offshore waters and for nearshore waters the values are 0.1 km, 0.1 km and 1 km for G, B and T levels, respectively. † In the GCOS documentation the unit for the horizontal resolution is given as km, but logically this would be in m at goal level.*

	ECV	Plankton			
	Product	**Phytoplankton carbon biomass**		**Phytoplankton pigment diversity***	
Requirement	**Level**	**GCOS**	**Users**	**GCOS**	**Users**
Horizontal resolution	G B T	100 m † - 2000 km	0.1-1 km 0.1-1 km 1-10 km	100 m † 1 km 2000 km	0.1-1 km 0.1-1 km 1-10 km
Temporal resolution	G B T	Weekly-seasonal - 10 months	1 day 1 day 1 week	Weekly-monthly 3 months 12 months	1 day 1 day 1 week
Required measurement uncertainty	G B T	- - 5 %	<10 % 10-25 % 25->50 %	- - 5 %	<10 % 10-25 % 25->50 %
Stability	G B T	- - -	1 % per decade 2 % per decade 5 % per decade	- - -	1 % per decade 2-5 % per decade 5 % per decade

2.2 Spatial and temporal resolution

The user consultation of PHYTO-CCI revealed that many users expect higher resolution of ocean biosphere ECV products than set out by GCOS, in line with what might be expected for ocean-colour products (Table 1). There were some differences between the EO scientist and modelling user groups in the required spatial and temporal resolution of the phytoplankton carbon biomass and pigment diversity products, with EO scientists generally requiring higher spatial and temporal resolution data, especially by those who work in more dynamic coastal regions, than ecosystem modellers, for whom the resolution of their models is often coarser than that of current ocean-colour products. Considering the outcomes of the user consultation and the computational and data storage requirements, the first version of the PHYTO-CCI dataset will be produced at 4 km spatial and monthly temporal resolution. Additional data at daily temporal resolution will be produced for match-up purposes, for algorithm development and validation of data products within PHYTO-CCI. The need for an experimental dataset of the pigment fucoxanthin at 8-day temporal resolution will be discussed in collaboration with the CRG, whom might need higher temporal resolution to derive phenology metrics in the coastal and off-shore waters of Portugal and south-west India. Data products of PHYTO-CCI will be provided globally with a standard geographical projection with World Geodetic System 1984 (WGS84) datum with a resolution of 8640 by 4320 pixels. Following OC-CCI, the data will also be provided with a global sinusoidal equal-area grid matching the NASA standard level-3 binned projection.

2.3 Error characterisation

The majority of users of ocean-colour data indicated that uncertainty estimates for the ocean biosphere ECV products are important. In the first version of the PHYTO-CCI dataset, the OC-CCI approach to pixel-by-pixel uncertainty estimates will be followed in which optical water classes are used to estimate the extent to which satellite observations of phytoplankton carbon and phytoplankton pigments are likely to differ from *in situ* observations (Moore *et al.*, 2009; Jackson *et al.,* 2017). In this approach, the bias and root mean square difference (RMSD) are estimated for each of the optical water classes identified and then assigned to each pixel using the fuzzy membership of each optical class for that pixel. The uncertainties for that pixel are then computed as weighted averages of the uncertainties of the classes for that pixel with the fuzzy membership as the weighting factor for each class. While this satisfies the user requirements for ocean-colour ECV products, the approach does not consider any sources of errors in the ocean-colour retrieval scheme explicitly (i.e., only implicitly by comparing remote sensing to *in situ* validation values, both of which naturally exhibit errors). Therefore, in the next version of the PHYTO-CCI dataset, an uncertainty analysis following the Guide to the expression of Uncertainty in Measurement (GUM) and its supplements (BIPM 2008a, 2008b, 2011) will be carried out, in collaboration with OC-CCI.

2.4 Long-term stability

Users indicated that long-term stability is an important feature of ECV products, especially in the context of climate research and the analysis of trends. Users indicated that they expect a stability of 5 % per decade at threshold level (Table 1). It has been shown that ocean colour is close to 1 % stability per decade (Ohring *et al.*, 2005), but there is limited evidence that in-water variables fall within this level of stability, especially those variables that are not based on band ratios algorithms. No specific information on stability is currently available for ocean-colour-derived phytoplankton carbon and pigment ECV products, and this will be assessed using the first version of the PHYTO-CCI dataset to guide future improvements.

3 Product format and access

3.1 Data format

The datasets of PHYTO-CCI will in the first instance be provided as netCDF files that are compliant with the Climate and Forecast Metadata Convention, i.e., CF-compliant netCDF format. The majority of users expressed their preference for this type of data format during the user consultation. The structure of the data files will be constrained by the appropriate conventions and an example is provided in Appendix I.

3.2 Metadata

The PHYTO-CCI data products will include discovery and usage metadata, following the approach of related ocean-colour products from OC-CCI. Discovery metadata includes higher level properties, such as data ownership and versioning, that allows users to locate specific data relevant to a search query. This type of metadata will be included within each data file following netCDF discovery metadata conventions (NCDISC, 2011). Usage metadata will include standard attributes for the interpretation of data variables, such as array dimensions, and additional elements that provide a more detailed description of what the data in each variable represents, and the spatial and temporal properties of the data. An example of the metadata that will be provided is given in Appendix I (i.e., example of metadata of chlorophyll-a from OC-CCI). PHYTO-CCI aims to provide data that is fully compliant with Climate and Forecast Metadata Convention (CF Metadata, 2011).

3.3 Filename convention

The file naming follows the CCI Guidelines for Data Producers, with the format being:

> ESACCI-PHYTO-<Processing Level>-<Product String>-<Data Type>-<Temporal resolution>-<Spatial resolution>-<Projection>-PML-<Additional Segregator>-<Indicative Date>-fv<File version>.nc

3.4 Data volume

It is estimated that the first PHYTO-CCI dataset will have a data volume of approximately 3 Tb. This includes four phytoplankton carbon variables (i.e., total concentration and three size classes) and eight pigment variables at monthly resolution between 1997-2025 at geographic and sinusoidal projections, each estimated to be around 100 Gb. An additional dataset for the pigment fucoxanthin at 8-day resolution is expected to be produced for the same time period, which is estimated to be around 300 Gb for geographic and sinusoidal projections each. During the user consultation, users indicated that large file sizes are of concern and therefore the data will be provided as individual files for each variable in addition to files that contain all variables.

3.5 Data access

The user consultation from PHYTO-CCI showed that users access ocean colour CCI data in various ways, i.e., through web browser, FTP and cloud services, and through different portals, including those of Plymouth Marine Laboratory (PML), ESA CCI and Copernicus Climate Change Services (C3S). For the first version of the PHYTO-CCI dataset, which is only available for project members and collaborators, the dataset will be made available through an FTP server. For public release of the dataset in the future, we will use methods currently in place for OC-CCI as the ocean-colour products are closely related and accessed by a similar user community.

3.6 Documentation

It became clear from the user consultation that appropriate documentation is required that is easily accessible. The PHYTO-CCI data products will therefore be accompanied by detailed documentation, including a product user guide, that will be made available on the CCI website. As is now standard in the CCI programme, all documents related to PHYTO-CCI, that form the project deliverables, will be made publicly available. These documents will detail algorithms used, approaches to uncertainties, dataset validation and quality assessment, among other information.

5 Technical summary

The data product specification for the first version of the PHYTO-CCI dataset is summarised in Table 2. Note that this version of the dataset is only available to the project team and their collaborators.

Table 2. Summary of the specification of version 1 of the PHYTO-CCI ECV dataset from ocean-colour observations.

Product details		
Technical point	**PHYTO-CCI implementation**	**Comments**
Spatial coverage	Global	
Spatial resolution	4 km (nominal at equator)	
Temporal coverage	1997-2025	
Temporal resolution	Monthly	Daily data will be produced for match-up purposes. An experimental dataset for fucoxanthin at 8-day resolution is expected to be needed for the CRG.
Products	Phytoplankton carbon (total and for pico-, nano- and microphytoplankton size classes) Phytoplankton pigments (19'-butanoyloxyfucoxanthin, 19'-hexanoyloxyfucoxanthin, alloxanthin, divinyl chlorophyll-a, chlorophyll-b, fucoxanthin, peridinin and zeaxanthin)	
Datum	WGS84	Standard datum
Map projection	Geographic and sinusoidal	The projections have the highest level of compatibility with most applications

Table 2. Continued.

Data format		
Technical point	**PHYTO-CCI implementation**	**Comments**
File format	NetCDF	CMIP and other required formats are expected for version 3, i.e., the final (public) dataset of PHYTO-CCI.
Convention compliance	NetCDF general conventions CF conventions CF-satellite conventions Unidata discovery convention	
Representation of uncertainty	RMSE and bias	
General		
Technical point	**PHYTO-CCI implementation**	**Comments**
Data volume	3 Tb	
Number of products per file	All, but also split into separate files for: phytoplankton carbon, phytoplankton pigments	Products subsets are provided as there are concerns about file size among users
Product versioning	By internal tagging (includes a unique identification per file)	
Naming convention	Follows CCI Guidelines for Data Producers	See Section 3.3
Product size for gridded data	Gridded 4 km data is 8640 by 4320 pixels	

6 References

BIPM (2008a). Evaluation of measurement data – Guide to expression of uncertainty in measurement. JCGM 100:2008. Available online at: https://www.bipm.org/documents/20126/2071204/JCGM_100_2008_E.pdf/cb0ef43f-baa5-11cf-3f85-4dcd86f77bd6

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CF Metadata (2011). NetCDF Climate and Forecast (CF) Metadata Convention. Available online at: https://cfconventions.org/

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Ohring G, Wielicki B, Spencer R, Emery B, Datla R (2005). Satellite Instrument Calibration for Measuring Global Climate Change: Report of a Workshop. Bulletin of the American Meteorological Society 86: 1303-1314. https://doi.org/10.1175/BAMS-86-9-1303

WMO (2022). GCOS ECVs Requirements (GCOS-245). Available online at: https://library.wmo.int/records/item/58111-the-2022-gcos-ecvs-requirements

Appendix I – Example of data structure and metadata

An example of the data structure and metadata from OC-CCI for chlorophyll-a is provided below, as an example of the structure used and metadata included in data files of PHYTO-CCI.

```
netcdf ESACCI-OC-L3S-CHLOR_A-MERGED-1M_MONTHLY_4km_SIN_PML_OCx-201005-fv6.0 {
dimensions:
	time = 1 ;
	bin_index = 23761676 ;
variables:
	float MERIS_nobs_sum(time, bin_index) ;
		MERIS_nobs_sum:_FillValue = 0.f ;
		MERIS_nobs_sum:coordinates = "lat lon" ;
		MERIS_nobs_sum:long_name = "Count of the number of observations from the MERIS sensor contributing to this bin cell" ;
		MERIS_nobs_sum:number_of_files_composited = 31 ;
	float MODISA_nobs_sum(time, bin_index) ;
		MODISA_nobs_sum:_FillValue = 0.f ;
		MODISA_nobs_sum:coordinates = "lat lon" ;
		MODISA_nobs_sum:long_name = "Count of the number of observations from the MODIS (Aqua) sensor contributing to this bin cell" ;
		MODISA_nobs_sum:number_of_files_composited = 31 ;
	float OLCI-A_nobs_sum(time, bin_index) ;
		OLCI-A_nobs_sum:_FillValue = 0.f ;
		OLCI-A_nobs_sum:coordinates = "lat lon" ;
		OLCI-A_nobs_sum:long_name = "Count of the number of observations from the OLCI (Sentinel-3a) sensor contributing to this bin cell" ;
		OLCI-A_nobs_sum:number_of_files_composited = 31 ;
	float OLCI-B_nobs_sum(time, bin_index) ;
		OLCI-B_nobs_sum:_FillValue = 0.f ;
		OLCI-B_nobs_sum:coordinates = "lat lon" ;
		OLCI-B_nobs_sum:long_name = "Count of the number of observations from the OLCI (Sentinel-3b) sensor contributing to this bin cell" ;
		OLCI-B_nobs_sum:number_of_files_composited = 31 ;
	float SeaWiFS_nobs_sum(time, bin_index) ;
		SeaWiFS_nobs_sum:_FillValue = 0.f ;
		SeaWiFS_nobs_sum:coordinates = "lat lon" ;
		SeaWiFS_nobs_sum:long_name = "Count of the number of observations from the SeaWiFS (GAC and LAC) sensor contributing to this bin cell" ;
		SeaWiFS_nobs_sum:number_of_files_composited = 31 ;
	float VIIRS_nobs_sum(time, bin_index) ;
		VIIRS_nobs_sum:_FillValue = 0.f ;
		VIIRS_nobs_sum:coordinates = "lat lon" ;
		VIIRS_nobs_sum:long_name = "Count of the number of observations from the VIIRS sensor contributing to this bin cell" ;
		VIIRS_nobs_sum:number_of_files_composited = 31 ;
	float chlor_a(time, bin_index) ;
		chlor_a:_FillValue = 9.96921e+36f ;
		chlor_a:ancillary_variables = "chlor_a_log10_rmsd chlor_a_log10_bias" ;
		chlor_a:coordinates = "lat lon" ;
		chlor_a:long_name = "Chlorophyll-a concentration in seawater (not log-transformed), generated by as a blended combination of OCI, OCI2, OC2 and OCx algorithms, depending on water class memberships" ;
		chlor_a:parameter_vocab_uri = "http://vocab.ndg.nerc.ac.uk/term/P011/current/CHLTVOLU" ;
		chlor_a:standard_name = "mass_concentration_of_chlorophyll_a_in_sea_water" ;
		chlor_a:units = "milligram m-3" ;
		chlor_a:units_nonstandard = "mg m^-3" ;
	float chlor_a_log10_bias(time, bin_index) ;
		chlor_a_log10_bias:_FillValue = 9.96921e+36f ;
		chlor_a_log10_bias:comment = "Uncertainty lookups derived from file: /data/datasets/CCI/v6.0-production/stage09b-uncertainty_tables/chlor_a/cci_chla_bias.dat" ;
		chlor_a_log10_bias:coordinates = "lat lon" ;
		chlor_a_log10_bias:long_name = "Bias of log10-transformed chlorophyll-a concentration in seawater." ;
		chlor_a_log10_bias:ref = "http://www.esa-oceancolour-cci.org/?q=webfm_send/581" ;
		chlor_a_log10_bias:rel = "uncertainty" ;
	float chlor_a_log10_rmsd(time, bin_index) ;
```

```
		chlor_a_log10_rmsd:_FillValue = 9.96921e+36f ;
		chlor_a_log10_rmsd:comment = "Uncertainty lookups derived from file: /data/datasets/CCI/v6.0-production/stage09b-uncertainty_tables/chlor_a/cci_chla_rmsd.dat" ;
		chlor_a_log10_rmsd:coordinates = "lat lon" ;
		chlor_a_log10_rmsd:long_name = "Root-mean-square-difference of log10-transformed chlorophyll-a concentration in seawater." ;
		chlor_a_log10_rmsd:ref = "http://www.esa-oceancolour-cci.org/?q=webfm_send/581" ;
		chlor_a_log10_rmsd:rel = "uncertainty" ;
	int crs(time) ;
		crs:grid_mapping_name = "1D binned sinusoidal" ;
		crs:number_of_latitude_rows = 4320 ;
		crs:total_number_of_bins = 23761676 ;
	float lat(bin_index) ;
		lat:standard_name = "latitude" ;
		lat:units = "degrees_north" ;
		lat:axis = "Y" ;
	float lon(bin_index) ;
		lon:standard_name = "longitude" ;
		lon:units = "degrees_east" ;
		lon:axis = "X" ;
	int time(time) ;
		time:axis = "T" ;
		time:standard_name = "time" ;
		time:units = "days since 1970-01-01 00:00:00" ;
	float total_nobs_sum(time, bin_index) ;
		total_nobs_sum:_FillValue = 0.f ;
		total_nobs_sum:coordinates = "lat lon" ;
		total_nobs_sum:long_name = "Count of the total number of observations contributing to this bin cell" ;
		total_nobs_sum:number_of_files_composited = 31 ;

// global attributes:
		:Conventions = "CF-1.7" ;
		:Metadata_Conventions = "Unidata Dataset Discovery v1.0" ;
		:cdm_data_type = "Grid" ;
		:comment = "See summary attribute" ;
		:creator_email = "help@esa-oceancolour-cci.org" ;
		:creator_name = "Plymouth Marine Laboratory" ;
		:creator_url = "http://esa-oceancolour-cci.org" ;
		:geospatial_lat_max = 90.f ;
		:geospatial_lat_min = -90.f ;
		:geospatial_lat_resolution = ".041666666666666666" ;
		:geospatial_lat_units = "decimal degrees north" ;
		:geospatial_lon_max = 180.f ;
		:geospatial_lon_min = -180.f ;
		:geospatial_lon_resolution = ".041666666666666666" ;
		:geospatial_lon_units = "decimal degrees east" ;
		:geospatial_vertical_max = 0.f ;
		:geospatial_vertical_min = 0.f ;
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		:institution = "Plymouth Marine Laboratory" ;
		:keywords = "satellite,observation,ocean,ocean colour" ;
		:keywords_vocabulary = "none" ;
		:naming_authority = "uk.ac.pml" ;
		:number_of_bands_used_to_classify = "4" ;
		:number_of_optical_water_types = "14" ;
		:platform = "Orbview-2,Aqua,Envisat,Suomi-NPP, Sentinel-3a, Sentinel-3b" ;
		:processing_level = "Level-3 binned" ;
		:product_version = "6.0" ;
		:sensor = "SeaWiFS,MODIS,MERIS,VIIRS,OLCI" ;
		:sensors_present = " MERIS MODISA SeaWiFS" ;
		:spatial_resolution = "4km bin cells" ;
		:standard_name_vocabulary = "NetCDF Climate and Forecast (CF) Metadata Conventions Version 1.7" ;
		:NCO = "netCDF Operators version 4.7.5 (Homepage = http://nco.sf.net, Code = http://github.com/nco/nco)" ;
		:number_of_files_composited = 31 ;
		:creation_date = "Mon Aug 15 08:59:17 2022" ;
		:date_created = "Mon Aug 15 08:59:17 2022" ;
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:time_coverage_resolution = "P1M" ;
:time_coverage_duration = "P1M" ;
:start_date = "01-MAY-2010 00:00:00.000000" ;
:stop_date = "31-MAY-2010 23:59:00.000000" ;
:time_coverage_start = "201005010000Z" ;
:time_coverage_end = "201005312359Z" ;
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:license = "ESA CCI, EOCIS, and C3S Data Policy: free and open access. When referencing, please use: Ocean Colour Climate Change Initiative dataset, Version 6.0, European Space Agency, available online at https://climate.esa.int/en/projects/ocean-colour/. We would also appreciate being notified of publications so that we can list them on the project website at https://climate.esa.int/en/projects/ocean-colour/, https://eocis.org/, https://climate.copernicus.eu/" ;
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:title = "ESA CCI, EOCIS Ocean Colour Product, and Copernicus Climate Change Service" ;

:summary = "Data products generated by the Ocean Colour component of the European Space Agency Climate Change Initiative project. These files are daily composites of merged sensor (MERIS, MODIS Aqua, SeaWiFS LAC & GAC, VIIRS, OLCI) products. MODIS Aqua and SeaWiFS were band-shifted and bias-corrected to MERIS bands and values using a temporally and spatially varying scheme based on the overlap years of 2003-2007. VIIRS was band-shifted and bias-corrected in a second stage against the MODIS Rrs that had already been corrected to MERIS levels, for the overlap period 2012-2013; and at the third stage OLCI was bias corrected against already corrected MODIS, for overlap period 2016-07-01 to 2019-06-30. VIIRS, MODIS, SeaWiFS and MERIS Rrs were derived from a combination of NASA\'s l2gen (for basic sensor geometry corrections, etc) and HYGEOS Polymer v4.12 (for atmospheric correction). OLCI Rrs were sourced at L1b (already geometrically corrected) and processed with polymer. The Rrs were binned to a sinusoidal 1km level-3 grid, and later to 1km geographic projection, by Brockmann Consult\'s SNAP. Derived products were generally computed with the standard algorithms through SeaDAS. QAA IOPs were derived using the standard SeaDAS algorithm but with a modified backscattering table to match that used in the bandshifting. The final chlorophyll is a combination of OCI, OCI2, OC2 and OCx, depending on the water class memberships. Uncertainty estimates were added using the fuzzy water classifier and uncertainty estimation algorithm of Tim Moore as documented in Jackson et al (2017)." ;

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